



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:54 PM EDT

PDB ID : 7C52 / pdb\_00007c52  
Title : Co-crystal structure of a photosynthetic LH1-RC in complex with electron donor HiPIP  
Authors : Yu, L.-J.; Wang-Otomo, Z.-Y.  
Deposited on : 2020-05-18  
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

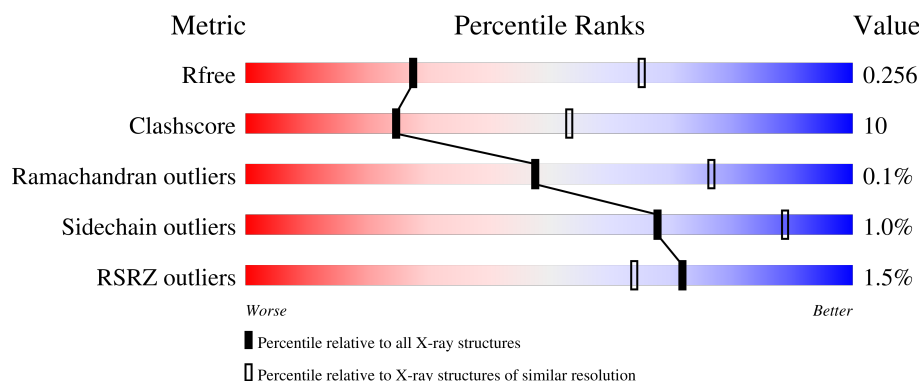
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                 |
|-----|-------|--------|--------------------------------------------------|
| 1   | C     | 311    | <div> <div>0%</div> <div>92% 8%</div> </div>     |
| 2   | L     | 281    | <div> <div>2%</div> <div>87% 12%</div> </div>    |
| 3   | M     | 325    | <div> <div>0%</div> <div>84% 14% .</div> </div>  |
| 4   | H     | 259    | <div> <div>2%</div> <div>87% 11% .</div> </div>  |
| 5   | 1     | 61     | <div> <div>3%</div> <div>79% 13% 8%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | 3     | 61     |                  |
| 5   | 5     | 61     |                  |
| 5   | 7     | 61     |                  |
| 5   | 9     | 61     |                  |
| 5   | A     | 61     |                  |
| 5   | D     | 61     |                  |
| 5   | F     | 61     |                  |
| 5   | I     | 61     |                  |
| 5   | K     | 61     |                  |
| 5   | O     | 61     |                  |
| 5   | Q     | 61     |                  |
| 5   | S     | 61     |                  |
| 5   | U     | 61     |                  |
| 5   | W     | 61     |                  |
| 5   | Y     | 61     |                  |
| 6   | 0     | 47     |                  |
| 6   | 2     | 47     |                  |
| 6   | 4     | 47     |                  |
| 6   | 6     | 47     |                  |
| 6   | 8     | 47     |                  |
| 6   | B     | 47     |                  |
| 6   | E     | 47     |                  |
| 6   | G     | 47     |                  |
| 6   | J     | 47     |                  |
| 6   | N     | 47     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 6   | P     | 47     |  |
| 6   | R     | 47     |  |
| 6   | T     | 47     |  |
| 6   | V     | 47     |  |
| 6   | X     | 47     |  |
| 6   | Z     | 47     |  |
| 7   | b     | 83     |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21  | PEF  | 1     | 103 | -         | X        | -       | -                |
| 21  | PEF  | 3     | 104 | -         | X        | -       | -                |
| 21  | PEF  | H     | 302 | -         | X        | -       | -                |
| 21  | PEF  | I     | 103 | -         | X        | -       | -                |
| 21  | PEF  | M     | 407 | -         | X        | -       | -                |
| 21  | PEF  | M     | 409 | -         | X        | -       | -                |
| 21  | PEF  | W     | 105 | -         | X        | -       | -                |
| 21  | PEF  | W     | 106 | -         | X        | -       | -                |

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 27405 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     | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2417  | 1524 | 424 | 453 | 16 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | L     | 280      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2236  | 1505 | 359 | 361 | 11 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | M     | 318      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2555  | 1715 | 417 | 412 | 11 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | H     | 255      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1973  | 1269 | 337 | 361 | 6 |         |         |       |

- Molecule 5 is a protein called LH1 alpha polypeptide.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 5   | A     | 54       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 434   | 290 | 70 | 73 | 1 |         |         |       |
| 5   | D     | 55       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 445   | 296 | 72 | 76 | 1 |         |         |       |
| 5   | F     | 55       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 445   | 296 | 72 | 76 | 1 |         |         |       |
| 5   | I     | 57       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 460   | 305 | 74 | 79 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 5   | K     | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 454   | 301 | 74 | 78 | 1 |         |         |       |
| 5   | O     | 56       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 455   | 303 | 73 | 76 | 3 |         |         |       |
| 5   | Q     | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 457   | 303 | 74 | 78 | 2 |         |         |       |
| 5   | S     | 56       | Total | C   | N  | O  | S | 0       | 3       | 0     |
|     |       |          | 465   | 310 | 74 | 79 | 2 |         |         |       |
| 5   | U     | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 466   | 309 | 76 | 79 | 2 |         |         |       |
| 5   | W     | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 451   | 300 | 74 | 76 | 1 |         |         |       |
| 5   | Y     | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 457   | 303 | 74 | 78 | 2 |         |         |       |
| 5   | 1     | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 447   | 297 | 73 | 76 | 1 |         |         |       |
| 5   | 3     | 56       | Total | C   | N  | O  | S | 0       | 1       | 0     |
|     |       |          | 455   | 303 | 73 | 76 | 3 |         |         |       |
| 5   | 5     | 54       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 434   | 290 | 70 | 73 | 1 |         |         |       |
| 5   | 7     | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 457   | 303 | 74 | 78 | 2 |         |         |       |
| 5   | 9     | 57       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 457   | 303 | 74 | 78 | 2 |         |         |       |

- Molecule 6 is a protein called LH1 beta polypeptide.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | B     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | E     | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 326   | 222 | 50 | 52 | 2 |         |         |       |
| 6   | G     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | J     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | N     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | P     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | R     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 345   | 234 | 53 | 56 | 2 |         |         |       |

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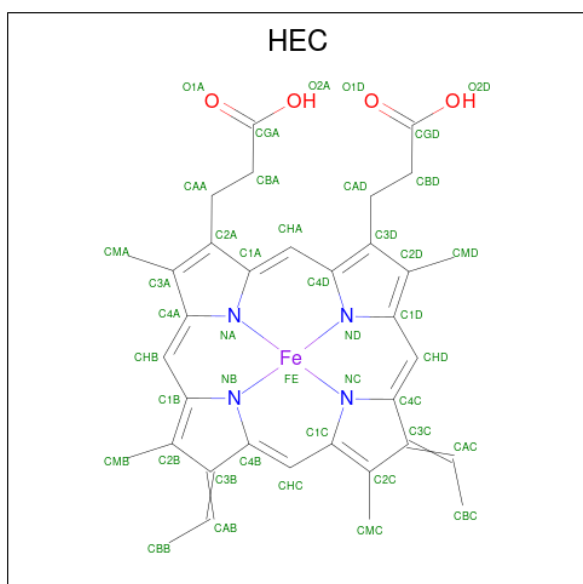
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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | T     | 43       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 360   | 243 | 56 | 59 | 2 |         |         |       |
| 6   | V     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | X     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 345   | 234 | 53 | 56 | 2 |         |         |       |
| 6   | Z     | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 337   | 228 | 52 | 55 | 2 |         |         |       |
| 6   | 2     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 345   | 234 | 53 | 56 | 2 |         |         |       |
| 6   | 4     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | 6     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 351   | 237 | 54 | 58 | 2 |         |         |       |
| 6   | 8     | 41       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 345   | 234 | 53 | 56 | 2 |         |         |       |
| 6   | 0     | 43       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 360   | 243 | 56 | 59 | 2 |         |         |       |

- Molecule 7 is a protein called High-potential iron-sulfur protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | b     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 616   | 383 | 110 | 118 | 5 |         |         |       |

- Molecule 8 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 8   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 8   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 8   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 8   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

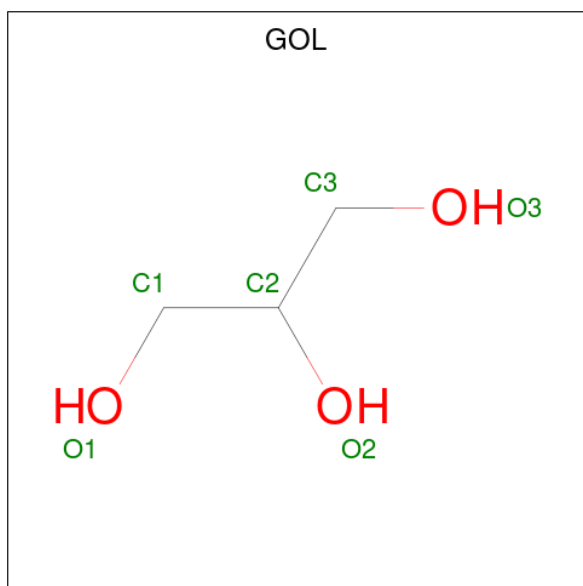
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 9   | C     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | A     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | D     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | F     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | I     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | K     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | O     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | Q     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | S     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | U     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | W     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | Y     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | 1     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | 3     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | 5     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 9   | 7     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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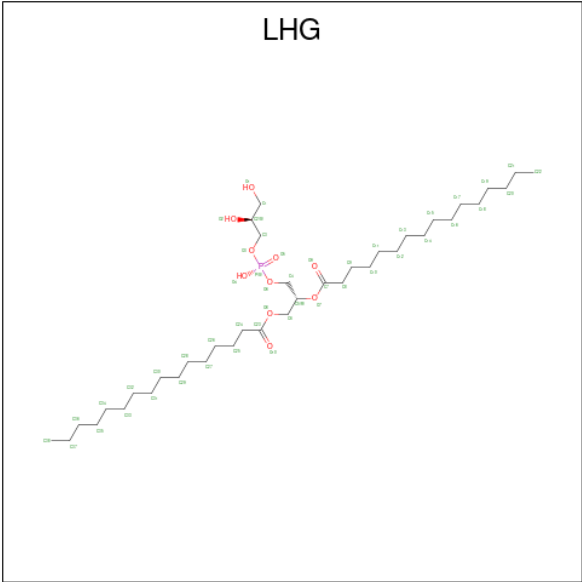
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | 9     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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



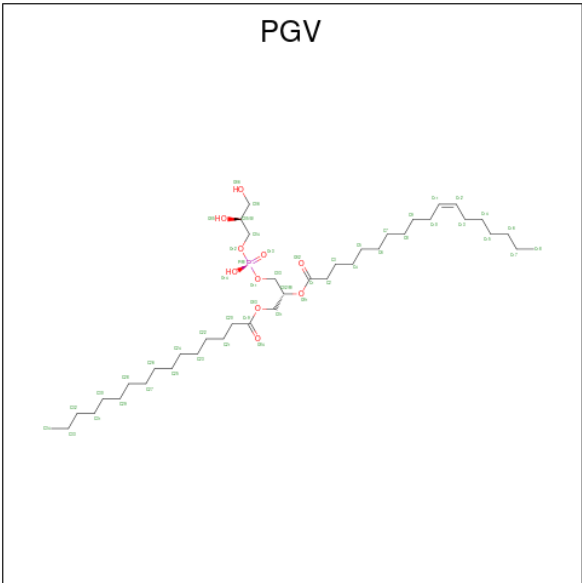
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 10  | H     | 1        | Total | C | O | 0    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

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 11  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 9     | 8 | 1 |         |         |

- Molecule 12 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



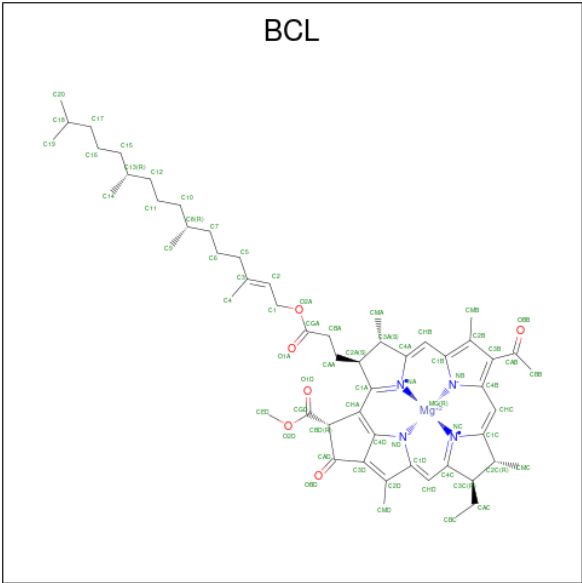
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12  | C     | 1        | Total | C  | O  |   | 0       | 0       |
|     |       |          | 21    | 17 | 4  |   |         |         |
| 12  | L     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 12  | L     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 44    | 33 | 10 | 1 |         |         |
| 12  | M     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 46    | 37 | 8  | 1 |         |         |
| 12  | M     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |         |
| 12  | H     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 36    | 25 | 10 | 1 |         |         |
| 12  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 35    | 24 | 10 | 1 |         |         |
| 12  | 1     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 31    | 20 | 10 | 1 |         |         |
| 12  | 3     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |         |
| 12  | 9     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 33    | 22 | 10 | 1 |         |         |

- Molecule 13 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 13  | L     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |
| 13  | L     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |
| 13  | L     | 1        | Total | C  | Mg | N | O       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6       |         |

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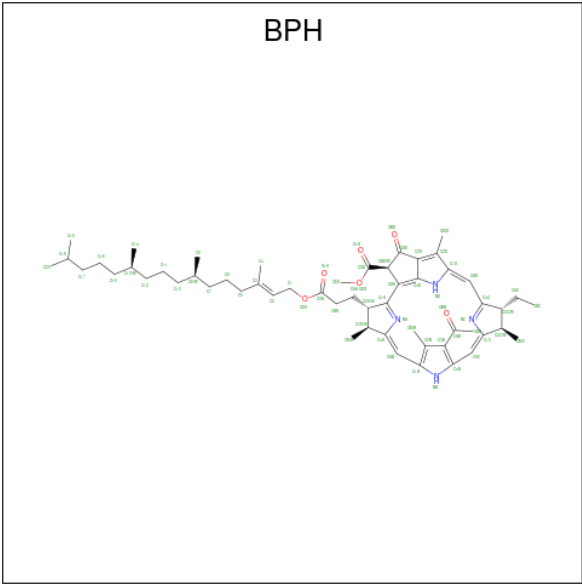
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 13  | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | D     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | D     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | F     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | F     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | I     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | J     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | O     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | P     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | Q     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | Q     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | S     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | S     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | U     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | U     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | W     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 13  | W     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |

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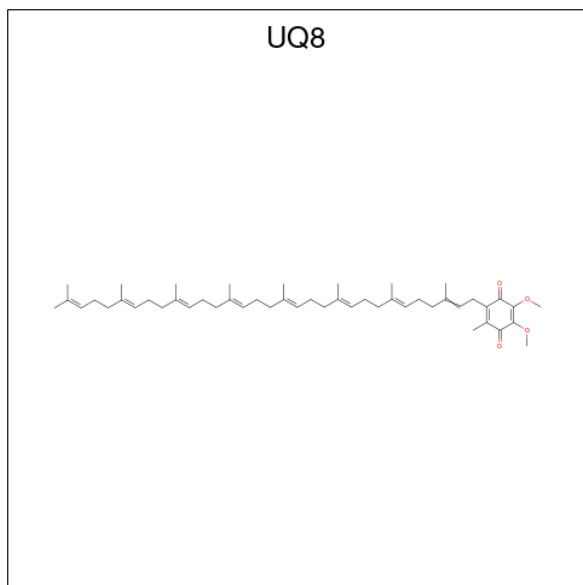
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 13  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | Y     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 1     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 2     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 3     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 4     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 5     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 5     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 7     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |         |
| 13  | 7     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 9     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 13  | 9     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |

- Molecule 14 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



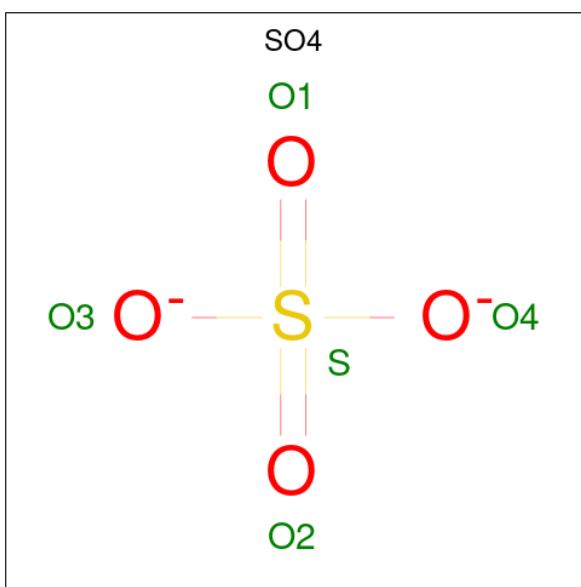
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 14  | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |
| 14  | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |

- Molecule 15 is Ubiquinone-8 (CCD ID: UQ8) (formula: C<sub>49</sub>H<sub>74</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 15  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 29 | 4 |         |         |
| 15  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 53    | 49 | 4 |         |         |
| 15  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 33    | 29 | 4 |         |         |
| 15  | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 14 | 4 |         |         |
| 15  | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 18    | 14 | 4 |         |         |

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

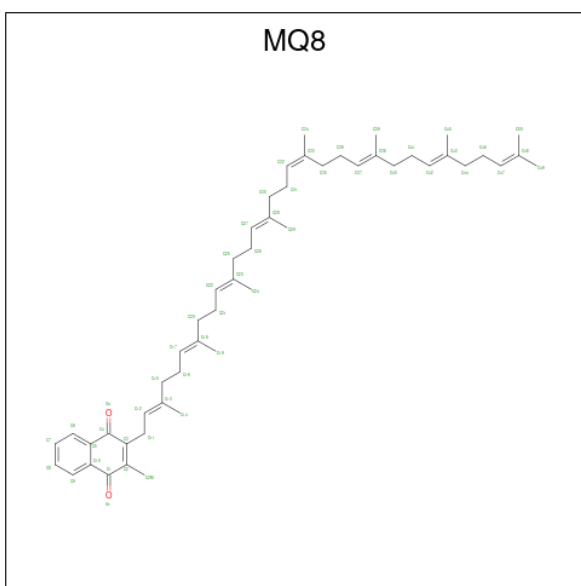


| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 16  | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 17 is FE (III) ION (CCD ID: FE) (formula: Fe).

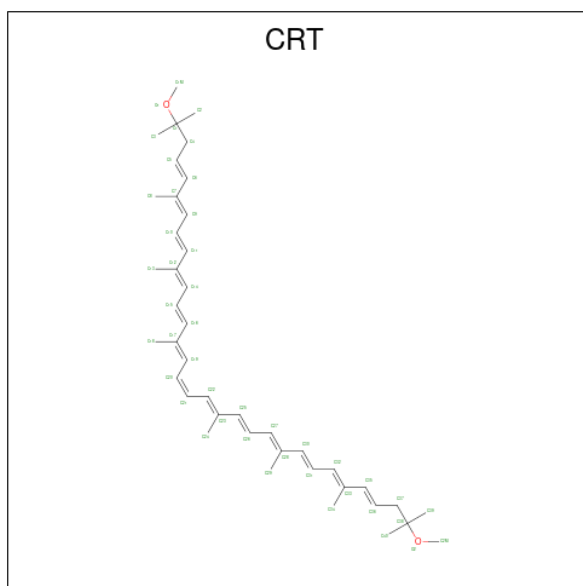
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | M     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 18 is MENAQUINONE 8 (CCD ID: MQ8) (formula: C<sub>51</sub>H<sub>72</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 18  | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 53    | 51 | 2 |         |         |

- Molecule 19 is SPIRILLOXANTHIN (CCD ID: CRT) (formula:  $C_{42}H_{60}O_2$ ).



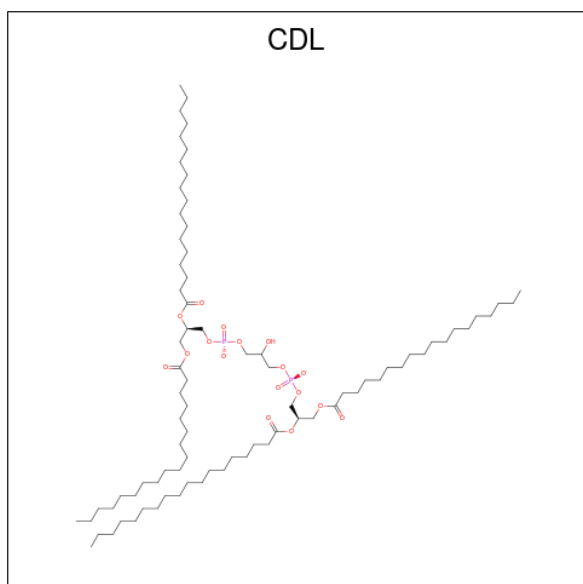
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 19  | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | T     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | V     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | W     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 19  | Z     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | 2     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | 3     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | 4     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | 8     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |
| 19  | 0     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 44    | 42 | 2 |         |         |

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



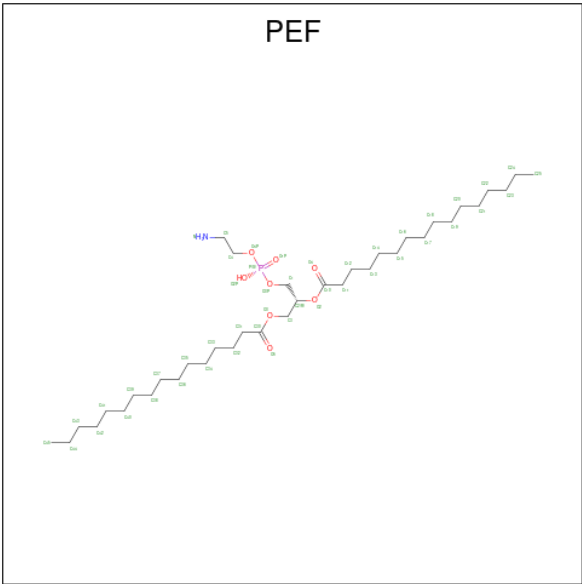
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20  | M     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |         |
| 20  | M     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 39    | 21 | 16 | 2 |         |         |
| 20  | H     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 79    | 60 | 17 | 2 |         |         |
| 20  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 21 | 17 | 2 |         |         |
| 20  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 64    | 45 | 17 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20  | O     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 86    | 67 | 17 | 2 |         |         |
| 20  | S     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 75    | 56 | 17 | 2 |         |         |
| 20  | U     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 62    | 43 | 17 | 2 |         |         |
| 20  | Y     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 40    | 21 | 17 | 2 |         |         |
| 20  | 1     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 13    | 5  | 7  | 1 |         |         |

- Molecule 21 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



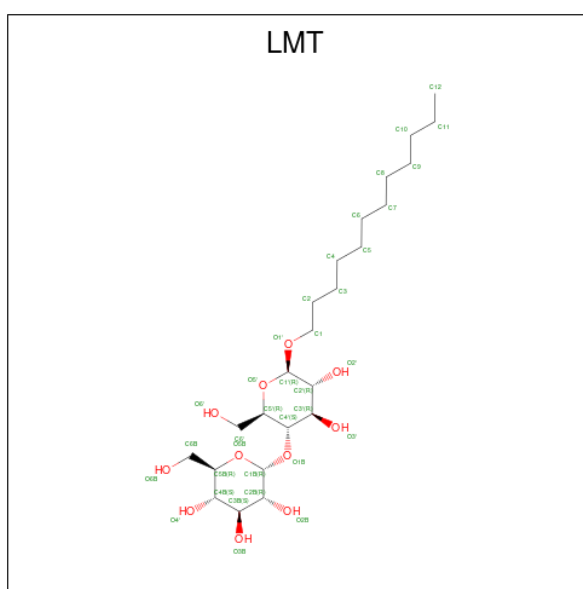
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 21  | M     | 1        | Total | O  | P |   | 0       | 0       |
|     |       |          | 5     | 4  | 1 |   |         |         |
| 21  | M     | 1        | Total | O  | P |   | 0       | 0       |
|     |       |          | 5     | 4  | 1 |   |         |         |
| 21  | M     | 1        | Total | O  | P |   | 0       | 0       |
|     |       |          | 5     | 4  | 1 |   |         |         |
| 21  | H     | 1        | Total | O  | P |   | 0       | 0       |
|     |       |          | 5     | 4  | 1 |   |         |         |
| 21  | I     | 1        | Total | O  | P |   | 0       | 0       |
|     |       |          | 5     | 4  | 1 |   |         |         |
| 21  | K     | 1        | Total | C  | N | O | P       |         |
|     |       |          | 27    | 17 | 1 | 8 | 1       |         |

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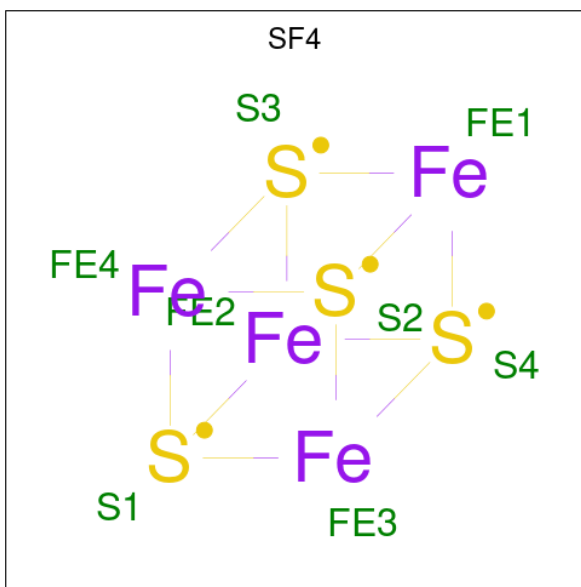
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 21  | W     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 21  | W     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 21  | 1     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 21  | 3     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 22 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 22  | M     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |
| 22  | H     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ) (labeled as "Ligand of Interest" by depositor).

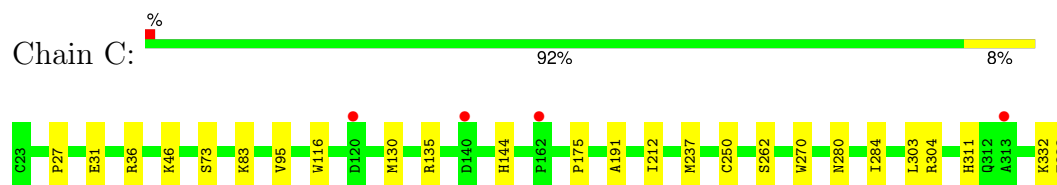


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 23  | b     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

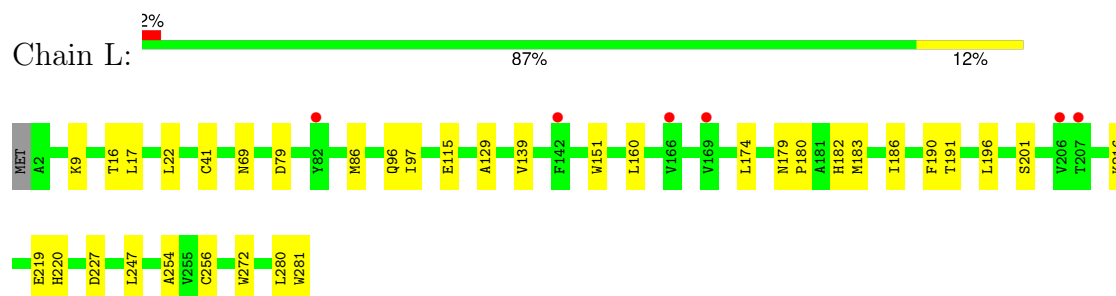
### 3 Residue-property plots [i](#)

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.

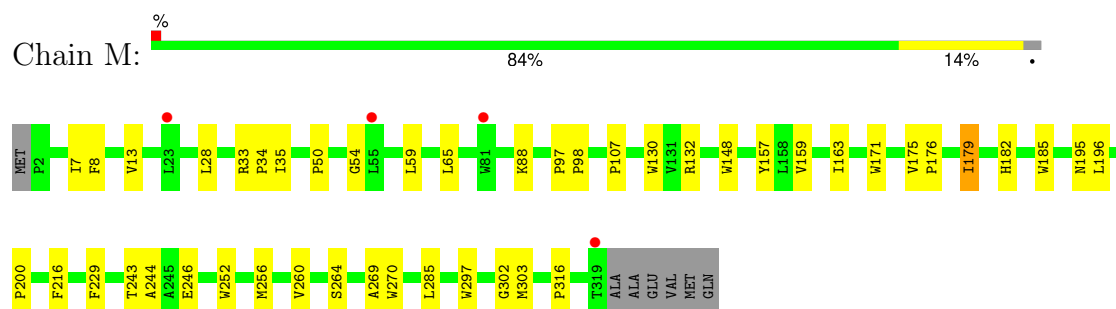
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



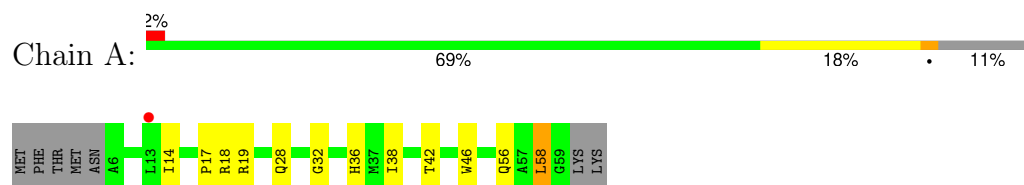
- Molecule 2: Photosynthetic reaction center L subunit



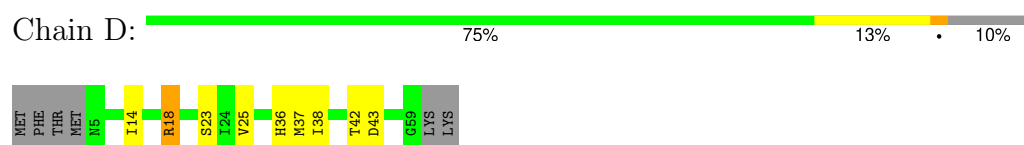
- Molecule 3: Photosynthetic reaction center M subunit



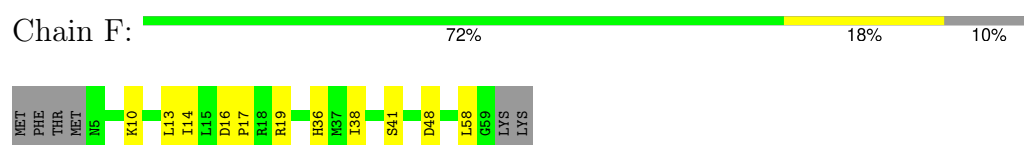
- Molecule 5: LH1 alpha polypeptide



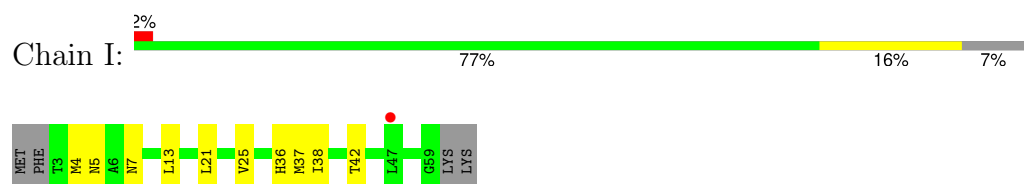
- Molecule 5: LH1 alpha polypeptide



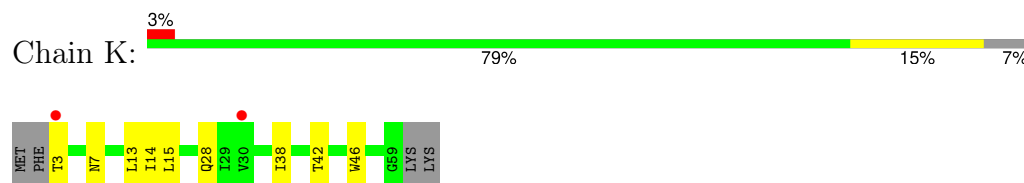
- Molecule 5: LH1 alpha polypeptide



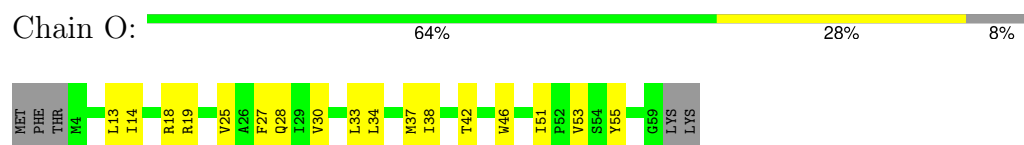
- Molecule 5: LH1 alpha polypeptide



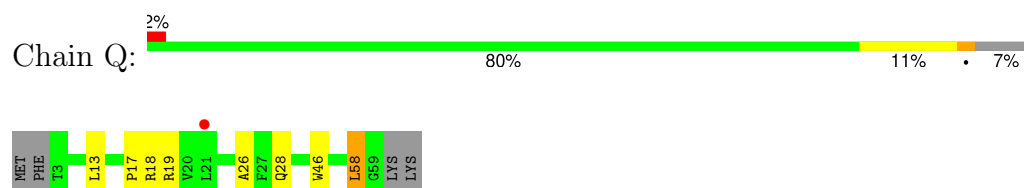
- Molecule 5: LH1 alpha polypeptide



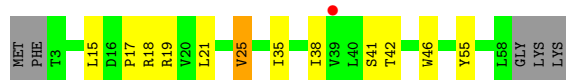
- Molecule 5: LH1 alpha polypeptide



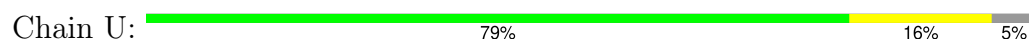
- Molecule 5: LH1 alpha polypeptide



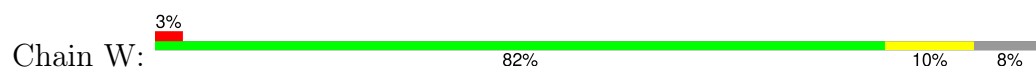
- Molecule 5: LH1 alpha polypeptide



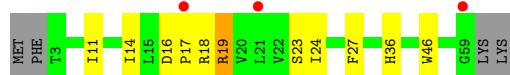
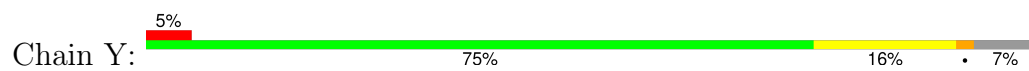
- Molecule 5: LH1 alpha polypeptide



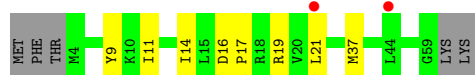
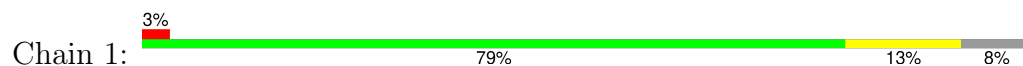
- Molecule 5: LH1 alpha polypeptide



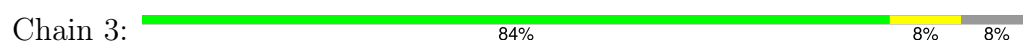
- Molecule 5: LH1 alpha polypeptide



- Molecule 5: LH1 alpha polypeptide



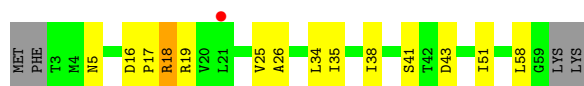
- Molecule 5: LH1 alpha polypeptide



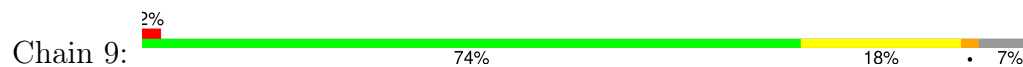
- Molecule 5: LH1 alpha polypeptide



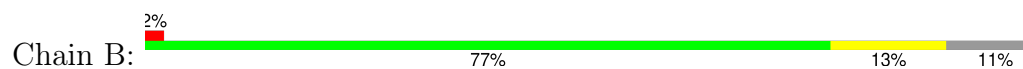
- Molecule 5: LH1 alpha polypeptide



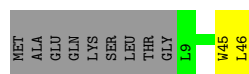
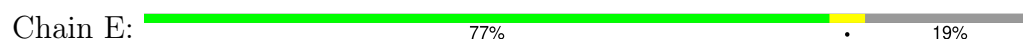
- Molecule 5: LH1 alpha polypeptide



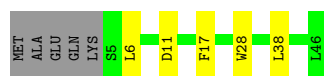
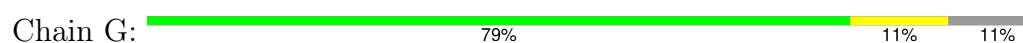
- Molecule 6: LH1 beta polypeptide



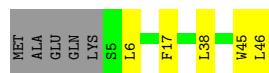
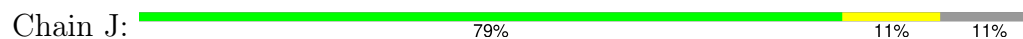
- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide



- Molecule 6: LH1 beta polypeptide

Chain P:  72% 17% 11%



- Molecule 6: LH1 beta polypeptide

Chain R:  74% 11% 13%



- Molecule 6: LH1 beta polypeptide

Chain T:  2% 81% 11% 9%



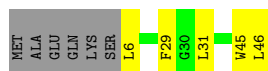
- Molecule 6: LH1 beta polypeptide

Chain V:  81% 9% 11%



- Molecule 6: LH1 beta polypeptide

Chain X:  77% 11% 13%



- Molecule 6: LH1 beta polypeptide

Chain Z:  66% 19% 15%



- Molecule 6: LH1 beta polypeptide

Chain 2:  62% 26% 13%



- Molecule 6: LH1 beta polypeptide

Chain 4:  70% 19% 11%



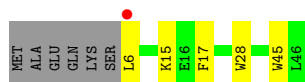
- Molecule 6: LH1 beta polypeptide

Chain 6:  74% 13% 11%



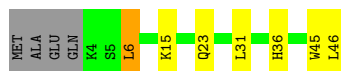
- Molecule 6: LH1 beta polypeptide

Chain 8:  2% 77% 11% 13%



- Molecule 6: LH1 beta polypeptide

Chain 0:  77% 13% 9%



- Molecule 7: High-potential iron-sulfur protein

Chain b:  2% 81% 18%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 96.44Å 183.34Å 123.86Å<br>90.00° 112.58° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.99 – 2.89<br>29.99 – 2.89                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.6 (29.99-2.89)<br>97.5 (29.99-2.89)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.35 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1_3660                                          | Depositor        |
| R, $R_{free}$                                                           | 0.219 , 0.248<br>0.226 , 0.256                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4316 reflections (4.88%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 103.8                                                       | Xtriage          |
| Anisotropy                                                              | 0.047                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 54.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | 0.030 for h,-k,-h-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 27405                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 128.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: BPH, UQ8, GOL, HEC, CRT, SF4, FE, SO4, CDL, LHG, CA, BCL, PEF, MQ8, LMT, PGV

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     | 0.17         | 0/2487       | 0.50        | 0/3396       |
| 2   | L     | 0.17         | 0/2326       | 0.48        | 0/3177       |
| 3   | M     | 0.17         | 0/2658       | 0.45        | 0/3637       |
| 4   | H     | 0.21         | 0/2031       | 0.53        | 0/2769       |
| 5   | 1     | 0.34         | 0/456        | 0.59        | 0/625        |
| 5   | 3     | 0.19         | 0/467        | 0.46        | 0/638        |
| 5   | 5     | 0.48         | 1/443 (0.2%) | 0.78        | 2/607 (0.3%) |
| 5   | 7     | 0.52         | 1/466 (0.2%) | 0.67        | 3/638 (0.5%) |
| 5   | 9     | 0.24         | 0/466        | 0.58        | 0/638        |
| 5   | A     | 0.16         | 0/443        | 0.50        | 0/607        |
| 5   | D     | 0.25         | 0/457        | 0.62        | 2/626 (0.3%) |
| 5   | F     | 0.27         | 0/457        | 0.61        | 0/626        |
| 5   | I     | 0.20         | 0/472        | 0.53        | 0/646        |
| 5   | K     | 0.14         | 0/463        | 0.44        | 0/635        |
| 5   | O     | 0.21         | 0/467        | 0.60        | 0/638        |
| 5   | Q     | 0.16         | 0/466        | 0.53        | 1/638 (0.2%) |
| 5   | S     | 0.25         | 0/480        | 0.55        | 0/658        |
| 5   | U     | 0.28         | 0/475        | 0.62        | 0/649        |
| 5   | W     | 0.23         | 0/460        | 0.58        | 1/629 (0.2%) |
| 5   | Y     | 0.57         | 2/466 (0.4%) | 0.63        | 2/638 (0.3%) |
| 6   | 0     | 0.14         | 0/373        | 0.39        | 0/506        |
| 6   | 2     | 0.15         | 0/358        | 0.39        | 0/487        |
| 6   | 4     | 0.14         | 0/364        | 0.40        | 0/495        |
| 6   | 6     | 0.19         | 0/364        | 0.46        | 0/495        |
| 6   | 8     | 0.15         | 0/358        | 0.44        | 0/487        |
| 6   | B     | 0.12         | 0/364        | 0.38        | 0/495        |
| 6   | E     | 0.15         | 0/339        | 0.42        | 0/461        |
| 6   | G     | 0.12         | 0/364        | 0.39        | 0/495        |
| 6   | J     | 0.16         | 0/364        | 0.43        | 0/495        |
| 6   | N     | 0.17         | 0/364        | 0.38        | 0/495        |
| 6   | P     | 0.12         | 0/364        | 0.33        | 0/495        |
| 6   | R     | 0.13         | 0/358        | 0.33        | 0/487        |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 6   | T     | 0.13         | 0/373          | 0.42        | 0/506           |
| 6   | V     | 0.19         | 0/364          | 0.36        | 0/495           |
| 6   | X     | 0.15         | 0/358          | 0.39        | 0/487           |
| 6   | Z     | 0.13         | 0/350          | 0.33        | 0/476           |
| 7   | b     | 0.17         | 0/631          | 0.48        | 0/859           |
| All | All   | 0.22         | 4/23316 (0.0%) | 0.50        | 11/31831 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | 7     | 18  | ARG  | CG-CD  | -8.82 | 1.25        | 1.52     |
| 5   | Y     | 19  | ARG  | CG-CD  | -8.09 | 1.28        | 1.52     |
| 5   | 5     | 19  | ARG  | CZ-NH1 | 5.88  | 1.41        | 1.32     |
| 5   | Y     | 19  | ARG  | CB-CG  | -5.44 | 1.36        | 1.52     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 5   | 7     | 18  | ARG  | CB-CG-CD  | -8.19 | 92.46       | 111.30   |
| 5   | 5     | 19  | ARG  | CG-CD-NE  | -6.69 | 97.28       | 112.00   |
| 5   | Y     | 19  | ARG  | CG-CD-NE  | -5.99 | 98.82       | 112.00   |
| 5   | 7     | 18  | ARG  | NE-CZ-NH2 | -5.79 | 113.99      | 119.20   |
| 5   | 7     | 18  | ARG  | CD-NE-CZ  | -5.77 | 116.32      | 124.40   |
| 5   | Y     | 19  | ARG  | CD-NE-CZ  | -5.45 | 116.78      | 124.40   |
| 5   | 5     | 19  | ARG  | NE-CZ-NH2 | -5.37 | 114.36      | 119.20   |
| 5   | D     | 18  | ARG  | NE-CZ-NH2 | 5.23  | 123.91      | 119.20   |
| 5   | Q     | 18  | ARG  | CB-CA-C   | 5.17  | 119.07      | 110.90   |
| 5   | W     | 18  | ARG  | NE-CZ-NH1 | -5.08 | 116.42      | 121.50   |
| 5   | D     | 18  | ARG  | CD-NE-CZ  | -5.04 | 117.34      | 124.40   |

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     | 2417  | 0        | 2328     | 19      | 0            |
| 2   | L     | 2236  | 0        | 2201     | 33      | 0            |
| 3   | M     | 2555  | 0        | 2528     | 39      | 0            |
| 4   | H     | 1973  | 0        | 1968     | 37      | 0            |
| 5   | 1     | 447   | 0        | 468      | 18      | 0            |
| 5   | 3     | 455   | 0        | 484      | 6       | 0            |
| 5   | 5     | 434   | 0        | 460      | 22      | 0            |
| 5   | 7     | 457   | 0        | 482      | 22      | 0            |
| 5   | 9     | 457   | 0        | 482      | 14      | 0            |
| 5   | A     | 434   | 0        | 460      | 14      | 0            |
| 5   | D     | 445   | 0        | 471      | 12      | 0            |
| 5   | F     | 445   | 0        | 471      | 12      | 0            |
| 5   | I     | 460   | 0        | 487      | 10      | 0            |
| 5   | K     | 454   | 0        | 475      | 8       | 0            |
| 5   | O     | 455   | 0        | 484      | 18      | 0            |
| 5   | Q     | 457   | 0        | 482      | 8       | 0            |
| 5   | S     | 465   | 0        | 494      | 18      | 0            |
| 5   | U     | 466   | 0        | 495      | 18      | 0            |
| 5   | W     | 451   | 0        | 479      | 5       | 0            |
| 5   | Y     | 457   | 0        | 482      | 14      | 0            |
| 6   | 0     | 360   | 0        | 352      | 9       | 0            |
| 6   | 2     | 345   | 0        | 334      | 15      | 0            |
| 6   | 4     | 351   | 0        | 339      | 9       | 0            |
| 6   | 6     | 351   | 0        | 339      | 9       | 0            |
| 6   | 8     | 345   | 0        | 334      | 5       | 0            |
| 6   | B     | 351   | 0        | 339      | 7       | 0            |
| 6   | E     | 326   | 0        | 313      | 1       | 0            |
| 6   | G     | 351   | 0        | 339      | 6       | 0            |
| 6   | J     | 351   | 0        | 339      | 5       | 0            |
| 6   | N     | 351   | 0        | 339      | 10      | 0            |
| 6   | P     | 351   | 0        | 339      | 8       | 0            |
| 6   | R     | 345   | 0        | 334      | 6       | 0            |
| 6   | T     | 360   | 0        | 352      | 6       | 0            |
| 6   | V     | 351   | 0        | 339      | 6       | 0            |
| 6   | X     | 345   | 0        | 334      | 7       | 0            |
| 6   | Z     | 337   | 0        | 323      | 15      | 0            |
| 7   | b     | 616   | 0        | 589      | 11      | 0            |
| 8   | C     | 172   | 0        | 120      | 5       | 0            |
| 9   | 1     | 1     | 0        | 0        | 0       | 0            |
| 9   | 3     | 1     | 0        | 0        | 0       | 0            |
| 9   | 5     | 1     | 0        | 0        | 0       | 0            |
| 9   | 7     | 1     | 0        | 0        | 0       | 0            |
| 9   | 9     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | A     | 1     | 0        | 0        | 0       | 0            |
| 9   | C     | 1     | 0        | 0        | 0       | 0            |
| 9   | D     | 1     | 0        | 0        | 0       | 0            |
| 9   | F     | 1     | 0        | 0        | 0       | 0            |
| 9   | I     | 1     | 0        | 0        | 0       | 0            |
| 9   | K     | 1     | 0        | 0        | 0       | 0            |
| 9   | O     | 1     | 0        | 0        | 0       | 0            |
| 9   | Q     | 1     | 0        | 0        | 0       | 0            |
| 9   | S     | 1     | 0        | 0        | 0       | 0            |
| 9   | U     | 1     | 0        | 0        | 0       | 0            |
| 9   | W     | 1     | 0        | 0        | 0       | 0            |
| 9   | Y     | 1     | 0        | 0        | 0       | 0            |
| 10  | C     | 6     | 0        | 8        | 1       | 0            |
| 10  | H     | 6     | 0        | 8        | 0       | 0            |
| 11  | C     | 9     | 0        | 12       | 0       | 0            |
| 12  | 1     | 31    | 0        | 32       | 1       | 0            |
| 12  | 3     | 51    | 0        | 76       | 6       | 0            |
| 12  | 9     | 33    | 0        | 36       | 5       | 0            |
| 12  | C     | 21    | 0        | 23       | 0       | 0            |
| 12  | D     | 35    | 0        | 40       | 2       | 0            |
| 12  | H     | 36    | 0        | 42       | 2       | 0            |
| 12  | L     | 87    | 0        | 120      | 12      | 0            |
| 12  | M     | 83    | 0        | 116      | 8       | 0            |
| 13  | 1     | 66    | 0        | 74       | 5       | 0            |
| 13  | 2     | 66    | 0        | 74       | 10      | 0            |
| 13  | 3     | 66    | 0        | 74       | 3       | 0            |
| 13  | 4     | 66    | 0        | 74       | 6       | 0            |
| 13  | 5     | 132   | 0        | 148      | 6       | 0            |
| 13  | 7     | 127   | 0        | 135      | 10      | 0            |
| 13  | 9     | 132   | 0        | 148      | 8       | 0            |
| 13  | A     | 132   | 0        | 148      | 9       | 0            |
| 13  | D     | 132   | 0        | 148      | 4       | 0            |
| 13  | F     | 132   | 0        | 148      | 11      | 0            |
| 13  | I     | 66    | 0        | 74       | 3       | 0            |
| 13  | J     | 66    | 0        | 74       | 3       | 0            |
| 13  | K     | 132   | 0        | 148      | 8       | 0            |
| 13  | L     | 198   | 0        | 222      | 12      | 0            |
| 13  | M     | 66    | 0        | 74       | 0       | 0            |
| 13  | O     | 66    | 0        | 74       | 6       | 0            |
| 13  | P     | 66    | 0        | 74       | 5       | 0            |
| 13  | Q     | 132   | 0        | 148      | 9       | 0            |
| 13  | S     | 132   | 0        | 148      | 10      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | U     | 132   | 0        | 148      | 12      | 0            |
| 13  | W     | 132   | 0        | 148      | 11      | 0            |
| 13  | Y     | 132   | 0        | 148      | 16      | 0            |
| 14  | L     | 65    | 0        | 74       | 4       | 0            |
| 14  | M     | 65    | 0        | 74       | 7       | 0            |
| 15  | L     | 137   | 0        | 167      | 19      | 0            |
| 15  | M     | 18    | 0        | 15       | 1       | 0            |
| 16  | L     | 5     | 0        | 0        | 0       | 0            |
| 17  | M     | 1     | 0        | 0        | 0       | 0            |
| 18  | M     | 53    | 0        | 72       | 5       | 0            |
| 19  | O     | 44    | 0        | 60       | 5       | 0            |
| 19  | 2     | 44    | 0        | 60       | 6       | 0            |
| 19  | 3     | 44    | 0        | 60       | 2       | 0            |
| 19  | 4     | 44    | 0        | 60       | 6       | 0            |
| 19  | 8     | 44    | 0        | 60       | 5       | 0            |
| 19  | A     | 44    | 0        | 60       | 8       | 0            |
| 19  | B     | 44    | 0        | 60       | 6       | 0            |
| 19  | G     | 44    | 0        | 60       | 5       | 0            |
| 19  | J     | 44    | 0        | 60       | 2       | 0            |
| 19  | M     | 44    | 0        | 60       | 7       | 0            |
| 19  | N     | 44    | 0        | 60       | 4       | 0            |
| 19  | O     | 44    | 0        | 60       | 0       | 0            |
| 19  | P     | 44    | 0        | 60       | 4       | 0            |
| 19  | T     | 44    | 0        | 60       | 3       | 0            |
| 19  | V     | 44    | 0        | 60       | 3       | 0            |
| 19  | W     | 44    | 0        | 60       | 1       | 0            |
| 19  | Z     | 44    | 0        | 60       | 5       | 0            |
| 20  | 1     | 13    | 0        | 7        | 0       | 0            |
| 20  | D     | 104   | 0        | 96       | 10      | 0            |
| 20  | H     | 79    | 0        | 105      | 6       | 0            |
| 20  | M     | 139   | 0        | 184      | 7       | 0            |
| 20  | O     | 86    | 0        | 119      | 13      | 0            |
| 20  | S     | 75    | 0        | 94       | 12      | 0            |
| 20  | U     | 62    | 0        | 68       | 9       | 0            |
| 20  | Y     | 40    | 0        | 24       | 3       | 0            |
| 21  | 1     | 5     | 0        | 0        | 2       | 0            |
| 21  | 3     | 5     | 0        | 0        | 0       | 0            |
| 21  | H     | 5     | 0        | 0        | 0       | 0            |
| 21  | I     | 5     | 0        | 0        | 0       | 0            |
| 21  | K     | 27    | 0        | 27       | 2       | 0            |
| 21  | M     | 15    | 0        | 0        | 0       | 0            |
| 21  | W     | 10    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | H     | 35    | 0        | 46       | 8       | 0            |
| 22  | M     | 35    | 0        | 46       | 0       | 0            |
| 23  | b     | 8     | 0        | 0        | 0       | 0            |
| All | All   | 27405 | 0        | 28180    | 542     | 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 10.

All (542) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:16:ASP:HB3    | 5:1:19:ARG:HE     | 1.25                     | 1.00              |
| 5:U:11:ILE:HD12   | 5:U:14:ILE:HD11   | 1.48                     | 0.94              |
| 4:H:258:LEU:O     | 5:5:19:ARG:NH2    | 2.10                     | 0.85              |
| 5:D:18:ARG:NH1    | 20:D:105:CDL:OB4  | 2.13                     | 0.82              |
| 2:L:96:GLN:HG2    | 15:L:309:UQ8:H4M  | 1.63                     | 0.80              |
| 5:S:19:ARG:HH11   | 20:S:104:CDL:PB2  | 2.05                     | 0.79              |
| 5:U:18:ARG:NH1    | 20:U:104:CDL:O1   | 2.15                     | 0.78              |
| 5:1:11:ILE:HD12   | 5:1:14:ILE:HD11   | 1.65                     | 0.78              |
| 5:D:18:ARG:NH2    | 20:D:105:CDL:OA3  | 2.16                     | 0.78              |
| 5:5:16:ASP:HB3    | 5:5:19:ARG:NH1    | 2.00                     | 0.76              |
| 5:1:19:ARG:NH1    | 21:1:103:PEF:O2P  | 2.19                     | 0.76              |
| 5:A:19:ARG:NH2    | 20:D:105:CDL:O1   | 2.16                     | 0.76              |
| 5:1:16:ASP:HB3    | 5:1:19:ARG:NE     | 2.02                     | 0.74              |
| 6:6:6:LEU:CB      | 5:7:18:ARG:HH22   | 1.99                     | 0.74              |
| 4:H:44:ASP:H      | 12:9:104:PGV:H062 | 1.52                     | 0.74              |
| 5:U:18:ARG:HH12   | 20:U:104:CDL:C1   | 2.01                     | 0.73              |
| 13:P:102:BCL:H42  | 13:Q:101:BCL:H202 | 1.70                     | 0.72              |
| 2:L:17:LEU:O      | 4:H:258:LEU:N     | 2.21                     | 0.72              |
| 5:U:18:ARG:NH1    | 20:U:104:CDL:C1   | 2.53                     | 0.72              |
| 6:6:6:LEU:HB2     | 5:7:18:ARG:HH22   | 1.57                     | 0.70              |
| 6:4:17:PHE:HA     | 19:4:101:CRT:H6   | 1.74                     | 0.68              |
| 4:H:258:LEU:O     | 5:5:19:ARG:CZ     | 2.41                     | 0.68              |
| 4:H:45:ARG:NH1    | 5:A:14:ILE:O      | 2.28                     | 0.67              |
| 5:D:25:VAL:HG11   | 20:D:105:CDL:H521 | 1.75                     | 0.67              |
| 5:S:18:ARG:HH22   | 5:S:19:ARG:HE     | 1.42                     | 0.67              |
| 2:L:86[B]:MET:HG2 | 5:7:41:SER:HB3    | 1.77                     | 0.67              |
| 5:K:15:LEU:HD23   | 5:O:18:ARG:HG3    | 1.77                     | 0.66              |
| 6:2:17:PHE:HA     | 19:2:101:CRT:H6   | 1.76                     | 0.66              |
| 5:5:16:ASP:OD1    | 5:5:18:ARG:HG2    | 1.96                     | 0.66              |
| 3:M:28:LEU:HD12   | 3:M:54:GLY:HA2    | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:308:PGV:H202 | 12:M:410:PGV:H222 | 1.79                     | 0.64              |
| 5:D:14:ILE:HD11   | 19:G:101:CRT:H23  | 1.77                     | 0.64              |
| 6:2:29:PHE:CE1    | 13:2:102:BCL:H2   | 2.32                     | 0.64              |
| 3:M:130:TRP:HZ3   | 20:O:104:CDL:H511 | 1.62                     | 0.64              |
| 19:3:103:CRT:H371 | 13:7:101:BCL:HMB2 | 1.78                     | 0.64              |
| 13:W:104:BCL:H51  | 13:Y:101:BCL:H162 | 1.78                     | 0.64              |
| 2:L:180:PRO:HA    | 2:L:183:MET:HE3   | 1.80                     | 0.64              |
| 4:H:45:ARG:HD3    | 4:H:53:VAL:HG11   | 1.80                     | 0.63              |
| 5:F:10:LYS:NZ     | 6:G:11:ASP:OD1    | 2.30                     | 0.63              |
| 13:U:103:BCL:H2   | 6:V:29:PHE:CE1    | 2.34                     | 0.63              |
| 5:1:16:ASP:CB     | 5:1:19:ARG:HH11   | 2.13                     | 0.62              |
| 13:Y:103:BCL:H2   | 6:Z:29:PHE:CE1    | 2.35                     | 0.62              |
| 6:4:29:PHE:CE1    | 13:4:102:BCL:H11  | 2.35                     | 0.62              |
| 14:L:303:BPH:HBB3 | 14:L:303:BPH:HHC  | 1.82                     | 0.61              |
| 12:L:307:PGV:H62  | 12:D:106:PGV:H62  | 1.82                     | 0.61              |
| 12:3:105:PGV:H251 | 5:5:37:MET:HG3    | 1.83                     | 0.61              |
| 5:Y:18:ARG:HH12   | 20:Y:104:CDL:CB2  | 2.14                     | 0.60              |
| 2:L:17:LEU:HD22   | 4:H:258:LEU:HD11  | 1.84                     | 0.60              |
| 12:L:308:PGV:H62  | 4:H:258:LEU:HD12  | 1.83                     | 0.60              |
| 13:4:102:BCL:H42  | 13:5:101:BCL:H162 | 1.83                     | 0.60              |
| 5:O:25:VAL:HG11   | 20:O:104:CDL:H331 | 1.82                     | 0.60              |
| 1:C:116:TRP:NE1   | 7:b:79:THR:OG1    | 2.32                     | 0.60              |
| 3:M:200:PRO:HB3   | 12:H:303:PGV:H22  | 1.84                     | 0.59              |
| 5:Q:28:GLN:HB3    | 13:Q:101:BCL:H42  | 1.83                     | 0.59              |
| 13:S:101:BCL:HMA3 | 13:S:101:BCL:H203 | 1.85                     | 0.59              |
| 2:L:16:THR:OG1    | 4:H:257:PRO:HB3   | 2.03                     | 0.59              |
| 5:S:18:ARG:HH22   | 5:S:19:ARG:NE     | 2.00                     | 0.59              |
| 6:2:29:PHE:CD1    | 13:2:102:BCL:H2   | 2.37                     | 0.59              |
| 5:Y:36:HIS:CE1    | 13:Y:103:BCL:HMD3 | 2.38                     | 0.58              |
| 6:Z:17:PHE:HA     | 19:Z:101:CRT:H6   | 1.85                     | 0.58              |
| 4:H:45:ARG:NH2    | 6:B:6:LEU:O       | 2.33                     | 0.58              |
| 19:B:101:CRT:H1M1 | 5:9:14:ILE:HD11   | 1.85                     | 0.58              |
| 6:6:6:LEU:HD22    | 5:7:18:ARG:HH12   | 1.68                     | 0.58              |
| 18:M:404:MQ8:H241 | 20:H:305:CDL:H772 | 1.85                     | 0.58              |
| 20:O:104:CDL:H531 | 20:O:104:CDL:H371 | 1.85                     | 0.58              |
| 20:H:305:CDL:OA3  | 5:A:19:ARG:NH2    | 2.36                     | 0.58              |
| 6:P:17:PHE:HA     | 19:P:101:CRT:H6   | 1.86                     | 0.57              |
| 19:2:101:CRT:H342 | 13:3:101:BCL:HBA2 | 1.85                     | 0.57              |
| 3:M:157:TYR:CZ    | 19:M:405:CRT:H293 | 2.39                     | 0.57              |
| 6:B:45:TRP:CD1    | 6:B:46:LEU:HG     | 2.40                     | 0.57              |
| 19:B:101:CRT:H372 | 5:D:36:HIS:CG     | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:45:ARG:NH2    | 4:H:53:VAL:HG21   | 2.20                     | 0.57              |
| 5:1:16:ASP:HB2    | 5:1:19:ARG:HH11   | 1.69                     | 0.57              |
| 5:Y:11:ILE:HD12   | 5:Y:14:ILE:HD11   | 1.85                     | 0.57              |
| 5:U:18:ARG:NH1    | 20:U:104:CDL:H1   | 2.19                     | 0.57              |
| 19:A:104:CRT:H27  | 13:D:103:BCL:O1A  | 2.05                     | 0.56              |
| 5:1:16:ASP:CB     | 5:1:19:ARG:HE     | 2.11                     | 0.56              |
| 13:S:103:BCL:H42  | 13:U:101:BCL:H151 | 1.87                     | 0.56              |
| 5:Y:19:ARG:NH2    | 20:Y:104:CDL:O1   | 2.38                     | 0.56              |
| 13:L:305:BCL:H161 | 15:L:311:UQ8:H3M  | 1.86                     | 0.56              |
| 6:B:21:PHE:HA     | 19:B:101:CRT:H14  | 1.87                     | 0.56              |
| 5:D:18:ARG:NH1    | 20:D:105:CDL:HB21 | 2.21                     | 0.56              |
| 5:F:16:ASP:HB3    | 5:F:19:ARG:HE     | 1.71                     | 0.56              |
| 5:7:35:ILE:HG12   | 19:8:101:CRT:H403 | 1.88                     | 0.56              |
| 7:b:33:ARG:NH1    | 7:b:78:TRP:O      | 2.38                     | 0.56              |
| 5:7:5:ASN:ND2     | 6:0:23:GLN:OE1    | 2.38                     | 0.55              |
| 20:H:305:CDL:H862 | 20:H:305:CDL:H592 | 1.87                     | 0.55              |
| 13:F:103:BCL:O1A  | 19:G:101:CRT:H27  | 2.07                     | 0.55              |
| 5:W:46:TRP:CE2    | 13:W:101:BCL:H2C  | 2.41                     | 0.55              |
| 5:9:53:VAL:CG2    | 5:9:58:LEU:HD11   | 2.36                     | 0.55              |
| 3:M:65:LEU:HD21   | 14:M:402:BPH:H112 | 1.89                     | 0.55              |
| 3:M:171:TRP:HZ2   | 19:M:405:CRT:H402 | 1.72                     | 0.55              |
| 19:A:104:CRT:H27  | 13:D:103:BCL:H12  | 1.88                     | 0.55              |
| 5:D:38:ILE:O      | 5:D:42:THR:HG23   | 2.07                     | 0.55              |
| 5:7:16:ASP:OD1    | 5:7:18:ARG:HG2    | 2.07                     | 0.55              |
| 2:L:151:TRP:HE1   | 15:L:309:UQ8:H3MA | 1.71                     | 0.55              |
| 14:M:402:BPH:HBC3 | 14:M:402:BPH:HHD  | 1.88                     | 0.55              |
| 5:I:21:LEU:HD21   | 19:J:101:CRT:C14  | 2.37                     | 0.55              |
| 2:L:190:PHE:HB3   | 14:M:402:BPH:CBB  | 2.37                     | 0.54              |
| 5:7:43:ASP:HB2    | 5:9:48:ASP:OD1    | 2.07                     | 0.54              |
| 5:W:36:HIS:CE1    | 13:W:104:BCL:HMD3 | 2.42                     | 0.54              |
| 5:5:7:ASN:HB3     | 5:5:10:LYS:HD2    | 1.88                     | 0.54              |
| 1:C:27:PRO:HG3    | 12:3:105:PGV:H32  | 1.90                     | 0.54              |
| 4:H:258:LEU:HA    | 5:5:19:ARG:NH2    | 2.23                     | 0.54              |
| 19:2:101:CRT:H27  | 13:2:102:BCL:O1A  | 2.07                     | 0.54              |
| 2:L:201:SER:HG    | 3:M:270:TRP:CD1   | 2.25                     | 0.54              |
| 13:W:104:BCL:H2C  | 6:X:45:TRP:CE2    | 2.43                     | 0.54              |
| 19:Z:101:CRT:H292 | 13:1:101:BCL:H51  | 1.90                     | 0.54              |
| 4:H:58:PHE:HB3    | 20:D:105:CDL:H122 | 1.88                     | 0.53              |
| 19:A:104:CRT:H371 | 13:F:101:BCL:HMB2 | 1.90                     | 0.53              |
| 5:1:16:ASP:HB2    | 5:1:19:ARG:NH1    | 2.22                     | 0.53              |
| 5:D:43:ASP:N      | 5:F:48:ASP:OD1    | 2.37                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:R:44:PRO:O      | 5:S:55:TYR:OH     | 2.26                     | 0.53              |
| 5:U:25:VAL:HG11   | 20:U:104:CDL:H122 | 1.91                     | 0.53              |
| 13:Q:101:BCL:H141 | 13:Q:101:BCL:H203 | 1.89                     | 0.53              |
| 3:M:59:LEU:HD13   | 5:Q:26:ALA:HA     | 1.90                     | 0.53              |
| 5:S:19:ARG:NH1    | 20:S:104:CDL:OB5  | 2.42                     | 0.53              |
| 13:U:103:BCL:H92  | 6:V:32:VAL:HG12   | 1.91                     | 0.53              |
| 19:V:101:CRT:H371 | 13:W:101:BCL:HMB2 | 1.90                     | 0.53              |
| 13:Y:103:BCL:H2   | 6:Z:29:PHE:CD1    | 2.44                     | 0.53              |
| 6:N:43:ARG:HG3    | 5:O:55:TYR:CZ     | 2.44                     | 0.53              |
| 5:W:13:LEU:O      | 6:X:6:LEU:HB3     | 2.09                     | 0.52              |
| 6:4:40:TRP:CE2    | 13:4:102:BCL:H18  | 2.44                     | 0.52              |
| 2:L:182:HIS:CE1   | 2:L:186:ILE:HD11  | 2.44                     | 0.52              |
| 20:D:104:CDL:OB4  | 5:F:19:ARG:HG2    | 2.09                     | 0.52              |
| 13:A:103:BCL:H2C  | 6:B:45:TRP:CE2    | 2.45                     | 0.52              |
| 19:4:101:CRT:H27  | 13:4:102:BCL:O1A  | 2.10                     | 0.52              |
| 5:7:51:ILE:HD11   | 5:9:58:LEU:O      | 2.10                     | 0.52              |
| 13:K:103:BCL:H202 | 6:N:40:TRP:CE2    | 2.45                     | 0.52              |
| 5:F:36:HIS:CE1    | 13:F:103:BCL:HMD3 | 2.44                     | 0.52              |
| 5:U:23:SER:OG     | 20:U:104:CDL:H712 | 2.10                     | 0.52              |
| 5:O:19:ARG:NH1    | 20:O:104:CDL:PB2  | 2.83                     | 0.52              |
| 5:S:19:ARG:NH2    | 20:S:104:CDL:OB9  | 2.43                     | 0.52              |
| 6:2:43:ARG:HG3    | 5:3:55:TYR:CZ     | 2.44                     | 0.52              |
| 1:C:175:PRO:HB2   | 5:S:41[B]:SER:O   | 2.10                     | 0.51              |
| 5:Y:23:SER:HB3    | 13:1:101:BCL:H172 | 1.91                     | 0.51              |
| 3:M:34:PRO:HG3    | 3:M:50:PRO:HD3    | 1.92                     | 0.51              |
| 1:C:284:ILE:HG21  | 1:C:304:ARG:HB3   | 1.93                     | 0.51              |
| 12:L:307:PGV:H82  | 5:D:37:MET:HE1    | 1.92                     | 0.51              |
| 15:L:309:UQ8:H28  | 5:7:26:ALA:HB1    | 1.93                     | 0.51              |
| 4:H:35:LYS:HB3    | 4:H:61:LEU:HD22   | 1.91                     | 0.51              |
| 1:C:135:ARG:HB3   | 1:C:332:LYS:HG3   | 1.91                     | 0.51              |
| 1:C:175:PRO:HB2   | 5:S:41[A]:SER:O   | 2.10                     | 0.51              |
| 13:5:101:BCL:H43  | 6:6:28:TRP:CZ2    | 2.46                     | 0.51              |
| 5:D:23:SER:OG     | 20:D:105:CDL:OA9  | 2.25                     | 0.51              |
| 13:L:302:BCL:H152 | 14:L:303:BPH:H3A  | 1.92                     | 0.51              |
| 3:M:8:PHE:CD1     | 20:M:412:CDL:H512 | 2.45                     | 0.51              |
| 3:M:256:MET:CE    | 18:M:404:MQ8:H142 | 2.41                     | 0.51              |
| 19:B:101:CRT:C1M  | 5:9:14:ILE:HD11   | 2.41                     | 0.51              |
| 1:C:280:ASN:OD1   | 1:C:304:ARG:HB2   | 2.11                     | 0.51              |
| 13:F:103:BCL:H13  | 13:F:103:BCL:HBB2 | 1.93                     | 0.51              |
| 1:C:191:ALA:HB3   | 1:C:237:MET:HE3   | 1.93                     | 0.50              |
| 13:A:103:BCL:H12  | 19:B:101:CRT:H27  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:48:ARG:HE     | 6:0:6:LEU:HD12    | 1.77                     | 0.50              |
| 13:9:103:BCL:O1A  | 19:0:101:CRT:H27  | 2.11                     | 0.50              |
| 5:3:51:ILE:HD13   | 5:5:58:LEU:HD23   | 1.92                     | 0.50              |
| 5:K:28:GLN:HB3    | 13:K:101:BCL:H12  | 1.93                     | 0.50              |
| 5:S:21:LEU:O      | 5:S:25:VAL:HG13   | 2.12                     | 0.50              |
| 6:2:21:PHE:CD2    | 19:2:101:CRT:H14  | 2.47                     | 0.50              |
| 4:H:17:TRP:CD1    | 22:H:304:LMT:H61  | 2.47                     | 0.50              |
| 2:L:9:LYS:HA      | 4:H:87:VAL:HG13   | 1.93                     | 0.50              |
| 5:U:11:ILE:CD1    | 5:U:14:ILE:HD11   | 2.32                     | 0.50              |
| 6:2:40:TRP:CE2    | 13:2:102:BCL:H18  | 2.47                     | 0.50              |
| 13:2:102:BCL:HED3 | 13:2:102:BCL:HBA2 | 1.93                     | 0.50              |
| 2:L:17:LEU:N      | 2:L:115:GLU:OE1   | 2.38                     | 0.49              |
| 6:G:17:PHE:HB2    | 19:G:101:CRT:H21A | 1.94                     | 0.49              |
| 13:9:103:BCL:H2C  | 6:0:45:TRP:CE2    | 2.47                     | 0.49              |
| 2:L:196:LEU:HD11  | 3:M:269:ALA:HB1   | 1.94                     | 0.49              |
| 15:L:309:UQ8:H46A | 6:6:21:PHE:HE1    | 1.76                     | 0.49              |
| 4:H:258:LEU:C     | 5:5:19:ARG:NH2    | 2.70                     | 0.49              |
| 13:7:103:BCL:H2C  | 6:8:45:TRP:CD2    | 2.47                     | 0.49              |
| 20:M:406:CDL:H571 | 20:M:406:CDL:H342 | 1.94                     | 0.49              |
| 5:Y:17:PRO:HB3    | 6:Z:17:PHE:CE2    | 2.48                     | 0.49              |
| 4:H:156:VAL:HG21  | 4:H:184:VAL:HG22  | 1.95                     | 0.49              |
| 13:7:103:BCL:H2C  | 6:8:45:TRP:CE2    | 2.47                     | 0.49              |
| 13:L:305:BCL:H203 | 15:L:311:UQ8:H3MA | 1.94                     | 0.49              |
| 3:M:35:ILE:HD11   | 12:M:411:PGV:H21  | 1.94                     | 0.49              |
| 13:W:104:BCL:H11  | 6:X:29:PHE:CE1    | 2.48                     | 0.49              |
| 5:1:17:PRO:HG2    | 6:2:9:LEU:HD21    | 1.95                     | 0.49              |
| 5:I:36:HIS:CE1    | 13:J:102:BCL:HMD3 | 2.48                     | 0.49              |
| 13:K:103:BCL:O1A  | 19:N:101:CRT:H27  | 2.13                     | 0.49              |
| 6:Z:21:PHE:CD2    | 19:Z:101:CRT:H14  | 2.48                     | 0.49              |
| 6:2:45:TRP:CD1    | 6:2:46:LEU:HG     | 2.48                     | 0.48              |
| 5:I:38:ILE:HG12   | 21:K:104:PEF:H312 | 1.95                     | 0.48              |
| 5:A:28:GLN:HB3    | 13:A:101:BCL:H12  | 1.95                     | 0.48              |
| 13:W:101:BCL:H171 | 6:X:31:LEU:HD21   | 1.96                     | 0.48              |
| 13:Y:103:BCL:O1A  | 19:Z:101:CRT:H27  | 2.13                     | 0.48              |
| 5:5:51:ILE:HD13   | 5:7:58:LEU:HD23   | 1.95                     | 0.48              |
| 5:5:51:ILE:CD1    | 5:7:58:LEU:HD23   | 2.44                     | 0.48              |
| 4:H:18:ALA:HB2    | 22:H:304:LMT:H121 | 1.94                     | 0.48              |
| 19:P:101:CRT:H27  | 13:P:102:BCL:O1A  | 2.13                     | 0.48              |
| 5:U:19:ARG:HD2    | 20:U:104:CDL:HB61 | 1.95                     | 0.48              |
| 13:5:103:BCL:H162 | 13:5:103:BCL:H141 | 1.62                     | 0.48              |
| 5:7:17:PRO:HB3    | 6:8:17:PHE:CE2    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:L:309:UQ8:H26  | 5:7:26:ALA:HB1    | 1.96                     | 0.48              |
| 6:J:17:PHE:HA     | 19:J:101:CRT:H6   | 1.95                     | 0.48              |
| 13:Q:101:BCL:H43  | 6:R:28:TRP:CZ2    | 2.47                     | 0.48              |
| 5:Y:24:ILE:HG12   | 13:1:101:BCL:H112 | 1.96                     | 0.48              |
| 13:5:103:BCL:H11  | 6:6:29:PHE:CE1    | 2.49                     | 0.48              |
| 7:b:43:CYS:HB2    | 7:b:71:VAL:HA     | 1.96                     | 0.48              |
| 2:L:129:ALA:HB1   | 2:L:247:LEU:HD21  | 1.95                     | 0.48              |
| 22:H:304:LMT:H6D  | 5:F:41[A]:SER:HA  | 1.95                     | 0.48              |
| 13:I:101:BCL:HMA3 | 13:I:101:BCL:H203 | 1.95                     | 0.48              |
| 6:P:21:PHE:CD1    | 19:P:101:CRT:H14  | 2.49                     | 0.48              |
| 5:1:19:ARG:NH2    | 21:1:103:PEF:O1P  | 2.46                     | 0.48              |
| 20:M:406:CDL:H351 | 20:M:406:CDL:H621 | 1.94                     | 0.47              |
| 5:I:5:ASN:OD1     | 5:I:7:ASN:N       | 2.40                     | 0.47              |
| 20:O:104:CDL:H401 | 20:O:104:CDL:H551 | 1.96                     | 0.47              |
| 5:1:17:PRO:HG2    | 6:2:9:LEU:CD2     | 2.44                     | 0.47              |
| 5:1:37:MET:SD     | 12:1:105:PGV:H232 | 2.55                     | 0.47              |
| 3:M:256:MET:HE3   | 18:M:404:MQ8:H142 | 1.96                     | 0.47              |
| 19:M:405:CRT:H21A | 15:M:413:UQ8:H1MA | 1.96                     | 0.47              |
| 5:I:13:LEU:O      | 6:J:6:LEU:HB3     | 2.13                     | 0.47              |
| 13:K:101:BCL:H43  | 6:N:28:TRP:CZ2    | 2.49                     | 0.47              |
| 13:S:101:BCL:H13  | 13:S:101:BCL:H102 | 1.60                     | 0.47              |
| 5:I:5:ASN:ND2     | 6:N:23:GLN:OE1    | 2.44                     | 0.47              |
| 5:Q:13:LEU:O      | 6:R:6:LEU:HA      | 2.15                     | 0.47              |
| 6:Z:46:LEU:HB3    | 6:2:42:TYR:CE1    | 2.49                     | 0.47              |
| 3:M:130:TRP:CZ3   | 20:O:104:CDL:H511 | 2.46                     | 0.47              |
| 5:K:13:LEU:HB3    | 6:N:5:SER:HB2     | 1.96                     | 0.47              |
| 20:S:104:CDL:H121 | 20:S:104:CDL:H341 | 1.97                     | 0.47              |
| 5:1:17:PRO:HB3    | 6:2:17:PHE:CZ     | 2.50                     | 0.47              |
| 7:b:48:PHE:HD1    | 7:b:62:GLN:HE21   | 1.61                     | 0.47              |
| 1:C:144:HIS:HE1   | 8:C:504:HEC:NC    | 2.09                     | 0.47              |
| 6:6:9:LEU:HD22    | 6:6:13:GLU:HB3    | 1.95                     | 0.47              |
| 7:b:48:PHE:O      | 7:b:62:GLN:HG3    | 2.15                     | 0.47              |
| 12:L:307:PGV:H202 | 5:D:37:MET:HE2    | 1.95                     | 0.47              |
| 3:M:260:VAL:HB    | 3:M:264:SER:OG    | 2.15                     | 0.47              |
| 4:H:60:ASP:OD1    | 4:H:61:LEU:N      | 2.40                     | 0.47              |
| 5:O:19:ARG:NH1    | 20:O:104:CDL:OB3  | 2.43                     | 0.47              |
| 2:L:96:GLN:CG     | 15:L:309:UQ8:H4M  | 2.39                     | 0.47              |
| 13:L:305:BCL:H72  | 14:M:402:BPH:HMB2 | 1.96                     | 0.47              |
| 5:Q:19:ARG:HG2    | 20:S:104:CDL:HA4  | 1.97                     | 0.47              |
| 5:S:17:PRO:HB3    | 6:T:17:PHE:CE2    | 2.50                     | 0.47              |
| 5:A:18:ARG:NH1    | 12:9:104:PGV:H012 | 2.29                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:A:104:CRT:H372 | 5:F:36:HIS:CD2    | 2.50                     | 0.46              |
| 3:M:252:TRP:CE3   | 3:M:256:MET:HE2   | 2.51                     | 0.46              |
| 13:F:103:BCL:H51  | 13:I:101:BCL:H171 | 1.96                     | 0.46              |
| 6:N:21:PHE:CD2    | 19:N:101:CRT:H14  | 2.50                     | 0.46              |
| 5:O:13:LEU:HB3    | 6:P:5:SER:HB2     | 1.97                     | 0.46              |
| 5:U:11:ILE:HD12   | 5:U:14:ILE:CD1    | 2.33                     | 0.46              |
| 2:L:191:THR:OG1   | 13:L:305:BCL:H12  | 2.16                     | 0.46              |
| 13:L:301:BCL:H13  | 13:L:301:BCL:H172 | 1.71                     | 0.46              |
| 14:L:303:BPH:HHC  | 14:L:303:BPH:CBB  | 2.45                     | 0.46              |
| 22:H:304:LMT:H6D  | 5:F:41[B]:SER:HA  | 1.96                     | 0.46              |
| 20:O:104:CDL:H522 | 20:O:104:CDL:H131 | 1.97                     | 0.46              |
| 2:L:179:ASN:HB3   | 2:L:182:HIS:HB3   | 1.97                     | 0.46              |
| 5:S:38:ILE:O      | 5:S:42:THR:HG23   | 2.16                     | 0.46              |
| 13:U:103:BCL:HBA2 | 13:U:103:BCL:HED3 | 1.96                     | 0.46              |
| 5:D:18:ARG:HH22   | 20:D:105:CDL:PA1  | 2.39                     | 0.46              |
| 12:9:104:PGV:H041 | 12:9:104:PGV:H032 | 1.98                     | 0.46              |
| 2:L:160:LEU:HD12  | 3:M:303:MET:O     | 2.16                     | 0.46              |
| 5:S:18:ARG:HH12   | 5:S:19:ARG:CZ     | 2.29                     | 0.46              |
| 13:9:103:BCL:H2C  | 6:0:45:TRP:CD2    | 2.51                     | 0.46              |
| 3:M:179:ILE:O     | 3:M:182:HIS:ND1   | 2.39                     | 0.46              |
| 13:A:101:BCL:H203 | 13:A:101:BCL:HMA3 | 1.97                     | 0.46              |
| 6:T:45:TRP:CD1    | 6:T:46:LEU:HG     | 2.51                     | 0.46              |
| 13:W:104:BCL:H121 | 13:W:104:BCL:H161 | 1.74                     | 0.46              |
| 13:Y:103:BCL:H142 | 13:Y:103:BCL:H102 | 1.98                     | 0.46              |
| 5:3:37[B]:MET:SD  | 12:3:105:PGV:H12  | 2.56                     | 0.46              |
| 5:7:25:VAL:HG21   | 13:7:101:BCL:H13  | 1.97                     | 0.46              |
| 2:L:97:ILE:HG21   | 5:9:37:MET:HE1    | 1.96                     | 0.45              |
| 2:L:151:TRP:HB3   | 15:L:309:UQ8:H4MB | 1.98                     | 0.45              |
| 5:Q:28:GLN:CB     | 13:Q:101:BCL:H42  | 2.44                     | 0.45              |
| 2:L:41:CYS:SG     | 15:L:310:UQ8:H1MB | 2.57                     | 0.45              |
| 13:S:101:BCL:H43  | 6:T:28:TRP:CE2    | 2.51                     | 0.45              |
| 13:S:103:BCL:H2C  | 6:T:45:TRP:CD2    | 2.51                     | 0.45              |
| 5:3:51:ILE:HD11   | 5:5:58:LEU:HB3    | 1.99                     | 0.45              |
| 5:9:53:VAL:HG21   | 5:9:58:LEU:HD11   | 1.98                     | 0.45              |
| 5:O:19:ARG:NH1    | 20:O:104:CDL:OB4  | 2.49                     | 0.45              |
| 19:T:101:CRT:H243 | 20:U:104:CDL:H172 | 1.99                     | 0.45              |
| 5:5:19:ARG:HE     | 5:5:19:ARG:HB2    | 0.99                     | 0.45              |
| 2:L:281:TRP:CG    | 3:M:88:LYS:HB2    | 2.51                     | 0.45              |
| 13:L:301:BCL:H161 | 13:L:301:BCL:H192 | 1.67                     | 0.45              |
| 5:A:36:HIS:CG     | 19:0:101:CRT:H372 | 2.52                     | 0.45              |
| 6:P:29:PHE:CE1    | 13:P:102:BCL:H11  | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Y:18:ARG:NH2    | 5:Y:19:ARG:NH1    | 2.64                     | 0.45              |
| 13:Y:101:BCL:OBB  | 13:Y:101:BCL:HHC  | 2.17                     | 0.45              |
| 12:3:105:PGV:H212 | 12:3:105:PGV:H241 | 1.62                     | 0.45              |
| 20:S:104:CDL:H131 | 20:S:104:CDL:H171 | 1.98                     | 0.45              |
| 12:M:411:PGV:H261 | 12:M:411:PGV:H232 | 1.85                     | 0.45              |
| 6:V:17:PHE:HA     | 19:V:101:CRT:H6   | 1.98                     | 0.45              |
| 5:1:16:ASP:CB     | 5:1:19:ARG:NH1    | 2.78                     | 0.45              |
| 6:6:6:LEU:HB3     | 5:7:18:ARG:HH22   | 1.80                     | 0.45              |
| 2:L:69:ASN:ND2    | 3:M:302:GLY:O     | 2.48                     | 0.45              |
| 15:L:310:UQ8:H15  | 15:L:310:UQ8:H12  | 1.68                     | 0.45              |
| 3:M:285:LEU:HD21  | 21:K:104:PEF:H141 | 1.99                     | 0.45              |
| 6:2:29:PHE:O      | 6:2:33:VAL:HG23   | 2.16                     | 0.45              |
| 3:M:13:VAL:HG12   | 4:H:144:ILE:HD13  | 1.99                     | 0.45              |
| 5:A:58:LEU:HA     | 5:A:58:LEU:HD13   | 1.65                     | 0.45              |
| 5:1:16:ASP:CB     | 5:1:19:ARG:NE     | 2.77                     | 0.45              |
| 5:7:19:ARG:HA     | 5:7:19:ARG:HD3    | 1.71                     | 0.45              |
| 1:C:311:HIS:CE1   | 8:C:504:HEC:NA    | 2.84                     | 0.45              |
| 5:I:21:LEU:O      | 5:I:25:VAL:HG23   | 2.17                     | 0.45              |
| 6:P:40:TRP:CE2    | 13:P:102:BCL:H18  | 2.51                     | 0.45              |
| 3:M:7:ILE:HD12    | 12:M:410:PGV:H92  | 1.98                     | 0.45              |
| 13:D:103:BCL:HHC  | 13:D:103:BCL:OBB  | 2.17                     | 0.45              |
| 13:D:103:BCL:H202 | 6:G:38:LEU:HD13   | 1.98                     | 0.45              |
| 5:U:28:GLN:CB     | 13:U:101:BCL:H42  | 2.47                     | 0.45              |
| 13:W:104:BCL:H2C  | 6:X:45:TRP:CD2    | 2.52                     | 0.45              |
| 13:Y:101:BCL:H43  | 6:Z:28:TRP:CE2    | 2.52                     | 0.45              |
| 5:K:38:ILE:O      | 5:K:42:THR:HG23   | 2.16                     | 0.44              |
| 5:1:9:TYR:CE1     | 6:2:15:LYS:HG3    | 2.52                     | 0.44              |
| 13:5:103:BCL:H162 | 13:5:103:BCL:H192 | 1.85                     | 0.44              |
| 5:7:38:ILE:O      | 5:7:41:SER:OG     | 2.34                     | 0.44              |
| 13:7:103:BCL:H112 | 13:7:103:BCL:H152 | 1.45                     | 0.44              |
| 7:b:33:ARG:HA     | 7:b:34:PRO:HD3    | 1.88                     | 0.44              |
| 15:L:309:UQ8:H27  | 15:L:309:UQ8:H30  | 1.80                     | 0.44              |
| 15:L:310:UQ8:H25  | 15:L:310:UQ8:H22  | 1.68                     | 0.44              |
| 6:J:46:LEU:HB3    | 6:N:42:TYR:CE1    | 2.51                     | 0.44              |
| 13:K:103:BCL:H11  | 6:N:29:PHE:CE1    | 2.51                     | 0.44              |
| 13:2:102:BCL:HHC  | 13:2:102:BCL:OBB  | 2.17                     | 0.44              |
| 14:L:303:BPH:H172 | 12:L:307:PGV:H342 | 1.99                     | 0.44              |
| 13:5:101:BCL:H142 | 13:5:101:BCL:H111 | 1.86                     | 0.44              |
| 13:A:101:BCL:H62  | 13:A:101:BCL:H41  | 1.81                     | 0.44              |
| 13:O:101:BCL:H62  | 13:O:101:BCL:H41  | 1.78                     | 0.44              |
| 5:1:16:ASP:H      | 5:1:19:ARG:HH11   | 1.65                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:17:TRP:CG     | 22:H:304:LMT:H61  | 2.52                     | 0.44              |
| 22:H:304:LMT:H71  | 5:F:38:ILE:HG12   | 1.99                     | 0.44              |
| 5:K:46:TRP:CE2    | 13:K:101:BCL:H2C  | 2.52                     | 0.44              |
| 3:M:175:VAL:HG22  | 3:M:185:TRP:CE2   | 2.52                     | 0.44              |
| 4:H:205:LYS:HA    | 4:H:205:LYS:HD2   | 1.88                     | 0.44              |
| 5:O:34:LEU:HA     | 5:O:37[A]:MET:HE2 | 2.00                     | 0.44              |
| 13:2:102:BCL:H52  | 13:2:102:BCL:H12  | 1.76                     | 0.44              |
| 13:O:101:BCL:H43  | 6:P:28:TRP:CZ2    | 2.52                     | 0.44              |
| 13:3:101:BCL:H41  | 13:3:101:BCL:H62  | 1.76                     | 0.44              |
| 6:4:6:LEU:HD23    | 5:5:18:ARG:HH21   | 1.82                     | 0.44              |
| 5:9:46:TRP:CE2    | 13:9:101:BCL:H2C  | 2.53                     | 0.44              |
| 13:A:101:BCL:HMB1 | 19:0:101:CRT:H371 | 2.00                     | 0.44              |
| 5:O:27:PHE:HB2    | 20:O:104:CDL:H762 | 2.00                     | 0.44              |
| 6:Z:45:TRP:CD1    | 6:Z:46:LEU:HG     | 2.53                     | 0.44              |
| 12:L:308:PGV:C11  | 15:L:309:UQ8:H26A | 2.48                     | 0.44              |
| 15:L:310:UQ8:H10  | 15:L:310:UQ8:H7A  | 1.55                     | 0.44              |
| 5:5:16:ASP:HB3    | 5:5:19:ARG:CZ     | 2.47                     | 0.44              |
| 5:5:17:PRO:HB3    | 6:6:17:PHE:CZ     | 2.53                     | 0.44              |
| 13:L:305:BCL:H161 | 13:L:305:BCL:H141 | 1.49                     | 0.43              |
| 18:M:404:MQ8:H412 | 18:M:404:MQ8:H441 | 1.77                     | 0.43              |
| 19:M:405:CRT:H20  | 19:M:405:CRT:H181 | 1.84                     | 0.43              |
| 5:S:19:ARG:NH2    | 20:S:104:CDL:CB7  | 2.81                     | 0.43              |
| 13:S:101:BCL:H43  | 6:T:28:TRP:CZ2    | 2.53                     | 0.43              |
| 13:W:101:BCL:H62  | 13:W:101:BCL:H41  | 1.73                     | 0.43              |
| 13:Y:103:BCL:OB   | 13:Y:103:BCL:HH   | 2.18                     | 0.43              |
| 6:Z:46:LEU:HB3    | 6:2:42:TYR:CZ     | 2.53                     | 0.43              |
| 6:4:21:PHE:HA     | 19:4:101:CRT:H14  | 1.99                     | 0.43              |
| 1:C:31:GLU:OE2    | 10:C:506:GOL:H2   | 2.18                     | 0.43              |
| 12:M:411:PGV:P    | 20:S:104:CDL:HB31 | 2.58                     | 0.43              |
| 5:K:14:ILE:HG22   | 5:O:18:ARG:HB2    | 2.00                     | 0.43              |
| 5:O:38:ILE:O      | 5:O:42:THR:HG23   | 2.18                     | 0.43              |
| 5:O:46:TRP:CE2    | 13:O:101:BCL:H2C  | 2.54                     | 0.43              |
| 13:O:101:BCL:O1D  | 13:O:101:BCL:H202 | 2.18                     | 0.43              |
| 5:W:21:LEU:HD23   | 5:W:21:LEU:HA     | 1.90                     | 0.43              |
| 1:C:130:MET:HB3   | 8:C:502:HEC:C4B   | 2.47                     | 0.43              |
| 18:M:404:MQ8:H312 | 18:M:404:MQ8:H351 | 1.78                     | 0.43              |
| 4:H:9:ILE:HA      | 4:H:13:GLN:OE1    | 2.18                     | 0.43              |
| 5:A:46:TRP:HA     | 6:B:43:ARG:HH12   | 1.82                     | 0.43              |
| 13:J:102:BCL:H111 | 13:J:102:BCL:H152 | 1.67                     | 0.43              |
| 19:T:101:CRT:H372 | 5:U:36:HIS:CD2    | 2.54                     | 0.43              |
| 1:C:46:LYS:HD3    | 12:3:105:PGV:H062 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:L:309:UQ8:H32  | 15:L:309:UQ8:H35  | 1.78                     | 0.43              |
| 20:M:406:CDL:H202 | 4:H:25:GLY:HA3    | 2.00                     | 0.43              |
| 5:O:51:ILE:HD11   | 5:Q:58:LEU:HB2    | 2.01                     | 0.43              |
| 13:2:102:BCL:H192 | 13:2:102:BCL:H162 | 1.74                     | 0.43              |
| 6:0:45:TRP:CD1    | 6:0:46:LEU:HG     | 2.53                     | 0.43              |
| 1:C:303:LEU:HB2   | 8:C:502:HEC:HBD1  | 2.01                     | 0.43              |
| 20:H:305:CDL:H172 | 20:H:305:CDL:H202 | 1.86                     | 0.43              |
| 19:A:104:CRT:H372 | 5:F:36:HIS:CG     | 2.54                     | 0.43              |
| 19:N:101:CRT:H10  | 19:N:101:CRT:H81  | 1.85                     | 0.43              |
| 6:8:15:LYS:HA     | 6:8:15:LYS:HD2    | 1.80                     | 0.43              |
| 2:L:219:GLU:OE1   | 2:L:219:GLU:N     | 2.45                     | 0.43              |
| 20:H:305:CDL:H862 | 20:H:305:CDL:H831 | 1.81                     | 0.43              |
| 13:F:103:BCL:H193 | 6:J:38:LEU:HD13   | 2.01                     | 0.43              |
| 5:U:23:SER:HA     | 20:U:104:CDL:H731 | 2.00                     | 0.43              |
| 5:Y:19:ARG:NH2    | 20:Y:104:CDL:OA2  | 2.49                     | 0.43              |
| 5:1:21:LEU:HD23   | 5:1:21:LEU:HA     | 1.78                     | 0.43              |
| 13:7:101:BCL:H61  | 13:7:101:BCL:H41  | 1.96                     | 0.43              |
| 2:L:190:PHE:CD2   | 14:M:402:BPH:HBB1 | 2.54                     | 0.43              |
| 5:O:28:GLN:CB     | 13:O:101:BCL:H42  | 2.49                     | 0.43              |
| 6:Z:31:LEU:HD23   | 6:Z:31:LEU:HA     | 1.68                     | 0.43              |
| 19:Z:101:CRT:H10  | 19:Z:101:CRT:H81  | 1.84                     | 0.43              |
| 5:9:49:ASP:O      | 5:9:51:ILE:HG13   | 2.18                     | 0.43              |
| 7:b:57:ASP:O      | 7:b:70:ASN:HA     | 2.19                     | 0.43              |
| 13:L:305:BCL:OBB  | 19:M:405:CRT:H243 | 2.19                     | 0.43              |
| 3:M:98:PRO:CG     | 3:M:107:PRO:HG3   | 2.48                     | 0.43              |
| 4:H:258:LEU:HA    | 5:5:19:ARG:HH21   | 1.83                     | 0.43              |
| 20:O:104:CDL:H342 | 20:O:104:CDL:H311 | 1.80                     | 0.43              |
| 13:4:102:BCL:HHC  | 13:4:102:BCL:OBB  | 2.18                     | 0.43              |
| 15:L:304:UQ8:H7   | 15:L:304:UQ8:H10  | 1.75                     | 0.43              |
| 19:M:405:CRT:H2M3 | 5:O:38:ILE:HA     | 2.00                     | 0.43              |
| 4:H:48:ARG:NE     | 6:0:6:LEU:HD12    | 2.33                     | 0.43              |
| 13:U:101:BCL:HED1 | 6:V:28:TRP:CZ3    | 2.54                     | 0.43              |
| 6:X:46:LEU:HB3    | 6:Z:42:TYR:CE1    | 2.53                     | 0.43              |
| 19:0:101:CRT:H10  | 19:0:101:CRT:H81  | 1.90                     | 0.43              |
| 7:b:49:MET:HE2    | 7:b:49:MET:HB3    | 1.92                     | 0.43              |
| 4:H:100:LEU:HB2   | 4:H:111:PHE:CZ    | 2.53                     | 0.42              |
| 5:U:46:TRP:CE2    | 13:U:101:BCL:H2C  | 2.54                     | 0.42              |
| 6:X:31:LEU:HD12   | 6:X:31:LEU:HA     | 1.91                     | 0.42              |
| 5:5:51:ILE:HD11   | 5:7:58:LEU:HB3    | 2.01                     | 0.42              |
| 15:L:310:UQ8:H16A | 5:7:34:LEU:HD13   | 2.00                     | 0.42              |
| 6:J:45:TRP:CD2    | 13:J:102:BCL:H2C  | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Q:17:PRO:HB3    | 6:R:17:PHE:CZ     | 2.54                     | 0.42              |
| 13:Q:103:BCL:H2C  | 6:R:45:TRP:CD2    | 2.55                     | 0.42              |
| 6:4:44:PRO:O      | 5:5:55:TYR:OH     | 2.33                     | 0.42              |
| 19:8:101:CRT:H36  | 19:8:101:CRT:H341 | 1.91                     | 0.42              |
| 7:b:53:VAL:HB     | 7:b:60:GLY:HA3    | 2.00                     | 0.42              |
| 2:L:139:VAL:HG21  | 2:L:254:ALA:HB1   | 2.02                     | 0.42              |
| 19:4:101:CRT:H10  | 19:4:101:CRT:H81  | 1.84                     | 0.42              |
| 7:b:58:TRP:HA     | 7:b:69:ILE:O      | 2.19                     | 0.42              |
| 3:M:243:THR:HB    | 4:H:117:PRO:HD2   | 2.02                     | 0.42              |
| 14:M:402:BPH:H161 | 20:S:104:CDL:H752 | 2.00                     | 0.42              |
| 13:A:103:BCL:H161 | 13:A:103:BCL:H192 | 1.66                     | 0.42              |
| 19:B:101:CRT:H10  | 19:B:101:CRT:H81  | 1.84                     | 0.42              |
| 5:Y:27:PHE:HB2    | 13:1:101:BCL:H152 | 2.00                     | 0.42              |
| 13:1:101:BCL:HHC  | 13:1:101:BCL:OBB  | 2.20                     | 0.42              |
| 5:9:35:ILE:O      | 5:9:39:VAL:HG23   | 2.19                     | 0.42              |
| 5:9:46:TRP:CD2    | 13:9:101:BCL:H2C  | 2.55                     | 0.42              |
| 4:H:214:ILE:HB    | 4:H:218:HIS:HB2   | 2.01                     | 0.42              |
| 5:A:18:ARG:HD3    | 6:0:6:LEU:HD22    | 2.01                     | 0.42              |
| 19:W:102:CRT:H10  | 19:W:102:CRT:H81  | 1.91                     | 0.42              |
| 5:5:35:ILE:O      | 5:5:39:VAL:HG23   | 2.19                     | 0.42              |
| 5:S:46:TRP:CD2    | 13:S:101:BCL:H2C  | 2.55                     | 0.42              |
| 20:S:104:CDL:H362 | 20:S:104:CDL:C14  | 2.50                     | 0.42              |
| 5:W:28:GLN:HB3    | 13:W:101:BCL:H12  | 2.02                     | 0.42              |
| 3:M:196:LEU:HD12  | 3:M:196:LEU:HA    | 1.82                     | 0.42              |
| 3:M:200:PRO:HG3   | 3:M:297:TRP:CH2   | 2.54                     | 0.42              |
| 4:H:17:TRP:NE1    | 22:H:304:LMT:H41  | 2.35                     | 0.42              |
| 12:L:307:PGV:H222 | 12:L:307:PGV:H251 | 1.82                     | 0.42              |
| 12:M:410:PGV:H312 | 12:M:410:PGV:H281 | 1.88                     | 0.42              |
| 5:A:17:PRO:HB3    | 6:B:17:PHE:CZ     | 2.54                     | 0.42              |
| 5:Q:46:TRP:CE2    | 13:Q:101:BCL:H2C  | 2.55                     | 0.42              |
| 6:4:32:VAL:HG12   | 13:4:102:BCL:H61  | 2.01                     | 0.42              |
| 13:7:101:BCL:H43  | 6:8:28:TRP:CH2    | 2.55                     | 0.42              |
| 5:I:38:ILE:O      | 5:I:42:THR:HG23   | 2.19                     | 0.42              |
| 13:P:102:BCL:H192 | 13:P:102:BCL:H152 | 2.01                     | 0.42              |
| 8:C:503:HEC:HBB1  | 2:L:174:LEU:HD22  | 2.02                     | 0.41              |
| 5:K:46:TRP:CD2    | 13:K:101:BCL:H2C  | 2.55                     | 0.41              |
| 13:K:101:BCL:HMD3 | 6:N:36:HIS:CE1    | 2.55                     | 0.41              |
| 6:P:37:LEU:HD23   | 6:P:37:LEU:HA     | 1.87                     | 0.41              |
| 13:Y:103:BCL:H193 | 6:Z:40:TRP:CH2    | 2.55                     | 0.41              |
| 6:4:45:TRP:CD1    | 6:4:46:LEU:HG     | 2.54                     | 0.41              |
| 1:C:73:SER:HB2    | 1:C:83:LYS:HB3    | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:308:PGV:H52  | 12:L:308:PGV:H81  | 1.73                     | 0.41              |
| 4:H:119:ARG:HD2   | 4:H:237:ASP:CG    | 2.45                     | 0.41              |
| 13:I:101:BCL:HHC  | 13:I:101:BCL:OBB  | 2.20                     | 0.41              |
| 5:O:18:ARG:HD2    | 20:O:104:CDL:HA21 | 2.02                     | 0.41              |
| 13:7:103:BCL:HBA2 | 13:7:103:BCL:HED3 | 2.02                     | 0.41              |
| 2:L:179:ASN:HB3   | 2:L:182:HIS:CB    | 2.49                     | 0.41              |
| 12:L:307:PGV:H42  | 12:D:106:PGV:H51  | 2.01                     | 0.41              |
| 3:M:33:ARG:HD3    | 12:M:411:PGV:H062 | 2.01                     | 0.41              |
| 4:H:17:TRP:CE2    | 22:H:304:LMT:H41  | 2.54                     | 0.41              |
| 12:H:303:PGV:H262 | 20:H:305:CDL:H841 | 2.01                     | 0.41              |
| 13:O:101:BCL:HHC  | 13:O:101:BCL:OBB  | 2.21                     | 0.41              |
| 5:S:46:TRP:CE2    | 13:S:101:BCL:H2C  | 2.55                     | 0.41              |
| 13:U:101:BCL:HHC  | 13:U:101:BCL:OBB  | 2.19                     | 0.41              |
| 5:Y:36:HIS:NE2    | 13:Y:103:BCL:HMD3 | 2.35                     | 0.41              |
| 13:Y:103:BCL:HED1 | 6:Z:28:TRP:HZ2    | 1.86                     | 0.41              |
| 2:L:216:LYS:HD2   | 2:L:220:HIS:CD2   | 2.56                     | 0.41              |
| 13:L:305:BCL:OBB  | 13:L:305:BCL:HHC  | 2.21                     | 0.41              |
| 5:A:38:ILE:O      | 5:A:42:THR:HG23   | 2.20                     | 0.41              |
| 19:N:101:CRT:H241 | 19:N:101:CRT:H26  | 1.85                     | 0.41              |
| 13:Q:101:BCL:H141 | 13:Q:101:BCL:H162 | 1.72                     | 0.41              |
| 13:Y:103:BCL:H52  | 13:Y:103:BCL:H12  | 1.81                     | 0.41              |
| 6:2:21:PHE:HA     | 19:2:101:CRT:H11  | 2.03                     | 0.41              |
| 19:3:103:CRT:H10  | 19:3:103:CRT:H81  | 1.79                     | 0.41              |
| 5:5:10:LYS:HB2    | 19:8:101:CRT:H5   | 2.02                     | 0.41              |
| 5:9:15:LEU:HD13   | 12:9:104:PGV:H261 | 2.01                     | 0.41              |
| 13:A:101:BCL:HHB  | 19:0:101:CRT:H35  | 2.02                     | 0.41              |
| 19:A:104:CRT:H36  | 19:A:104:CRT:H341 | 1.88                     | 0.41              |
| 6:E:45:TRP:CD1    | 6:E:46:LEU:HG     | 2.56                     | 0.41              |
| 5:F:17:PRO:HB3    | 6:G:17:PHE:CZ     | 2.56                     | 0.41              |
| 6:N:45:TRP:CD1    | 6:N:46:LEU:HG     | 2.55                     | 0.41              |
| 13:S:103:BCL:H93  | 13:S:103:BCL:H61  | 1.61                     | 0.41              |
| 13:U:103:BCL:O1A  | 19:V:101:CRT:H27  | 2.20                     | 0.41              |
| 19:4:101:CRT:H26  | 19:4:101:CRT:H241 | 1.91                     | 0.41              |
| 6:0:15:LYS:HD2    | 6:0:15:LYS:HA     | 1.88                     | 0.41              |
| 13:L:301:BCL:H151 | 12:L:307:PGV:H321 | 2.02                     | 0.41              |
| 19:M:405:CRT:H10  | 19:M:405:CRT:H81  | 1.87                     | 0.41              |
| 5:O:30:VAL:HG11   | 20:O:104:CDL:H601 | 2.02                     | 0.41              |
| 19:T:101:CRT:C31  | 13:U:101:BCL:HBA2 | 2.50                     | 0.41              |
| 13:Y:103:BCL:H141 | 6:Z:45:TRP:CZ2    | 2.55                     | 0.41              |
| 5:7:35:ILE:HD12   | 13:7:103:BCL:O1D  | 2.21                     | 0.41              |
| 13:9:103:BCL:H101 | 6:0:36:HIS:CD2    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:36:ARG:HB3    | 2:L:79:ASP:OD1    | 2.21                     | 0.41              |
| 1:C:250:CYS:O     | 1:C:262:SER:HB3   | 2.21                     | 0.41              |
| 1:C:270:TRP:CG    | 3:M:316:PRO:HG2   | 2.55                     | 0.41              |
| 19:2:101:CRT:H35  | 13:3:101:BCL:HMB1 | 2.02                     | 0.41              |
| 13:7:101:BCL:OBB  | 13:7:101:BCL:HHC  | 2.21                     | 0.41              |
| 12:L:308:PGV:C20  | 12:M:410:PGV:H222 | 2.49                     | 0.41              |
| 15:L:310:UQ8:H12  | 15:L:310:UQ8:H10A | 1.84                     | 0.41              |
| 20:S:104:CDL:H362 | 20:S:104:CDL:H142 | 2.03                     | 0.41              |
| 6:4:21:PHE:CD2    | 19:4:101:CRT:H14  | 2.55                     | 0.41              |
| 19:8:101:CRT:H20  | 19:8:101:CRT:H181 | 1.94                     | 0.41              |
| 3:M:130:TRP:CH2   | 20:M:406:CDL:H781 | 2.56                     | 0.41              |
| 3:M:229:PHE:HB2   | 3:M:244:ALA:HB2   | 2.02                     | 0.41              |
| 5:A:56:GLN:HE22   | 5:9:49:ASP:HB3    | 1.85                     | 0.41              |
| 19:A:104:CRT:H10  | 19:A:104:CRT:H81  | 1.80                     | 0.41              |
| 20:D:105:CDL:H741 | 12:9:104:PGV:H42  | 2.02                     | 0.41              |
| 5:F:13:LEU:O      | 6:G:6:LEU:HB3     | 2.21                     | 0.41              |
| 19:G:101:CRT:H20  | 19:G:101:CRT:H181 | 1.90                     | 0.41              |
| 5:O:33:LEU:O      | 5:O:37[A]:MET:HG3 | 2.20                     | 0.41              |
| 5:S:15:LEU:HD23   | 5:U:18:ARG:HG3    | 2.03                     | 0.41              |
| 5:U:17:PRO:HB3    | 6:V:17:PHE:CE2    | 2.56                     | 0.41              |
| 5:Y:16:ASP:OD2    | 5:Y:19:ARG:HG2    | 2.20                     | 0.41              |
| 13:2:102:BCL:H62  | 13:2:102:BCL:H41  | 1.92                     | 0.41              |
| 5:3:19:ARG:HD3    | 5:3:19:ARG:HA     | 1.95                     | 0.41              |
| 1:C:95:VAL:HG21   | 7:b:63:LEU:O      | 2.21                     | 0.41              |
| 2:L:227:ASP:O     | 3:M:132:ARG:NH2   | 2.54                     | 0.41              |
| 19:A:104:CRT:H35  | 13:F:101:BCL:HBB  | 2.02                     | 0.41              |
| 5:U:17:PRO:HB3    | 6:V:17:PHE:CZ     | 2.55                     | 0.41              |
| 5:Y:19:ARG:HA     | 5:Y:19:ARG:HD3    | 1.75                     | 0.41              |
| 5:5:38:ILE:O      | 5:5:42:THR:HG23   | 2.21                     | 0.41              |
| 3:M:97:PRO:HD3    | 3:M:176:PRO:HB3   | 2.02                     | 0.40              |
| 3:M:159:VAL:HA    | 3:M:163:ILE:HB    | 2.03                     | 0.40              |
| 13:F:101:BCL:H43  | 6:G:28:TRP:CZ2    | 2.56                     | 0.40              |
| 5:S:17:PRO:HB3    | 6:T:17:PHE:CZ     | 2.56                     | 0.40              |
| 13:U:103:BCL:H161 | 13:U:103:BCL:H192 | 1.79                     | 0.40              |
| 5:Y:46:TRP:CE3    | 13:Y:101:BCL:HAC2 | 2.56                     | 0.40              |
| 13:2:102:BCL:HBB2 | 13:2:102:BCL:H121 | 2.03                     | 0.40              |
| 3:M:246:GLU:OE2   | 4:H:117:PRO:HD3   | 2.21                     | 0.40              |
| 13:F:101:BCL:H141 | 13:F:101:BCL:H161 | 1.88                     | 0.40              |
| 5:U:36:HIS:CG     | 13:U:103:BCL:HMD1 | 2.56                     | 0.40              |
| 19:8:101:CRT:H371 | 13:9:101:BCL:HMB1 | 2.02                     | 0.40              |
| 4:H:65:LYS:HE2    | 4:H:67:PHE:CZ     | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:A:32:GLY:HA2    | 13:A:103:BCL:O1D  | 2.21                     | 0.40              |
| 13:F:103:BCL:H152 | 13:F:103:BCL:H112 | 1.80                     | 0.40              |
| 19:P:101:CRT:H20  | 19:P:101:CRT:H181 | 1.96                     | 0.40              |
| 13:Y:101:BCL:H171 | 6:Z:31:LEU:HD13   | 2.04                     | 0.40              |
| 5:3:41:SER:O      | 12:3:105:PGV:H011 | 2.21                     | 0.40              |
| 5:9:46:TRP:NE1    | 13:9:101:BCL:HHC  | 2.37                     | 0.40              |
| 2:L:22:LEU:HB2    | 5:7:19:ARG:HB2    | 2.04                     | 0.40              |
| 14:M:402:BPH:H141 | 20:S:104:CDL:H751 | 2.03                     | 0.40              |
| 5:I:37:MET:HE2    | 5:I:37:MET:HA     | 2.04                     | 0.40              |
| 2:L:183:MET:HE1   | 2:L:272:TRP:CZ2   | 2.57                     | 0.40              |
| 13:L:302:BCL:HHC  | 13:L:302:BCL:OBB  | 2.21                     | 0.40              |
| 3:M:8:PHE:HB2     | 20:M:412:CDL:HB22 | 2.02                     | 0.40              |
| 3:M:148:TRP:HE1   | 20:M:406:CDL:H711 | 1.86                     | 0.40              |
| 4:H:31:ARG:HA     | 4:H:31:ARG:HD2    | 1.86                     | 0.40              |
| 5:A:17:PRO:HB3    | 6:B:17:PHE:CE1    | 2.56                     | 0.40              |
| 13:F:103:BCL:H161 | 13:F:103:BCL:H192 | 1.83                     | 0.40              |
| 19:G:101:CRT:H2M3 | 5:I:37:MET:HE3    | 2.04                     | 0.40              |
| 5:K:7:ASN:HB2     | 6:P:20:ILE:HD11   | 2.03                     | 0.40              |
| 13:Q:103:BCL:HAA1 | 6:R:32:VAL:HG11   | 2.02                     | 0.40              |
| 5:S:35:ILE:HD12   | 13:S:103:BCL:O1D  | 2.22                     | 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     | 309/311 (99%) | 296 (96%)  | 13 (4%) | 0        | 100         | 100 |
| 2   | L     | 279/281 (99%) | 272 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 3   | M     | 318/325 (98%) | 311 (98%)  | 5 (2%)  | 2 (1%)   | 21          | 51  |
| 4   | H     | 255/259 (98%) | 254 (100%) | 1 (0%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 5   | 1     | 54/61 (88%) | 54 (100%) | 0       | 0        | 100         | 100 |
| 5   | 3     | 55/61 (90%) | 54 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | 5     | 52/61 (85%) | 50 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 5   | 7     | 55/61 (90%) | 55 (100%) | 0       | 0        | 100         | 100 |
| 5   | 9     | 55/61 (90%) | 54 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | A     | 52/61 (85%) | 51 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | D     | 54/61 (88%) | 54 (100%) | 0       | 0        | 100         | 100 |
| 5   | F     | 54/61 (88%) | 52 (96%)  | 1 (2%)  | 1 (2%)   | 6           | 23  |
| 5   | I     | 56/61 (92%) | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | K     | 55/61 (90%) | 55 (100%) | 0       | 0        | 100         | 100 |
| 5   | O     | 55/61 (90%) | 54 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | Q     | 55/61 (90%) | 55 (100%) | 0       | 0        | 100         | 100 |
| 5   | S     | 57/61 (93%) | 57 (100%) | 0       | 0        | 100         | 100 |
| 5   | U     | 56/61 (92%) | 55 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 5   | W     | 54/61 (88%) | 54 (100%) | 0       | 0        | 100         | 100 |
| 5   | Y     | 55/61 (90%) | 54 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | 0     | 41/47 (87%) | 41 (100%) | 0       | 0        | 100         | 100 |
| 6   | 2     | 39/47 (83%) | 39 (100%) | 0       | 0        | 100         | 100 |
| 6   | 4     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | 6     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | 8     | 39/47 (83%) | 39 (100%) | 0       | 0        | 100         | 100 |
| 6   | B     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | E     | 36/47 (77%) | 36 (100%) | 0       | 0        | 100         | 100 |
| 6   | G     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | J     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | N     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | P     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | R     | 39/47 (83%) | 39 (100%) | 0       | 0        | 100         | 100 |
| 6   | T     | 41/47 (87%) | 41 (100%) | 0       | 0        | 100         | 100 |
| 6   | V     | 40/47 (85%) | 40 (100%) | 0       | 0        | 100         | 100 |
| 6   | X     | 39/47 (83%) | 39 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 6   | Z     | 38/47 (81%)     | 38 (100%)  | 0       | 0        | 100         | 100 |
| 7   | b     | 81/83 (98%)     | 79 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| All | All   | 2748/2987 (92%) | 2707 (98%) | 38 (1%) | 3 (0%)   | 48          | 77  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 58  | LEU  |
| 3   | M     | 195 | ASN  |
| 3   | M     | 179 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | C     | 260/260 (100%) | 258 (99%)  | 2 (1%)   | 73          | 90  |
| 2   | L     | 229/229 (100%) | 227 (99%)  | 2 (1%)   | 70          | 90  |
| 3   | M     | 258/261 (99%)  | 257 (100%) | 1 (0%)   | 84          | 94  |
| 4   | H     | 210/211 (100%) | 209 (100%) | 1 (0%)   | 81          | 93  |
| 5   | 1     | 50/56 (89%)    | 50 (100%)  | 0        | 100         | 100 |
| 5   | 3     | 52/56 (93%)    | 52 (100%)  | 0        | 100         | 100 |
| 5   | 5     | 49/56 (88%)    | 49 (100%)  | 0        | 100         | 100 |
| 5   | 7     | 52/56 (93%)    | 52 (100%)  | 0        | 100         | 100 |
| 5   | 9     | 52/56 (93%)    | 50 (96%)   | 2 (4%)   | 29          | 64  |
| 5   | A     | 49/56 (88%)    | 48 (98%)   | 1 (2%)   | 48          | 78  |
| 5   | D     | 51/56 (91%)    | 51 (100%)  | 0        | 100         | 100 |
| 5   | F     | 51/56 (91%)    | 50 (98%)   | 1 (2%)   | 48          | 78  |
| 5   | I     | 53/56 (95%)    | 52 (98%)   | 1 (2%)   | 50          | 79  |
| 5   | K     | 51/56 (91%)    | 50 (98%)   | 1 (2%)   | 48          | 78  |
| 5   | O     | 52/56 (93%)    | 50 (96%)   | 2 (4%)   | 29          | 64  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 5   | Q     | 52/56 (93%)     | 51 (98%)   | 1 (2%)   | 50          | 79  |
| 5   | S     | 54/56 (96%)     | 53 (98%)   | 1 (2%)   | 50          | 79  |
| 5   | U     | 53/56 (95%)     | 53 (100%)  | 0        | 100         | 100 |
| 5   | W     | 51/56 (91%)     | 51 (100%)  | 0        | 100         | 100 |
| 5   | Y     | 52/56 (93%)     | 52 (100%)  | 0        | 100         | 100 |
| 6   | 0     | 36/39 (92%)     | 34 (94%)   | 2 (6%)   | 19          | 50  |
| 6   | 2     | 34/39 (87%)     | 33 (97%)   | 1 (3%)   | 37          | 71  |
| 6   | 4     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | 6     | 35/39 (90%)     | 34 (97%)   | 1 (3%)   | 37          | 71  |
| 6   | 8     | 34/39 (87%)     | 33 (97%)   | 1 (3%)   | 37          | 71  |
| 6   | B     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | E     | 32/39 (82%)     | 32 (100%)  | 0        | 100         | 100 |
| 6   | G     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | J     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | N     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | P     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | R     | 34/39 (87%)     | 33 (97%)   | 1 (3%)   | 37          | 71  |
| 6   | T     | 36/39 (92%)     | 35 (97%)   | 1 (3%)   | 38          | 72  |
| 6   | V     | 35/39 (90%)     | 35 (100%)  | 0        | 100         | 100 |
| 6   | X     | 34/39 (87%)     | 34 (100%)  | 0        | 100         | 100 |
| 6   | Z     | 33/39 (85%)     | 33 (100%)  | 0        | 100         | 100 |
| 7   | b     | 61/61 (100%)    | 60 (98%)   | 1 (2%)   | 55          | 83  |
| All | All   | 2395/2542 (94%) | 2371 (99%) | 24 (1%)  | 68          | 89  |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 212 | ILE  |
| 1   | C     | 333 | THR  |
| 2   | L     | 256 | CYS  |
| 2   | L     | 280 | LEU  |
| 3   | M     | 216 | PHE  |
| 4   | H     | 237 | ASP  |
| 5   | A     | 58  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 14  | ILE  |
| 5   | I     | 4   | MET  |
| 5   | K     | 3   | THR  |
| 5   | O     | 14  | ILE  |
| 5   | O     | 53  | VAL  |
| 5   | Q     | 58  | LEU  |
| 6   | R     | 6   | LEU  |
| 5   | S     | 25  | VAL  |
| 6   | T     | 31  | LEU  |
| 6   | 2     | 6   | LEU  |
| 6   | 6     | 6   | LEU  |
| 6   | 8     | 6   | LEU  |
| 5   | 9     | 3   | THR  |
| 5   | 9     | 53  | VAL  |
| 6   | 0     | 6   | LEU  |
| 6   | 0     | 31  | LEU  |
| 7   | b     | 33  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 42  | ASN  |
| 2   | L     | 172 | GLN  |
| 2   | L     | 175 | HIS  |
| 2   | L     | 210 | GLN  |
| 2   | L     | 222 | ASN  |
| 3   | M     | 80  | HIS  |
| 4   | H     | 7   | HIS  |
| 5   | D     | 7   | ASN  |
| 5   | I     | 7   | ASN  |
| 5   | Q     | 7   | ASN  |
| 5   | 5     | 7   | ASN  |
| 5   | 7     | 7   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 18 are monoatomic - leaving 102 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$ |
| 19  | CRT  | T     | 101 | -    | 43,43,43     | 0.76 | 0           | 48,54,54    | 1.86 | 16 (33%)    |
| 20  | CDL  | D     | 104 | -    | 39,39,99     | 1.45 | 4 (10%)     | 45,51,111   | 1.30 | 7 (15%)     |
| 20  | CDL  | S     | 104 | -    | 74,74,99     | 1.19 | 4 (5%)      | 80,86,111   | 1.37 | 9 (11%)     |
| 19  | CRT  | O     | 103 | -    | 43,43,43     | 0.68 | 0           | 48,54,54    | 1.88 | 13 (27%)    |
| 12  | PGV  | M     | 411 | -    | 36,36,50     | 1.06 | 2 (5%)      | 39,42,56    | 1.25 | 5 (12%)     |
| 13  | BCL  | U     | 103 | -    | 69,74,74     | 1.23 | 5 (7%)      | 79,115,115  | 1.53 | 14 (17%)    |
| 13  | BCL  | 3     | 101 | -    | 69,74,74     | 1.20 | 3 (4%)      | 79,115,115  | 1.91 | 16 (20%)    |
| 19  | CRT  | N     | 101 | -    | 43,43,43     | 0.71 | 0           | 48,54,54    | 2.14 | 15 (31%)    |
| 20  | CDL  | U     | 104 | -    | 61,61,99     | 1.19 | 4 (6%)      | 67,73,111   | 1.66 | 14 (20%)    |
| 21  | PEF  | W     | 106 | -    | 4,4,46       | 2.73 | 2 (50%)     | 6,6,51      | 1.90 | 2 (33%)     |
| 21  | PEF  | M     | 408 | -    | 4,4,46       | 1.76 | 2 (50%)     | 6,6,51      | 1.32 | 1 (16%)     |
| 13  | BCL  | F     | 101 | -    | 69,74,74     | 1.13 | 4 (5%)      | 79,115,115  | 1.68 | 16 (20%)    |
| 13  | BCL  | O     | 101 | -    | 69,74,74     | 1.12 | 4 (5%)      | 79,115,115  | 1.53 | 12 (15%)    |
| 12  | PGV  | L     | 308 | -    | 43,43,50     | 0.98 | 2 (4%)      | 46,49,56    | 1.14 | 3 (6%)      |
| 15  | UQ8  | L     | 311 | -    | 18,18,53     | 2.16 | 2 (11%)     | 24,25,67    | 1.06 | 2 (8%)      |
| 13  | BCL  | D     | 103 | -    | 69,74,74     | 1.14 | 4 (5%)      | 79,115,115  | 1.42 | 12 (15%)    |
| 12  | PGV  | H     | 303 | -    | 35,35,50     | 1.10 | 2 (5%)      | 38,41,56    | 1.21 | 4 (10%)     |
| 13  | BCL  | I     | 101 | -    | 69,74,74     | 1.18 | 6 (8%)      | 79,115,115  | 1.48 | 12 (15%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | SO4  | L     | 306 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.05 | 0        |
| 13  | BCL  | L     | 301 | -    | 69,74,74     | 1.12 | 4 (5%)   | 79,115,115  | 1.45 | 11 (13%) |
| 12  | PGV  | 9     | 104 | -    | 32,32,50     | 1.17 | 2 (6%)   | 35,38,56    | 1.34 | 6 (17%)  |
| 19  | CRT  | V     | 101 | -    | 43,43,43     | 0.65 | 0        | 48,54,54    | 2.02 | 15 (31%) |
| 8   | HEC  | C     | 503 | 1    | 46,50,50     | 1.71 | 10 (21%) | 58,82,82    | 1.67 | 12 (20%) |
| 13  | BCL  | Q     | 101 | -    | 69,74,74     | 1.15 | 3 (4%)   | 79,115,115  | 1.66 | 14 (17%) |
| 13  | BCL  | U     | 101 | -    | 69,74,74     | 1.16 | 3 (4%)   | 79,115,115  | 1.51 | 12 (15%) |
| 13  | BCL  | 1     | 101 | -    | 69,74,74     | 1.14 | 4 (5%)   | 79,115,115  | 1.53 | 10 (12%) |
| 13  | BCL  | 5     | 103 | -    | 69,74,74     | 1.15 | 5 (7%)   | 79,115,115  | 1.55 | 12 (15%) |
| 12  | PGV  | L     | 307 | -    | 42,42,50     | 0.99 | 2 (4%)   | 45,48,56    | 1.24 | 4 (8%)   |
| 13  | BCL  | 2     | 102 | -    | 69,74,74     | 1.26 | 6 (8%)   | 79,115,115  | 1.66 | 12 (15%) |
| 20  | CDL  | 1     | 104 | -    | 12,12,99     | 0.45 | 0        | 13,15,111   | 0.60 | 0        |
| 19  | CRT  | 4     | 101 | -    | 43,43,43     | 0.66 | 0        | 48,54,54    | 1.98 | 15 (31%) |
| 13  | BCL  | L     | 305 | -    | 69,74,74     | 1.12 | 4 (5%)   | 79,115,115  | 1.61 | 14 (17%) |
| 15  | UQ8  | L     | 304 | -    | 33,33,53     | 1.53 | 2 (6%)   | 42,43,67    | 1.79 | 10 (23%) |
| 13  | BCL  | A     | 101 | -    | 69,74,74     | 1.14 | 4 (5%)   | 79,115,115  | 1.55 | 13 (16%) |
| 15  | UQ8  | L     | 310 | -    | 33,33,53     | 1.52 | 2 (6%)   | 42,43,67    | 1.82 | 14 (33%) |
| 19  | CRT  | Z     | 101 | -    | 43,43,43     | 0.64 | 0        | 48,54,54    | 2.23 | 17 (35%) |
| 13  | BCL  | W     | 104 | -    | 69,74,74     | 1.15 | 4 (5%)   | 79,115,115  | 1.40 | 10 (12%) |
| 10  | GOL  | C     | 506 | -    | 5,5,5        | 0.93 | 0        | 5,5,5       | 1.08 | 0        |
| 19  | CRT  | P     | 101 | -    | 43,43,43     | 0.71 | 0        | 48,54,54    | 1.86 | 11 (22%) |
| 13  | BCL  | Y     | 103 | -    | 69,74,74     | 1.16 | 5 (7%)   | 79,115,115  | 1.55 | 15 (18%) |
| 11  | LHG  | C     | 507 | -    | 7,8,48       | 0.21 | 0        | 6,7,54      | 1.07 | 1 (16%)  |
| 14  | BPH  | M     | 402 | -    | 59,70,70     | 2.53 | 15 (25%) | 59,101,101  | 2.22 | 20 (33%) |
| 20  | CDL  | D     | 105 | -    | 63,63,99     | 1.08 | 4 (6%)   | 69,75,111   | 1.28 | 6 (8%)   |
| 13  | BCL  | M     | 401 | -    | 69,74,74     | 1.16 | 5 (7%)   | 79,115,115  | 1.44 | 10 (12%) |
| 12  | PGV  | C     | 508 | -    | 20,20,50     | 1.45 | 3 (15%)  | 22,22,56    | 1.52 | 3 (13%)  |
| 21  | PEF  | W     | 105 | -    | 4,4,46       | 2.78 | 2 (50%)  | 6,6,51      | 1.72 | 2 (33%)  |
| 19  | CRT  | 8     | 101 | -    | 43,43,43     | 0.71 | 0        | 48,54,54    | 1.85 | 15 (31%) |
| 20  | CDL  | M     | 412 | -    | 38,38,99     | 1.31 | 3 (7%)   | 43,49,111   | 1.29 | 5 (11%)  |
| 12  | PGV  | M     | 410 | -    | 45,45,50     | 1.06 | 2 (4%)   | 48,50,56    | 0.97 | 3 (6%)   |
| 19  | CRT  | J     | 101 | -    | 43,43,43     | 0.79 | 0        | 48,54,54    | 1.69 | 11 (22%) |
| 19  | CRT  | G     | 101 | -    | 43,43,43     | 0.66 | 0        | 48,54,54    | 1.91 | 13 (27%) |
| 13  | BCL  | P     | 102 | -    | 69,74,74     | 1.21 | 3 (4%)   | 79,115,115  | 1.67 | 14 (17%) |
| 13  | BCL  | J     | 102 | -    | 69,74,74     | 1.11 | 6 (8%)   | 79,115,115  | 1.48 | 13 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | CRT  | 2     | 101 | -    | 43,43,43     | 0.66 | 0        | 48,54,54    | 2.04 | 14 (29%) |
| 13  | BCL  | K     | 103 | -    | 69,74,74     | 1.14 | 4 (5%)   | 79,115,115  | 1.52 | 12 (15%) |
| 19  | CRT  | M     | 405 | -    | 43,43,43     | 0.72 | 0        | 48,54,54    | 1.90 | 13 (27%) |
| 13  | BCL  | W     | 101 | -    | 69,74,74     | 1.14 | 4 (5%)   | 79,115,115  | 1.47 | 12 (15%) |
| 13  | BCL  | 7     | 101 | -    | 64,69,74     | 1.20 | 4 (6%)   | 73,109,115  | 1.65 | 12 (16%) |
| 15  | UQ8  | L     | 309 | -    | 53,53,53     | 1.22 | 2 (3%)   | 66,67,67    | 1.76 | 20 (30%) |
| 21  | PEF  | I     | 103 | -    | 4,4,46       | 2.72 | 2 (50%)  | 6,6,51      | 1.90 | 2 (33%)  |
| 13  | BCL  | D     | 101 | -    | 69,74,74     | 1.14 | 3 (4%)   | 79,115,115  | 1.60 | 15 (18%) |
| 23  | SF4  | b     | 101 | 7    | 0,12,12      | -    | -        | -           | -    | -        |
| 21  | PEF  | H     | 302 | -    | 4,4,46       | 2.57 | 2 (50%)  | 6,6,51      | 2.53 | 2 (33%)  |
| 13  | BCL  | K     | 101 | -    | 69,74,74     | 1.16 | 5 (7%)   | 79,115,115  | 1.57 | 14 (17%) |
| 8   | HEC  | C     | 502 | 1    | 46,50,50     | 1.84 | 9 (19%)  | 58,82,82    | 1.71 | 13 (22%) |
| 22  | LMT  | H     | 304 | -    | 36,36,36     | 0.52 | 0        | 47,47,47    | 1.32 | 8 (17%)  |
| 13  | BCL  | 4     | 102 | -    | 69,74,74     | 1.14 | 5 (7%)   | 79,115,115  | 1.51 | 12 (15%) |
| 12  | PGV  | 1     | 105 | -    | 30,30,50     | 1.22 | 2 (6%)   | 33,36,56    | 1.19 | 2 (6%)   |
| 19  | CRT  | 0     | 101 | -    | 43,43,43     | 0.74 | 0        | 48,54,54    | 1.72 | 12 (25%) |
| 20  | CDL  | O     | 104 | -    | 85,85,99     | 1.00 | 4 (4%)   | 91,97,111   | 1.28 | 11 (12%) |
| 13  | BCL  | 5     | 101 | -    | 69,74,74     | 1.18 | 5 (7%)   | 79,115,115  | 1.61 | 15 (18%) |
| 8   | HEC  | C     | 501 | 1    | 46,50,50     | 1.96 | 8 (17%)  | 58,82,82    | 2.05 | 18 (31%) |
| 20  | CDL  | M     | 406 | -    | 99,99,99     | 0.93 | 4 (4%)   | 105,111,111 | 1.15 | 8 (7%)   |
| 21  | PEF  | K     | 104 | -    | 26,26,46     | 1.31 | 2 (7%)   | 29,31,51    | 1.29 | 3 (10%)  |
| 13  | BCL  | F     | 103 | -    | 69,74,74     | 1.14 | 4 (5%)   | 79,115,115  | 1.37 | 9 (11%)  |
| 13  | BCL  | S     | 101 | -    | 69,74,74     | 1.18 | 3 (4%)   | 79,115,115  | 1.44 | 11 (13%) |
| 13  | BCL  | Q     | 103 | -    | 69,74,74     | 1.17 | 4 (5%)   | 79,115,115  | 1.50 | 11 (13%) |
| 13  | BCL  | L     | 302 | -    | 69,74,74     | 1.12 | 4 (5%)   | 79,115,115  | 1.31 | 8 (10%)  |
| 13  | BCL  | 9     | 103 | -    | 69,74,74     | 1.18 | 3 (4%)   | 79,115,115  | 1.51 | 12 (15%) |
| 20  | CDL  | H     | 305 | -    | 78,78,99     | 1.05 | 4 (5%)   | 84,90,111   | 1.06 | 5 (5%)   |
| 22  | LMT  | M     | 414 | -    | 36,36,36     | 0.42 | 0        | 47,47,47    | 0.77 | 0        |
| 12  | PGV  | D     | 106 | -    | 34,34,50     | 1.12 | 2 (5%)   | 37,40,56    | 1.07 | 3 (8%)   |
| 19  | CRT  | A     | 104 | -    | 43,43,43     | 0.66 | 0        | 48,54,54    | 1.87 | 14 (29%) |
| 21  | PEF  | 1     | 103 | -    | 4,4,46       | 2.70 | 2 (50%)  | 6,6,51      | 2.87 | 3 (50%)  |
| 10  | GOL  | H     | 301 | -    | 5,5,5        | 0.96 | 0        | 5,5,5       | 1.02 | 0        |
| 13  | BCL  | Y     | 101 | -    | 69,74,74     | 1.13 | 5 (7%)   | 79,115,115  | 1.42 | 10 (12%) |
| 13  | BCL  | 7     | 103 | -    | 69,74,74     | 1.19 | 4 (5%)   | 79,115,115  | 1.35 | 10 (12%) |
| 21  | PEF  | 3     | 104 | -    | 4,4,46       | 2.72 | 2 (50%)  | 6,6,51      | 1.91 | 2 (33%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | HEC  | C     | 504 | 1    | 46,50,50     | 1.76 | 10 (21%) | 58,82,82    | 1.68 | 12 (20%) |
| 12  | PGV  | 3     | 105 | -    | 50,50,50     | 0.94 | 2 (4%)   | 53,56,56    | 0.99 | 3 (5%)   |
| 19  | CRT  | W     | 102 | -    | 43,43,43     | 0.72 | 0        | 48,54,54    | 1.88 | 14 (29%) |
| 19  | CRT  | B     | 101 | -    | 43,43,43     | 0.71 | 0        | 48,54,54    | 1.83 | 13 (27%) |
| 21  | PEF  | M     | 409 | -    | 4,4,46       | 2.73 | 2 (50%)  | 6,6,51      | 1.93 | 2 (33%)  |
| 15  | UQ8  | M     | 413 | -    | 18,18,53     | 2.20 | 2 (11%)  | 24,25,67    | 1.37 | 3 (12%)  |
| 13  | BCL  | A     | 103 | -    | 69,74,74     | 1.12 | 4 (5%)   | 79,115,115  | 1.37 | 10 (12%) |
| 13  | BCL  | S     | 103 | -    | 69,74,74     | 1.25 | 4 (5%)   | 79,115,115  | 1.72 | 13 (16%) |
| 13  | BCL  | 9     | 101 | -    | 69,74,74     | 1.13 | 4 (5%)   | 79,115,115  | 1.37 | 9 (11%)  |
| 20  | CDL  | Y     | 104 | -    | 39,39,99     | 1.48 | 5 (12%)  | 45,51,111   | 1.92 | 15 (33%) |
| 21  | PEF  | M     | 407 | -    | 4,4,46       | 2.73 | 2 (50%)  | 6,6,51      | 1.91 | 2 (33%)  |
| 19  | CRT  | 3     | 103 | -    | 43,43,43     | 0.67 | 0        | 48,54,54    | 1.99 | 16 (33%) |
| 18  | MQ8  | M     | 404 | -    | 54,54,54     | 1.38 | 2 (3%)   | 67,69,69    | 1.51 | 15 (22%) |
| 14  | BPH  | L     | 303 | -    | 59,70,70     | 2.65 | 15 (25%) | 59,101,101  | 2.00 | 12 (20%) |

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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 19  | CRT  | T     | 101 | -    | -       | 2/51/51/51    | -       |
| 20  | CDL  | D     | 104 | -    | -       | 22/50/50/110  | -       |
| 20  | CDL  | S     | 104 | -    | -       | 37/85/85/110  | -       |
| 19  | CRT  | O     | 103 | -    | -       | 0/51/51/51    | -       |
| 12  | PGV  | M     | 411 | -    | -       | 15/41/41/55   | -       |
| 13  | BCL  | U     | 103 | -    | -       | 13/41/137/137 | -       |
| 13  | BCL  | 3     | 101 | -    | -       | 17/41/137/137 | -       |
| 19  | CRT  | N     | 101 | -    | -       | 0/51/51/51    | -       |
| 20  | CDL  | U     | 104 | -    | -       | 28/71/71/110  | -       |
| 13  | BCL  | F     | 101 | -    | -       | 12/41/137/137 | -       |
| 13  | BCL  | O     | 101 | -    | -       | 6/41/137/137  | -       |
| 12  | PGV  | L     | 308 | -    | -       | 24/48/48/55   | -       |
| 15  | UQ8  | L     | 311 | -    | -       | 2/9/33/75     | 0/1/1/1 |
| 13  | BCL  | D     | 103 | -    | -       | 7/41/137/137  | -       |
| 12  | PGV  | H     | 303 | -    | -       | 10/40/40/55   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 13  | BCL  | I     | 101 | -    | -       | 6/41/137/137  | -       |
| 13  | BCL  | L     | 301 | -    | -       | 3/41/137/137  | -       |
| 12  | PGV  | 9     | 104 | -    | -       | 14/37/37/55   | -       |
| 19  | CRT  | V     | 101 | -    | -       | 5/51/51/51    | -       |
| 8   | HEC  | C     | 503 | 1    | -       | 4/14/54/54    | -       |
| 13  | BCL  | Q     | 101 | -    | -       | 15/41/137/137 | -       |
| 13  | BCL  | U     | 101 | -    | -       | 3/41/137/137  | -       |
| 13  | BCL  | 1     | 101 | -    | -       | 14/41/137/137 | -       |
| 13  | BCL  | 5     | 103 | -    | -       | 13/41/137/137 | -       |
| 12  | PGV  | L     | 307 | -    | -       | 20/47/47/55   | -       |
| 13  | BCL  | 2     | 102 | -    | -       | 14/41/137/137 | -       |
| 20  | CDL  | 1     | 104 | -    | -       | 6/13/13/110   | -       |
| 19  | CRT  | 4     | 101 | -    | -       | 1/51/51/51    | -       |
| 13  | BCL  | L     | 305 | -    | -       | 13/41/137/137 | -       |
| 15  | UQ8  | L     | 304 | -    | -       | 3/27/51/75    | 0/1/1/1 |
| 13  | BCL  | A     | 101 | -    | -       | 11/41/137/137 | -       |
| 15  | UQ8  | L     | 310 | -    | -       | 8/27/51/75    | 0/1/1/1 |
| 19  | CRT  | Z     | 101 | -    | -       | 0/51/51/51    | -       |
| 13  | BCL  | W     | 104 | -    | -       | 7/41/137/137  | -       |
| 10  | GOL  | C     | 506 | -    | -       | 2/4/4/4       | -       |
| 19  | CRT  | P     | 101 | -    | -       | 0/51/51/51    | -       |
| 13  | BCL  | Y     | 103 | -    | -       | 15/41/137/137 | -       |
| 11  | LHG  | C     | 507 | -    | -       | 3/6/6/53      | -       |
| 14  | BPH  | M     | 402 | -    | -       | 6/37/105/105  | 0/5/6/6 |
| 20  | CDL  | D     | 105 | -    | -       | 26/73/73/110  | -       |
| 13  | BCL  | M     | 401 | -    | -       | 4/41/137/137  | -       |
| 12  | PGV  | C     | 508 | -    | -       | 6/21/21/55    | -       |
| 19  | CRT  | 8     | 101 | -    | -       | 4/51/51/51    | -       |
| 20  | CDL  | M     | 412 | -    | -       | 6/48/48/110   | -       |
| 12  | PGV  | M     | 410 | -    | -       | 15/47/47/55   | -       |
| 19  | CRT  | J     | 101 | -    | -       | 2/51/51/51    | -       |
| 19  | CRT  | G     | 101 | -    | -       | 2/51/51/51    | -       |
| 13  | BCL  | P     | 102 | -    | -       | 12/41/137/137 | -       |
| 13  | BCL  | J     | 102 | -    | -       | 11/41/137/137 | -       |
| 19  | CRT  | 2     | 101 | -    | -       | 0/51/51/51    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 13  | BCL  | K     | 103 | -    | -       | 13/41/137/137  | -       |
| 19  | CRT  | M     | 405 | -    | -       | 6/51/51/51     | -       |
| 13  | BCL  | W     | 101 | -    | -       | 10/41/137/137  | -       |
| 13  | BCL  | 7     | 101 | -    | -       | 5/35/131/137   | -       |
| 15  | UQ8  | L     | 309 | -    | -       | 16/51/75/75    | 0/1/1/1 |
| 13  | BCL  | D     | 101 | -    | -       | 8/41/137/137   | -       |
| 23  | SF4  | b     | 101 | 7    | -       | -              | 0/6/5/5 |
| 13  | BCL  | K     | 101 | -    | -       | 10/41/137/137  | -       |
| 8   | HEC  | C     | 502 | 1    | -       | 9/14/54/54     | -       |
| 22  | LMT  | H     | 304 | -    | -       | 9/21/61/61     | 0/2/2/2 |
| 13  | BCL  | 4     | 102 | -    | -       | 13/41/137/137  | -       |
| 12  | PGV  | 1     | 105 | -    | -       | 9/35/35/55     | -       |
| 19  | CRT  | 0     | 101 | -    | -       | 4/51/51/51     | -       |
| 20  | CDL  | O     | 104 | -    | -       | 32/96/96/110   | -       |
| 13  | BCL  | 5     | 101 | -    | -       | 9/41/137/137   | -       |
| 8   | HEC  | C     | 501 | 1    | -       | 6/14/54/54     | -       |
| 20  | CDL  | M     | 406 | -    | -       | 46/110/110/110 | -       |
| 21  | PEF  | K     | 104 | -    | -       | 6/30/30/50     | -       |
| 13  | BCL  | F     | 103 | -    | -       | 10/41/137/137  | -       |
| 13  | BCL  | S     | 101 | -    | -       | 8/41/137/137   | -       |
| 13  | BCL  | Q     | 103 | -    | -       | 8/41/137/137   | -       |
| 13  | BCL  | L     | 302 | -    | -       | 1/41/137/137   | -       |
| 13  | BCL  | 9     | 103 | -    | -       | 10/41/137/137  | -       |
| 20  | CDL  | H     | 305 | -    | -       | 29/89/89/110   | -       |
| 22  | LMT  | M     | 414 | -    | -       | 6/21/61/61     | 0/2/2/2 |
| 12  | PGV  | D     | 106 | -    | -       | 15/39/39/55    | -       |
| 19  | CRT  | A     | 104 | -    | -       | 0/51/51/51     | -       |
| 10  | GOL  | H     | 301 | -    | -       | 2/4/4/4        | -       |
| 13  | BCL  | Y     | 101 | -    | -       | 8/41/137/137   | -       |
| 13  | BCL  | 7     | 103 | -    | -       | 11/41/137/137  | -       |
| 8   | HEC  | C     | 504 | 1    | -       | 8/14/54/54     | -       |
| 12  | PGV  | 3     | 105 | -    | -       | 17/55/55/55    | -       |
| 19  | CRT  | W     | 102 | -    | -       | 3/51/51/51     | -       |
| 19  | CRT  | B     | 101 | -    | -       | 5/51/51/51     | -       |
| 15  | UQ8  | M     | 413 | -    | -       | 0/9/33/75      | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 13  | BCL  | A     | 103 | -    | -       | 11/41/137/137 | -       |
| 13  | BCL  | S     | 103 | -    | -       | 17/41/137/137 | -       |
| 13  | BCL  | 9     | 101 | -    | -       | 16/41/137/137 | -       |
| 20  | CDL  | Y     | 104 | -    | -       | 20/50/50/110  | -       |
| 19  | CRT  | 3     | 103 | -    | -       | 0/51/51/51    | -       |
| 18  | MQ8  | M     | 404 | -    | -       | 2/47/67/67    | 0/2/2/2 |
| 14  | BPH  | L     | 303 | -    | -       | 5/37/105/105  | 0/5/6/6 |

All (307) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | L     | 303 | BPH  | C1B-C2B | 9.35 | 1.49        | 1.39     |
| 14  | L     | 303 | BPH  | C1D-C2D | 8.49 | 1.48        | 1.39     |
| 14  | M     | 402 | BPH  | C1B-C2B | 8.41 | 1.48        | 1.39     |
| 14  | M     | 402 | BPH  | C1D-C2D | 8.19 | 1.48        | 1.39     |
| 15  | M     | 413 | UQ8  | C6-C1   | 8.17 | 1.49        | 1.35     |
| 15  | L     | 311 | UQ8  | C6-C1   | 8.11 | 1.49        | 1.35     |
| 18  | M     | 404 | MQ8  | C3-C2   | 8.07 | 1.49        | 1.35     |
| 15  | L     | 304 | UQ8  | C6-C1   | 7.68 | 1.49        | 1.35     |
| 15  | L     | 310 | UQ8  | C6-C1   | 7.45 | 1.48        | 1.35     |
| 15  | L     | 309 | UQ8  | C6-C1   | 7.40 | 1.48        | 1.35     |
| 14  | L     | 303 | BPH  | C3B-C2B | 5.90 | 1.49        | 1.39     |
| 14  | L     | 303 | BPH  | C3B-C4B | 5.58 | 1.50        | 1.41     |
| 14  | M     | 402 | BPH  | C4D-CHA | 5.57 | 1.47        | 1.39     |
| 14  | L     | 303 | BPH  | C4D-CHA | 5.52 | 1.47        | 1.39     |
| 14  | M     | 402 | BPH  | C3D-C2D | 5.31 | 1.48        | 1.39     |
| 14  | L     | 303 | BPH  | C3D-C2D | 5.27 | 1.48        | 1.39     |
| 13  | S     | 103 | BCL  | MG-NA   | 5.21 | 2.18        | 2.06     |
| 20  | S     | 104 | CDL  | OB8-CB7 | 5.20 | 1.48        | 1.33     |
| 13  | 2     | 102 | BCL  | MG-NA   | 5.19 | 2.18        | 2.06     |
| 14  | L     | 303 | BPH  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 13  | Y     | 103 | BCL  | MG-NA   | 5.13 | 2.18        | 2.06     |
| 13  | U     | 103 | BCL  | MG-NA   | 5.13 | 2.18        | 2.06     |
| 14  | M     | 402 | BPH  | O2D-CGD | 5.11 | 1.45        | 1.33     |
| 18  | M     | 404 | MQ8  | C10-C5  | 5.09 | 1.49        | 1.40     |
| 14  | M     | 402 | BPH  | C3B-C4B | 5.09 | 1.49        | 1.41     |
| 13  | 3     | 101 | BCL  | MG-NA   | 5.09 | 2.18        | 2.06     |
| 13  | Q     | 103 | BCL  | MG-NA   | 5.08 | 2.18        | 2.06     |
| 13  | 5     | 103 | BCL  | MG-NA   | 5.08 | 2.18        | 2.06     |
| 14  | M     | 402 | BPH  | C3B-C2B | 5.07 | 1.48        | 1.39     |
| 13  | Y     | 101 | BCL  | MG-NA   | 5.03 | 2.18        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | 7     | 103 | BCL  | MG-NA   | 5.02  | 2.18        | 2.06     |
| 13  | A     | 103 | BCL  | MG-NA   | 5.01  | 2.18        | 2.06     |
| 13  | M     | 401 | BCL  | MG-NA   | 5.00  | 2.18        | 2.06     |
| 13  | W     | 104 | BCL  | MG-NA   | 4.98  | 2.18        | 2.06     |
| 14  | M     | 402 | BPH  | OBD-CAD | 4.98  | 1.28        | 1.22     |
| 14  | L     | 303 | BPH  | OBD-CAD | 4.97  | 1.28        | 1.22     |
| 13  | S     | 101 | BCL  | MG-NA   | 4.95  | 2.18        | 2.06     |
| 13  | P     | 102 | BCL  | MG-NA   | 4.93  | 2.18        | 2.06     |
| 13  | F     | 103 | BCL  | MG-NA   | 4.90  | 2.17        | 2.06     |
| 13  | 4     | 102 | BCL  | MG-NA   | 4.90  | 2.17        | 2.06     |
| 13  | K     | 103 | BCL  | MG-NA   | 4.89  | 2.17        | 2.06     |
| 13  | L     | 301 | BCL  | MG-NA   | 4.88  | 2.17        | 2.06     |
| 13  | J     | 102 | BCL  | MG-NA   | 4.87  | 2.17        | 2.06     |
| 13  | W     | 101 | BCL  | MG-NA   | 4.85  | 2.17        | 2.06     |
| 13  | 1     | 101 | BCL  | MG-NA   | 4.82  | 2.17        | 2.06     |
| 13  | 9     | 103 | BCL  | MG-NA   | 4.82  | 2.17        | 2.06     |
| 21  | 1     | 103 | PEF  | P-O1P   | 4.82  | 1.61        | 1.50     |
| 13  | U     | 101 | BCL  | MG-NA   | 4.80  | 2.17        | 2.06     |
| 13  | A     | 101 | BCL  | MG-NA   | 4.78  | 2.17        | 2.06     |
| 13  | D     | 101 | BCL  | MG-NA   | 4.76  | 2.17        | 2.06     |
| 13  | 5     | 101 | BCL  | MG-NA   | 4.76  | 2.17        | 2.06     |
| 13  | I     | 101 | BCL  | MG-NA   | 4.76  | 2.17        | 2.06     |
| 13  | D     | 103 | BCL  | MG-NA   | 4.75  | 2.17        | 2.06     |
| 21  | W     | 105 | PEF  | P-O1P   | 4.71  | 1.61        | 1.50     |
| 21  | M     | 409 | PEF  | P-O1P   | 4.71  | 1.61        | 1.50     |
| 13  | O     | 101 | BCL  | MG-NA   | 4.70  | 2.17        | 2.06     |
| 13  | 9     | 101 | BCL  | MG-NA   | 4.70  | 2.17        | 2.06     |
| 8   | C     | 501 | HEC  | CAC-C3C | 4.68  | 1.50        | 1.35     |
| 21  | W     | 106 | PEF  | P-O1P   | 4.68  | 1.61        | 1.50     |
| 21  | I     | 103 | PEF  | P-O1P   | 4.67  | 1.61        | 1.50     |
| 13  | 7     | 101 | BCL  | MG-NA   | 4.67  | 2.17        | 2.06     |
| 13  | K     | 101 | BCL  | MG-NA   | 4.67  | 2.17        | 2.06     |
| 21  | M     | 407 | PEF  | P-O1P   | 4.66  | 1.61        | 1.50     |
| 21  | 3     | 104 | PEF  | P-O1P   | 4.66  | 1.61        | 1.50     |
| 13  | F     | 101 | BCL  | MG-NA   | 4.64  | 2.17        | 2.06     |
| 8   | C     | 502 | HEC  | CBC-CAC | -4.59 | 1.32        | 1.49     |
| 13  | L     | 302 | BCL  | MG-NA   | 4.59  | 2.17        | 2.06     |
| 13  | L     | 305 | BCL  | MG-NA   | 4.58  | 2.17        | 2.06     |
| 13  | Q     | 101 | BCL  | MG-NA   | 4.56  | 2.17        | 2.06     |
| 21  | H     | 302 | PEF  | P-O1P   | 4.50  | 1.61        | 1.50     |
| 12  | M     | 410 | PGV  | O03-C19 | 4.50  | 1.46        | 1.33     |
| 20  | M     | 412 | CDL  | OA8-CA7 | 4.49  | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | K     | 104 | PEF  | O2-C10  | 4.46  | 1.46        | 1.34     |
| 20  | H     | 305 | CDL  | OA6-CA5 | 4.46  | 1.46        | 1.34     |
| 12  | 1     | 105 | PGV  | O03-C19 | 4.41  | 1.46        | 1.33     |
| 8   | C     | 504 | HEC  | CBB-CAB | -4.41 | 1.33        | 1.49     |
| 20  | M     | 406 | CDL  | OB8-CB7 | 4.41  | 1.46        | 1.33     |
| 20  | S     | 104 | CDL  | OA8-CA7 | 4.40  | 1.46        | 1.33     |
| 20  | U     | 104 | CDL  | OB8-CB7 | 4.38  | 1.46        | 1.33     |
| 8   | C     | 501 | HEC  | CBC-CAC | -4.37 | 1.33        | 1.49     |
| 12  | M     | 410 | PGV  | O01-C1  | 4.37  | 1.46        | 1.34     |
| 20  | H     | 305 | CDL  | OA8-CA7 | 4.36  | 1.46        | 1.33     |
| 20  | D     | 105 | CDL  | OA6-CA5 | 4.36  | 1.46        | 1.34     |
| 8   | C     | 501 | HEC  | CBB-CAB | -4.34 | 1.33        | 1.49     |
| 8   | C     | 502 | HEC  | C1A-C2A | -4.33 | 1.37        | 1.45     |
| 20  | U     | 104 | CDL  | OB6-CB5 | 4.33  | 1.44        | 1.35     |
| 12  | 9     | 104 | PGV  | O03-C19 | 4.33  | 1.46        | 1.33     |
| 8   | C     | 503 | HEC  | CBC-CAC | -4.33 | 1.33        | 1.49     |
| 20  | M     | 406 | CDL  | OB6-CB5 | 4.31  | 1.46        | 1.34     |
| 12  | 1     | 105 | PGV  | O01-C1  | 4.31  | 1.46        | 1.34     |
| 20  | D     | 105 | CDL  | OB8-CB7 | 4.31  | 1.45        | 1.33     |
| 20  | O     | 104 | CDL  | OA6-CA5 | 4.30  | 1.46        | 1.34     |
| 12  | D     | 106 | PGV  | O03-C19 | 4.30  | 1.45        | 1.33     |
| 20  | D     | 104 | CDL  | OA8-CA7 | 4.30  | 1.45        | 1.33     |
| 20  | O     | 104 | CDL  | OA8-CA7 | 4.29  | 1.45        | 1.33     |
| 8   | C     | 504 | HEC  | CAC-C3C | 4.29  | 1.48        | 1.35     |
| 8   | C     | 503 | HEC  | CBB-CAB | -4.29 | 1.33        | 1.49     |
| 14  | M     | 402 | BPH  | O2A-CGA | 4.28  | 1.45        | 1.33     |
| 20  | D     | 104 | CDL  | OB8-CB7 | 4.28  | 1.45        | 1.33     |
| 12  | 3     | 105 | PGV  | O03-C19 | 4.27  | 1.45        | 1.33     |
| 20  | Y     | 104 | CDL  | OB8-CB7 | 4.26  | 1.45        | 1.33     |
| 20  | H     | 305 | CDL  | OB8-CB7 | 4.26  | 1.45        | 1.33     |
| 12  | 3     | 105 | PGV  | O01-C1  | 4.25  | 1.46        | 1.34     |
| 12  | H     | 303 | PGV  | O01-C1  | 4.24  | 1.46        | 1.34     |
| 8   | C     | 501 | HEC  | C4D-ND  | -4.24 | 1.31        | 1.39     |
| 21  | K     | 104 | PEF  | O3-C30  | 4.21  | 1.45        | 1.33     |
| 20  | U     | 104 | CDL  | OA8-CA7 | 4.21  | 1.45        | 1.33     |
| 20  | Y     | 104 | CDL  | OB6-CB5 | 4.20  | 1.46        | 1.34     |
| 12  | L     | 308 | PGV  | O03-C19 | 4.19  | 1.45        | 1.33     |
| 12  | H     | 303 | PGV  | O03-C19 | 4.19  | 1.45        | 1.33     |
| 8   | C     | 504 | HEC  | CBC-CAC | -4.18 | 1.34        | 1.49     |
| 12  | C     | 508 | PGV  | O03-C19 | 4.17  | 1.45        | 1.33     |
| 20  | O     | 104 | CDL  | OB8-CB7 | 4.17  | 1.45        | 1.33     |
| 12  | M     | 411 | PGV  | O03-C19 | 4.16  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | 9     | 104 | PGV  | O01-C1  | 4.15  | 1.46        | 1.34     |
| 12  | L     | 307 | PGV  | O01-C1  | 4.15  | 1.46        | 1.34     |
| 20  | D     | 104 | CDL  | OA6-CA5 | 4.15  | 1.46        | 1.34     |
| 20  | M     | 406 | CDL  | OA8-CA7 | 4.15  | 1.45        | 1.33     |
| 20  | M     | 412 | CDL  | OA6-CA5 | 4.15  | 1.46        | 1.34     |
| 20  | M     | 412 | CDL  | OB6-CB5 | 4.14  | 1.46        | 1.34     |
| 20  | Y     | 104 | CDL  | OA6-CA5 | 4.13  | 1.45        | 1.34     |
| 20  | S     | 104 | CDL  | OB6-CB5 | 4.12  | 1.45        | 1.34     |
| 20  | S     | 104 | CDL  | OA6-CA5 | 4.11  | 1.45        | 1.34     |
| 12  | C     | 508 | PGV  | O01-C1  | 4.11  | 1.45        | 1.34     |
| 8   | C     | 502 | HEC  | CBB-CAB | -4.09 | 1.34        | 1.49     |
| 12  | D     | 106 | PGV  | O01-C1  | 4.09  | 1.45        | 1.34     |
| 8   | C     | 501 | HEC  | C4A-C3A | -4.09 | 1.37        | 1.45     |
| 12  | L     | 307 | PGV  | O03-C19 | 4.09  | 1.45        | 1.33     |
| 12  | L     | 308 | PGV  | O01-C1  | 4.07  | 1.45        | 1.34     |
| 8   | C     | 501 | HEC  | C1B-NB  | -4.06 | 1.32        | 1.39     |
| 12  | M     | 411 | PGV  | O01-C1  | 4.06  | 1.45        | 1.34     |
| 20  | D     | 104 | CDL  | OB6-CB5 | 4.05  | 1.45        | 1.34     |
| 20  | H     | 305 | CDL  | OB6-CB5 | 4.03  | 1.45        | 1.34     |
| 14  | L     | 303 | BPH  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 8   | C     | 503 | HEC  | CAC-C3C | 4.02  | 1.48        | 1.35     |
| 8   | C     | 504 | HEC  | CAB-C3B | 4.01  | 1.48        | 1.35     |
| 8   | C     | 503 | HEC  | CAB-C3B | 3.96  | 1.47        | 1.35     |
| 8   | C     | 502 | HEC  | CAB-C3B | 3.94  | 1.47        | 1.35     |
| 20  | M     | 406 | CDL  | OA6-CA5 | 3.92  | 1.45        | 1.34     |
| 20  | O     | 104 | CDL  | OB6-CB5 | 3.89  | 1.45        | 1.34     |
| 8   | C     | 502 | HEC  | C4A-C3A | -3.88 | 1.37        | 1.45     |
| 13  | U     | 103 | BCL  | MG-NC   | 3.87  | 2.15        | 2.06     |
| 20  | Y     | 104 | CDL  | OA8-CA7 | 3.85  | 1.44        | 1.33     |
| 13  | 3     | 101 | BCL  | MG-NC   | 3.84  | 2.15        | 2.06     |
| 20  | D     | 105 | CDL  | OB6-CB5 | 3.81  | 1.45        | 1.34     |
| 13  | 2     | 102 | BCL  | MG-NC   | 3.80  | 2.15        | 2.06     |
| 15  | L     | 309 | UQ8  | C4-C3   | 3.75  | 1.49        | 1.36     |
| 20  | U     | 104 | CDL  | OA6-CA5 | 3.72  | 1.44        | 1.34     |
| 8   | C     | 501 | HEC  | C1A-C2A | -3.70 | 1.38        | 1.45     |
| 8   | C     | 502 | HEC  | CAC-C3C | 3.69  | 1.47        | 1.35     |
| 13  | 5     | 101 | BCL  | MG-NC   | 3.67  | 2.15        | 2.06     |
| 13  | 1     | 101 | BCL  | MG-NC   | 3.64  | 2.14        | 2.06     |
| 13  | S     | 103 | BCL  | MG-NC   | 3.63  | 2.14        | 2.06     |
| 15  | M     | 413 | UQ8  | C4-C3   | 3.60  | 1.49        | 1.36     |
| 13  | Q     | 101 | BCL  | MG-NC   | 3.60  | 2.14        | 2.06     |
| 13  | W     | 104 | BCL  | MG-NC   | 3.59  | 2.14        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | 5     | 103 | BCL  | MG-NC   | 3.59  | 2.14        | 2.06     |
| 13  | O     | 101 | BCL  | MG-NC   | 3.59  | 2.14        | 2.06     |
| 15  | L     | 310 | UQ8  | C4-C3   | 3.57  | 1.49        | 1.36     |
| 13  | Y     | 101 | BCL  | MG-NC   | 3.57  | 2.14        | 2.06     |
| 14  | M     | 402 | BPH  | CHA-CBD | -3.56 | 1.47        | 1.51     |
| 13  | L     | 302 | BCL  | MG-NC   | 3.56  | 2.14        | 2.06     |
| 13  | 7     | 101 | BCL  | MG-NC   | 3.55  | 2.14        | 2.06     |
| 13  | Q     | 103 | BCL  | MG-NC   | 3.54  | 2.14        | 2.06     |
| 13  | 9     | 101 | BCL  | MG-NC   | 3.54  | 2.14        | 2.06     |
| 13  | W     | 101 | BCL  | MG-NC   | 3.53  | 2.14        | 2.06     |
| 8   | C     | 501 | HEC  | CAB-C3B | 3.53  | 1.46        | 1.35     |
| 15  | L     | 304 | UQ8  | C4-C3   | 3.52  | 1.49        | 1.36     |
| 13  | Y     | 103 | BCL  | MG-NC   | 3.51  | 2.14        | 2.06     |
| 14  | L     | 303 | BPH  | CHA-CBD | -3.51 | 1.47        | 1.51     |
| 13  | I     | 101 | BCL  | MG-NC   | 3.50  | 2.14        | 2.06     |
| 13  | S     | 101 | BCL  | MG-NC   | 3.49  | 2.14        | 2.06     |
| 13  | L     | 305 | BCL  | MG-NC   | 3.48  | 2.14        | 2.06     |
| 13  | U     | 101 | BCL  | MG-NC   | 3.48  | 2.14        | 2.06     |
| 15  | L     | 311 | UQ8  | C4-C3   | 3.46  | 1.48        | 1.36     |
| 13  | K     | 103 | BCL  | MG-NC   | 3.43  | 2.14        | 2.06     |
| 13  | P     | 102 | BCL  | MG-NC   | 3.41  | 2.14        | 2.06     |
| 13  | A     | 101 | BCL  | MG-NC   | 3.40  | 2.14        | 2.06     |
| 13  | D     | 103 | BCL  | MG-NC   | 3.37  | 2.14        | 2.06     |
| 13  | F     | 101 | BCL  | MG-NC   | 3.37  | 2.14        | 2.06     |
| 13  | K     | 101 | BCL  | MG-NC   | 3.35  | 2.14        | 2.06     |
| 13  | F     | 103 | BCL  | MG-NC   | 3.35  | 2.14        | 2.06     |
| 13  | A     | 103 | BCL  | MG-NC   | 3.32  | 2.14        | 2.06     |
| 13  | 4     | 102 | BCL  | MG-NC   | 3.32  | 2.14        | 2.06     |
| 13  | M     | 401 | BCL  | C3B-C4B | 3.27  | 1.47        | 1.41     |
| 13  | 9     | 103 | BCL  | MG-NC   | 3.27  | 2.14        | 2.06     |
| 13  | D     | 101 | BCL  | MG-NC   | 3.24  | 2.14        | 2.06     |
| 13  | 9     | 103 | BCL  | C3B-C4B | 3.23  | 1.47        | 1.41     |
| 13  | 7     | 103 | BCL  | MG-NC   | 3.23  | 2.13        | 2.06     |
| 13  | S     | 103 | BCL  | C3B-C4B | 3.19  | 1.47        | 1.41     |
| 13  | P     | 102 | BCL  | C3B-C4B | 3.19  | 1.47        | 1.41     |
| 13  | J     | 102 | BCL  | MG-NC   | 3.18  | 2.13        | 2.06     |
| 8   | C     | 502 | HEC  | C4D-ND  | -3.15 | 1.33        | 1.39     |
| 13  | 3     | 101 | BCL  | C3B-C4B | 3.13  | 1.47        | 1.41     |
| 13  | L     | 301 | BCL  | MG-NC   | 3.12  | 2.13        | 2.06     |
| 13  | Q     | 103 | BCL  | C3B-C4B | 3.09  | 1.47        | 1.41     |
| 13  | K     | 103 | BCL  | C3B-C4B | 3.06  | 1.47        | 1.41     |
| 8   | C     | 504 | HEC  | C4D-ND  | -3.05 | 1.33        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | 7     | 103 | BCL  | C3B-C4B | 3.05  | 1.47        | 1.41     |
| 13  | S     | 101 | BCL  | C3B-C4B | 3.01  | 1.47        | 1.41     |
| 13  | Q     | 101 | BCL  | C3B-C4B | 3.00  | 1.47        | 1.41     |
| 13  | F     | 101 | BCL  | C3B-C4B | 2.99  | 1.47        | 1.41     |
| 13  | A     | 103 | BCL  | C3B-C4B | 2.98  | 1.47        | 1.41     |
| 13  | U     | 103 | BCL  | C3B-C4B | 2.96  | 1.47        | 1.41     |
| 13  | A     | 101 | BCL  | C3B-C4B | 2.93  | 1.46        | 1.41     |
| 13  | M     | 401 | BCL  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 13  | 5     | 101 | BCL  | C3B-C4B | 2.91  | 1.46        | 1.41     |
| 13  | K     | 101 | BCL  | C3B-C4B | 2.90  | 1.46        | 1.41     |
| 13  | W     | 101 | BCL  | C3B-C4B | 2.90  | 1.46        | 1.41     |
| 13  | 7     | 101 | BCL  | C3B-C4B | 2.88  | 1.46        | 1.41     |
| 13  | L     | 302 | BCL  | C3B-C4B | 2.88  | 1.46        | 1.41     |
| 13  | F     | 103 | BCL  | C3B-C4B | 2.88  | 1.46        | 1.41     |
| 13  | 5     | 103 | BCL  | C3B-C4B | 2.87  | 1.46        | 1.41     |
| 13  | D     | 101 | BCL  | C3B-C4B | 2.86  | 1.46        | 1.41     |
| 13  | 9     | 101 | BCL  | C3B-C4B | 2.85  | 1.46        | 1.41     |
| 14  | L     | 303 | BPH  | C1D-ND  | -2.84 | 1.33        | 1.38     |
| 13  | 4     | 102 | BCL  | C3B-C4B | 2.83  | 1.46        | 1.41     |
| 13  | 2     | 102 | BCL  | O2A-CGA | -2.83 | 1.25        | 1.33     |
| 13  | J     | 102 | BCL  | C3B-C4B | 2.81  | 1.46        | 1.41     |
| 13  | D     | 103 | BCL  | C3B-C4B | 2.81  | 1.46        | 1.41     |
| 13  | W     | 104 | BCL  | C3B-C4B | 2.80  | 1.46        | 1.41     |
| 14  | M     | 402 | BPH  | C1D-ND  | -2.78 | 1.33        | 1.38     |
| 8   | C     | 503 | HEC  | C4D-ND  | -2.77 | 1.34        | 1.39     |
| 13  | O     | 101 | BCL  | C3B-C4B | 2.76  | 1.46        | 1.41     |
| 13  | U     | 101 | BCL  | C3B-C4B | 2.75  | 1.46        | 1.41     |
| 8   | C     | 502 | HEC  | C1D-ND  | -2.73 | 1.34        | 1.39     |
| 13  | Y     | 103 | BCL  | C3B-C4B | 2.73  | 1.46        | 1.41     |
| 8   | C     | 503 | HEC  | C1D-ND  | -2.71 | 1.34        | 1.39     |
| 13  | 2     | 102 | BCL  | C3B-C4B | 2.70  | 1.46        | 1.41     |
| 14  | L     | 303 | BPH  | C2C-C3C | -2.69 | 1.52        | 1.54     |
| 8   | C     | 504 | HEC  | C1D-ND  | -2.68 | 1.34        | 1.39     |
| 13  | 1     | 101 | BCL  | C3B-C4B | 2.68  | 1.46        | 1.41     |
| 13  | I     | 101 | BCL  | C3B-C4B | 2.66  | 1.46        | 1.41     |
| 13  | L     | 301 | BCL  | C3B-C4B | 2.65  | 1.46        | 1.41     |
| 8   | C     | 502 | HEC  | C1B-NB  | -2.62 | 1.34        | 1.39     |
| 14  | M     | 402 | BPH  | C2C-C3C | -2.61 | 1.52        | 1.54     |
| 13  | L     | 305 | BCL  | CHD-C1D | 2.61  | 1.43        | 1.38     |
| 8   | C     | 504 | HEC  | C1B-NB  | -2.60 | 1.34        | 1.39     |
| 13  | Y     | 101 | BCL  | C3B-C4B | 2.55  | 1.46        | 1.41     |
| 20  | D     | 105 | CDL  | OA8-CA7 | 2.54  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | C     | 504 | HEC  | C3C-C4C | -2.51 | 1.41        | 1.46     |
| 13  | A     | 101 | BCL  | CHD-C1D | 2.50  | 1.43        | 1.38     |
| 13  | M     | 401 | BCL  | CHD-C1D | 2.49  | 1.43        | 1.38     |
| 14  | L     | 303 | BPH  | C4B-NB  | -2.47 | 1.34        | 1.38     |
| 13  | 2     | 102 | BCL  | O1A-CGA | -2.47 | 1.15        | 1.22     |
| 13  | W     | 101 | BCL  | CHD-C1D | 2.44  | 1.43        | 1.38     |
| 8   | C     | 503 | HEC  | C4B-NB  | -2.39 | 1.35        | 1.39     |
| 13  | L     | 301 | BCL  | CHD-C1D | 2.39  | 1.43        | 1.38     |
| 13  | Y     | 103 | BCL  | C1D-C2D | -2.39 | 1.40        | 1.45     |
| 21  | W     | 105 | PEF  | P-O4P   | 2.38  | 1.61        | 1.54     |
| 13  | I     | 101 | BCL  | C1-C2   | 2.37  | 1.55        | 1.49     |
| 13  | U     | 103 | BCL  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 13  | Q     | 103 | BCL  | C1D-C2D | -2.36 | 1.40        | 1.45     |
| 14  | L     | 303 | BPH  | CBD-CGD | -2.36 | 1.49        | 1.52     |
| 21  | M     | 408 | PEF  | P-O4P   | 2.36  | 1.61        | 1.54     |
| 21  | I     | 103 | PEF  | P-O4P   | 2.35  | 1.61        | 1.54     |
| 21  | M     | 408 | PEF  | P-O3P   | 2.35  | 1.61        | 1.54     |
| 8   | C     | 503 | HEC  | C1B-NB  | -2.35 | 1.35        | 1.39     |
| 21  | W     | 106 | PEF  | P-O3P   | 2.34  | 1.61        | 1.54     |
| 21  | M     | 409 | PEF  | P-O4P   | 2.34  | 1.61        | 1.54     |
| 13  | L     | 302 | BCL  | CHD-C1D | 2.34  | 1.43        | 1.38     |
| 21  | M     | 407 | PEF  | P-O3P   | 2.34  | 1.61        | 1.54     |
| 21  | 3     | 104 | PEF  | P-O3P   | 2.33  | 1.61        | 1.54     |
| 13  | Y     | 101 | BCL  | CHD-C1D | 2.32  | 1.42        | 1.38     |
| 8   | C     | 503 | HEC  | C1A-C2A | -2.32 | 1.41        | 1.45     |
| 14  | M     | 402 | BPH  | CBD-CGD | -2.31 | 1.49        | 1.52     |
| 14  | L     | 303 | BPH  | C1B-NB  | -2.31 | 1.34        | 1.38     |
| 13  | D     | 103 | BCL  | C1D-C2D | -2.28 | 1.40        | 1.45     |
| 13  | 5     | 101 | BCL  | C5-C3   | 2.28  | 1.56        | 1.51     |
| 8   | C     | 504 | HEC  | C4B-NB  | -2.27 | 1.35        | 1.39     |
| 12  | C     | 508 | PGV  | O01-C02 | -2.27 | 1.43        | 1.47     |
| 13  | 7     | 103 | BCL  | C1D-C2D | -2.26 | 1.40        | 1.45     |
| 13  | 9     | 101 | BCL  | CHD-C1D | 2.23  | 1.42        | 1.38     |
| 13  | 1     | 101 | BCL  | CHD-C1D | 2.23  | 1.42        | 1.38     |
| 13  | 5     | 101 | BCL  | C1-C2   | 2.23  | 1.55        | 1.49     |
| 14  | M     | 402 | BPH  | C4B-NB  | -2.23 | 1.34        | 1.38     |
| 13  | I     | 101 | BCL  | CHD-C1D | 2.22  | 1.42        | 1.38     |
| 13  | U     | 103 | BCL  | C16-C15 | 2.21  | 1.61        | 1.52     |
| 13  | K     | 101 | BCL  | CHD-C1D | 2.21  | 1.42        | 1.38     |
| 13  | A     | 103 | BCL  | CHD-C1D | 2.20  | 1.42        | 1.38     |
| 13  | L     | 305 | BCL  | C3B-C4B | 2.19  | 1.45        | 1.41     |
| 13  | W     | 104 | BCL  | C1D-C2D | -2.18 | 1.41        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | 1     | 103 | PEF  | P-O4P   | 2.18  | 1.61        | 1.54     |
| 13  | O     | 101 | BCL  | CHD-C1D | 2.17  | 1.42        | 1.38     |
| 13  | K     | 101 | BCL  | C1-C2   | 2.16  | 1.55        | 1.49     |
| 8   | C     | 503 | HEC  | C4A-C3A | -2.16 | 1.41        | 1.45     |
| 13  | 4     | 102 | BCL  | C1D-C2D | -2.14 | 1.41        | 1.45     |
| 13  | Y     | 103 | BCL  | CHD-C1D | 2.14  | 1.42        | 1.38     |
| 8   | C     | 504 | HEC  | C1D-C2D | 2.12  | 1.48        | 1.43     |
| 20  | Y     | 104 | CDL  | PA1-OA5 | 2.11  | 1.67        | 1.59     |
| 13  | J     | 102 | BCL  | C1D-C2D | -2.11 | 1.41        | 1.45     |
| 13  | F     | 103 | BCL  | C1D-C2D | -2.11 | 1.41        | 1.45     |
| 13  | 2     | 102 | BCL  | CHD-C1D | 2.11  | 1.42        | 1.38     |
| 13  | 4     | 102 | BCL  | CHD-C1D | 2.10  | 1.42        | 1.38     |
| 13  | 7     | 101 | BCL  | CHD-C1D | 2.09  | 1.42        | 1.38     |
| 13  | I     | 101 | BCL  | C5-C3   | 2.09  | 1.55        | 1.51     |
| 13  | K     | 103 | BCL  | C1D-C2D | -2.07 | 1.41        | 1.45     |
| 14  | M     | 402 | BPH  | C1B-NB  | -2.07 | 1.34        | 1.38     |
| 13  | S     | 103 | BCL  | CHD-C1D | 2.06  | 1.42        | 1.38     |
| 13  | Y     | 101 | BCL  | C1D-ND  | 2.06  | 1.40        | 1.37     |
| 13  | M     | 401 | BCL  | C3D-C4D | -2.06 | 1.39        | 1.44     |
| 13  | 5     | 103 | BCL  | C1D-C2D | -2.06 | 1.41        | 1.45     |
| 13  | F     | 101 | BCL  | CHD-C1D | 2.05  | 1.42        | 1.38     |
| 13  | J     | 102 | BCL  | CHD-C1D | 2.05  | 1.42        | 1.38     |
| 21  | H     | 302 | PEF  | P-O4P   | 2.04  | 1.60        | 1.54     |
| 13  | 5     | 103 | BCL  | CHD-C1D | 2.01  | 1.42        | 1.38     |
| 13  | J     | 102 | BCL  | C3D-C4D | -2.01 | 1.39        | 1.44     |

All (971) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | 3     | 101 | BCL  | C1-O2A-CGA  | 8.48  | 137.19      | 116.65   |
| 19  | 2     | 101 | CRT  | C37-C36-C35 | -7.66 | 114.15      | 124.91   |
| 19  | Z     | 101 | CRT  | C4-C5-C6    | -7.65 | 114.16      | 124.91   |
| 14  | M     | 402 | BPH  | O2D-CGD-CBD | 7.40  | 119.07      | 110.95   |
| 13  | S     | 103 | BCL  | C1-O2A-CGA  | 7.09  | 133.82      | 116.65   |
| 13  | L     | 305 | BCL  | C1-C2-C3    | -6.59 | 115.40      | 126.20   |
| 13  | Q     | 101 | BCL  | C1-C2-C3    | -6.44 | 115.65      | 126.20   |
| 19  | O     | 103 | CRT  | C37-C36-C35 | -6.41 | 115.92      | 124.91   |
| 19  | M     | 405 | CRT  | C37-C36-C35 | -6.34 | 116.01      | 124.91   |
| 19  | N     | 101 | CRT  | C21-C22-C23 | -6.16 | 118.63      | 127.28   |
| 19  | V     | 101 | CRT  | C37-C36-C35 | -6.14 | 116.30      | 124.91   |
| 19  | G     | 101 | CRT  | C4-C5-C6    | -6.05 | 116.41      | 124.91   |
| 14  | M     | 402 | BPH  | C2B-C1B-NB  | 6.01  | 113.77      | 109.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | 1     | 101 | BCL  | C1-O2A-CGA  | 5.94  | 131.03      | 116.65   |
| 14  | L     | 303 | BPH  | CMC-C2C-C1C | 5.90  | 127.32      | 114.61   |
| 13  | 7     | 101 | BCL  | C1-C2-C3    | -5.89 | 116.55      | 126.20   |
| 13  | 2     | 102 | BCL  | C1-O2A-CGA  | 5.88  | 130.89      | 116.65   |
| 14  | M     | 402 | BPH  | CMC-C2C-C1C | 5.81  | 127.14      | 114.61   |
| 13  | 5     | 103 | BCL  | C1-C2-C3    | -5.75 | 116.78      | 126.20   |
| 20  | U     | 104 | CDL  | CB4-OB6-CB5 | -5.69 | 107.79      | 117.85   |
| 14  | M     | 402 | BPH  | C4A-C3A-C2A | -5.67 | 97.44       | 102.84   |
| 19  | 4     | 101 | CRT  | C37-C36-C35 | -5.63 | 117.00      | 124.91   |
| 19  | N     | 101 | CRT  | C37-C36-C35 | -5.61 | 117.03      | 124.91   |
| 19  | T     | 101 | CRT  | C37-C36-C35 | -5.61 | 117.04      | 124.91   |
| 19  | W     | 102 | CRT  | C37-C36-C35 | -5.57 | 117.09      | 124.91   |
| 13  | A     | 101 | BCL  | C4D-CHA-C1A | 5.53  | 127.84      | 121.24   |
| 8   | C     | 501 | HEC  | CHC-C4B-NB  | 5.48  | 130.42      | 124.45   |
| 13  | F     | 101 | BCL  | C4D-CHA-C1A | 5.45  | 127.75      | 121.24   |
| 19  | P     | 101 | CRT  | C21-C22-C23 | -5.45 | 119.64      | 127.28   |
| 13  | S     | 101 | BCL  | C4D-CHA-C1A | 5.44  | 127.74      | 121.24   |
| 13  | I     | 101 | BCL  | C4D-CHA-C1A | 5.43  | 127.72      | 121.24   |
| 13  | F     | 101 | BCL  | C1-O2A-CGA  | 5.43  | 129.80      | 116.65   |
| 13  | U     | 101 | BCL  | C4D-CHA-C1A | 5.42  | 127.71      | 121.24   |
| 21  | H     | 302 | PEF  | O3P-P-O2P   | 5.41  | 124.75      | 107.91   |
| 13  | M     | 401 | BCL  | C4D-CHA-C1A | 5.35  | 127.62      | 121.24   |
| 13  | D     | 101 | BCL  | C4D-CHA-C1A | 5.33  | 127.60      | 121.24   |
| 13  | 3     | 101 | BCL  | O2A-CGA-O1A | -5.30 | 110.38      | 123.63   |
| 13  | P     | 102 | BCL  | C1-C2-C3    | 5.29  | 134.86      | 126.20   |
| 13  | 5     | 101 | BCL  | C11-C10-C8  | -5.25 | 98.53       | 115.97   |
| 13  | L     | 301 | BCL  | C4D-CHA-C1A | 5.22  | 127.47      | 121.24   |
| 13  | K     | 101 | BCL  | C4D-CHA-C1A | 5.21  | 127.46      | 121.24   |
| 19  | 3     | 103 | CRT  | C37-C36-C35 | -5.21 | 117.60      | 124.91   |
| 14  | L     | 303 | BPH  | O2D-CGD-CBD | 5.19  | 116.64      | 110.95   |
| 19  | Z     | 101 | CRT  | C37-C36-C35 | -5.18 | 117.64      | 124.91   |
| 13  | 9     | 103 | BCL  | C4D-CHA-C1A | 5.17  | 127.42      | 121.24   |
| 13  | W     | 101 | BCL  | C4D-CHA-C1A | 5.16  | 127.40      | 121.24   |
| 13  | W     | 104 | BCL  | C4D-CHA-C1A | 5.16  | 127.40      | 121.24   |
| 13  | Q     | 101 | BCL  | C4D-CHA-C1A | 5.15  | 127.39      | 121.24   |
| 20  | Y     | 104 | CDL  | CA4-OA6-CA5 | -5.14 | 105.49      | 117.80   |
| 13  | 9     | 103 | BCL  | C1-O2A-CGA  | 5.14  | 129.09      | 116.65   |
| 13  | F     | 103 | BCL  | C4D-CHA-C1A | 5.12  | 127.35      | 121.24   |
| 13  | 4     | 102 | BCL  | C4D-CHA-C1A | 5.12  | 127.35      | 121.24   |
| 19  | Z     | 101 | CRT  | C21-C22-C23 | -5.11 | 120.11      | 127.28   |
| 13  | Y     | 103 | BCL  | C4D-CHA-C1A | 5.11  | 127.33      | 121.24   |
| 13  | O     | 101 | BCL  | C4D-CHA-C1A | 5.10  | 127.33      | 121.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | V     | 101 | CRT  | C4-C5-C6    | -5.09 | 117.77      | 124.91   |
| 13  | Y     | 101 | BCL  | C4D-CHA-C1A | 5.07  | 127.30      | 121.24   |
| 8   | C     | 504 | HEC  | CHC-C4B-NB  | 5.06  | 129.96      | 124.45   |
| 15  | L     | 304 | UQ8  | C15-C14-C16 | 5.05  | 123.99      | 115.23   |
| 19  | 8     | 101 | CRT  | C4-C5-C6    | -5.04 | 117.84      | 124.91   |
| 19  | N     | 101 | CRT  | C4-C5-C6    | -5.04 | 117.84      | 124.91   |
| 13  | 2     | 102 | BCL  | C4D-CHA-C1A | 5.02  | 127.23      | 121.24   |
| 19  | W     | 102 | CRT  | C21-C22-C23 | -5.02 | 120.24      | 127.28   |
| 13  | D     | 103 | BCL  | C4D-CHA-C1A | 5.01  | 127.22      | 121.24   |
| 13  | 9     | 101 | BCL  | C4D-CHA-C1A | 5.01  | 127.21      | 121.24   |
| 13  | 7     | 101 | BCL  | C4D-CHA-C1A | 5.00  | 127.21      | 121.24   |
| 8   | C     | 501 | HEC  | CHD-C4C-NC  | 4.98  | 129.88      | 124.45   |
| 20  | U     | 104 | CDL  | OB6-CB5-C51 | 4.96  | 119.92      | 111.09   |
| 8   | C     | 503 | HEC  | CHC-C4B-NB  | 4.95  | 129.85      | 124.45   |
| 13  | Q     | 103 | BCL  | C4D-CHA-C1A | 4.95  | 127.15      | 121.24   |
| 13  | 3     | 101 | BCL  | C4D-CHA-C1A | 4.95  | 127.15      | 121.24   |
| 19  | J     | 101 | CRT  | C37-C36-C35 | -4.95 | 117.96      | 124.91   |
| 13  | 2     | 102 | BCL  | C16-C15-C13 | -4.94 | 99.53       | 115.97   |
| 14  | L     | 303 | BPH  | C2B-C1B-NB  | 4.93  | 112.99      | 109.43   |
| 19  | V     | 101 | CRT  | C21-C22-C23 | -4.90 | 120.40      | 127.28   |
| 15  | L     | 310 | UQ8  | C7-C8-C9    | -4.90 | 118.39      | 126.83   |
| 20  | S     | 104 | CDL  | OB6-CB5-C51 | 4.90  | 122.07      | 111.48   |
| 13  | 3     | 101 | BCL  | O2A-CGA-CBA | 4.88  | 126.72      | 111.83   |
| 19  | B     | 101 | CRT  | C21-C22-C23 | -4.86 | 120.46      | 127.28   |
| 20  | D     | 105 | CDL  | OA6-CA5-C11 | 4.85  | 121.98      | 111.48   |
| 13  | S     | 103 | BCL  | C4D-CHA-C1A | 4.83  | 127.00      | 121.24   |
| 19  | M     | 405 | CRT  | C21-C22-C23 | -4.81 | 120.53      | 127.28   |
| 13  | 1     | 101 | BCL  | C4D-CHA-C1A | 4.79  | 126.95      | 121.24   |
| 13  | J     | 102 | BCL  | C4D-CHA-C1A | 4.74  | 126.90      | 121.24   |
| 21  | 1     | 103 | PEF  | O4P-P-O1P   | -4.74 | 94.18       | 110.95   |
| 8   | C     | 501 | HEC  | C2A-C1A-NA  | -4.72 | 105.77      | 110.32   |
| 13  | 7     | 103 | BCL  | C4D-CHA-C1A | 4.72  | 126.87      | 121.24   |
| 13  | L     | 302 | BCL  | C4D-CHA-C1A | 4.70  | 126.85      | 121.24   |
| 19  | B     | 101 | CRT  | C37-C36-C35 | -4.67 | 118.35      | 124.91   |
| 19  | 3     | 103 | CRT  | C21-C22-C23 | -4.67 | 120.72      | 127.28   |
| 13  | L     | 305 | BCL  | C4D-CHA-C1A | 4.66  | 126.81      | 121.24   |
| 13  | D     | 101 | BCL  | C17-C16-C15 | 4.63  | 134.03      | 113.28   |
| 13  | 5     | 101 | BCL  | C4D-CHA-C1A | 4.61  | 126.75      | 121.24   |
| 13  | U     | 103 | BCL  | C4D-CHA-C1A | 4.60  | 126.73      | 121.24   |
| 8   | C     | 502 | HEC  | CHC-C4B-NB  | 4.59  | 129.46      | 124.45   |
| 19  | P     | 101 | CRT  | C4-C5-C6    | -4.56 | 118.51      | 124.91   |
| 19  | P     | 101 | CRT  | C37-C36-C35 | -4.55 | 118.52      | 124.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | A     | 104 | CRT  | C4-C5-C6    | -4.55 | 118.53      | 124.91   |
| 19  | 4     | 101 | CRT  | C4-C5-C6    | -4.53 | 118.55      | 124.91   |
| 12  | L     | 307 | PGV  | O01-C1-C2   | 4.53  | 121.28      | 111.48   |
| 19  | 8     | 101 | CRT  | C21-C22-C23 | -4.51 | 120.96      | 127.28   |
| 13  | A     | 101 | BCL  | C1-O2A-CGA  | 4.49  | 127.52      | 116.65   |
| 19  | 2     | 101 | CRT  | C21-C22-C23 | -4.48 | 121.00      | 127.28   |
| 8   | C     | 503 | HEC  | CBB-CAB-C3B | -4.48 | 118.48      | 127.43   |
| 19  | 0     | 101 | CRT  | C21-C22-C23 | -4.47 | 121.02      | 127.28   |
| 13  | 5     | 103 | BCL  | C4D-CHA-C1A | 4.46  | 126.56      | 121.24   |
| 13  | K     | 103 | BCL  | C1-C2-C3    | -4.44 | 118.92      | 126.20   |
| 19  | O     | 103 | CRT  | C21-C22-C23 | -4.44 | 121.05      | 127.28   |
| 13  | S     | 103 | BCL  | C1-C2-C3    | -4.43 | 118.94      | 126.20   |
| 13  | A     | 103 | BCL  | C4D-CHA-C1A | 4.42  | 126.52      | 121.24   |
| 20  | O     | 104 | CDL  | OA6-CA5-C11 | 4.41  | 121.03      | 111.48   |
| 20  | M     | 406 | CDL  | OB6-CB5-C51 | 4.41  | 121.02      | 111.48   |
| 21  | K     | 104 | PEF  | O2-C10-C11  | 4.40  | 121.00      | 111.48   |
| 12  | H     | 303 | PGV  | O01-C1-C2   | 4.39  | 120.98      | 111.48   |
| 13  | P     | 102 | BCL  | C4A-NA-C1A  | 4.37  | 108.67      | 106.68   |
| 13  | P     | 102 | BCL  | C4D-CHA-C1A | 4.32  | 126.39      | 121.24   |
| 19  | 0     | 101 | CRT  | C37-C36-C35 | -4.30 | 118.88      | 124.91   |
| 20  | M     | 406 | CDL  | OA6-CA5-C11 | 4.28  | 120.74      | 111.48   |
| 8   | C     | 502 | HEC  | CHA-C1A-NA  | 4.27  | 129.10      | 124.45   |
| 13  | K     | 101 | BCL  | C11-C10-C8  | -4.27 | 101.79      | 115.97   |
| 8   | C     | 501 | HEC  | CBB-CAB-C3B | -4.26 | 118.92      | 127.43   |
| 12  | L     | 308 | PGV  | O01-C1-C2   | 4.26  | 120.70      | 111.48   |
| 19  | 3     | 103 | CRT  | C4-C5-C6    | -4.25 | 118.95      | 124.91   |
| 12  | 1     | 105 | PGV  | O01-C1-C2   | 4.24  | 120.65      | 111.48   |
| 12  | M     | 411 | PGV  | O01-C1-C2   | 4.21  | 120.59      | 111.48   |
| 19  | 0     | 101 | CRT  | C4-C5-C6    | -4.21 | 119.01      | 124.91   |
| 19  | G     | 101 | CRT  | C37-C36-C35 | -4.19 | 119.03      | 124.91   |
| 19  | 8     | 101 | CRT  | C37-C36-C35 | -4.19 | 119.03      | 124.91   |
| 13  | P     | 102 | BCL  | C6-C5-C3    | 4.15  | 123.58      | 113.47   |
| 19  | 3     | 103 | CRT  | C10-C9-C7   | -4.14 | 121.47      | 127.28   |
| 13  | U     | 101 | BCL  | C1-C2-C3    | -4.12 | 119.44      | 126.20   |
| 20  | O     | 104 | CDL  | CB4-OB6-CB5 | -4.11 | 107.95      | 117.80   |
| 13  | Y     | 101 | BCL  | C4A-NA-C1A  | 4.11  | 108.55      | 106.68   |
| 13  | J     | 102 | BCL  | C4A-NA-C1A  | 4.10  | 108.55      | 106.68   |
| 12  | 3     | 105 | PGV  | O01-C1-C2   | 4.09  | 120.34      | 111.48   |
| 19  | T     | 101 | CRT  | C21-C22-C23 | -4.09 | 121.55      | 127.28   |
| 12  | 9     | 104 | PGV  | O01-C1-C2   | 4.09  | 120.32      | 111.48   |
| 19  | A     | 104 | CRT  | C21-C22-C23 | -4.08 | 121.55      | 127.28   |
| 20  | S     | 104 | CDL  | CB4-OB6-CB5 | -4.08 | 108.03      | 117.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | U     | 104 | CDL  | CA6-CA4-CA3 | -4.07 | 102.28      | 111.78   |
| 13  | L     | 305 | BCL  | C1D-ND-C4D  | -4.07 | 103.46      | 106.31   |
| 8   | C     | 504 | HEC  | CHD-C4C-NC  | 4.07  | 128.88      | 124.45   |
| 18  | M     | 404 | MQ8  | C16-C17-C18 | -4.06 | 118.32      | 127.62   |
| 13  | 7     | 101 | BCL  | C4A-NA-C1A  | 4.06  | 108.53      | 106.68   |
| 8   | C     | 502 | HEC  | CBC-CAC-C3C | -4.04 | 119.36      | 127.43   |
| 20  | D     | 105 | CDL  | OB6-CB5-C51 | 4.04  | 120.21      | 111.48   |
| 13  | 3     | 101 | BCL  | CHD-C1D-ND  | -4.03 | 119.12      | 124.80   |
| 12  | C     | 508 | PGV  | O01-C1-C2   | 4.01  | 120.16      | 111.48   |
| 13  | 2     | 102 | BCL  | C4A-NA-C1A  | 4.01  | 108.51      | 106.68   |
| 13  | Q     | 101 | BCL  | CHD-C1D-ND  | -4.01 | 119.16      | 124.80   |
| 19  | A     | 104 | CRT  | C10-C9-C7   | -3.95 | 121.73      | 127.28   |
| 13  | O     | 101 | BCL  | CHD-C1D-ND  | -3.95 | 119.25      | 124.80   |
| 13  | K     | 103 | BCL  | C4D-CHA-C1A | 3.94  | 125.95      | 121.24   |
| 13  | L     | 301 | BCL  | C1D-ND-C4D  | -3.94 | 103.55      | 106.31   |
| 13  | 4     | 102 | BCL  | C4A-NA-C1A  | 3.94  | 108.48      | 106.68   |
| 13  | K     | 103 | BCL  | C4A-NA-C1A  | 3.94  | 108.48      | 106.68   |
| 13  | 1     | 101 | BCL  | C1-C2-C3    | 3.93  | 132.64      | 126.20   |
| 13  | U     | 103 | BCL  | C20-C18-C19 | -3.93 | 92.99       | 110.53   |
| 13  | F     | 101 | BCL  | CHD-C1D-ND  | -3.93 | 119.27      | 124.80   |
| 13  | S     | 103 | BCL  | C4A-NA-C1A  | 3.91  | 108.47      | 106.68   |
| 13  | Y     | 103 | BCL  | C4A-NA-C1A  | 3.91  | 108.47      | 106.68   |
| 20  | H     | 305 | CDL  | OB6-CB5-C51 | 3.91  | 119.95      | 111.48   |
| 21  | M     | 409 | PEF  | O3P-P-O2P   | 3.91  | 120.07      | 107.91   |
| 21  | 3     | 104 | PEF  | O4P-P-O2P   | 3.91  | 120.07      | 107.91   |
| 14  | M     | 402 | BPH  | C3D-C4D-ND  | 3.90  | 112.71      | 107.71   |
| 21  | M     | 407 | PEF  | O4P-P-O2P   | 3.90  | 120.03      | 107.91   |
| 13  | O     | 101 | BCL  | C4A-NA-C1A  | 3.89  | 108.45      | 106.68   |
| 19  | 4     | 101 | CRT  | C21-C22-C23 | -3.88 | 121.83      | 127.28   |
| 21  | I     | 103 | PEF  | O3P-P-O2P   | 3.88  | 120.00      | 107.91   |
| 13  | W     | 104 | BCL  | C4A-NA-C1A  | 3.87  | 108.44      | 106.68   |
| 19  | 2     | 101 | CRT  | C4-C5-C6    | -3.86 | 119.49      | 124.91   |
| 13  | Q     | 103 | BCL  | C1D-ND-C4D  | -3.86 | 103.61      | 106.31   |
| 13  | L     | 305 | BCL  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 13  | U     | 101 | BCL  | CHD-C1D-ND  | -3.86 | 119.37      | 124.80   |
| 21  | W     | 106 | PEF  | O4P-P-O2P   | 3.86  | 119.91      | 107.91   |
| 13  | D     | 101 | BCL  | CHD-C1D-ND  | -3.86 | 119.38      | 124.80   |
| 20  | S     | 104 | CDL  | OA6-CA5-C11 | 3.85  | 119.81      | 111.48   |
| 13  | A     | 103 | BCL  | C4A-NA-C1A  | 3.85  | 108.44      | 106.68   |
| 19  | G     | 101 | CRT  | C21-C22-C23 | -3.85 | 121.89      | 127.28   |
| 13  | Q     | 103 | BCL  | C4A-NA-C1A  | 3.84  | 108.43      | 106.68   |
| 20  | U     | 104 | CDL  | OA6-CA5-C11 | 3.84  | 119.78      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | A     | 101 | BCL  | CHD-C1D-ND  | -3.83 | 119.41      | 124.80   |
| 13  | U     | 103 | BCL  | C1D-ND-C4D  | -3.83 | 103.62      | 106.31   |
| 13  | 5     | 101 | BCL  | CHD-C1D-ND  | -3.83 | 119.41      | 124.80   |
| 13  | O     | 101 | BCL  | C11-C10-C8  | -3.82 | 103.26      | 115.97   |
| 13  | I     | 101 | BCL  | CHD-C1D-ND  | -3.82 | 119.43      | 124.80   |
| 14  | L     | 303 | BPH  | C4D-CHA-CBD | -3.81 | 106.63      | 108.45   |
| 13  | 9     | 101 | BCL  | C4A-NA-C1A  | 3.81  | 108.42      | 106.68   |
| 8   | C     | 503 | HEC  | CHA-C1A-NA  | 3.80  | 128.60      | 124.45   |
| 13  | D     | 101 | BCL  | C1D-ND-C4D  | -3.80 | 103.65      | 106.31   |
| 15  | L     | 304 | UQ8  | C7-C8-C9    | -3.80 | 120.29      | 126.83   |
| 13  | 5     | 101 | BCL  | C4A-NA-C1A  | 3.80  | 108.41      | 106.68   |
| 14  | L     | 303 | BPH  | C3D-C4D-ND  | 3.79  | 112.57      | 107.71   |
| 20  | D     | 105 | CDL  | CB4-OB6-CB5 | -3.79 | 108.73      | 117.80   |
| 13  | Q     | 101 | BCL  | C16-C15-C13 | -3.79 | 103.37      | 115.97   |
| 8   | C     | 504 | HEC  | CBB-CAB-C3B | -3.79 | 119.86      | 127.43   |
| 19  | W     | 102 | CRT  | C4-C5-C6    | -3.78 | 119.60      | 124.91   |
| 13  | 7     | 101 | BCL  | CHD-C1D-ND  | -3.78 | 119.48      | 124.80   |
| 19  | M     | 405 | CRT  | C4-C5-C6    | -3.78 | 119.61      | 124.91   |
| 13  | K     | 101 | BCL  | C1-O2A-CGA  | 3.77  | 125.77      | 116.65   |
| 13  | U     | 101 | BCL  | C4A-NA-C1A  | 3.77  | 108.40      | 106.68   |
| 13  | W     | 101 | BCL  | CHD-C1D-ND  | -3.76 | 119.51      | 124.80   |
| 13  | F     | 103 | BCL  | C4A-NA-C1A  | 3.76  | 108.39      | 106.68   |
| 13  | U     | 101 | BCL  | C1D-ND-C4D  | -3.76 | 103.67      | 106.31   |
| 13  | 1     | 101 | BCL  | CHD-C1D-ND  | -3.75 | 119.52      | 124.80   |
| 22  | H     | 304 | LMT  | C3'-C4'-C5' | -3.74 | 102.64      | 110.93   |
| 13  | L     | 302 | BCL  | CHD-C1D-ND  | -3.73 | 119.56      | 124.80   |
| 13  | L     | 301 | BCL  | CHD-C1D-ND  | -3.72 | 119.56      | 124.80   |
| 19  | Z     | 101 | CRT  | C20-C19-C17 | -3.72 | 122.06      | 127.28   |
| 13  | D     | 101 | BCL  | C4A-NA-C1A  | 3.72  | 108.38      | 106.68   |
| 13  | J     | 102 | BCL  | C1-C2-C3    | -3.70 | 120.14      | 126.20   |
| 13  | M     | 401 | BCL  | CHD-C1D-ND  | -3.69 | 119.61      | 124.80   |
| 19  | T     | 101 | CRT  | C10-C9-C7   | -3.69 | 122.11      | 127.28   |
| 20  | O     | 104 | CDL  | OB6-CB5-C51 | 3.68  | 119.44      | 111.48   |
| 13  | K     | 103 | BCL  | C1D-ND-C4D  | -3.68 | 103.73      | 106.31   |
| 13  | Y     | 101 | BCL  | C1D-ND-C4D  | -3.68 | 103.73      | 106.31   |
| 14  | L     | 303 | BPH  | CBC-CAC-C3C | -3.67 | 106.55      | 113.78   |
| 13  | K     | 101 | BCL  | CHD-C1D-ND  | -3.67 | 119.64      | 124.80   |
| 13  | K     | 101 | BCL  | C1D-ND-C4D  | -3.66 | 103.74      | 106.31   |
| 13  | P     | 102 | BCL  | C1D-ND-C4D  | -3.65 | 103.75      | 106.31   |
| 13  | Y     | 103 | BCL  | C1-O2A-CGA  | 3.65  | 125.48      | 116.65   |
| 13  | 5     | 103 | BCL  | C4A-NA-C1A  | 3.65  | 108.34      | 106.68   |
| 14  | L     | 303 | BPH  | C1A-C2A-C3A | -3.65 | 99.37       | 102.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | M     | 406 | CDL  | CA4-OA6-CA5 | -3.64 | 109.08      | 117.80   |
| 13  | K     | 101 | BCL  | C4A-NA-C1A  | 3.63  | 108.34      | 106.68   |
| 13  | 5     | 103 | BCL  | C1D-ND-C4D  | -3.63 | 103.76      | 106.31   |
| 13  | 7     | 103 | BCL  | C4A-NA-C1A  | 3.63  | 108.33      | 106.68   |
| 13  | Y     | 101 | BCL  | CHD-C1D-ND  | -3.62 | 119.71      | 124.80   |
| 13  | M     | 401 | BCL  | C4A-NA-C1A  | 3.62  | 108.33      | 106.68   |
| 21  | 1     | 103 | PEF  | O3P-P-O2P   | 3.61  | 119.14      | 107.91   |
| 19  | N     | 101 | CRT  | C10-C9-C7   | -3.61 | 122.22      | 127.28   |
| 13  | 7     | 101 | BCL  | C1D-ND-C4D  | -3.59 | 103.79      | 106.31   |
| 20  | S     | 104 | CDL  | OB8-CB7-C71 | 3.58  | 122.76      | 111.83   |
| 13  | S     | 101 | BCL  | CHD-C1D-ND  | -3.58 | 119.76      | 124.80   |
| 13  | U     | 103 | BCL  | CHD-C1D-ND  | -3.54 | 119.82      | 124.80   |
| 19  | O     | 103 | CRT  | C4-C5-C6    | -3.53 | 119.95      | 124.91   |
| 13  | 4     | 102 | BCL  | C1-C2-C3    | 3.52  | 131.97      | 126.20   |
| 13  | 9     | 101 | BCL  | CHD-C1D-ND  | -3.52 | 119.84      | 124.80   |
| 13  | F     | 101 | BCL  | C4A-NA-C1A  | 3.52  | 108.28      | 106.68   |
| 13  | 9     | 103 | BCL  | CHD-C1D-ND  | -3.52 | 119.85      | 124.80   |
| 13  | A     | 101 | BCL  | C4A-NA-C1A  | 3.52  | 108.28      | 106.68   |
| 8   | C     | 501 | HEC  | CBC-CAC-C3C | -3.52 | 120.41      | 127.43   |
| 13  | I     | 101 | BCL  | C1D-ND-C4D  | -3.51 | 103.85      | 106.31   |
| 13  | W     | 104 | BCL  | CHD-C1D-ND  | -3.51 | 119.87      | 124.80   |
| 19  | 2     | 101 | CRT  | C10-C9-C7   | -3.50 | 122.36      | 127.28   |
| 13  | 2     | 102 | BCL  | C1D-ND-C4D  | -3.50 | 103.85      | 106.31   |
| 13  | Q     | 101 | BCL  | C1D-ND-C4D  | -3.50 | 103.86      | 106.31   |
| 13  | 5     | 101 | BCL  | C1D-ND-C4D  | -3.50 | 103.86      | 106.31   |
| 13  | 2     | 102 | BCL  | CHD-C1D-ND  | -3.50 | 119.88      | 124.80   |
| 19  | 4     | 101 | CRT  | C10-C9-C7   | -3.50 | 122.37      | 127.28   |
| 20  | H     | 305 | CDL  | OA6-CA5-C11 | 3.49  | 119.04      | 111.48   |
| 8   | C     | 503 | HEC  | CBC-CAC-C3C | -3.49 | 120.45      | 127.43   |
| 13  | F     | 103 | BCL  | C1D-ND-C4D  | -3.49 | 103.87      | 106.31   |
| 20  | Y     | 104 | CDL  | OA6-CA5-C11 | 3.48  | 123.73      | 110.93   |
| 13  | S     | 103 | BCL  | C1D-ND-C4D  | -3.48 | 103.87      | 106.31   |
| 13  | 3     | 101 | BCL  | C1D-ND-C4D  | -3.48 | 103.87      | 106.31   |
| 15  | L     | 304 | UQ8  | C16-C14-C13 | -3.47 | 113.37      | 121.17   |
| 13  | K     | 103 | BCL  | CHD-C1D-ND  | -3.47 | 119.92      | 124.80   |
| 13  | 5     | 101 | BCL  | C1-C2-C3    | -3.47 | 120.52      | 126.20   |
| 13  | 5     | 103 | BCL  | CHD-C1D-ND  | -3.45 | 119.94      | 124.80   |
| 21  | W     | 105 | PEF  | O3P-P-O2P   | 3.44  | 118.61      | 107.91   |
| 13  | S     | 101 | BCL  | C1D-ND-C4D  | -3.44 | 103.90      | 106.31   |
| 13  | W     | 104 | BCL  | C1D-ND-C4D  | -3.43 | 103.90      | 106.31   |
| 13  | Q     | 103 | BCL  | CHD-C1D-ND  | -3.43 | 119.97      | 124.80   |
| 19  | N     | 101 | CRT  | C21-C20-C19 | -3.43 | 116.50      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | L     | 309 | UQ8  | C7-C8-C9    | -3.43 | 120.92      | 126.83   |
| 20  | M     | 412 | CDL  | OB6-CB5-C51 | 3.43  | 118.90      | 111.48   |
| 19  | Z     | 101 | CRT  | C10-C9-C7   | -3.42 | 122.49      | 127.28   |
| 13  | M     | 401 | BCL  | C1D-ND-C4D  | -3.41 | 103.92      | 106.31   |
| 13  | O     | 101 | BCL  | C1D-ND-C4D  | -3.40 | 103.92      | 106.31   |
| 22  | H     | 304 | LMT  | C1B-O5B-C5B | 3.40  | 120.36      | 113.72   |
| 13  | D     | 101 | BCL  | C1-O2A-CGA  | 3.40  | 124.88      | 116.65   |
| 12  | M     | 410 | PGV  | O01-C1-C2   | 3.40  | 118.83      | 111.48   |
| 13  | F     | 101 | BCL  | C1D-ND-C4D  | -3.39 | 103.93      | 106.31   |
| 13  | M     | 401 | BCL  | CHA-C1A-NA  | -3.39 | 118.71      | 126.39   |
| 13  | W     | 101 | BCL  | C1D-ND-C4D  | -3.39 | 103.93      | 106.31   |
| 13  | D     | 103 | BCL  | C4A-NA-C1A  | 3.39  | 108.22      | 106.68   |
| 13  | 9     | 103 | BCL  | C1D-ND-C4D  | -3.38 | 103.94      | 106.31   |
| 15  | L     | 304 | UQ8  | C7-C6-C1    | -3.38 | 119.09      | 124.89   |
| 8   | C     | 502 | HEC  | CBB-CAB-C3B | -3.38 | 120.67      | 127.43   |
| 19  | M     | 405 | CRT  | C20-C19-C17 | -3.38 | 122.53      | 127.28   |
| 13  | P     | 102 | BCL  | CHD-C1D-ND  | -3.38 | 120.05      | 124.80   |
| 13  | 1     | 101 | BCL  | C1D-ND-C4D  | -3.38 | 103.94      | 106.31   |
| 12  | D     | 106 | PGV  | O01-C1-C2   | 3.37  | 118.78      | 111.48   |
| 8   | C     | 504 | HEC  | CBC-CAC-C3C | -3.37 | 120.70      | 127.43   |
| 13  | F     | 103 | BCL  | CHD-C1D-ND  | -3.37 | 120.06      | 124.80   |
| 13  | 7     | 103 | BCL  | C1D-ND-C4D  | -3.37 | 103.95      | 106.31   |
| 12  | C     | 508 | PGV  | C02-O01-C1  | -3.37 | 112.93      | 117.78   |
| 13  | U     | 103 | BCL  | C4A-NA-C1A  | 3.36  | 108.21      | 106.68   |
| 19  | P     | 101 | CRT  | C32-C31-C30 | -3.36 | 113.46      | 123.20   |
| 13  | S     | 103 | BCL  | CHD-C1D-ND  | -3.36 | 120.07      | 124.80   |
| 13  | D     | 103 | BCL  | C1D-ND-C4D  | -3.36 | 103.95      | 106.31   |
| 13  | P     | 102 | BCL  | C1-O2A-CGA  | 3.36  | 124.78      | 116.65   |
| 20  | O     | 104 | CDL  | OB8-CB7-C71 | 3.36  | 122.07      | 111.83   |
| 13  | 9     | 103 | BCL  | C4A-NA-C1A  | 3.35  | 108.21      | 106.68   |
| 19  | O     | 103 | CRT  | C21-C20-C19 | -3.35 | 116.67      | 123.52   |
| 13  | A     | 101 | BCL  | C1D-ND-C4D  | -3.35 | 103.97      | 106.31   |
| 20  | M     | 406 | CDL  | OA8-CA7-C31 | 3.34  | 122.03      | 111.83   |
| 19  | N     | 101 | CRT  | C32-C31-C30 | -3.34 | 113.52      | 123.20   |
| 13  | Q     | 101 | BCL  | C4A-NA-C1A  | 3.34  | 108.20      | 106.68   |
| 19  | B     | 101 | CRT  | C4-C5-C6    | -3.34 | 120.23      | 124.91   |
| 15  | L     | 309 | UQ8  | O5-C5-C6    | -3.32 | 115.37      | 121.79   |
| 19  | V     | 101 | CRT  | C20-C19-C17 | -3.32 | 122.63      | 127.28   |
| 12  | 9     | 104 | PGV  | O03-C19-C20 | 3.31  | 121.92      | 111.83   |
| 13  | 1     | 101 | BCL  | C4A-NA-C1A  | 3.31  | 108.19      | 106.68   |
| 13  | 9     | 101 | BCL  | C1D-ND-C4D  | -3.31 | 103.99      | 106.31   |
| 13  | J     | 102 | BCL  | CHA-C1A-NA  | -3.30 | 118.91      | 126.39   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | A     | 103 | BCL  | CHD-C1D-ND  | -3.30 | 120.16      | 124.80   |
| 13  | W     | 101 | BCL  | C4A-NA-C1A  | 3.29  | 108.18      | 106.68   |
| 13  | 4     | 102 | BCL  | C1D-ND-C4D  | -3.29 | 104.01      | 106.31   |
| 13  | I     | 101 | BCL  | C4A-NA-C1A  | 3.28  | 108.17      | 106.68   |
| 14  | M     | 402 | BPH  | CMC-C2C-C3C | 3.28  | 126.79      | 114.13   |
| 19  | 4     | 101 | CRT  | C20-C19-C17 | -3.28 | 122.68      | 127.28   |
| 14  | L     | 303 | BPH  | C4A-C3A-C2A | -3.26 | 99.74       | 102.84   |
| 15  | L     | 309 | UQ8  | C12-C13-C14 | -3.26 | 120.17      | 127.62   |
| 20  | O     | 104 | CDL  | OA8-CA7-C31 | 3.25  | 121.76      | 111.83   |
| 13  | 7     | 103 | BCL  | CHA-C1A-NA  | -3.24 | 119.04      | 126.39   |
| 19  | A     | 104 | CRT  | C37-C36-C35 | -3.24 | 120.36      | 124.91   |
| 12  | M     | 411 | PGV  | C02-O01-C1  | -3.24 | 110.05      | 117.80   |
| 13  | S     | 101 | BCL  | C1-C2-C3    | -3.23 | 120.90      | 126.20   |
| 13  | D     | 103 | BCL  | CHD-C1D-ND  | -3.23 | 120.26      | 124.80   |
| 13  | 4     | 102 | BCL  | CHD-C1D-ND  | -3.23 | 120.26      | 124.80   |
| 13  | K     | 103 | BCL  | CHA-C1A-NA  | -3.23 | 119.08      | 126.39   |
| 19  | T     | 101 | CRT  | C5-C6-C7    | -3.23 | 121.02      | 125.89   |
| 13  | Y     | 103 | BCL  | C1D-ND-C4D  | -3.22 | 104.05      | 106.31   |
| 13  | U     | 103 | BCL  | CHA-C1A-NA  | -3.22 | 119.09      | 126.39   |
| 13  | 4     | 102 | BCL  | CHA-C1A-NA  | -3.22 | 119.09      | 126.39   |
| 13  | A     | 103 | BCL  | C1D-ND-C4D  | -3.22 | 104.05      | 106.31   |
| 19  | J     | 101 | CRT  | C10-C9-C7   | -3.22 | 122.76      | 127.28   |
| 13  | 3     | 101 | BCL  | CHA-C1A-NA  | -3.22 | 119.10      | 126.39   |
| 13  | 5     | 103 | BCL  | CHA-C1A-NA  | -3.21 | 119.12      | 126.39   |
| 13  | L     | 302 | BCL  | C1D-ND-C4D  | -3.21 | 104.06      | 106.31   |
| 14  | L     | 303 | BPH  | CMC-C2C-C3C | 3.20  | 126.49      | 114.13   |
| 13  | Y     | 103 | BCL  | CHA-C1A-NA  | -3.20 | 119.15      | 126.39   |
| 15  | L     | 310 | UQ8  | C12-C13-C14 | -3.20 | 120.31      | 127.62   |
| 13  | F     | 103 | BCL  | CHA-C1A-NA  | -3.19 | 119.17      | 126.39   |
| 15  | L     | 309 | UQ8  | C35-C34-C36 | 3.18  | 120.75      | 115.23   |
| 13  | D     | 101 | BCL  | CHA-C1A-NA  | -3.17 | 119.20      | 126.39   |
| 19  | 4     | 101 | CRT  | C32-C31-C30 | -3.17 | 114.02      | 123.20   |
| 20  | Y     | 104 | CDL  | OB8-CB7-C71 | 3.17  | 120.77      | 111.15   |
| 13  | J     | 102 | BCL  | C2A-C1A-CHA | 3.16  | 129.35      | 123.87   |
| 20  | M     | 412 | CDL  | OA8-CA7-C31 | 3.16  | 120.74      | 111.15   |
| 8   | C     | 502 | HEC  | CHA-C4D-ND  | 3.16  | 129.59      | 123.86   |
| 20  | Y     | 104 | CDL  | OA2-PA1-OA3 | -3.15 | 96.45       | 108.94   |
| 8   | C     | 501 | HEC  | CHD-C4C-C3C | -3.14 | 119.91      | 125.21   |
| 13  | J     | 102 | BCL  | CHD-C1D-ND  | -3.14 | 120.38      | 124.80   |
| 13  | W     | 101 | BCL  | C17-C16-C15 | 3.14  | 127.36      | 113.28   |
| 13  | Y     | 103 | BCL  | O2A-CGA-O1A | -3.13 | 115.79      | 123.63   |
| 14  | M     | 402 | BPH  | CBA-CAA-C2A | -3.13 | 104.55      | 113.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | J     | 102 | BCL  | C1D-ND-C4D  | -3.13 | 104.12      | 106.31   |
| 15  | L     | 310 | UQ8  | C7-C6-C1    | -3.12 | 119.54      | 124.89   |
| 13  | A     | 103 | BCL  | CHA-C1A-NA  | -3.12 | 119.33      | 126.39   |
| 13  | S     | 103 | BCL  | CHA-C1A-NA  | -3.11 | 119.35      | 126.39   |
| 19  | Z     | 101 | CRT  | C32-C31-C30 | -3.11 | 114.20      | 123.20   |
| 13  | Q     | 103 | BCL  | CHA-C1A-NA  | -3.11 | 119.36      | 126.39   |
| 13  | O     | 101 | BCL  | C1-C2-C3    | -3.09 | 121.13      | 126.20   |
| 13  | P     | 102 | BCL  | CHA-C1A-NA  | -3.09 | 119.40      | 126.39   |
| 19  | G     | 101 | CRT  | C26-C27-C28 | -3.09 | 122.95      | 127.28   |
| 13  | 7     | 103 | BCL  | CHD-C1D-ND  | -3.09 | 120.46      | 124.80   |
| 13  | D     | 103 | BCL  | CHA-C1A-NA  | -3.08 | 119.42      | 126.39   |
| 13  | W     | 101 | BCL  | C1-C2-C3    | -3.07 | 121.17      | 126.20   |
| 19  | A     | 104 | CRT  | C36-C35-C33 | -3.06 | 121.26      | 125.89   |
| 14  | M     | 402 | BPH  | CBC-CAC-C3C | -3.06 | 107.75      | 113.78   |
| 13  | Y     | 103 | BCL  | CHD-C1D-ND  | -3.06 | 120.49      | 124.80   |
| 19  | B     | 101 | CRT  | C32-C31-C30 | -3.06 | 114.33      | 123.20   |
| 19  | B     | 101 | CRT  | C10-C9-C7   | -3.06 | 122.99      | 127.28   |
| 20  | S     | 104 | CDL  | OA8-CA7-C31 | 3.06  | 121.17      | 111.83   |
| 13  | 9     | 103 | BCL  | C1-C2-C3    | -3.05 | 121.19      | 126.20   |
| 19  | 4     | 101 | CRT  | C26-C27-C28 | -3.05 | 122.99      | 127.28   |
| 20  | Y     | 104 | CDL  | PA1-OA2-CA2 | 3.05  | 138.82      | 121.35   |
| 13  | U     | 103 | BCL  | C2A-C1A-CHA | 3.05  | 129.15      | 123.87   |
| 20  | S     | 104 | CDL  | CB6-CB4-CB3 | 3.04  | 118.87      | 111.78   |
| 13  | 9     | 103 | BCL  | CHA-C1A-NA  | -3.04 | 119.51      | 126.39   |
| 13  | 7     | 103 | BCL  | C2A-C1A-CHA | 3.03  | 129.13      | 123.87   |
| 19  | N     | 101 | CRT  | C29-C28-C30 | 3.03  | 122.72      | 118.09   |
| 19  | J     | 101 | CRT  | C5-C6-C7    | -3.03 | 121.32      | 125.89   |
| 13  | 5     | 103 | BCL  | C17-C16-C15 | 3.02  | 126.83      | 113.28   |
| 19  | M     | 405 | CRT  | C10-C9-C7   | -3.02 | 123.04      | 127.28   |
| 13  | W     | 104 | BCL  | CHA-C1A-NA  | -3.02 | 119.55      | 126.39   |
| 18  | M     | 404 | MQ8  | C29-C28-C30 | 3.02  | 120.47      | 115.23   |
| 13  | 2     | 102 | BCL  | CHA-C1A-NA  | -3.02 | 119.56      | 126.39   |
| 21  | 1     | 103 | PEF  | O4P-P-O3P   | 3.02  | 117.30      | 107.91   |
| 13  | F     | 101 | BCL  | O2A-CGA-O1A | -3.01 | 116.09      | 123.63   |
| 13  | L     | 301 | BCL  | C4A-NA-C1A  | 3.00  | 108.05      | 106.68   |
| 20  | Y     | 104 | CDL  | OA6-CA4-CA3 | 3.00  | 119.11      | 108.34   |
| 13  | 4     | 102 | BCL  | C2A-C1A-CHA | 3.00  | 129.07      | 123.87   |
| 13  | S     | 101 | BCL  | CHA-C1A-NA  | -2.99 | 119.62      | 126.39   |
| 13  | Q     | 101 | BCL  | C17-C16-C15 | -2.99 | 99.88       | 113.28   |
| 15  | L     | 309 | UQ8  | C15-C14-C16 | 2.99  | 120.42      | 115.23   |
| 19  | 4     | 101 | CRT  | C5-C6-C7    | -2.99 | 121.38      | 125.89   |
| 19  | M     | 405 | CRT  | C14-C15-C16 | -2.98 | 114.57      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | D     | 104 | CDL  | OA8-CA7-C31 | 2.98  | 120.19      | 111.15   |
| 20  | D     | 105 | CDL  | OB8-CB7-C71 | 2.98  | 120.91      | 111.83   |
| 15  | L     | 309 | UQ8  | C37-C38-C39 | -2.98 | 120.81      | 127.62   |
| 13  | L     | 305 | BCL  | CAB-C3B-C2B | 2.96  | 133.89      | 127.74   |
| 19  | 8     | 101 | CRT  | C21-C20-C19 | -2.95 | 117.47      | 123.52   |
| 19  | 3     | 103 | CRT  | C21-C20-C19 | -2.95 | 117.48      | 123.52   |
| 13  | L     | 301 | BCL  | CHA-C1A-NA  | -2.95 | 119.71      | 126.39   |
| 15  | L     | 304 | UQ8  | C10-C9-C11  | 2.95  | 120.34      | 115.23   |
| 13  | F     | 101 | BCL  | O2A-CGA-CBA | 2.94  | 120.81      | 111.83   |
| 18  | M     | 404 | MQ8  | C45-C43-C44 | 2.94  | 120.33      | 115.23   |
| 8   | C     | 501 | HEC  | CHA-C1A-C2A | 2.94  | 129.51      | 124.86   |
| 13  | Y     | 103 | BCL  | C2A-C1A-CHA | 2.93  | 128.95      | 123.87   |
| 15  | L     | 309 | UQ8  | C1M-C1-C6   | -2.93 | 119.64      | 124.45   |
| 20  | Y     | 104 | CDL  | OA6-CA5-OA7 | -2.92 | 116.87      | 123.70   |
| 19  | P     | 101 | CRT  | C21-C20-C19 | -2.92 | 117.54      | 123.52   |
| 19  | 3     | 103 | CRT  | C14-C15-C16 | -2.92 | 114.75      | 123.20   |
| 20  | D     | 104 | CDL  | OB8-CB7-C71 | 2.91  | 119.98      | 111.15   |
| 19  | Z     | 101 | CRT  | C14-C15-C16 | -2.91 | 114.77      | 123.20   |
| 20  | U     | 104 | CDL  | OB8-CB7-C71 | 2.91  | 120.70      | 111.83   |
| 19  | 8     | 101 | CRT  | C10-C9-C7   | -2.91 | 123.20      | 127.28   |
| 19  | T     | 101 | CRT  | C14-C15-C16 | -2.90 | 114.81      | 123.20   |
| 13  | A     | 101 | BCL  | CHA-C1A-NA  | -2.90 | 119.83      | 126.39   |
| 13  | I     | 101 | BCL  | CHA-C1A-NA  | -2.89 | 119.84      | 126.39   |
| 12  | L     | 307 | PGV  | C02-O01-C1  | -2.89 | 110.87      | 117.80   |
| 13  | O     | 101 | BCL  | C1-O2A-CGA  | 2.89  | 123.64      | 116.65   |
| 13  | S     | 103 | BCL  | C6-C5-C3    | 2.89  | 120.50      | 113.47   |
| 15  | L     | 310 | UQ8  | C1M-C1-C6   | -2.88 | 119.71      | 124.45   |
| 13  | K     | 103 | BCL  | C2A-C1A-CHA | 2.88  | 128.87      | 123.87   |
| 20  | Y     | 104 | CDL  | O1-C1-CA2   | 2.88  | 119.64      | 109.70   |
| 18  | M     | 404 | MQ8  | C41-C42-C43 | -2.88 | 121.04      | 127.62   |
| 20  | M     | 412 | CDL  | CA4-OA6-CA5 | -2.87 | 110.92      | 117.80   |
| 13  | S     | 101 | BCL  | C4A-NA-C1A  | 2.87  | 107.99      | 106.68   |
| 12  | L     | 308 | PGV  | O03-C19-C20 | 2.87  | 120.59      | 111.83   |
| 19  | W     | 102 | CRT  | C21-C20-C19 | -2.87 | 117.65      | 123.52   |
| 19  | A     | 104 | CRT  | C14-C15-C16 | -2.87 | 114.90      | 123.20   |
| 13  | P     | 102 | BCL  | C2A-C1A-CHA | 2.86  | 128.83      | 123.87   |
| 8   | C     | 501 | HEC  | CHD-C1D-ND  | 2.86  | 129.04      | 123.86   |
| 13  | D     | 103 | BCL  | C1-O2A-CGA  | 2.85  | 123.56      | 116.65   |
| 13  | Q     | 103 | BCL  | C2A-C1A-CHA | 2.85  | 128.81      | 123.87   |
| 13  | Y     | 101 | BCL  | CHA-C1A-NA  | -2.85 | 119.94      | 126.39   |
| 19  | V     | 101 | CRT  | C14-C15-C16 | -2.84 | 114.96      | 123.20   |
| 19  | J     | 101 | CRT  | C21-C22-C23 | -2.84 | 123.30      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | H     | 305 | CDL  | OA8-CA7-C31 | 2.84  | 120.48      | 111.83   |
| 12  | L     | 307 | PGV  | O03-C19-C20 | 2.83  | 120.47      | 111.83   |
| 13  | Q     | 101 | BCL  | CHA-C1A-NA  | -2.83 | 119.98      | 126.39   |
| 13  | Y     | 103 | BCL  | O2A-CGA-CBA | 2.83  | 120.47      | 111.83   |
| 13  | Q     | 103 | BCL  | C16-C15-C13 | 2.83  | 125.37      | 115.97   |
| 8   | C     | 502 | HEC  | CHB-C1B-NB  | 2.82  | 128.98      | 123.86   |
| 19  | M     | 405 | CRT  | C31-C32-C33 | -2.82 | 123.32      | 127.28   |
| 20  | U     | 104 | CDL  | OA8-CA7-C31 | 2.82  | 120.44      | 111.83   |
| 13  | A     | 103 | BCL  | C2A-C1A-CHA | 2.82  | 128.76      | 123.87   |
| 13  | 1     | 101 | BCL  | CHA-C1A-NA  | -2.82 | 120.01      | 126.39   |
| 13  | 3     | 101 | BCL  | C4A-NA-C1A  | 2.82  | 107.96      | 106.68   |
| 13  | D     | 103 | BCL  | C1-C2-C3    | -2.81 | 121.58      | 126.20   |
| 13  | L     | 302 | BCL  | CHA-C1A-NA  | -2.81 | 120.02      | 126.39   |
| 13  | 9     | 101 | BCL  | CHA-C1A-NA  | -2.80 | 120.04      | 126.39   |
| 12  | H     | 303 | PGV  | C02-O01-C1  | -2.80 | 111.08      | 117.80   |
| 20  | M     | 412 | CDL  | CB3-CB4-CB6 | -2.80 | 105.33      | 111.80   |
| 8   | C     | 504 | HEC  | CHA-C1A-NA  | 2.80  | 127.50      | 124.45   |
| 15  | M     | 413 | UQ8  | C7-C6-C1    | -2.80 | 120.09      | 124.89   |
| 13  | U     | 101 | BCL  | CHA-C1A-NA  | -2.80 | 120.06      | 126.39   |
| 15  | L     | 309 | UQ8  | C22-C23-C24 | -2.79 | 121.23      | 127.62   |
| 13  | S     | 103 | BCL  | C2A-C1A-CHA | 2.79  | 128.71      | 123.87   |
| 15  | L     | 310 | UQ8  | O5-C5-C6    | -2.78 | 116.42      | 121.79   |
| 20  | Y     | 104 | CDL  | OA8-CA7-C31 | 2.78  | 119.58      | 111.15   |
| 13  | I     | 101 | BCL  | C1-C2-C3    | -2.77 | 121.65      | 126.20   |
| 13  | F     | 103 | BCL  | C2A-C1A-CHA | 2.77  | 128.68      | 123.87   |
| 20  | Y     | 104 | CDL  | OA5-PA1-OA3 | 2.77  | 119.92      | 108.94   |
| 13  | 7     | 101 | BCL  | CHA-C1A-NA  | -2.77 | 120.11      | 126.39   |
| 19  | 2     | 101 | CRT  | C32-C31-C30 | -2.77 | 115.19      | 123.20   |
| 13  | F     | 101 | BCL  | CHA-C1A-NA  | -2.76 | 120.14      | 126.39   |
| 20  | U     | 104 | CDL  | CB2-C1-CA2  | 2.76  | 120.59      | 112.65   |
| 13  | L     | 305 | BCL  | CHA-C1A-NA  | -2.76 | 120.15      | 126.39   |
| 13  | W     | 104 | BCL  | C2A-C1A-CHA | 2.75  | 128.64      | 123.87   |
| 19  | G     | 101 | CRT  | C20-C19-C17 | -2.75 | 123.42      | 127.28   |
| 12  | L     | 308 | PGV  | C02-O01-C1  | -2.75 | 111.22      | 117.80   |
| 13  | K     | 103 | BCL  | C1-O2A-CGA  | 2.74  | 123.29      | 116.65   |
| 19  | Z     | 101 | CRT  | C21-C20-C19 | -2.74 | 117.92      | 123.52   |
| 8   | C     | 501 | HEC  | CHB-C1B-C2B | -2.74 | 119.49      | 127.43   |
| 19  | V     | 101 | CRT  | C32-C31-C30 | -2.73 | 115.28      | 123.20   |
| 19  | B     | 101 | CRT  | C21-C20-C19 | -2.73 | 117.93      | 123.52   |
| 13  | K     | 101 | BCL  | CHA-C1A-NA  | -2.72 | 120.22      | 126.39   |
| 18  | M     | 404 | MQ8  | C24-C23-C25 | 2.72  | 119.95      | 115.23   |
| 19  | P     | 101 | CRT  | C29-C28-C30 | 2.72  | 122.25      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | D     | 106 | PGV  | O03-C19-C20 | 2.72  | 120.13      | 111.83   |
| 13  | W     | 101 | BCL  | CHA-C1A-NA  | -2.72 | 120.23      | 126.39   |
| 13  | P     | 102 | BCL  | CAA-CBA-CGA | -2.72 | 105.49      | 113.21   |
| 13  | U     | 103 | BCL  | C17-C16-C15 | -2.71 | 101.11      | 113.28   |
| 8   | C     | 501 | HEC  | CHB-C1B-NB  | 2.71  | 128.78      | 123.86   |
| 8   | C     | 503 | HEC  | CHD-C4C-NC  | 2.71  | 127.41      | 124.45   |
| 19  | 2     | 101 | CRT  | C5-C6-C7    | -2.71 | 121.80      | 125.89   |
| 13  | L     | 301 | BCL  | C2A-C1A-CHA | 2.71  | 128.57      | 123.87   |
| 15  | L     | 309 | UQ8  | C17-C18-C19 | -2.71 | 121.42      | 127.62   |
| 20  | D     | 104 | CDL  | OA6-CA5-C11 | 2.71  | 120.88      | 110.93   |
| 19  | A     | 104 | CRT  | C21-C20-C19 | -2.71 | 117.98      | 123.52   |
| 15  | L     | 310 | UQ8  | C15-C14-C16 | 2.71  | 119.93      | 115.23   |
| 15  | L     | 304 | UQ8  | C1M-C1-C6   | -2.71 | 120.00      | 124.45   |
| 18  | M     | 404 | MQ8  | C11-C3-C2   | -2.70 | 120.25      | 124.89   |
| 13  | F     | 101 | BCL  | C11-C10-C8  | -2.70 | 106.98      | 115.97   |
| 15  | L     | 310 | UQ8  | C10-C9-C11  | 2.70  | 119.92      | 115.23   |
| 13  | O     | 101 | BCL  | CHA-C1A-NA  | -2.70 | 120.28      | 126.39   |
| 22  | H     | 304 | LMT  | C1'-C2'-C3' | 2.70  | 115.68      | 110.01   |
| 13  | 5     | 101 | BCL  | CHA-C1A-NA  | -2.70 | 120.28      | 126.39   |
| 19  | G     | 101 | CRT  | C14-C15-C16 | -2.69 | 115.40      | 123.20   |
| 20  | M     | 406 | CDL  | OB8-CB7-C71 | 2.69  | 120.03      | 111.83   |
| 8   | C     | 502 | HEC  | C2A-C1A-NA  | -2.69 | 107.73      | 110.32   |
| 20  | U     | 104 | CDL  | CA4-OA6-CA5 | -2.68 | 111.37      | 117.80   |
| 20  | O     | 104 | CDL  | CA4-OA6-CA5 | -2.68 | 111.38      | 117.80   |
| 19  | W     | 102 | CRT  | C10-C9-C7   | -2.68 | 123.52      | 127.28   |
| 15  | L     | 310 | UQ8  | C20-C19-C21 | 2.67  | 119.87      | 115.23   |
| 15  | L     | 309 | UQ8  | C30-C29-C31 | 2.67  | 119.86      | 115.23   |
| 13  | 5     | 101 | BCL  | C4-C3-C5    | -2.66 | 110.61      | 115.23   |
| 19  | 3     | 103 | CRT  | C18-C17-C16 | 2.66  | 122.16      | 118.09   |
| 19  | 0     | 101 | CRT  | C10-C9-C7   | -2.66 | 123.55      | 127.28   |
| 19  | G     | 101 | CRT  | C32-C31-C30 | -2.65 | 115.51      | 123.20   |
| 13  | Y     | 101 | BCL  | CAB-C3B-C2B | 2.65  | 133.25      | 127.74   |
| 19  | 2     | 101 | CRT  | C21-C20-C19 | -2.65 | 118.09      | 123.52   |
| 15  | L     | 309 | UQ8  | C10-C9-C11  | 2.65  | 119.83      | 115.23   |
| 13  | L     | 305 | BCL  | C11-C12-C13 | -2.65 | 107.17      | 115.97   |
| 19  | 3     | 103 | CRT  | C5-C6-C7    | -2.65 | 121.89      | 125.89   |
| 13  | I     | 101 | BCL  | C11-C10-C8  | -2.64 | 107.19      | 115.97   |
| 12  | 1     | 105 | PGV  | O03-C19-C20 | 2.64  | 119.87      | 111.83   |
| 13  | L     | 302 | BCL  | C2A-C1A-CHA | 2.63  | 128.44      | 123.87   |
| 12  | H     | 303 | PGV  | O03-C19-C20 | 2.63  | 119.86      | 111.83   |
| 19  | O     | 103 | CRT  | C32-C31-C30 | -2.63 | 115.58      | 123.20   |
| 20  | S     | 104 | CDL  | CB6-OB8-CB7 | 2.63  | 126.73      | 117.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | L     | 301 | BCL  | CAB-C3B-C2B | 2.63  | 133.20      | 127.74   |
| 19  | P     | 101 | CRT  | C10-C9-C7   | -2.63 | 123.59      | 127.28   |
| 19  | A     | 104 | CRT  | C32-C31-C30 | -2.63 | 115.59      | 123.20   |
| 8   | C     | 504 | HEC  | CHD-C1D-ND  | 2.62  | 128.62      | 123.86   |
| 13  | U     | 103 | BCL  | C16-C15-C13 | -2.62 | 107.25      | 115.97   |
| 13  | 5     | 103 | BCL  | C2A-C1A-CHA | 2.62  | 128.42      | 123.87   |
| 8   | C     | 501 | HEC  | CHC-C1C-C2C | -2.62 | 119.82      | 127.43   |
| 8   | C     | 503 | HEC  | CHD-C1D-ND  | 2.60  | 128.58      | 123.86   |
| 15  | L     | 309 | UQ8  | C20-C19-C21 | 2.60  | 119.74      | 115.23   |
| 20  | M     | 406 | CDL  | OA8-CA7-OA9 | -2.60 | 117.12      | 123.63   |
| 19  | 4     | 101 | CRT  | C14-C15-C16 | -2.60 | 115.67      | 123.20   |
| 8   | C     | 504 | HEC  | CHB-C1B-NB  | 2.59  | 128.56      | 123.86   |
| 19  | 4     | 101 | CRT  | C34-C33-C35 | 2.59  | 122.04      | 118.09   |
| 21  | H     | 302 | PEF  | O4P-P-O1P   | -2.58 | 101.81      | 110.95   |
| 22  | H     | 304 | LMT  | O1B-C4'-C3' | 2.58  | 113.78      | 107.23   |
| 19  | W     | 102 | CRT  | C32-C31-C30 | -2.57 | 115.75      | 123.20   |
| 19  | T     | 101 | CRT  | C32-C31-C30 | -2.56 | 115.77      | 123.20   |
| 19  | 8     | 101 | CRT  | C32-C31-C30 | -2.56 | 115.77      | 123.20   |
| 19  | B     | 101 | CRT  | C29-C28-C30 | 2.56  | 122.00      | 118.09   |
| 19  | 2     | 101 | CRT  | C34-C33-C35 | 2.56  | 122.00      | 118.09   |
| 14  | M     | 402 | BPH  | C4-C3-C2    | -2.56 | 117.05      | 123.63   |
| 19  | V     | 101 | CRT  | C9-C10-C11  | -2.56 | 115.79      | 123.20   |
| 19  | T     | 101 | CRT  | C29-C28-C30 | 2.56  | 121.99      | 118.09   |
| 20  | Y     | 104 | CDL  | OB6-CB5-C51 | 2.55  | 120.29      | 110.93   |
| 15  | M     | 413 | UQ8  | C4M-O4-C4   | 2.55  | 125.42      | 116.47   |
| 13  | L     | 305 | BCL  | C2A-C1A-CHA | 2.55  | 128.29      | 123.87   |
| 22  | H     | 304 | LMT  | C4B-C3B-C2B | -2.55 | 106.36      | 110.83   |
| 13  | Q     | 103 | BCL  | C1-C2-C3    | -2.55 | 122.03      | 126.20   |
| 19  | W     | 102 | CRT  | C9-C10-C11  | -2.54 | 115.83      | 123.20   |
| 20  | Y     | 104 | CDL  | CA6-CA4-CA3 | -2.54 | 105.86      | 111.78   |
| 19  | 3     | 103 | CRT  | C32-C31-C30 | -2.54 | 115.85      | 123.20   |
| 15  | L     | 309 | UQ8  | C8-C7-C6    | -2.53 | 105.84      | 112.08   |
| 8   | C     | 502 | HEC  | CHB-C1B-C2B | -2.53 | 120.07      | 127.43   |
| 13  | S     | 103 | BCL  | CMB-C2B-C1B | -2.53 | 121.56      | 125.42   |
| 19  | B     | 101 | CRT  | C26-C27-C28 | -2.53 | 123.73      | 127.28   |
| 13  | D     | 103 | BCL  | C2A-C1A-CHA | 2.53  | 128.26      | 123.87   |
| 13  | 2     | 102 | BCL  | CAB-C3B-C2B | 2.53  | 132.99      | 127.74   |
| 21  | M     | 408 | PEF  | O2P-P-O1P   | 2.52  | 119.88      | 110.95   |
| 19  | M     | 405 | CRT  | C5-C6-C7    | -2.52 | 122.08      | 125.89   |
| 13  | W     | 101 | BCL  | C1C-NC-C4C  | 2.52  | 107.83      | 106.68   |
| 13  | M     | 401 | BCL  | C4D-C3D-CAD | -2.52 | 105.37      | 108.11   |
| 13  | S     | 101 | BCL  | CMB-C2B-C1B | -2.52 | 121.59      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | 3     | 103 | CRT  | C27-C26-C25 | -2.51 | 115.91      | 123.20   |
| 19  | N     | 101 | CRT  | C27-C26-C25 | -2.51 | 115.92      | 123.20   |
| 20  | H     | 305 | CDL  | CB4-OB6-CB5 | -2.51 | 111.79      | 117.80   |
| 13  | 9     | 103 | BCL  | C2A-C1A-CHA | 2.51  | 128.22      | 123.87   |
| 13  | 9     | 103 | BCL  | CMB-C2B-C1B | -2.51 | 121.60      | 125.42   |
| 19  | T     | 101 | CRT  | C21-C20-C19 | -2.50 | 118.39      | 123.52   |
| 19  | 2     | 101 | CRT  | C35-C33-C32 | -2.50 | 115.07      | 119.01   |
| 15  | L     | 309 | UQ8  | C40-C39-C41 | 2.50  | 119.57      | 115.23   |
| 20  | U     | 104 | CDL  | PA1-OA5-CA3 | -2.50 | 107.01      | 121.35   |
| 13  | M     | 401 | BCL  | CMB-C2B-C1B | -2.50 | 121.61      | 125.42   |
| 13  | K     | 103 | BCL  | CMB-C2B-C1B | -2.50 | 121.62      | 125.42   |
| 8   | C     | 501 | HEC  | CHC-C1C-NC  | 2.50  | 128.39      | 123.86   |
| 18  | M     | 404 | MQ8  | C34-C33-C35 | 2.49  | 119.56      | 115.23   |
| 8   | C     | 504 | HEC  | CHA-C4D-ND  | 2.49  | 128.38      | 123.86   |
| 22  | H     | 304 | LMT  | O5'-C1'-C2' | 2.49  | 115.49      | 110.37   |
| 20  | M     | 412 | CDL  | OA6-CA5-C11 | 2.49  | 120.08      | 110.93   |
| 13  | U     | 101 | BCL  | C16-C15-C13 | 2.49  | 124.24      | 115.97   |
| 19  | W     | 102 | CRT  | C14-C15-C16 | -2.49 | 116.00      | 123.20   |
| 19  | W     | 102 | CRT  | C20-C19-C17 | -2.49 | 123.79      | 127.28   |
| 15  | L     | 311 | UQ8  | C10-C9-C11  | 2.49  | 120.31      | 114.59   |
| 19  | G     | 101 | CRT  | C9-C10-C11  | -2.49 | 116.00      | 123.20   |
| 19  | N     | 101 | CRT  | C34-C33-C35 | 2.48  | 121.88      | 118.09   |
| 19  | J     | 101 | CRT  | C14-C15-C16 | -2.48 | 116.01      | 123.20   |
| 18  | M     | 404 | MQ8  | C26-C27-C28 | -2.48 | 121.95      | 127.62   |
| 13  | I     | 101 | BCL  | C4-C3-C5    | -2.48 | 110.93      | 115.23   |
| 13  | D     | 103 | BCL  | CAB-C3B-C2B | 2.48  | 132.89      | 127.74   |
| 13  | U     | 101 | BCL  | C4-C3-C5    | -2.47 | 110.94      | 115.23   |
| 19  | B     | 101 | CRT  | C5-C6-C7    | -2.47 | 122.16      | 125.89   |
| 13  | A     | 101 | BCL  | C6-C5-C3    | 2.47  | 119.48      | 113.47   |
| 13  | I     | 101 | BCL  | CAB-C3B-C2B | 2.47  | 132.87      | 127.74   |
| 19  | A     | 104 | CRT  | C20-C19-C17 | -2.46 | 123.82      | 127.28   |
| 19  | Z     | 101 | CRT  | C18-C17-C16 | 2.46  | 121.85      | 118.09   |
| 19  | 3     | 103 | CRT  | C20-C19-C17 | -2.46 | 123.83      | 127.28   |
| 19  | J     | 101 | CRT  | C32-C31-C30 | -2.46 | 116.08      | 123.20   |
| 13  | 9     | 103 | BCL  | C16-C15-C13 | 2.46  | 124.14      | 115.97   |
| 14  | L     | 303 | BPH  | CED-O2D-CGD | 2.46  | 121.49      | 115.92   |
| 19  | T     | 101 | CRT  | C1-C4-C5    | 2.46  | 119.36      | 112.98   |
| 13  | S     | 101 | BCL  | C4-C3-C5    | -2.45 | 110.97      | 115.23   |
| 12  | M     | 410 | PGV  | O03-C19-C20 | 2.45  | 119.31      | 111.83   |
| 20  | D     | 104 | CDL  | CA4-OA6-CA5 | -2.45 | 111.93      | 117.80   |
| 13  | U     | 101 | BCL  | CAB-C3B-C2B | 2.45  | 132.84      | 127.74   |
| 13  | F     | 101 | BCL  | C1-C2-C3    | -2.45 | 122.19      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | 0     | 101 | CRT  | C36-C35-C33 | -2.44 | 122.20      | 125.89   |
| 13  | J     | 102 | BCL  | O2A-CGA-O1A | -2.44 | 117.52      | 123.63   |
| 19  | T     | 101 | CRT  | C13-C12-C11 | 2.44  | 121.82      | 118.09   |
| 13  | L     | 305 | BCL  | C6-C7-C8    | 2.44  | 124.08      | 115.97   |
| 8   | C     | 502 | HEC  | CHB-C4A-NA  | 2.44  | 127.11      | 124.45   |
| 13  | U     | 103 | BCL  | CMB-C2B-C1B | -2.44 | 121.70      | 125.42   |
| 8   | C     | 503 | HEC  | CHB-C1B-NB  | 2.44  | 128.28      | 123.86   |
| 13  | 9     | 101 | BCL  | C2A-C1A-CHA | 2.44  | 128.10      | 123.87   |
| 20  | S     | 104 | CDL  | OB6-CB5-OB7 | -2.44 | 118.00      | 123.70   |
| 22  | H     | 304 | LMT  | O5B-C5B-C4B | 2.44  | 114.09      | 109.70   |
| 13  | Y     | 103 | BCL  | CAB-C3B-C2B | 2.44  | 132.81      | 127.74   |
| 19  | O     | 103 | CRT  | C34-C33-C35 | 2.43  | 121.80      | 118.09   |
| 19  | Z     | 101 | CRT  | C26-C27-C28 | -2.43 | 123.87      | 127.28   |
| 15  | L     | 309 | UQ8  | C3M-O3-C3   | 2.43  | 125.01      | 116.47   |
| 19  | V     | 101 | CRT  | C26-C27-C28 | -2.43 | 123.87      | 127.28   |
| 8   | C     | 503 | HEC  | CHA-C4D-ND  | 2.43  | 128.26      | 123.86   |
| 21  | M     | 409 | PEF  | O4P-P-O1P   | -2.42 | 102.38      | 110.95   |
| 13  | 5     | 101 | BCL  | CMB-C2B-C1B | -2.42 | 121.73      | 125.42   |
| 19  | J     | 101 | CRT  | C18-C17-C16 | 2.42  | 121.78      | 118.09   |
| 13  | U     | 103 | BCL  | C19-C18-C17 | -2.42 | 97.23       | 111.55   |
| 15  | L     | 310 | UQ8  | C22-C23-C24 | -2.41 | 119.59      | 127.64   |
| 14  | L     | 303 | BPH  | CBA-CAA-C2A | -2.41 | 106.67      | 113.78   |
| 13  | A     | 101 | BCL  | C2A-C1A-CHA | 2.41  | 128.05      | 123.87   |
| 13  | 4     | 102 | BCL  | CAB-C3B-C2B | 2.41  | 132.75      | 127.74   |
| 15  | L     | 310 | UQ8  | O4-C4-C5    | 2.41  | 124.77      | 116.64   |
| 19  | 0     | 101 | CRT  | C32-C31-C30 | -2.41 | 116.22      | 123.20   |
| 13  | D     | 101 | BCL  | C2A-C1A-CHA | 2.40  | 128.04      | 123.87   |
| 19  | 8     | 101 | CRT  | C29-C28-C30 | 2.40  | 121.76      | 118.09   |
| 19  | M     | 405 | CRT  | C13-C12-C11 | 2.40  | 121.75      | 118.09   |
| 19  | O     | 103 | CRT  | C27-C26-C25 | -2.40 | 116.25      | 123.20   |
| 13  | D     | 101 | BCL  | CMB-C2B-C1B | -2.40 | 121.77      | 125.42   |
| 19  | Z     | 101 | CRT  | C27-C26-C25 | -2.40 | 116.26      | 123.20   |
| 19  | 2     | 101 | CRT  | C20-C19-C17 | -2.39 | 123.92      | 127.28   |
| 13  | W     | 101 | BCL  | CAB-C3B-C2B | 2.39  | 132.71      | 127.74   |
| 19  | V     | 101 | CRT  | C21-C20-C19 | -2.39 | 118.63      | 123.52   |
| 13  | K     | 101 | BCL  | C11-C12-C13 | -2.39 | 108.02      | 115.97   |
| 19  | Z     | 101 | CRT  | C29-C28-C30 | 2.39  | 121.73      | 118.09   |
| 19  | N     | 101 | CRT  | C18-C17-C16 | 2.39  | 121.73      | 118.09   |
| 19  | J     | 101 | CRT  | C13-C12-C11 | 2.38  | 121.73      | 118.09   |
| 19  | N     | 101 | CRT  | C20-C19-C17 | -2.38 | 123.94      | 127.28   |
| 19  | 8     | 101 | CRT  | C18-C17-C16 | 2.38  | 121.73      | 118.09   |
| 8   | C     | 504 | HEC  | CHB-C1B-C2B | -2.38 | 120.52      | 127.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | Q     | 101 | BCL  | CMB-C2B-C1B | -2.38 | 121.80      | 125.42   |
| 15  | L     | 309 | UQ8  | C25-C24-C26 | 2.38  | 119.36      | 115.23   |
| 19  | 8     | 101 | CRT  | C9-C10-C11  | -2.37 | 116.33      | 123.20   |
| 19  | M     | 405 | CRT  | C18-C17-C16 | 2.37  | 121.71      | 118.09   |
| 19  | W     | 102 | CRT  | C27-C26-C25 | -2.37 | 116.33      | 123.20   |
| 13  | A     | 101 | BCL  | C1C-NC-C4C  | 2.37  | 107.76      | 106.68   |
| 13  | D     | 101 | BCL  | CAB-C3B-C2B | 2.37  | 132.67      | 127.74   |
| 13  | 4     | 102 | BCL  | CMB-C2B-C1B | -2.37 | 121.81      | 125.42   |
| 13  | W     | 101 | BCL  | OBB-CAB-CBB | -2.37 | 114.46      | 119.77   |
| 13  | Y     | 103 | BCL  | CMB-C2B-C1B | -2.37 | 121.81      | 125.42   |
| 19  | G     | 101 | CRT  | C29-C28-C30 | 2.37  | 121.71      | 118.09   |
| 19  | 4     | 101 | CRT  | C21-C20-C19 | -2.37 | 118.67      | 123.52   |
| 13  | Q     | 101 | BCL  | C2A-C1A-CHA | 2.37  | 127.97      | 123.87   |
| 19  | A     | 104 | CRT  | C27-C26-C25 | -2.37 | 116.34      | 123.20   |
| 20  | H     | 305 | CDL  | OB8-CB7-C71 | 2.37  | 119.05      | 111.83   |
| 13  | 9     | 101 | BCL  | CAB-C3B-C2B | 2.37  | 132.66      | 127.74   |
| 13  | Q     | 101 | BCL  | CBA-CAA-C2A | -2.36 | 106.76      | 113.79   |
| 13  | 2     | 102 | BCL  | C2A-C1A-CHA | 2.36  | 127.97      | 123.87   |
| 15  | L     | 310 | UQ8  | C4M-O4-C4   | 2.36  | 124.78      | 116.47   |
| 19  | N     | 101 | CRT  | C30-C28-C27 | -2.36 | 115.30      | 119.01   |
| 19  | T     | 101 | CRT  | C8-C7-C9    | -2.36 | 118.99      | 122.82   |
| 13  | O     | 101 | BCL  | CAB-C3B-C2B | 2.36  | 132.64      | 127.74   |
| 8   | C     | 503 | HEC  | C4B-NB-C1B  | 2.36  | 109.66      | 105.82   |
| 21  | W     | 106 | PEF  | O3P-P-O1P   | -2.36 | 102.62      | 110.95   |
| 13  | P     | 102 | BCL  | CMB-C2B-C1B | -2.35 | 121.83      | 125.42   |
| 13  | 3     | 101 | BCL  | CMB-C2B-C1B | -2.35 | 121.83      | 125.42   |
| 20  | D     | 104 | CDL  | OB6-CB5-C51 | 2.35  | 119.57      | 110.93   |
| 13  | 1     | 101 | BCL  | CAB-C3B-C2B | 2.35  | 132.62      | 127.74   |
| 12  | C     | 508 | PGV  | O03-C19-C20 | 2.35  | 119.00      | 111.83   |
| 13  | 7     | 101 | BCL  | CBA-CAA-C2A | -2.35 | 106.81      | 113.79   |
| 8   | C     | 501 | HEC  | CAD-CBD-CGD | 2.35  | 119.89      | 113.67   |
| 13  | A     | 103 | BCL  | CMB-C2B-C1B | -2.35 | 121.85      | 125.42   |
| 13  | 5     | 103 | BCL  | CMB-C2B-C1B | -2.35 | 121.85      | 125.42   |
| 21  | M     | 407 | PEF  | O3P-P-O1P   | -2.35 | 102.66      | 110.95   |
| 13  | J     | 102 | BCL  | CMB-C2B-C1B | -2.34 | 121.85      | 125.42   |
| 13  | 7     | 103 | BCL  | CMB-C2B-C1B | -2.34 | 121.85      | 125.42   |
| 12  | M     | 410 | PGV  | O14-P-O13   | 2.34  | 119.96      | 110.83   |
| 13  | Q     | 103 | BCL  | CMB-C2B-C1B | -2.34 | 121.86      | 125.42   |
| 13  | K     | 101 | BCL  | CAB-C3B-C2B | 2.34  | 132.60      | 127.74   |
| 19  | W     | 102 | CRT  | C13-C12-C11 | 2.34  | 121.66      | 118.09   |
| 13  | U     | 101 | BCL  | OBB-CAB-CBB | -2.34 | 114.54      | 119.77   |
| 13  | L     | 305 | BCL  | C4A-NA-C1A  | 2.34  | 107.75      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | I     | 103 | PEF  | O4P-P-O1P   | -2.33 | 102.71      | 110.95   |
| 21  | 3     | 104 | PEF  | O3P-P-O1P   | -2.33 | 102.71      | 110.95   |
| 13  | 5     | 101 | BCL  | C11-C12-C13 | -2.32 | 108.24      | 115.97   |
| 19  | A     | 104 | CRT  | C29-C28-C30 | 2.32  | 121.64      | 118.09   |
| 12  | M     | 411 | PGV  | O03-C19-C20 | 2.32  | 118.91      | 111.83   |
| 13  | D     | 101 | BCL  | C11-C10-C8  | -2.32 | 108.25      | 115.97   |
| 20  | U     | 104 | CDL  | OB6-CB5-OB7 | -2.32 | 118.52      | 122.99   |
| 13  | W     | 104 | BCL  | CAB-C3B-C2B | 2.32  | 132.56      | 127.74   |
| 19  | V     | 101 | CRT  | C34-C33-C35 | 2.32  | 121.63      | 118.09   |
| 15  | L     | 309 | UQ8  | C7-C6-C1    | -2.32 | 120.92      | 124.89   |
| 13  | M     | 401 | BCL  | OBB-CAB-CBB | -2.31 | 114.59      | 119.77   |
| 19  | 0     | 101 | CRT  | C21-C20-C19 | -2.31 | 118.79      | 123.52   |
| 19  | 3     | 103 | CRT  | C13-C12-C11 | 2.31  | 121.62      | 118.09   |
| 13  | L     | 301 | BCL  | OBB-CAB-CBB | -2.31 | 114.60      | 119.77   |
| 13  | A     | 101 | BCL  | CMB-C2B-C1B | -2.31 | 121.91      | 125.42   |
| 13  | Y     | 101 | BCL  | OBB-CAB-CBB | -2.31 | 114.60      | 119.77   |
| 15  | M     | 413 | UQ8  | C10-C9-C11  | 2.31  | 119.90      | 114.59   |
| 19  | 3     | 103 | CRT  | C31-C32-C33 | -2.31 | 124.04      | 127.28   |
| 21  | K     | 104 | PEF  | O3-C30-C31  | 2.30  | 118.86      | 111.83   |
| 13  | 9     | 101 | BCL  | OBB-CAB-CBB | -2.30 | 114.61      | 119.77   |
| 19  | 8     | 101 | CRT  | C27-C26-C25 | -2.30 | 116.53      | 123.20   |
| 8   | C     | 502 | HEC  | CHD-C4C-NC  | 2.30  | 126.96      | 124.45   |
| 13  | K     | 101 | BCL  | CMB-C2B-C1B | -2.30 | 121.92      | 125.42   |
| 13  | Q     | 101 | BCL  | C4-C3-C5    | -2.30 | 111.24      | 115.23   |
| 19  | 8     | 101 | CRT  | C14-C15-C16 | -2.30 | 116.54      | 123.20   |
| 8   | C     | 504 | HEC  | C4B-NB-C1B  | 2.30  | 109.57      | 105.82   |
| 19  | B     | 101 | CRT  | C34-C33-C35 | 2.30  | 121.60      | 118.09   |
| 19  | 4     | 101 | CRT  | C13-C12-C11 | 2.30  | 121.60      | 118.09   |
| 19  | N     | 101 | CRT  | C14-C15-C16 | -2.30 | 116.55      | 123.20   |
| 18  | M     | 404 | MQ8  | C50-C48-C49 | 2.30  | 119.87      | 114.59   |
| 14  | M     | 402 | BPH  | O2D-CGD-O1D | -2.30 | 119.38      | 123.85   |
| 13  | K     | 101 | BCL  | OBB-CAB-CBB | -2.29 | 114.63      | 119.77   |
| 13  | 7     | 101 | BCL  | CAB-C3B-C2B | 2.29  | 132.51      | 127.74   |
| 13  | 3     | 101 | BCL  | C11-C10-C8  | -2.29 | 108.35      | 115.97   |
| 13  | L     | 302 | BCL  | CAB-C3B-C2B | 2.29  | 132.50      | 127.74   |
| 13  | L     | 302 | BCL  | CMB-C2B-C1B | -2.29 | 121.94      | 125.42   |
| 13  | O     | 101 | BCL  | CMB-C2B-C1B | -2.29 | 121.94      | 125.42   |
| 20  | O     | 104 | CDL  | O1-C1-CA2   | -2.29 | 101.79      | 109.70   |
| 15  | L     | 309 | UQ8  | C46-C44-C45 | 2.29  | 119.85      | 114.59   |
| 8   | C     | 502 | HEC  | C4B-NB-C1B  | 2.29  | 109.55      | 105.82   |
| 13  | D     | 103 | BCL  | CMB-C2B-C1B | -2.28 | 121.94      | 125.42   |
| 13  | I     | 101 | BCL  | C2A-C1A-CHA | 2.28  | 127.83      | 123.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | L     | 304 | UQ8  | C25-C24-C26 | 2.28  | 119.84      | 114.59   |
| 13  | 2     | 102 | BCL  | OBB-CAB-CBB | -2.28 | 114.66      | 119.77   |
| 19  | 0     | 101 | CRT  | C27-C26-C25 | -2.28 | 116.59      | 123.20   |
| 19  | 8     | 101 | CRT  | C20-C19-C17 | -2.28 | 124.08      | 127.28   |
| 19  | O     | 103 | CRT  | C18-C17-C16 | 2.28  | 121.57      | 118.09   |
| 13  | 4     | 102 | BCL  | OBB-CAB-CBB | -2.28 | 114.66      | 119.77   |
| 19  | O     | 103 | CRT  | C9-C10-C11  | -2.28 | 116.60      | 123.20   |
| 14  | M     | 402 | BPH  | C4-C3-C5    | 2.28  | 119.18      | 115.23   |
| 13  | S     | 103 | BCL  | OBB-CAB-CBB | -2.28 | 114.67      | 119.77   |
| 13  | A     | 101 | BCL  | OBB-CAB-CBB | -2.28 | 114.67      | 119.77   |
| 13  | F     | 103 | BCL  | CAB-C3B-C2B | 2.27  | 132.46      | 127.74   |
| 13  | 3     | 101 | BCL  | OBB-CAB-CBB | -2.27 | 114.68      | 119.77   |
| 19  | A     | 104 | CRT  | C18-C17-C16 | 2.27  | 121.56      | 118.09   |
| 13  | 9     | 103 | BCL  | OBB-CAB-CBB | -2.27 | 114.69      | 119.77   |
| 13  | F     | 101 | BCL  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 13  | F     | 101 | BCL  | C1C-NC-C4C  | 2.27  | 107.71      | 106.68   |
| 19  | 3     | 103 | CRT  | C29-C28-C30 | 2.27  | 121.55      | 118.09   |
| 13  | D     | 103 | BCL  | OBB-CAB-CBB | -2.27 | 114.69      | 119.77   |
| 13  | D     | 101 | BCL  | OBB-CAB-CBB | -2.27 | 114.69      | 119.77   |
| 14  | M     | 402 | BPH  | C2D-C1D-ND  | 2.27  | 111.07      | 109.43   |
| 19  | P     | 101 | CRT  | C18-C17-C16 | 2.27  | 121.55      | 118.09   |
| 13  | F     | 101 | BCL  | C6-C5-C3    | 2.26  | 118.98      | 113.47   |
| 19  | V     | 101 | CRT  | C13-C12-C11 | 2.26  | 121.54      | 118.09   |
| 13  | F     | 103 | BCL  | CMB-C2B-C1B | -2.26 | 121.98      | 125.42   |
| 22  | H     | 304 | LMT  | O5'-C5'-C6' | 2.26  | 112.04      | 106.44   |
| 13  | P     | 102 | BCL  | C17-C16-C15 | -2.26 | 103.16      | 113.28   |
| 19  | G     | 101 | CRT  | C13-C12-C11 | 2.26  | 121.53      | 118.09   |
| 13  | F     | 101 | BCL  | OBB-CAB-CBB | -2.25 | 114.72      | 119.77   |
| 18  | M     | 404 | MQ8  | C39-C38-C40 | 2.25  | 119.14      | 115.23   |
| 19  | 2     | 101 | CRT  | C14-C15-C16 | -2.25 | 116.67      | 123.20   |
| 13  | Y     | 103 | BCL  | OBB-CAB-CBB | -2.25 | 114.72      | 119.77   |
| 12  | 9     | 104 | PGV  | O03-C19-O04 | -2.25 | 117.99      | 123.63   |
| 13  | 9     | 101 | BCL  | CMB-C2B-C1B | -2.25 | 121.99      | 125.42   |
| 19  | B     | 101 | CRT  | C18-C17-C16 | 2.25  | 121.53      | 118.09   |
| 19  | Z     | 101 | CRT  | C34-C33-C35 | 2.25  | 121.53      | 118.09   |
| 13  | L     | 302 | BCL  | OBB-CAB-CBB | -2.25 | 114.73      | 119.77   |
| 19  | 8     | 101 | CRT  | C8-C7-C6    | 2.25  | 121.52      | 118.09   |
| 13  | 5     | 101 | BCL  | C2A-C1A-CHA | 2.25  | 127.77      | 123.87   |
| 13  | Q     | 101 | BCL  | OBB-CAB-CBB | -2.25 | 114.74      | 119.77   |
| 13  | 3     | 101 | BCL  | C1-C2-C3    | -2.24 | 122.52      | 126.20   |
| 18  | M     | 404 | MQ8  | C21-C22-C23 | -2.24 | 122.49      | 127.62   |
| 13  | J     | 102 | BCL  | CAB-C3B-C2B | 2.24  | 132.40      | 127.74   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | 2     | 102 | BCL  | CMB-C2B-C1B | -2.24 | 122.01      | 125.42   |
| 13  | I     | 101 | BCL  | OBB-CAB-CBB | -2.24 | 114.75      | 119.77   |
| 19  | G     | 101 | CRT  | C18-C17-C16 | 2.24  | 121.51      | 118.09   |
| 13  | S     | 101 | BCL  | C1-O2A-CGA  | 2.24  | 122.07      | 116.65   |
| 13  | 5     | 101 | BCL  | OBB-CAB-CBB | -2.23 | 114.77      | 119.77   |
| 12  | 9     | 104 | PGV  | C03-C02-C01 | -2.23 | 106.58      | 111.78   |
| 13  | K     | 101 | BCL  | C1C-NC-C4C  | 2.23  | 107.70      | 106.68   |
| 20  | O     | 104 | CDL  | OB8-CB7-OB9 | -2.23 | 118.05      | 123.63   |
| 19  | V     | 101 | CRT  | C29-C28-C30 | 2.23  | 121.49      | 118.09   |
| 19  | V     | 101 | CRT  | C18-C17-C16 | 2.23  | 121.49      | 118.09   |
| 19  | M     | 405 | CRT  | C9-C10-C11  | -2.23 | 116.75      | 123.20   |
| 13  | W     | 101 | BCL  | CMB-C2B-C1B | -2.23 | 122.03      | 125.42   |
| 19  | J     | 101 | CRT  | C8-C7-C9    | -2.22 | 119.22      | 122.82   |
| 13  | P     | 102 | BCL  | OBB-CAB-CBB | -2.22 | 114.79      | 119.77   |
| 13  | 7     | 101 | BCL  | OBB-CAB-CBB | -2.22 | 114.79      | 119.77   |
| 19  | G     | 101 | CRT  | C21-C20-C19 | -2.22 | 118.98      | 123.52   |
| 14  | M     | 402 | BPH  | C1-O2A-CGA  | 2.22  | 122.02      | 116.65   |
| 13  | W     | 104 | BCL  | OBB-CAB-CBB | -2.22 | 114.80      | 119.77   |
| 19  | T     | 101 | CRT  | C18-C17-C16 | 2.21  | 121.47      | 118.09   |
| 12  | L     | 307 | PGV  | O01-C1-O02  | -2.21 | 118.53      | 123.70   |
| 13  | A     | 103 | BCL  | CAB-C3B-C2B | 2.21  | 132.34      | 127.74   |
| 8   | C     | 504 | HEC  | CAA-CBA-CGA | -2.21 | 107.80      | 113.67   |
| 19  | Z     | 101 | CRT  | C8-C7-C6    | 2.21  | 121.47      | 118.09   |
| 13  | U     | 103 | BCL  | OBB-CAB-CBB | -2.21 | 114.81      | 119.77   |
| 20  | D     | 105 | CDL  | OA6-CA5-OA7 | -2.21 | 118.53      | 123.70   |
| 14  | M     | 402 | BPH  | CMA-C3A-C4A | -2.21 | 109.85      | 114.61   |
| 19  | V     | 101 | CRT  | C10-C9-C7   | -2.21 | 124.18      | 127.28   |
| 13  | K     | 101 | BCL  | C4-C3-C5    | -2.21 | 111.40      | 115.23   |
| 19  | W     | 102 | CRT  | C29-C28-C30 | 2.20  | 121.45      | 118.09   |
| 13  | J     | 102 | BCL  | OBB-CAB-CBB | -2.20 | 114.83      | 119.77   |
| 13  | A     | 103 | BCL  | OBB-CAB-CBB | -2.20 | 114.84      | 119.77   |
| 13  | 1     | 101 | BCL  | OBB-CAB-CBB | -2.20 | 114.84      | 119.77   |
| 13  | W     | 104 | BCL  | O2A-CGA-O1A | -2.20 | 118.12      | 123.63   |
| 13  | F     | 101 | BCL  | C2A-C1A-CHA | 2.20  | 127.68      | 123.87   |
| 13  | 3     | 101 | BCL  | C16-C15-C13 | 2.20  | 123.27      | 115.97   |
| 13  | K     | 103 | BCL  | OBB-CAB-CBB | -2.20 | 114.85      | 119.77   |
| 13  | W     | 101 | BCL  | C11-C10-C8  | -2.20 | 108.66      | 115.97   |
| 21  | W     | 105 | PEF  | O4P-P-O1P   | -2.20 | 103.18      | 110.95   |
| 13  | 5     | 101 | BCL  | C5-C3-C2    | 2.20  | 126.10      | 121.17   |
| 13  | A     | 101 | BCL  | CAB-C3B-C2B | 2.20  | 132.31      | 127.74   |
| 13  | W     | 104 | BCL  | CMB-C2B-C1B | -2.20 | 122.08      | 125.42   |
| 13  | 7     | 101 | BCL  | CMB-C2B-C1B | -2.20 | 122.08      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | A     | 103 | BCL  | C11-C12-C13 | -2.19 | 108.67      | 115.97   |
| 13  | F     | 103 | BCL  | OBB-CAB-CBB | -2.19 | 114.86      | 119.77   |
| 13  | S     | 101 | BCL  | C2A-C1A-CHA | 2.19  | 127.67      | 123.87   |
| 19  | J     | 101 | CRT  | C29-C28-C30 | 2.19  | 121.43      | 118.09   |
| 19  | A     | 104 | CRT  | C9-C10-C11  | -2.19 | 116.86      | 123.20   |
| 13  | L     | 301 | BCL  | C1-C2-C3    | -2.19 | 122.61      | 126.20   |
| 14  | L     | 303 | BPH  | C3B-C4B-NB  | 2.19  | 111.23      | 108.05   |
| 13  | J     | 102 | BCL  | C17-C16-C15 | -2.19 | 103.48      | 113.28   |
| 19  | W     | 102 | CRT  | C5-C6-C7    | -2.19 | 122.59      | 125.89   |
| 13  | F     | 101 | BCL  | CAB-C3B-C2B | 2.19  | 132.28      | 127.74   |
| 14  | M     | 402 | BPH  | O1D-CGD-CBD | -2.18 | 121.41      | 124.72   |
| 13  | 7     | 103 | BCL  | OBB-CAB-CBB | -2.18 | 114.88      | 119.77   |
| 19  | G     | 101 | CRT  | C8-C7-C6    | 2.18  | 121.42      | 118.09   |
| 13  | K     | 101 | BCL  | C2A-C1A-CHA | 2.18  | 127.65      | 123.87   |
| 13  | 1     | 101 | BCL  | CMB-C2B-C1B | -2.18 | 122.10      | 125.42   |
| 15  | L     | 310 | UQ8  | C25-C24-C26 | 2.18  | 119.61      | 114.59   |
| 13  | O     | 101 | BCL  | OBB-CAB-CBB | -2.18 | 114.89      | 119.77   |
| 12  | 3     | 105 | PGV  | O03-C19-C20 | 2.18  | 118.47      | 111.83   |
| 19  | 4     | 101 | CRT  | C29-C28-C30 | 2.17  | 121.41      | 118.09   |
| 13  | 5     | 101 | BCL  | CAB-C3B-C2B | 2.17  | 132.25      | 127.74   |
| 13  | Y     | 103 | BCL  | C16-C15-C13 | 2.17  | 123.18      | 115.97   |
| 13  | Y     | 103 | BCL  | C6-C7-C8    | -2.17 | 108.75      | 115.97   |
| 19  | 3     | 103 | CRT  | C34-C33-C35 | 2.17  | 121.40      | 118.09   |
| 13  | M     | 401 | BCL  | C2A-C1A-CHA | 2.17  | 127.63      | 123.87   |
| 13  | D     | 101 | BCL  | C16-C15-C13 | 2.17  | 123.16      | 115.97   |
| 13  | M     | 401 | BCL  | C16-C15-C13 | -2.16 | 108.77      | 115.97   |
| 11  | C     | 507 | LHG  | C27-C26-C25 | -2.16 | 103.44      | 114.37   |
| 18  | M     | 404 | MQ8  | C2M-C2-C3   | -2.16 | 120.90      | 124.45   |
| 20  | D     | 105 | CDL  | CA4-OA6-CA5 | -2.16 | 112.62      | 117.80   |
| 19  | B     | 101 | CRT  | C20-C19-C17 | -2.16 | 124.25      | 127.28   |
| 13  | Q     | 103 | BCL  | C4D-C3D-CAD | -2.16 | 105.76      | 108.11   |
| 20  | U     | 104 | CDL  | OB8-CB6-CB4 | 2.16  | 114.62      | 108.40   |
| 8   | C     | 501 | HEC  | C4B-NB-C1B  | 2.16  | 109.34      | 105.82   |
| 13  | P     | 102 | BCL  | CAB-C3B-C2B | 2.16  | 132.23      | 127.74   |
| 13  | D     | 101 | BCL  | C6-C5-C3    | 2.16  | 118.72      | 113.47   |
| 13  | S     | 101 | BCL  | OBB-CAB-CBB | -2.16 | 114.94      | 119.77   |
| 13  | A     | 101 | BCL  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 13  | L     | 301 | BCL  | C17-C16-C15 | -2.16 | 103.62      | 113.28   |
| 19  | B     | 101 | CRT  | C14-C15-C16 | -2.15 | 116.96      | 123.20   |
| 13  | I     | 101 | BCL  | CMB-C2B-C1B | -2.15 | 122.14      | 125.42   |
| 13  | Q     | 101 | BCL  | CAB-C3B-C2B | 2.15  | 132.21      | 127.74   |
| 19  | T     | 101 | CRT  | C34-C33-C35 | 2.15  | 121.37      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | 0     | 101 | CRT  | C31-C32-C33 | -2.15 | 124.26      | 127.28   |
| 8   | C     | 501 | HEC  | CHA-C4D-ND  | 2.15  | 127.76      | 123.86   |
| 13  | Y     | 101 | BCL  | CMB-C2B-C1B | -2.15 | 122.15      | 125.42   |
| 13  | 5     | 103 | BCL  | C16-C15-C13 | -2.15 | 108.83      | 115.97   |
| 20  | U     | 104 | CDL  | OB4-PB2-OB3 | 2.15  | 122.43      | 112.44   |
| 13  | K     | 103 | BCL  | CAB-C3B-C2B | 2.14  | 132.20      | 127.74   |
| 20  | U     | 104 | CDL  | O1-C1-CB2   | -2.14 | 102.29      | 109.70   |
| 12  | 9     | 104 | PGV  | O03-C01-C02 | 2.14  | 114.58      | 108.40   |
| 15  | L     | 304 | UQ8  | C7-C6-C5    | 2.14  | 121.00      | 118.52   |
| 13  | Y     | 101 | BCL  | C6-C5-C3    | 2.14  | 118.68      | 113.47   |
| 13  | D     | 103 | BCL  | C17-C16-C15 | -2.14 | 103.69      | 113.28   |
| 13  | S     | 103 | BCL  | C9-C8-C10   | -2.14 | 103.64      | 111.27   |
| 19  | T     | 101 | CRT  | C9-C10-C11  | -2.14 | 117.00      | 123.20   |
| 8   | C     | 504 | HEC  | C4C-NC-C1C  | 2.14  | 109.31      | 105.82   |
| 19  | P     | 101 | CRT  | C27-C26-C25 | -2.14 | 117.01      | 123.20   |
| 13  | U     | 101 | BCL  | CMB-C2B-C1B | -2.14 | 122.17      | 125.42   |
| 12  | M     | 411 | PGV  | O14-P-O13   | 2.14  | 122.38      | 112.44   |
| 13  | J     | 102 | BCL  | O2A-CGA-CBA | 2.14  | 118.34      | 111.83   |
| 19  | N     | 101 | CRT  | C13-C12-C11 | 2.13  | 121.35      | 118.09   |
| 13  | 5     | 103 | BCL  | CAB-C3B-C2B | 2.13  | 132.17      | 127.74   |
| 13  | L     | 301 | BCL  | CMB-C2B-C1B | -2.13 | 122.17      | 125.42   |
| 8   | C     | 502 | HEC  | CHA-C4D-C3D | -2.13 | 120.63      | 125.30   |
| 19  | 8     | 101 | CRT  | C15-C14-C12 | -2.13 | 124.29      | 127.28   |
| 20  | U     | 104 | CDL  | OA6-CA5-OA7 | -2.13 | 118.73      | 123.70   |
| 19  | T     | 101 | CRT  | C27-C26-C25 | -2.13 | 117.03      | 123.20   |
| 14  | M     | 402 | BPH  | C3B-C4B-NB  | 2.13  | 111.15      | 108.05   |
| 19  | M     | 405 | CRT  | C27-C26-C25 | -2.13 | 117.04      | 123.20   |
| 20  | O     | 104 | CDL  | OA6-CA5-OA7 | -2.13 | 118.74      | 123.70   |
| 19  | O     | 103 | CRT  | C14-C15-C16 | -2.13 | 117.04      | 123.20   |
| 19  | A     | 104 | CRT  | C5-C6-C7    | -2.13 | 122.68      | 125.89   |
| 8   | C     | 503 | HEC  | O2D-CGD-CBD | 2.12  | 120.71      | 114.00   |
| 8   | C     | 501 | HEC  | C4A-NA-C1A  | 2.12  | 109.28      | 105.82   |
| 8   | C     | 501 | HEC  | CAD-C3D-C4D | 2.12  | 129.08      | 124.94   |
| 13  | 5     | 101 | BCL  | C16-C15-C13 | 2.12  | 123.02      | 115.97   |
| 13  | D     | 101 | BCL  | C1C-NC-C4C  | 2.12  | 107.65      | 106.68   |
| 12  | H     | 303 | PGV  | O01-C1-O02  | -2.12 | 118.75      | 123.70   |
| 15  | L     | 310 | UQ8  | C17-C18-C19 | -2.12 | 122.77      | 127.62   |
| 20  | O     | 104 | CDL  | CB2-C1-CA2  | -2.12 | 106.55      | 112.65   |
| 8   | C     | 503 | HEC  | CHB-C1B-C2B | -2.12 | 121.28      | 127.43   |
| 19  | P     | 101 | CRT  | C14-C15-C16 | -2.12 | 117.06      | 123.20   |
| 19  | 2     | 101 | CRT  | C18-C17-C16 | 2.12  | 121.32      | 118.09   |
| 13  | L     | 305 | BCL  | C1C-NC-C4C  | 2.11  | 107.64      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | D     | 104 | CDL  | OA6-CA5-OA7 | -2.11 | 118.77      | 123.70   |
| 13  | U     | 103 | BCL  | CAB-C3B-C2B | 2.11  | 132.13      | 127.74   |
| 20  | S     | 104 | CDL  | PB2-OB5-CB3 | 2.11  | 133.45      | 121.35   |
| 19  | T     | 101 | CRT  | C6-C7-C9    | 2.11  | 122.33      | 119.01   |
| 14  | M     | 402 | BPH  | C4D-CHA-CBD | -2.11 | 107.44      | 108.45   |
| 20  | D     | 104 | CDL  | CB4-OB6-CB5 | -2.11 | 112.74      | 117.80   |
| 19  | O     | 101 | CRT  | C13-C12-C11 | 2.11  | 121.31      | 118.09   |
| 15  | L     | 310 | UQ8  | O4-C4-C3    | -2.11 | 115.66      | 123.64   |
| 19  | 4     | 101 | CRT  | C26-C25-C23 | -2.11 | 120.58      | 126.36   |
| 13  | 3     | 101 | BCL  | C2A-C1A-CHA | 2.11  | 127.52      | 123.87   |
| 19  | 4     | 101 | CRT  | C9-C10-C11  | -2.10 | 117.11      | 123.20   |
| 12  | D     | 106 | PGV  | C02-O01-C1  | -2.10 | 112.77      | 117.80   |
| 19  | 3     | 103 | CRT  | C9-C10-C11  | -2.10 | 117.12      | 123.20   |
| 20  | Y     | 104 | CDL  | OA4-PA1-OA3 | 2.10  | 122.21      | 112.44   |
| 19  | Z     | 101 | CRT  | C9-C10-C11  | -2.10 | 117.12      | 123.20   |
| 20  | Y     | 104 | CDL  | CB4-OB6-CB5 | -2.10 | 112.78      | 117.80   |
| 18  | M     | 404 | MQ8  | C31-C32-C33 | -2.10 | 122.82      | 127.62   |
| 19  | M     | 405 | CRT  | C24-C23-C22 | -2.09 | 119.42      | 122.82   |
| 15  | L     | 304 | UQ8  | C12-C11-C9  | -2.09 | 106.25      | 113.19   |
| 13  | L     | 305 | BCL  | CAC-C3C-C4C | 2.09  | 117.22      | 112.58   |
| 13  | 2     | 102 | BCL  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 13  | L     | 305 | BCL  | C16-C15-C13 | -2.09 | 109.02      | 115.97   |
| 8   | C     | 502 | HEC  | CHD-C1D-ND  | 2.09  | 127.65      | 123.86   |
| 13  | Q     | 103 | BCL  | OBB-CAB-CBB | -2.09 | 115.09      | 119.77   |
| 13  | Y     | 101 | BCL  | C2A-C1A-CHA | 2.09  | 127.49      | 123.87   |
| 14  | M     | 402 | BPH  | CGD-CBD-CAD | -2.09 | 104.09      | 110.85   |
| 13  | 4     | 102 | BCL  | C16-C15-C13 | -2.08 | 109.04      | 115.97   |
| 13  | 5     | 103 | BCL  | OBB-CAB-CBB | -2.08 | 115.11      | 119.77   |
| 13  | 9     | 103 | BCL  | CAB-C3B-C2B | 2.08  | 132.06      | 127.74   |
| 19  | W     | 102 | CRT  | C18-C17-C16 | 2.08  | 121.26      | 118.09   |
| 14  | M     | 402 | BPH  | CMB-C2B-C3B | 2.08  | 128.83      | 124.68   |
| 13  | 7     | 103 | BCL  | C1-O2A-CGA  | 2.08  | 121.67      | 116.65   |
| 20  | O     | 104 | CDL  | OA8-CA7-OA9 | -2.07 | 118.44      | 123.63   |
| 12  | 9     | 104 | PGV  | C02-O01-C1  | -2.07 | 112.83      | 117.80   |
| 19  | O     | 103 | CRT  | C29-C28-C30 | 2.07  | 121.25      | 118.09   |
| 19  | 8     | 101 | CRT  | C36-C35-C33 | -2.07 | 122.76      | 125.89   |
| 19  | Z     | 101 | CRT  | C13-C12-C11 | 2.07  | 121.25      | 118.09   |
| 8   | C     | 503 | HEC  | C4C-NC-C1C  | 2.07  | 109.19      | 105.82   |
| 13  | U     | 101 | BCL  | C2A-C1A-CHA | 2.07  | 127.46      | 123.87   |
| 8   | C     | 501 | HEC  | O2A-CGA-CBA | 2.07  | 120.53      | 114.00   |
| 13  | 4     | 102 | BCL  | C4D-C3D-CAD | -2.07 | 105.86      | 108.11   |
| 19  | O     | 103 | CRT  | C10-C9-C7   | -2.06 | 124.38      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | S     | 103 | BCL  | CAB-C3B-C2B | 2.06  | 132.03      | 127.74   |
| 12  | M     | 411 | PGV  | O01-C1-O02  | -2.06 | 118.89      | 123.70   |
| 19  | 2     | 101 | CRT  | C27-C26-C25 | -2.06 | 117.23      | 123.20   |
| 19  | N     | 101 | CRT  | C8-C7-C9    | -2.06 | 119.48      | 122.82   |
| 18  | M     | 404 | MQ8  | C46-C47-C48 | -2.06 | 120.78      | 127.64   |
| 19  | V     | 101 | CRT  | C27-C26-C25 | -2.06 | 117.24      | 123.20   |
| 15  | L     | 304 | UQ8  | C20-C19-C21 | 2.05  | 118.79      | 115.23   |
| 19  | J     | 101 | CRT  | C21-C20-C19 | -2.05 | 119.32      | 123.52   |
| 13  | K     | 103 | BCL  | C11-C12-C13 | -2.05 | 109.16      | 115.97   |
| 13  | U     | 103 | BCL  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 19  | P     | 101 | CRT  | C9-C10-C11  | -2.04 | 117.28      | 123.20   |
| 19  | 0     | 101 | CRT  | C9-C10-C11  | -2.04 | 117.28      | 123.20   |
| 13  | 3     | 101 | BCL  | CBA-CAA-C2A | 2.04  | 119.87      | 113.79   |
| 18  | M     | 404 | MQ8  | C14-C13-C15 | 2.04  | 118.77      | 115.23   |
| 13  | 3     | 101 | BCL  | CAB-C3B-C2B | 2.04  | 131.98      | 127.74   |
| 19  | O     | 103 | CRT  | C13-C12-C11 | 2.04  | 121.20      | 118.09   |
| 13  | L     | 305 | BCL  | OB8-CAB-CBB | -2.04 | 115.20      | 119.77   |
| 13  | 7     | 101 | BCL  | C4-C3-C5    | -2.04 | 111.69      | 115.23   |
| 15  | L     | 309 | UQ8  | C27-C28-C29 | -2.04 | 122.96      | 127.62   |
| 15  | L     | 309 | UQ8  | C42-C43-C44 | -2.04 | 120.85      | 127.64   |
| 14  | M     | 402 | BPH  | C4C-C3C-C2C | -2.03 | 100.91      | 102.84   |
| 19  | 2     | 101 | CRT  | C29-C28-C30 | 2.03  | 121.19      | 118.09   |
| 13  | Y     | 103 | BCL  | C11-C12-C13 | -2.03 | 109.22      | 115.97   |
| 20  | M     | 406 | CDL  | C12-C11-CA5 | -2.03 | 106.27      | 113.69   |
| 19  | Z     | 101 | CRT  | C31-C32-C33 | -2.02 | 124.44      | 127.28   |
| 13  | 7     | 103 | BCL  | CAB-C3B-C2B | 2.02  | 131.94      | 127.74   |
| 19  | 0     | 101 | CRT  | C14-C15-C16 | -2.02 | 117.36      | 123.20   |
| 20  | M     | 406 | CDL  | CB4-OB6-CB5 | -2.02 | 112.97      | 117.80   |
| 13  | O     | 101 | BCL  | C2A-C1A-CHA | 2.01  | 127.36      | 123.87   |
| 20  | Y     | 104 | CDL  | OB8-CB7-OB9 | -2.01 | 118.59      | 123.63   |
| 15  | L     | 311 | UQ8  | C6-C1-C2    | 2.01  | 120.75      | 119.17   |
| 12  | 3     | 105 | PGV  | C02-O01-C1  | -2.01 | 112.99      | 117.80   |
| 21  | K     | 104 | PEF  | O2-C10-O4   | -2.01 | 119.02      | 123.70   |
| 13  | 7     | 101 | BCL  | C2A-C1A-CHA | 2.00  | 127.34      | 123.87   |

There are no chirality outliers.

All (892) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | C     | 501 | HEC  | C2B-C3B-CAB-CBB |
| 8   | C     | 501 | HEC  | C4B-C3B-CAB-CBB |
| 8   | C     | 501 | HEC  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 8   | C     | 501 | HEC  | C4C-C3C-CAC-CBC |
| 8   | C     | 502 | HEC  | C2B-C3B-CAB-CBB |
| 8   | C     | 502 | HEC  | C4B-C3B-CAB-CBB |
| 8   | C     | 502 | HEC  | C2C-C3C-CAC-CBC |
| 8   | C     | 502 | HEC  | C4C-C3C-CAC-CBC |
| 8   | C     | 503 | HEC  | C2B-C3B-CAB-CBB |
| 8   | C     | 503 | HEC  | C4B-C3B-CAB-CBB |
| 8   | C     | 503 | HEC  | C2C-C3C-CAC-CBC |
| 8   | C     | 503 | HEC  | C4C-C3C-CAC-CBC |
| 8   | C     | 504 | HEC  | C2B-C3B-CAB-CBB |
| 8   | C     | 504 | HEC  | C4B-C3B-CAB-CBB |
| 8   | C     | 504 | HEC  | C2C-C3C-CAC-CBC |
| 8   | C     | 504 | HEC  | C4C-C3C-CAC-CBC |
| 10  | H     | 301 | GOL  | C1-C2-C3-O3     |
| 12  | C     | 508 | PGV  | O02-C1-O01-C02  |
| 12  | L     | 308 | PGV  | C03-O11-P-O12   |
| 12  | L     | 308 | PGV  | C03-O11-P-O14   |
| 12  | L     | 308 | PGV  | C04-O12-P-O11   |
| 12  | L     | 308 | PGV  | O12-C04-C05-O05 |
| 12  | M     | 410 | PGV  | C03-O11-P-O12   |
| 12  | M     | 411 | PGV  | C04-C05-C06-O06 |
| 12  | H     | 303 | PGV  | C03-O11-P-O13   |
| 12  | H     | 303 | PGV  | C04-O12-P-O14   |
| 12  | D     | 106 | PGV  | C03-O11-P-O12   |
| 12  | D     | 106 | PGV  | O12-C04-C05-O05 |
| 12  | 1     | 105 | PGV  | C03-O11-P-O12   |
| 12  | 1     | 105 | PGV  | C03-O11-P-O13   |
| 12  | 1     | 105 | PGV  | C04-O12-P-O13   |
| 12  | 3     | 105 | PGV  | C03-O11-P-O12   |
| 12  | 3     | 105 | PGV  | C03-O11-P-O13   |
| 12  | 3     | 105 | PGV  | C03-O11-P-O14   |
| 12  | 3     | 105 | PGV  | O12-C04-C05-C06 |
| 13  | L     | 305 | BCL  | C4C-C3C-CAC-CBC |
| 13  | M     | 401 | BCL  | CAD-CBD-CGD-O1D |
| 13  | M     | 401 | BCL  | CAD-CBD-CGD-O2D |
| 13  | A     | 101 | BCL  | C14-C13-C15-C16 |
| 13  | A     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | F     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 13  | F     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | I     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 13  | J     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 13  | J     | 102 | BCL  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | J     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 13  | K     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | Q     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | Q     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | S     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | U     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | U     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | U     | 103 | BCL  | C11-C10-C8-C9   |
| 13  | W     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 13  | W     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 13  | W     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | W     | 104 | BCL  | C1A-C2A-CAA-CBA |
| 13  | Y     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 13  | Y     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 13  | Y     | 103 | BCL  | C2C-C3C-CAC-CBC |
| 13  | Y     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | 1     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 13  | 1     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 13  | 2     | 102 | BCL  | C2C-C3C-CAC-CBC |
| 13  | 2     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 13  | 2     | 102 | BCL  | C11-C10-C8-C9   |
| 13  | 3     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | 3     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | 4     | 102 | BCL  | C11-C10-C8-C9   |
| 13  | 5     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | 7     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | 7     | 103 | BCL  | C11-C10-C8-C9   |
| 13  | 9     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | 9     | 103 | BCL  | C2C-C3C-CAC-CBC |
| 13  | 9     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 14  | M     | 402 | BPH  | C2C-C3C-CAC-CBC |
| 19  | M     | 405 | CRT  | O1-C1-C4-C5     |
| 19  | M     | 405 | CRT  | C2-C1-C4-C5     |
| 19  | M     | 405 | CRT  | C3-C1-C4-C5     |
| 19  | M     | 405 | CRT  | C39-C38-O2-C2M  |
| 20  | M     | 406 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | M     | 406 | CDL  | CB2-OB2-PB2-OB4 |
| 20  | M     | 406 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | M     | 406 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | M     | 406 | CDL  | OB7-CB5-OB6-CB4 |
| 20  | M     | 406 | CDL  | C51-CB5-OB6-CB4 |
| 20  | M     | 412 | CDL  | CB2-OB2-PB2-OB5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | M     | 412 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | M     | 412 | CDL  | CB3-OB5-PB2-OB4 |
| 20  | H     | 305 | CDL  | O1-C1-CB2-OB2   |
| 20  | H     | 305 | CDL  | CA2-C1-CB2-OB2  |
| 20  | H     | 305 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | H     | 305 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | H     | 305 | CDL  | CA3-OA5-PA1-OA2 |
| 20  | H     | 305 | CDL  | CA3-OA5-PA1-OA3 |
| 20  | H     | 305 | CDL  | CA3-OA5-PA1-OA4 |
| 20  | H     | 305 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | H     | 305 | CDL  | CB3-OB5-PB2-OB4 |
| 20  | D     | 104 | CDL  | O1-C1-CA2-OA2   |
| 20  | D     | 104 | CDL  | O1-C1-CB2-OB2   |
| 20  | D     | 104 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | D     | 104 | CDL  | CA3-OA5-PA1-OA4 |
| 20  | D     | 104 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | D     | 104 | CDL  | CB2-OB2-PB2-OB4 |
| 20  | D     | 104 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | D     | 104 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | D     | 104 | CDL  | CB3-OB5-PB2-OB4 |
| 20  | D     | 104 | CDL  | C71-CB7-OB8-CB6 |
| 20  | D     | 105 | CDL  | CB2-C1-CA2-OA2  |
| 20  | D     | 105 | CDL  | O1-C1-CB2-OB2   |
| 20  | D     | 105 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | D     | 105 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | D     | 105 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | D     | 105 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | D     | 105 | CDL  | C11-CA5-OA6-CA4 |
| 20  | D     | 105 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | D     | 105 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | D     | 105 | CDL  | CB3-OB5-PB2-OB4 |
| 20  | O     | 104 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | O     | 104 | CDL  | OB7-CB5-OB6-CB4 |
| 20  | S     | 104 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | S     | 104 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | S     | 104 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | S     | 104 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | S     | 104 | CDL  | OB5-CB3-CB4-OB6 |
| 20  | S     | 104 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | U     | 104 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | U     | 104 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | U     | 104 | CDL  | CA2-OA2-PA1-OA5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | U     | 104 | CDL  | CB3-OB5-PB2-OB3 |
| 20  | U     | 104 | CDL  | OB5-CB3-CB4-OB6 |
| 20  | Y     | 104 | CDL  | O1-C1-CB2-OB2   |
| 20  | Y     | 104 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | Y     | 104 | CDL  | CA2-OA2-PA1-OA4 |
| 20  | Y     | 104 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | Y     | 104 | CDL  | CA3-OA5-PA1-OA3 |
| 20  | Y     | 104 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | Y     | 104 | CDL  | CB2-OB2-PB2-OB4 |
| 20  | Y     | 104 | CDL  | CB2-OB2-PB2-OB5 |
| 20  | Y     | 104 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | Y     | 104 | CDL  | CB3-OB5-PB2-OB3 |
| 20  | 1     | 104 | CDL  | CB3-OB5-PB2-OB2 |
| 20  | 1     | 104 | CDL  | CB3-OB5-PB2-OB3 |
| 20  | 1     | 104 | CDL  | CB3-OB5-PB2-OB4 |
| 20  | 1     | 104 | CDL  | CB3-CB4-CB6-OB8 |
| 20  | U     | 104 | CDL  | C51-CB5-OB6-CB4 |
| 20  | D     | 104 | CDL  | OB9-CB7-OB8-CB6 |
| 12  | C     | 508 | PGV  | O04-C19-O03-C01 |
| 12  | D     | 106 | PGV  | O04-C19-O03-C01 |
| 13  | 9     | 103 | BCL  | C3-C5-C6-C7     |
| 12  | C     | 508 | PGV  | C20-C19-O03-C01 |
| 12  | D     | 106 | PGV  | C20-C19-O03-C01 |
| 12  | C     | 508 | PGV  | C2-C1-O01-C02   |
| 20  | O     | 104 | CDL  | C51-CB5-OB6-CB4 |
| 13  | A     | 101 | BCL  | C4-C3-C5-C6     |
| 15  | L     | 304 | UQ8  | C15-C14-C16-C17 |
| 15  | L     | 309 | UQ8  | C35-C34-C36-C37 |
| 15  | L     | 310 | UQ8  | C12-C11-C9-C10  |
| 13  | A     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | Q     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | W     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | 7     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | L     | 304 | UQ8  | C13-C14-C16-C17 |
| 15  | L     | 309 | UQ8  | C33-C34-C36-C37 |
| 15  | L     | 310 | UQ8  | C12-C11-C9-C8   |
| 13  | 3     | 101 | BCL  | C3-C5-C6-C7     |
| 20  | U     | 104 | CDL  | OA9-CA7-OA8-CA6 |
| 12  | 9     | 104 | PGV  | O12-C04-C05-O05 |
| 20  | M     | 406 | CDL  | O1-C1-CA2-OA2   |
| 20  | S     | 104 | CDL  | O1-C1-CB2-OB2   |
| 20  | O     | 104 | CDL  | C31-CA7-OA8-CA6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | 3     | 105 | PGV  | C2-C1-O01-C02   |
| 12  | 9     | 104 | PGV  | C2-C1-O01-C02   |
| 12  | L     | 308 | PGV  | C19-C20-C21-C22 |
| 20  | U     | 104 | CDL  | C31-CA7-OA8-CA6 |
| 13  | 1     | 101 | BCL  | C4-C3-C5-C6     |
| 14  | M     | 402 | BPH  | C4-C3-C5-C6     |
| 13  | 1     | 101 | BCL  | C2-C3-C5-C6     |
| 20  | O     | 104 | CDL  | OA9-CA7-OA8-CA6 |
| 18  | M     | 404 | MQ8  | C33-C35-C36-C37 |
| 18  | M     | 404 | MQ8  | C38-C40-C41-C42 |
| 22  | M     | 414 | LMT  | O5'-C1'-O1'-C1  |
| 22  | H     | 304 | LMT  | O5'-C1'-O1'-C1  |
| 22  | H     | 304 | LMT  | O5'-C5'-C6'-O6' |
| 12  | 9     | 104 | PGV  | O02-C1-O01-C02  |
| 12  | L     | 308 | PGV  | O12-C04-C05-C06 |
| 12  | D     | 106 | PGV  | O12-C04-C05-C06 |
| 20  | M     | 406 | CDL  | CB2-C1-CA2-OA2  |
| 20  | D     | 104 | CDL  | CB2-C1-CA2-OA2  |
| 20  | S     | 104 | CDL  | CA2-C1-CB2-OB2  |
| 14  | M     | 402 | BPH  | C2-C3-C5-C6     |
| 13  | P     | 102 | BCL  | C3-C5-C6-C7     |
| 13  | L     | 305 | BCL  | C6-C7-C8-C9     |
| 13  | L     | 305 | BCL  | C14-C13-C15-C16 |
| 13  | A     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | F     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | F     | 103 | BCL  | C11-C10-C8-C9   |
| 13  | K     | 101 | BCL  | C14-C13-C15-C16 |
| 13  | K     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | K     | 103 | BCL  | C11-C10-C8-C9   |
| 13  | P     | 102 | BCL  | C6-C7-C8-C9     |
| 13  | P     | 102 | BCL  | C11-C10-C8-C9   |
| 13  | Q     | 101 | BCL  | C11-C12-C13-C14 |
| 13  | Q     | 103 | BCL  | C14-C13-C15-C16 |
| 13  | S     | 101 | BCL  | C14-C13-C15-C16 |
| 13  | U     | 103 | BCL  | C11-C12-C13-C14 |
| 13  | W     | 104 | BCL  | C6-C7-C8-C9     |
| 13  | Y     | 103 | BCL  | C14-C13-C15-C16 |
| 13  | 2     | 102 | BCL  | C6-C7-C8-C9     |
| 13  | 3     | 101 | BCL  | C14-C13-C15-C16 |
| 13  | 5     | 103 | BCL  | C11-C12-C13-C14 |
| 13  | 7     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | 9     | 103 | BCL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | M     | 414 | LMT  | C2'-C1'-O1'-C1  |
| 22  | H     | 304 | LMT  | C2'-C1'-O1'-C1  |
| 19  | B     | 101 | CRT  | C5-C6-C7-C8     |
| 19  | 8     | 101 | CRT  | C10-C11-C12-C13 |
| 13  | 4     | 102 | BCL  | C8-C10-C11-C12  |
| 12  | 3     | 105 | PGV  | O02-C1-O01-C02  |
| 20  | H     | 305 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | U     | 104 | CDL  | OB7-CB5-OB6-CB4 |
| 13  | P     | 102 | BCL  | C8-C10-C11-C12  |
| 13  | Q     | 101 | BCL  | C5-C6-C7-C8     |
| 10  | C     | 506 | GOL  | O1-C1-C2-O2     |
| 13  | 3     | 101 | BCL  | C5-C6-C7-C8     |
| 13  | S     | 101 | BCL  | CBD-CGD-O2D-CED |
| 13  | 9     | 101 | BCL  | CBD-CGD-O2D-CED |
| 13  | 9     | 101 | BCL  | C11-C10-C8-C7   |
| 15  | L     | 304 | UQ8  | C14-C16-C17-C18 |
| 13  | W     | 104 | BCL  | C8-C10-C11-C12  |
| 13  | 5     | 101 | BCL  | C5-C6-C7-C8     |
| 15  | L     | 309 | UQ8  | C3-C4-O4-C4M    |
| 15  | L     | 310 | UQ8  | C3-C4-O4-C4M    |
| 13  | P     | 102 | BCL  | C5-C6-C7-C8     |
| 13  | O     | 101 | BCL  | C13-C15-C16-C17 |
| 12  | 9     | 104 | PGV  | C1-C2-C3-C4     |
| 20  | O     | 104 | CDL  | C31-C32-C33-C34 |
| 13  | F     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | 1     | 101 | BCL  | C5-C6-C7-C8     |
| 13  | 1     | 101 | BCL  | C13-C15-C16-C17 |
| 12  | M     | 411 | PGV  | O12-C04-C05-O05 |
| 12  | 3     | 105 | PGV  | O12-C04-C05-O05 |
| 20  | D     | 105 | CDL  | O1-C1-CA2-OA2   |
| 20  | O     | 104 | CDL  | O1-C1-CB2-OB2   |
| 20  | S     | 104 | CDL  | O1-C1-CA2-OA2   |
| 20  | H     | 305 | CDL  | CB5-C51-C52-C53 |
| 13  | I     | 101 | BCL  | C5-C6-C7-C8     |
| 13  | S     | 101 | BCL  | C5-C6-C7-C8     |
| 13  | 7     | 101 | BCL  | C8-C10-C11-C12  |
| 13  | A     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | S     | 103 | BCL  | C5-C6-C7-C8     |
| 14  | M     | 402 | BPH  | C5-C6-C7-C8     |
| 22  | H     | 304 | LMT  | C4'-C5'-C6'-O6' |
| 20  | Y     | 104 | CDL  | C11-CA5-OA6-CA4 |
| 13  | Y     | 103 | BCL  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | M     | 411 | PGV  | O12-C04-C05-C06 |
| 20  | D     | 104 | CDL  | CA2-C1-CB2-OB2  |
| 20  | D     | 105 | CDL  | CA2-C1-CB2-OB2  |
| 20  | O     | 104 | CDL  | CA2-C1-CB2-OB2  |
| 20  | S     | 104 | CDL  | CB2-C1-CA2-OA2  |
| 12  | M     | 410 | PGV  | C20-C19-O03-C01 |
| 20  | M     | 406 | CDL  | C31-CA7-OA8-CA6 |
| 13  | Y     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | 1     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | 5     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | W     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | W     | 104 | BCL  | C13-C15-C16-C17 |
| 13  | Y     | 103 | BCL  | C13-C15-C16-C17 |
| 13  | Y     | 103 | BCL  | C15-C16-C17-C18 |
| 13  | A     | 103 | BCL  | C13-C15-C16-C17 |
| 13  | Q     | 103 | BCL  | C13-C15-C16-C17 |
| 13  | J     | 102 | BCL  | C15-C16-C17-C18 |
| 13  | U     | 101 | BCL  | C5-C6-C7-C8     |
| 12  | L     | 307 | PGV  | C2-C1-O01-C02   |
| 20  | O     | 104 | CDL  | C11-CA5-OA6-CA4 |
| 12  | L     | 307 | PGV  | O02-C1-O01-C02  |
| 15  | L     | 310 | UQ8  | C9-C11-C12-C13  |
| 13  | Q     | 103 | BCL  | C10-C11-C12-C13 |
| 19  | W     | 102 | CRT  | C15-C16-C17-C18 |
| 19  | 0     | 101 | CRT  | C5-C6-C7-C8     |
| 19  | 8     | 101 | CRT  | C10-C11-C12-C14 |
| 13  | Q     | 101 | BCL  | C15-C16-C17-C18 |
| 20  | M     | 406 | CDL  | C71-C72-C73-C74 |
| 10  | C     | 506 | GOL  | O1-C1-C2-C3     |
| 13  | 9     | 101 | BCL  | C16-C17-C18-C19 |
| 13  | 3     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 13  | Q     | 101 | BCL  | C10-C11-C12-C13 |
| 20  | O     | 104 | CDL  | CA7-C31-C32-C33 |
| 13  | F     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | I     | 101 | BCL  | C16-C17-C18-C19 |
| 13  | P     | 102 | BCL  | C16-C17-C18-C20 |
| 13  | Q     | 101 | BCL  | C16-C17-C18-C19 |
| 13  | 9     | 101 | BCL  | C16-C17-C18-C20 |
| 14  | L     | 303 | BPH  | C16-C17-C18-C19 |
| 12  | M     | 410 | PGV  | O04-C19-O03-C01 |
| 13  | 2     | 102 | BCL  | C13-C15-C16-C17 |
| 20  | S     | 104 | CDL  | C37-C38-C39-C40 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | U     | 104 | CDL  | C14-C15-C16-C17 |
| 20  | M     | 406 | CDL  | C40-C41-C42-C43 |
| 20  | U     | 104 | CDL  | C33-C34-C35-C36 |
| 20  | O     | 104 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | Y     | 104 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | 1     | 104 | CDL  | OB6-CB4-CB6-OB8 |
| 12  | 1     | 105 | PGV  | C19-C20-C21-C22 |
| 13  | 5     | 101 | BCL  | C16-C17-C18-C19 |
| 20  | M     | 406 | CDL  | C14-C15-C16-C17 |
| 20  | M     | 406 | CDL  | C51-C52-C53-C54 |
| 13  | U     | 103 | BCL  | C8-C10-C11-C12  |
| 13  | 7     | 103 | BCL  | C10-C11-C12-C13 |
| 20  | M     | 406 | CDL  | C11-CA5-OA6-CA4 |
| 12  | 9     | 104 | PGV  | C19-C20-C21-C22 |
| 13  | F     | 103 | BCL  | C10-C11-C12-C13 |
| 12  | L     | 308 | PGV  | C7-C8-C9-C10    |
| 20  | M     | 406 | CDL  | C34-C35-C36-C37 |
| 13  | K     | 103 | BCL  | C3-C5-C6-C7     |
| 13  | F     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | S     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | U     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | W     | 104 | BCL  | C3A-C2A-CAA-CBA |
| 13  | 5     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | 9     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 20  | D     | 105 | CDL  | C59-C60-C61-C62 |
| 13  | 1     | 101 | BCL  | C10-C11-C12-C13 |
| 20  | M     | 406 | CDL  | OA9-CA7-OA8-CA6 |
| 20  | S     | 104 | CDL  | C35-C36-C37-C38 |
| 20  | M     | 406 | CDL  | C12-C13-C14-C15 |
| 20  | H     | 305 | CDL  | C11-C12-C13-C14 |
| 20  | H     | 305 | CDL  | C78-C79-C80-C81 |
| 12  | M     | 410 | PGV  | C30-C31-C32-C33 |
| 22  | M     | 414 | LMT  | C5-C6-C7-C8     |
| 13  | S     | 103 | BCL  | C16-C17-C18-C20 |
| 20  | S     | 104 | CDL  | CB5-C51-C52-C53 |
| 13  | U     | 103 | BCL  | C10-C11-C12-C13 |
| 12  | 1     | 105 | PGV  | C3-C4-C5-C6     |
| 12  | L     | 307 | PGV  | C19-C20-C21-C22 |
| 20  | O     | 104 | CDL  | CB7-C71-C72-C73 |
| 13  | 4     | 102 | BCL  | C5-C6-C7-C8     |
| 13  | D     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | 3     | 101 | BCL  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | M     | 406 | CDL  | C61-C62-C63-C64 |
| 20  | S     | 104 | CDL  | CA5-C11-C12-C13 |
| 13  | A     | 103 | BCL  | C11-C10-C8-C9   |
| 13  | S     | 103 | BCL  | C11-C10-C8-C9   |
| 12  | L     | 307 | PGV  | C24-C25-C26-C27 |
| 12  | L     | 307 | PGV  | C23-C24-C25-C26 |
| 13  | F     | 101 | BCL  | C5-C6-C7-C8     |
| 20  | H     | 305 | CDL  | C71-CB7-OB8-CB6 |
| 13  | P     | 102 | BCL  | C16-C17-C18-C19 |
| 12  | D     | 106 | PGV  | C2-C1-O01-C02   |
| 20  | U     | 104 | CDL  | C11-CA5-OA6-CA4 |
| 20  | M     | 406 | CDL  | C17-C18-C19-C20 |
| 20  | U     | 104 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | O     | 104 | CDL  | C33-C34-C35-C36 |
| 19  | 8     | 101 | CRT  | C15-C16-C17-C18 |
| 20  | S     | 104 | CDL  | C14-C15-C16-C17 |
| 21  | K     | 104 | PEF  | C30-C31-C32-C33 |
| 13  | Y     | 103 | BCL  | C3-C5-C6-C7     |
| 13  | K     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | S     | 103 | BCL  | C16-C17-C18-C19 |
| 13  | K     | 101 | BCL  | C4-C3-C5-C6     |
| 14  | L     | 303 | BPH  | C4-C3-C5-C6     |
| 12  | L     | 307 | PGV  | C29-C30-C31-C32 |
| 13  | 4     | 102 | BCL  | C3-C5-C6-C7     |
| 13  | 9     | 101 | BCL  | C5-C6-C7-C8     |
| 20  | S     | 104 | CDL  | C73-C74-C75-C76 |
| 20  | M     | 406 | CDL  | OA7-CA5-OA6-CA4 |
| 20  | U     | 104 | CDL  | OA5-CA3-CA4-OA6 |
| 12  | L     | 307 | PGV  | C26-C27-C28-C29 |
| 20  | O     | 104 | CDL  | C60-C61-C62-C63 |
| 12  | 1     | 105 | PGV  | C2-C1-O01-C02   |
| 20  | D     | 104 | CDL  | C11-CA5-OA6-CA4 |
| 13  | W     | 101 | BCL  | C5-C6-C7-C8     |
| 13  | Q     | 101 | BCL  | C16-C17-C18-C20 |
| 20  | M     | 406 | CDL  | CB5-C51-C52-C53 |
| 20  | M     | 406 | CDL  | C42-C43-C44-C45 |
| 13  | A     | 103 | BCL  | C3-C5-C6-C7     |
| 12  | 3     | 105 | PGV  | C7-C8-C9-C10    |
| 20  | S     | 104 | CDL  | C72-C73-C74-C75 |
| 12  | 3     | 105 | PGV  | C13-C14-C15-C16 |
| 20  | H     | 305 | CDL  | C59-C60-C61-C62 |
| 20  | D     | 105 | CDL  | C71-C72-C73-C74 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | D     | 106 | PGV  | C4-C5-C6-C7     |
| 12  | L     | 308 | PGV  | C23-C24-C25-C26 |
| 12  | 9     | 104 | PGV  | C22-C23-C24-C25 |
| 20  | U     | 104 | CDL  | C71-C72-C73-C74 |
| 20  | M     | 406 | CDL  | C20-C21-C22-C23 |
| 12  | M     | 411 | PGV  | C27-C28-C29-C30 |
| 10  | H     | 301 | GOL  | O2-C2-C3-O3     |
| 12  | M     | 411 | PGV  | O05-C05-C06-O06 |
| 13  | D     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | K     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | P     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 13  | S     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | P     | 102 | BCL  | C13-C15-C16-C17 |
| 12  | M     | 410 | PGV  | C6-C7-C8-C9     |
| 12  | 3     | 105 | PGV  | C11-C10-C9-C8   |
| 12  | M     | 410 | PGV  | C2-C3-C4-C5     |
| 12  | M     | 411 | PGV  | C29-C30-C31-C32 |
| 12  | M     | 410 | PGV  | C01-C02-C03-O11 |
| 20  | S     | 104 | CDL  | OA5-CA3-CA4-CA6 |
| 13  | A     | 103 | BCL  | C6-C7-C8-C10    |
| 13  | D     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | D     | 103 | BCL  | C12-C13-C15-C16 |
| 13  | F     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | F     | 103 | BCL  | C6-C7-C8-C10    |
| 13  | K     | 103 | BCL  | C6-C7-C8-C10    |
| 13  | P     | 102 | BCL  | C6-C7-C8-C10    |
| 13  | A     | 103 | BCL  | C2C-C3C-CAC-CBC |
| 13  | I     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 19  | B     | 101 | CRT  | C2-C1-C4-C5     |
| 19  | B     | 101 | CRT  | C3-C1-C4-C5     |
| 19  | J     | 101 | CRT  | C2-C1-C4-C5     |
| 19  | 0     | 101 | CRT  | C2-C1-C4-C5     |
| 11  | C     | 507 | LHG  | C25-C26-C27-C28 |
| 12  | 3     | 105 | PGV  | C19-C20-C21-C22 |
| 13  | S     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | F     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | J     | 102 | BCL  | C6-C7-C8-C9     |
| 13  | Q     | 103 | BCL  | C11-C10-C8-C9   |
| 22  | M     | 414 | LMT  | O5'-C5'-C6'-O6' |
| 21  | K     | 104 | PEF  | C31-C30-O3-C3   |
| 12  | M     | 410 | PGV  | C13-C14-C15-C16 |
| 13  | Q     | 101 | BCL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | S     | 104 | CDL  | C52-C53-C54-C55 |
| 13  | W     | 104 | BCL  | C10-C11-C12-C13 |
| 12  | M     | 410 | PGV  | C21-C22-C23-C24 |
| 20  | M     | 406 | CDL  | CA3-CA4-CA6-OA8 |
| 20  | M     | 406 | CDL  | CB3-CB4-CB6-OB8 |
| 20  | S     | 104 | CDL  | CA3-CA4-CA6-OA8 |
| 20  | S     | 104 | CDL  | CB3-CB4-CB6-OB8 |
| 13  | 9     | 101 | BCL  | O1D-CGD-O2D-CED |
| 20  | U     | 104 | CDL  | CA5-C11-C12-C13 |
| 13  | S     | 101 | BCL  | O1D-CGD-O2D-CED |
| 22  | M     | 414 | LMT  | C4-C5-C6-C7     |
| 14  | L     | 303 | BPH  | C2-C3-C5-C6     |
| 13  | L     | 305 | BCL  | C13-C15-C16-C17 |
| 13  | Y     | 101 | BCL  | C15-C16-C17-C18 |
| 20  | H     | 305 | CDL  | OB9-CB7-OB8-CB6 |
| 12  | M     | 410 | PGV  | C03-O11-P-O13   |
| 20  | D     | 105 | CDL  | C75-C76-C77-C78 |
| 22  | H     | 304 | LMT  | O1'-C1-C2-C3    |
| 20  | M     | 406 | CDL  | C52-C53-C54-C55 |
| 12  | M     | 410 | PGV  | C19-C20-C21-C22 |
| 20  | U     | 104 | CDL  | C15-C16-C17-C18 |
| 12  | 9     | 104 | PGV  | O12-C04-C05-C06 |
| 20  | M     | 406 | CDL  | OB5-CB3-CB4-OB6 |
| 14  | L     | 303 | BPH  | C8-C10-C11-C12  |
| 12  | 9     | 104 | PGV  | C20-C19-O03-C01 |
| 20  | O     | 104 | CDL  | C17-C18-C19-C20 |
| 20  | S     | 104 | CDL  | C59-C60-C61-C62 |
| 20  | M     | 406 | CDL  | C31-C32-C33-C34 |
| 20  | S     | 104 | CDL  | C51-C52-C53-C54 |
| 20  | M     | 406 | CDL  | C53-C54-C55-C56 |
| 12  | D     | 106 | PGV  | O02-C1-O01-C02  |
| 20  | S     | 104 | CDL  | C74-C75-C76-C77 |
| 20  | U     | 104 | CDL  | CB7-C71-C72-C73 |
| 13  | 3     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 19  | M     | 405 | CRT  | C40-C38-O2-C2M  |
| 13  | S     | 101 | BCL  | C10-C11-C12-C13 |
| 13  | L     | 305 | BCL  | C16-C17-C18-C20 |
| 15  | L     | 309 | UQ8  | C40-C39-C41-C42 |
| 13  | D     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | D     | 103 | BCL  | C14-C13-C15-C16 |
| 13  | K     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | 3     | 101 | BCL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | 3     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | 5     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | 9     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | 9     | 101 | BCL  | C11-C12-C13-C14 |
| 13  | A     | 103 | BCL  | C10-C11-C12-C13 |
| 13  | I     | 101 | BCL  | C16-C17-C18-C20 |
| 13  | 7     | 103 | BCL  | C15-C16-C17-C18 |
| 22  | H     | 304 | LMT  | C11-C10-C9-C8   |
| 12  | H     | 303 | PGV  | C01-C02-C03-O11 |
| 12  | D     | 106 | PGV  | C01-C02-C03-O11 |
| 20  | O     | 104 | CDL  | OA5-CA3-CA4-CA6 |
| 20  | S     | 104 | CDL  | OB5-CB3-CB4-CB6 |
| 20  | U     | 104 | CDL  | OA5-CA3-CA4-CA6 |
| 20  | U     | 104 | CDL  | OB5-CB3-CB4-CB6 |
| 13  | A     | 101 | BCL  | C12-C13-C15-C16 |
| 13  | D     | 103 | BCL  | C6-C7-C8-C10    |
| 13  | J     | 102 | BCL  | C12-C13-C15-C16 |
| 13  | K     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | Q     | 103 | BCL  | C11-C10-C8-C7   |
| 13  | U     | 103 | BCL  | C11-C10-C8-C7   |
| 13  | 2     | 102 | BCL  | C11-C10-C8-C7   |
| 13  | 2     | 102 | BCL  | C12-C13-C15-C16 |
| 13  | 3     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | 4     | 102 | BCL  | C11-C10-C8-C7   |
| 13  | 5     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | 7     | 103 | BCL  | C11-C10-C8-C7   |
| 13  | 9     | 101 | BCL  | C11-C12-C13-C15 |
| 13  | Q     | 101 | BCL  | C13-C15-C16-C17 |
| 13  | 9     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | S     | 103 | BCL  | O1A-CGA-O2A-C1  |
| 21  | K     | 104 | PEF  | O5-C30-O3-C3    |
| 13  | D     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | J     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 13  | 3     | 101 | BCL  | C3A-C2A-CAA-CBA |
| 13  | S     | 101 | BCL  | C13-C15-C16-C17 |
| 12  | M     | 411 | PGV  | C21-C22-C23-C24 |
| 19  | G     | 101 | CRT  | C15-C16-C17-C18 |
| 19  | V     | 101 | CRT  | C5-C6-C7-C8     |
| 12  | 1     | 105 | PGV  | O02-C1-O01-C02  |
| 12  | L     | 308 | PGV  | C4-C5-C6-C7     |
| 20  | H     | 305 | CDL  | CB3-CB4-CB6-OB8 |
| 20  | D     | 104 | CDL  | CB3-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | O     | 104 | CDL  | CB3-CB4-CB6-OB8 |
| 13  | J     | 102 | BCL  | C13-C15-C16-C17 |
| 20  | M     | 406 | CDL  | C80-C81-C82-C83 |
| 20  | M     | 406 | CDL  | C38-C39-C40-C41 |
| 12  | D     | 106 | PGV  | O01-C02-C03-O11 |
| 20  | M     | 406 | CDL  | OA5-CA3-CA4-OA6 |
| 20  | D     | 105 | CDL  | OB5-CB3-CB4-OB6 |
| 20  | Y     | 104 | CDL  | OB5-CB3-CB4-OB6 |
| 13  | A     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | 5     | 103 | BCL  | C10-C11-C12-C13 |
| 12  | 9     | 104 | PGV  | C23-C24-C25-C26 |
| 20  | O     | 104 | CDL  | C77-C78-C79-C80 |
| 20  | O     | 104 | CDL  | C76-C77-C78-C79 |
| 12  | H     | 303 | PGV  | O03-C01-C02-O01 |
| 20  | M     | 406 | CDL  | OA6-CA4-CA6-OA8 |
| 20  | D     | 104 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | O     | 104 | CDL  | OB6-CB4-CB6-OB8 |
| 22  | M     | 414 | LMT  | C2-C3-C4-C5     |
| 13  | F     | 103 | BCL  | C3-C5-C6-C7     |
| 12  | L     | 308 | PGV  | C26-C27-C28-C29 |
| 15  | L     | 310 | UQ8  | C5-C4-O4-C4M    |
| 13  | 1     | 101 | BCL  | C16-C17-C18-C20 |
| 14  | L     | 303 | BPH  | C16-C17-C18-C20 |
| 20  | H     | 305 | CDL  | CA5-C11-C12-C13 |
| 13  | Y     | 103 | BCL  | C11-C12-C13-C14 |
| 13  | 1     | 101 | BCL  | C6-C7-C8-C9     |
| 13  | 5     | 103 | BCL  | C11-C10-C8-C9   |
| 22  | H     | 304 | LMT  | C6-C7-C8-C9     |
| 15  | L     | 310 | UQ8  | C14-C16-C17-C18 |
| 13  | D     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | S     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | 4     | 102 | BCL  | C4C-C3C-CAC-CBC |
| 13  | 5     | 103 | BCL  | C4C-C3C-CAC-CBC |
| 13  | 7     | 101 | BCL  | C4C-C3C-CAC-CBC |
| 13  | D     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | 5     | 101 | BCL  | C16-C17-C18-C20 |
| 12  | 3     | 105 | PGV  | C20-C19-O03-C01 |
| 13  | L     | 305 | BCL  | C6-C7-C8-C10    |
| 13  | L     | 305 | BCL  | C11-C12-C13-C15 |
| 13  | J     | 102 | BCL  | C6-C7-C8-C10    |
| 13  | U     | 103 | BCL  | C11-C12-C13-C15 |
| 13  | Y     | 103 | BCL  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | 1     | 101 | BCL  | C6-C7-C8-C10    |
| 13  | 3     | 101 | BCL  | C6-C7-C8-C10    |
| 13  | 3     | 101 | BCL  | C12-C13-C15-C16 |
| 13  | 4     | 102 | BCL  | C6-C7-C8-C10    |
| 13  | 7     | 103 | BCL  | C6-C7-C8-C10    |
| 13  | 9     | 101 | BCL  | C6-C7-C8-C10    |
| 13  | D     | 101 | BCL  | C5-C6-C7-C8     |
| 13  | S     | 103 | BCL  | C8-C10-C11-C12  |
| 19  | B     | 101 | CRT  | C5-C6-C7-C9     |
| 19  | 0     | 101 | CRT  | C5-C6-C7-C9     |
| 20  | D     | 105 | CDL  | C72-C73-C74-C75 |
| 20  | D     | 104 | CDL  | OA7-CA5-OA6-CA4 |
| 13  | 5     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | D     | 101 | BCL  | C2-C3-C5-C6     |
| 20  | O     | 104 | CDL  | C11-C12-C13-C14 |
| 20  | D     | 105 | CDL  | C15-C16-C17-C18 |
| 13  | W     | 101 | BCL  | C10-C11-C12-C13 |
| 13  | 5     | 103 | BCL  | C13-C15-C16-C17 |
| 12  | 9     | 104 | PGV  | O04-C19-O03-C01 |
| 21  | K     | 104 | PEF  | C32-C33-C34-C35 |
| 13  | S     | 103 | BCL  | CBA-CGA-O2A-C1  |
| 12  | L     | 308 | PGV  | C31-C32-C33-C34 |
| 12  | L     | 308 | PGV  | C2-C3-C4-C5     |
| 13  | 4     | 102 | BCL  | C15-C16-C17-C18 |
| 12  | H     | 303 | PGV  | O01-C02-C03-O11 |
| 20  | O     | 104 | CDL  | OA5-CA3-CA4-OA6 |
| 20  | S     | 104 | CDL  | OA5-CA3-CA4-OA6 |
| 12  | M     | 411 | PGV  | O03-C01-C02-C03 |
| 13  | S     | 103 | BCL  | C15-C16-C17-C18 |
| 13  | Y     | 101 | BCL  | C5-C6-C7-C8     |
| 20  | M     | 406 | CDL  | C35-C36-C37-C38 |
| 13  | K     | 101 | BCL  | C2-C3-C5-C6     |
| 12  | D     | 106 | PGV  | O03-C01-C02-O01 |
| 20  | M     | 406 | CDL  | OB6-CB4-CB6-OB8 |
| 20  | S     | 104 | CDL  | OA6-CA4-CA6-OA8 |
| 20  | M     | 406 | CDL  | C44-C45-C46-C47 |
| 13  | L     | 305 | BCL  | C5-C6-C7-C8     |
| 13  | L     | 305 | BCL  | C11-C12-C13-C14 |
| 13  | U     | 101 | BCL  | C14-C13-C15-C16 |
| 13  | 1     | 101 | BCL  | C16-C17-C18-C19 |
| 12  | H     | 303 | PGV  | C5-C6-C7-C8     |
| 13  | U     | 103 | BCL  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | L     | 305 | BCL  | C16-C17-C18-C19 |
| 13  | F     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | F     | 103 | BCL  | C13-C15-C16-C17 |
| 13  | 7     | 103 | BCL  | C16-C17-C18-C19 |
| 13  | L     | 301 | BCL  | C15-C16-C17-C18 |
| 11  | C     | 507 | LHG  | C23-C24-C25-C26 |
| 12  | M     | 410 | PGV  | C14-C15-C16-C17 |
| 12  | L     | 307 | PGV  | C25-C26-C27-C28 |
| 13  | A     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | Y     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | 2     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 13  | 4     | 102 | BCL  | C1A-C2A-CAA-CBA |
| 13  | 7     | 103 | BCL  | C1A-C2A-CAA-CBA |
| 13  | Q     | 101 | BCL  | O1D-CGD-O2D-CED |
| 12  | L     | 307 | PGV  | C20-C19-O03-C01 |
| 13  | 2     | 102 | BCL  | CBA-CGA-O2A-C1  |
| 19  | G     | 101 | CRT  | C15-C16-C17-C19 |
| 19  | W     | 102 | CRT  | C15-C16-C17-C19 |
| 19  | 8     | 101 | CRT  | C15-C16-C17-C19 |
| 20  | M     | 406 | CDL  | OB5-CB3-CB4-CB6 |
| 20  | D     | 105 | CDL  | OB5-CB3-CB4-CB6 |
| 20  | S     | 104 | CDL  | OB9-CB7-OB8-CB6 |
| 13  | K     | 101 | BCL  | C12-C13-C15-C16 |
| 20  | U     | 104 | CDL  | C34-C35-C36-C37 |
| 13  | L     | 305 | BCL  | C2C-C3C-CAC-CBC |
| 13  | F     | 101 | BCL  | C2C-C3C-CAC-CBC |
| 13  | K     | 103 | BCL  | C2C-C3C-CAC-CBC |
| 13  | U     | 103 | BCL  | C2C-C3C-CAC-CBC |
| 19  | J     | 101 | CRT  | C3-C1-C4-C5     |
| 19  | W     | 102 | CRT  | C2-C1-C4-C5     |
| 19  | 0     | 101 | CRT  | C3-C1-C4-C5     |
| 14  | M     | 402 | BPH  | C8-C10-C11-C12  |
| 12  | 3     | 105 | PGV  | O04-C19-O03-C01 |
| 13  | K     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | Q     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 12  | M     | 410 | PGV  | O01-C02-C03-O11 |
| 20  | Y     | 104 | CDL  | OA5-CA3-CA4-OA6 |
| 12  | L     | 308 | PGV  | C2-C1-O01-C02   |
| 13  | D     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | J     | 102 | BCL  | C14-C13-C15-C16 |
| 13  | 4     | 102 | BCL  | C6-C7-C8-C9     |
| 13  | 9     | 101 | BCL  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | K     | 103 | BCL  | C10-C11-C12-C13 |
| 12  | L     | 307 | PGV  | C5-C6-C7-C8     |
| 13  | S     | 103 | BCL  | C10-C11-C12-C13 |
| 13  | 9     | 101 | BCL  | C8-C10-C11-C12  |
| 12  | H     | 303 | PGV  | C20-C21-C22-C23 |
| 12  | D     | 106 | PGV  | O03-C01-C02-C03 |
| 13  | F     | 101 | BCL  | CBD-CGD-O2D-CED |
| 12  | L     | 308 | PGV  | O02-C1-O01-C02  |
| 15  | L     | 309 | UQ8  | C5-C4-O4-C4M    |
| 15  | L     | 311 | UQ8  | C5-C4-O4-C4M    |
| 20  | M     | 406 | CDL  | C13-C14-C15-C16 |
| 12  | L     | 308 | PGV  | C21-C22-C23-C24 |
| 12  | L     | 307 | PGV  | C03-O11-P-O13   |
| 12  | L     | 308 | PGV  | C03-O11-P-O13   |
| 12  | L     | 308 | PGV  | C04-O12-P-O13   |
| 12  | D     | 106 | PGV  | C03-O11-P-O13   |
| 12  | 3     | 105 | PGV  | C04-O12-P-O11   |
| 12  | 3     | 105 | PGV  | C04-O12-P-O14   |
| 15  | L     | 309 | UQ8  | C4-C3-O3-C3M    |
| 20  | M     | 406 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | M     | 406 | CDL  | CB3-OB5-PB2-OB3 |
| 20  | M     | 412 | CDL  | CA3-OA5-PA1-OA3 |
| 20  | M     | 412 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | M     | 412 | CDL  | CB3-OB5-PB2-OB3 |
| 20  | H     | 305 | CDL  | CA2-OA2-PA1-OA3 |
| 20  | D     | 104 | CDL  | CA2-OA2-PA1-OA5 |
| 20  | D     | 104 | CDL  | CA3-OA5-PA1-OA2 |
| 20  | D     | 104 | CDL  | CA3-OA5-PA1-OA3 |
| 20  | D     | 105 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | S     | 104 | CDL  | CB3-OB5-PB2-OB3 |
| 20  | U     | 104 | CDL  | CB2-OB2-PB2-OB3 |
| 20  | Y     | 104 | CDL  | CA3-OA5-PA1-OA2 |
| 20  | Y     | 104 | CDL  | CA3-OA5-PA1-OA4 |
| 20  | Y     | 104 | CDL  | CB3-OB5-PB2-OB4 |
| 12  | 3     | 105 | PGV  | C21-C22-C23-C24 |
| 13  | M     | 401 | BCL  | C13-C15-C16-C17 |
| 13  | O     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | 2     | 102 | BCL  | C4-C3-C5-C6     |
| 14  | M     | 402 | BPH  | C15-C16-C17-C18 |
| 12  | M     | 411 | PGV  | C02-C03-O11-P   |
| 20  | O     | 104 | CDL  | C1-CB2-OB2-PB2  |
| 20  | O     | 104 | CDL  | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | L     | 308 | PGV  | C3-C4-C5-C6     |
| 12  | D     | 106 | PGV  | C19-C20-C21-C22 |
| 13  | K     | 101 | BCL  | C5-C6-C7-C8     |
| 20  | U     | 104 | CDL  | CA6-CA4-OA6-CA5 |
| 12  | L     | 307 | PGV  | C7-C8-C9-C10    |
| 12  | L     | 308 | PGV  | C01-C02-C03-O11 |
| 20  | M     | 406 | CDL  | OA5-CA3-CA4-CA6 |
| 20  | Y     | 104 | CDL  | OA5-CA3-CA4-CA6 |
| 12  | D     | 106 | PGV  | C1-C2-C3-C4     |
| 13  | F     | 101 | BCL  | CBA-CGA-O2A-C1  |
| 13  | Q     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | W     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | 2     | 102 | BCL  | C14-C13-C15-C16 |
| 13  | 5     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | Q     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | Q     | 103 | BCL  | C12-C13-C15-C16 |
| 20  | Y     | 104 | CDL  | CA2-C1-CB2-OB2  |
| 20  | O     | 104 | CDL  | C57-C58-C59-C60 |
| 12  | L     | 308 | PGV  | C1-C2-C3-C4     |
| 12  | H     | 303 | PGV  | C3-C4-C5-C6     |
| 22  | H     | 304 | LMT  | C1-C2-C3-C4     |
| 20  | M     | 406 | CDL  | C73-C74-C75-C76 |
| 12  | 1     | 105 | PGV  | O03-C01-C02-O01 |
| 13  | W     | 101 | BCL  | C15-C16-C17-C18 |
| 11  | C     | 507 | LHG  | C26-C27-C28-C29 |
| 20  | O     | 104 | CDL  | C18-C19-C20-C21 |
| 20  | S     | 104 | CDL  | C16-C17-C18-C19 |
| 13  | Y     | 101 | BCL  | C4-C3-C5-C6     |
| 13  | M     | 401 | BCL  | CAA-CBA-CGA-O2A |
| 13  | 5     | 103 | BCL  | C15-C16-C17-C18 |
| 21  | K     | 104 | PEF  | O4-C10-O2-C2    |
| 20  | S     | 104 | CDL  | C71-CB7-OB8-CB6 |
| 20  | S     | 104 | CDL  | C58-C59-C60-C61 |
| 13  | A     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | Y     | 103 | BCL  | CBA-CGA-O2A-C1  |
| 12  | L     | 307 | PGV  | C27-C28-C29-C30 |
| 20  | D     | 105 | CDL  | C71-CB7-OB8-CB6 |
| 13  | F     | 101 | BCL  | O1D-CGD-O2D-CED |
| 12  | L     | 307 | PGV  | O04-C19-O03-C01 |
| 20  | D     | 105 | CDL  | C73-C74-C75-C76 |
| 12  | M     | 411 | PGV  | C28-C29-C30-C31 |
| 13  | 2     | 102 | BCL  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | C     | 508 | PGV  | C3-C4-C5-C6     |
| 13  | Q     | 101 | BCL  | C11-C12-C13-C15 |
| 13  | W     | 104 | BCL  | C6-C7-C8-C10    |
| 13  | 7     | 103 | BCL  | C11-C12-C13-C15 |
| 13  | L     | 305 | BCL  | C3-C5-C6-C7     |
| 20  | H     | 305 | CDL  | C79-C80-C81-C82 |
| 13  | K     | 103 | BCL  | C4-C3-C5-C6     |
| 13  | P     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 15  | L     | 309 | UQ8  | C30-C29-C31-C32 |
| 15  | L     | 309 | UQ8  | C20-C19-C21-C22 |
| 12  | M     | 411 | PGV  | C20-C21-C22-C23 |
| 20  | M     | 406 | CDL  | C77-C78-C79-C80 |
| 20  | O     | 104 | CDL  | C37-C38-C39-C40 |
| 12  | H     | 303 | PGV  | C02-C03-O11-P   |
| 19  | V     | 101 | CRT  | C10-C11-C12-C13 |
| 13  | 5     | 103 | BCL  | C4-C3-C5-C6     |
| 13  | 5     | 103 | BCL  | C3-C5-C6-C7     |
| 13  | 1     | 101 | BCL  | C11-C10-C8-C9   |
| 13  | 4     | 102 | BCL  | C14-C13-C15-C16 |
| 13  | 7     | 101 | BCL  | C11-C10-C8-C9   |
| 8   | C     | 502 | HEC  | CAA-CBA-CGA-O1A |
| 13  | 5     | 101 | BCL  | C3-C5-C6-C7     |
| 13  | S     | 103 | BCL  | C4-C3-C5-C6     |
| 8   | C     | 501 | HEC  | CAA-CBA-CGA-O1A |
| 8   | C     | 501 | HEC  | CAA-CBA-CGA-O2A |
| 13  | L     | 302 | BCL  | C2A-CAA-CBA-CGA |
| 12  | C     | 508 | PGV  | O03-C01-C02-O01 |
| 13  | 3     | 101 | BCL  | C1A-C2A-CAA-CBA |
| 12  | L     | 307 | PGV  | C28-C29-C30-C31 |
| 21  | K     | 104 | PEF  | C11-C10-O2-C2   |
| 8   | C     | 502 | HEC  | CAA-CBA-CGA-O2A |
| 8   | C     | 502 | HEC  | CAD-CBD-CGD-O1D |
| 20  | S     | 104 | CDL  | C40-C41-C42-C43 |
| 12  | L     | 307 | PGV  | C05-C04-O12-P   |
| 12  | H     | 303 | PGV  | C2-C3-C4-C5     |
| 15  | L     | 310 | UQ8  | C15-C14-C16-C17 |
| 20  | Y     | 104 | CDL  | OB5-CB3-CB4-CB6 |
| 15  | L     | 309 | UQ8  | C28-C29-C31-C32 |
| 15  | L     | 309 | UQ8  | C18-C19-C21-C22 |
| 8   | C     | 504 | HEC  | CAD-CBD-CGD-O1D |
| 13  | O     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | L     | 305 | BCL  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | A     | 101 | BCL  | C6-C7-C8-C10    |
| 13  | K     | 103 | BCL  | C11-C10-C8-C7   |
| 13  | S     | 101 | BCL  | C12-C13-C15-C16 |
| 13  | W     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | 4     | 102 | BCL  | C11-C12-C13-C15 |
| 13  | 9     | 103 | BCL  | C11-C10-C8-C7   |
| 12  | M     | 410 | PGV  | C31-C32-C33-C34 |
| 19  | T     | 101 | CRT  | C5-C6-C7-C8     |
| 13  | K     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | K     | 103 | BCL  | C15-C16-C17-C18 |
| 22  | H     | 304 | LMT  | O5B-C1B-O1B-C4' |
| 15  | L     | 309 | UQ8  | C25-C24-C26-C27 |
| 12  | 9     | 104 | PGV  | C02-C03-O11-P   |
| 12  | L     | 307 | PGV  | C30-C31-C32-C33 |
| 13  | F     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | 5     | 101 | BCL  | C2-C3-C5-C6     |
| 15  | L     | 309 | UQ8  | C38-C39-C41-C42 |
| 8   | C     | 504 | HEC  | CAD-CBD-CGD-O2D |
| 20  | D     | 105 | CDL  | OB9-CB7-OB8-CB6 |
| 8   | C     | 502 | HEC  | CAD-CBD-CGD-O2D |
| 20  | H     | 305 | CDL  | OA7-CA5-OA6-CA4 |
| 15  | L     | 309 | UQ8  | C15-C14-C16-C17 |
| 13  | P     | 102 | BCL  | C15-C16-C17-C18 |
| 20  | U     | 104 | CDL  | C36-C37-C38-C39 |
| 20  | D     | 105 | CDL  | C61-C62-C63-C64 |
| 13  | L     | 301 | BCL  | C13-C15-C16-C17 |
| 13  | 1     | 101 | BCL  | O1A-CGA-O2A-C1  |
| 20  | S     | 104 | CDL  | C32-C31-CA7-OA8 |
| 12  | 9     | 104 | PGV  | C20-C21-C22-C23 |
| 20  | H     | 305 | CDL  | OB5-CB3-CB4-CB6 |
| 20  | O     | 104 | CDL  | OA6-CA4-CA6-OA8 |
| 15  | L     | 310 | UQ8  | C13-C14-C16-C17 |
| 20  | D     | 104 | CDL  | C1-CA2-OA2-PA1  |
| 13  | S     | 103 | BCL  | C11-C12-C13-C14 |
| 13  | U     | 103 | BCL  | C6-C7-C8-C9     |
| 13  | 9     | 103 | BCL  | C11-C12-C13-C14 |
| 12  | M     | 411 | PGV  | C22-C23-C24-C25 |
| 13  | 9     | 101 | BCL  | C2-C1-O2A-CGA   |
| 13  | A     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | Y     | 103 | BCL  | C3A-C2A-CAA-CBA |
| 13  | 2     | 102 | BCL  | C3A-C2A-CAA-CBA |
| 13  | 7     | 103 | BCL  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | U     | 104 | CDL  | C72-C71-CB7-OB8 |
| 20  | H     | 305 | CDL  | CA6-CA4-OA6-CA5 |
| 20  | O     | 104 | CDL  | CA6-CA4-OA6-CA5 |
| 20  | H     | 305 | CDL  | OB5-CB3-CB4-OB6 |
| 12  | L     | 308 | PGV  | C22-C23-C24-C25 |
| 15  | L     | 309 | UQ8  | C34-C36-C37-C38 |
| 20  | U     | 104 | CDL  | CB3-CB4-CB6-OB8 |
| 13  | Q     | 101 | BCL  | C3-C5-C6-C7     |
| 13  | 9     | 103 | BCL  | C4-C3-C5-C6     |
| 20  | 1     | 104 | CDL  | O1-C1-CB2-OB2   |
| 20  | S     | 104 | CDL  | C72-C71-CB7-OB8 |
| 13  | 3     | 101 | BCL  | CAA-CBA-CGA-O2A |
| 19  | V     | 101 | CRT  | C5-C6-C7-C9     |
| 19  | B     | 101 | CRT  | O1-C1-C4-C5     |
| 15  | L     | 309 | UQ8  | C23-C24-C26-C27 |
| 13  | A     | 101 | BCL  | C11-C10-C8-C7   |
| 13  | D     | 101 | BCL  | C6-C7-C8-C10    |
| 13  | S     | 103 | BCL  | C11-C12-C13-C15 |
| 13  | U     | 103 | BCL  | C6-C7-C8-C10    |
| 13  | Y     | 103 | BCL  | C12-C13-C15-C16 |
| 13  | 9     | 103 | BCL  | C11-C12-C13-C15 |
| 20  | H     | 305 | CDL  | C11-CA5-OA6-CA4 |
| 12  | 3     | 105 | PGV  | C9-C10-C11-C12  |
| 13  | K     | 101 | BCL  | C2-C1-O2A-CGA   |
| 13  | 7     | 103 | BCL  | C2-C1-O2A-CGA   |
| 12  | M     | 411 | PGV  | C05-C04-O12-P   |
| 15  | L     | 309 | UQ8  | C29-C31-C32-C33 |
| 20  | M     | 406 | CDL  | C74-C75-C76-C77 |
| 20  | H     | 305 | CDL  | C81-C82-C83-C84 |
| 20  | S     | 104 | CDL  | C13-C14-C15-C16 |
| 12  | L     | 307 | PGV  | O01-C1-C2-C3    |
| 12  | M     | 411 | PGV  | C20-C19-O03-C01 |
| 20  | U     | 104 | CDL  | C40-C41-C42-C43 |
| 12  | L     | 308 | PGV  | O03-C19-C20-C21 |
| 12  | 9     | 104 | PGV  | O03-C19-C20-C21 |
| 20  | O     | 104 | CDL  | OB5-CB3-CB4-OB6 |
| 12  | L     | 307 | PGV  | C22-C23-C24-C25 |
| 13  | K     | 103 | BCL  | C2-C3-C5-C6     |
| 13  | O     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | S     | 103 | BCL  | C2-C3-C5-C6     |
| 13  | Y     | 101 | BCL  | C2-C3-C5-C6     |
| 13  | 2     | 102 | BCL  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | 5     | 103 | BCL  | C2-C3-C5-C6     |
| 20  | D     | 105 | CDL  | C76-C77-C78-C79 |
| 8   | C     | 504 | HEC  | CAA-CBA-CGA-O2A |
| 13  | 4     | 102 | BCL  | C11-C12-C13-C14 |
| 20  | H     | 305 | CDL  | C1-CA2-OA2-PA1  |
| 20  | U     | 104 | CDL  | CA3-CA4-CA6-OA8 |
| 20  | M     | 406 | CDL  | C39-C40-C41-C42 |
| 13  | A     | 103 | BCL  | C4-C3-C5-C6     |
| 13  | 9     | 101 | BCL  | C4-C3-C5-C6     |
| 12  | M     | 410 | PGV  | O03-C01-C02-O01 |
| 13  | A     | 101 | BCL  | C2-C1-O2A-CGA   |
| 13  | F     | 103 | BCL  | C2-C1-O2A-CGA   |
| 13  | O     | 101 | BCL  | C6-C7-C8-C10    |
| 13  | 5     | 103 | BCL  | C11-C12-C13-C15 |
| 20  | O     | 104 | CDL  | CA3-CA4-OA6-CA5 |
| 15  | L     | 311 | UQ8  | C3-C4-O4-C4M    |
| 13  | 9     | 101 | BCL  | C10-C11-C12-C13 |
| 20  | D     | 104 | CDL  | C32-C31-CA7-OA8 |
| 12  | L     | 308 | PGV  | O01-C1-C2-C3    |
| 13  | L     | 301 | BCL  | C16-C17-C18-C19 |
| 20  | M     | 406 | CDL  | C72-C73-C74-C75 |
| 13  | 3     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | D     | 101 | BCL  | C16-C17-C18-C20 |
| 13  | Y     | 103 | BCL  | C16-C17-C18-C19 |
| 19  | M     | 405 | CRT  | C35-C36-C37-C38 |
| 8   | C     | 504 | HEC  | CAA-CBA-CGA-O1A |
| 19  | T     | 101 | CRT  | C27-C28-C30-C31 |
| 19  | V     | 101 | CRT  | C10-C11-C12-C14 |
| 19  | V     | 101 | CRT  | C15-C16-C17-C19 |
| 19  | 4     | 101 | CRT  | C15-C16-C17-C19 |
| 13  | F     | 103 | BCL  | C15-C16-C17-C18 |
| 12  | 1     | 105 | PGV  | O01-C1-C2-C3    |
| 12  | M     | 411 | PGV  | O04-C19-O03-C01 |
| 12  | L     | 308 | PGV  | O04-C19-C20-C21 |
| 12  | 9     | 104 | PGV  | O04-C19-C20-C21 |
| 20  | S     | 104 | CDL  | C72-C71-CB7-OB9 |
| 13  | I     | 101 | BCL  | C15-C16-C17-C18 |
| 13  | Y     | 101 | BCL  | C10-C11-C12-C13 |
| 20  | O     | 104 | CDL  | CA4-CA3-OA5-PA1 |
| 20  | H     | 305 | CDL  | C31-C32-C33-C34 |
| 13  | A     | 101 | BCL  | CAD-CBD-CGD-O2D |
| 13  | Y     | 103 | BCL  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | O     | 101 | BCL  | C5-C6-C7-C8     |
| 8   | C     | 502 | HEC  | C3D-CAD-CBD-CGD |
| 20  | D     | 105 | CDL  | OA5-CA3-CA4-CA6 |
| 12  | L     | 307 | PGV  | O02-C1-C2-C3    |
| 13  | U     | 101 | BCL  | C11-C10-C8-C7   |
| 20  | H     | 305 | CDL  | C71-C72-C73-C74 |
| 13  | J     | 102 | BCL  | CAA-CBA-CGA-O1A |

There are no ring outliers.

83 monomers are involved in 342 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 19  | T     | 101 | CRT  | 3       | 0            |
| 20  | D     | 104 | CDL  | 1       | 0            |
| 20  | S     | 104 | CDL  | 12      | 0            |
| 12  | M     | 411 | PGV  | 4       | 0            |
| 13  | U     | 103 | BCL  | 6       | 0            |
| 13  | 3     | 101 | BCL  | 3       | 0            |
| 19  | N     | 101 | CRT  | 4       | 0            |
| 20  | U     | 104 | CDL  | 9       | 0            |
| 13  | F     | 101 | BCL  | 4       | 0            |
| 13  | O     | 101 | BCL  | 6       | 0            |
| 12  | L     | 308 | PGV  | 5       | 0            |
| 15  | L     | 311 | UQ8  | 2       | 0            |
| 13  | D     | 103 | BCL  | 4       | 0            |
| 12  | H     | 303 | PGV  | 2       | 0            |
| 13  | I     | 101 | BCL  | 3       | 0            |
| 13  | L     | 301 | BCL  | 3       | 0            |
| 12  | 9     | 104 | PGV  | 5       | 0            |
| 19  | V     | 101 | CRT  | 3       | 0            |
| 8   | C     | 503 | HEC  | 1       | 0            |
| 13  | Q     | 101 | BCL  | 7       | 0            |
| 13  | U     | 101 | BCL  | 6       | 0            |
| 13  | 1     | 101 | BCL  | 5       | 0            |
| 13  | 5     | 103 | BCL  | 3       | 0            |
| 12  | L     | 307 | PGV  | 7       | 0            |
| 13  | 2     | 102 | BCL  | 10      | 0            |
| 19  | 4     | 101 | CRT  | 6       | 0            |
| 13  | L     | 305 | BCL  | 7       | 0            |
| 15  | L     | 304 | UQ8  | 1       | 0            |
| 13  | A     | 101 | BCL  | 5       | 0            |
| 15  | L     | 310 | UQ8  | 6       | 0            |

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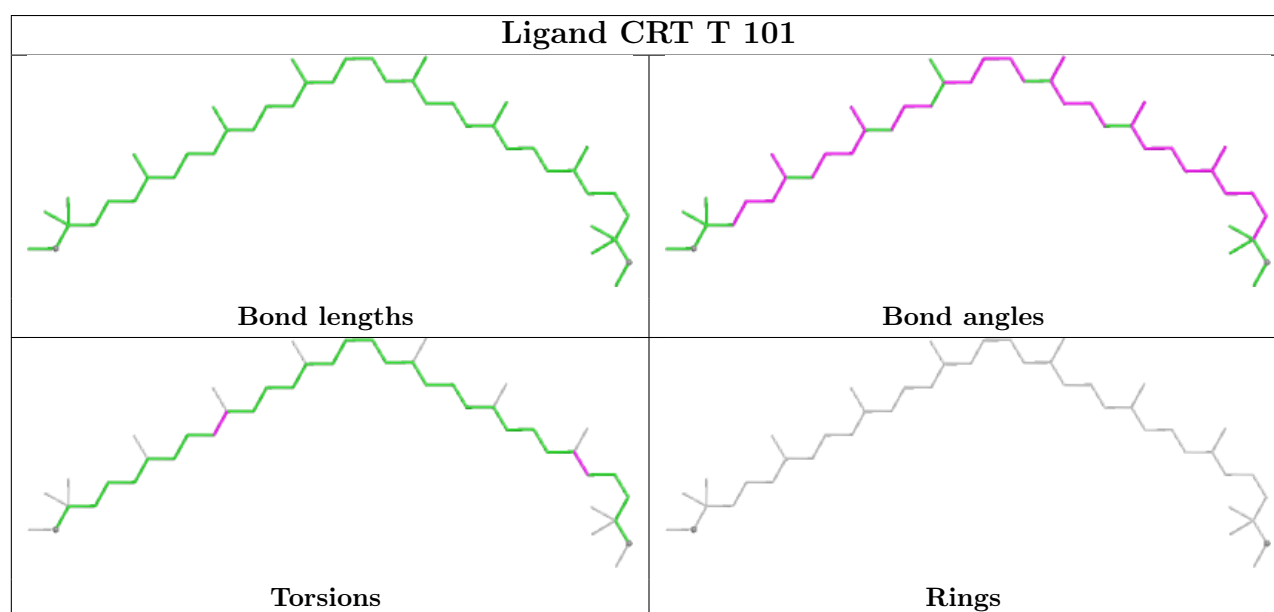
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 19  | Z     | 101 | CRT  | 5       | 0            |
| 13  | W     | 104 | BCL  | 6       | 0            |
| 10  | C     | 506 | GOL  | 1       | 0            |
| 19  | P     | 101 | CRT  | 4       | 0            |
| 13  | Y     | 103 | BCL  | 11      | 0            |
| 14  | M     | 402 | BPH  | 7       | 0            |
| 20  | D     | 105 | CDL  | 9       | 0            |
| 19  | 8     | 101 | CRT  | 5       | 0            |
| 20  | M     | 412 | CDL  | 2       | 0            |
| 12  | M     | 410 | PGV  | 4       | 0            |
| 19  | J     | 101 | CRT  | 2       | 0            |
| 19  | G     | 101 | CRT  | 5       | 0            |
| 13  | P     | 102 | BCL  | 5       | 0            |
| 13  | J     | 102 | BCL  | 3       | 0            |
| 19  | 2     | 101 | CRT  | 6       | 0            |
| 13  | K     | 103 | BCL  | 3       | 0            |
| 19  | M     | 405 | CRT  | 7       | 0            |
| 13  | W     | 101 | BCL  | 5       | 0            |
| 13  | 7     | 101 | BCL  | 5       | 0            |
| 15  | L     | 309 | UQ8  | 10      | 0            |
| 13  | K     | 101 | BCL  | 5       | 0            |
| 8   | C     | 502 | HEC  | 2       | 0            |
| 22  | H     | 304 | LMT  | 8       | 0            |
| 13  | 4     | 102 | BCL  | 6       | 0            |
| 12  | 1     | 105 | PGV  | 1       | 0            |
| 19  | 0     | 101 | CRT  | 5       | 0            |
| 20  | O     | 104 | CDL  | 13      | 0            |
| 13  | 5     | 101 | BCL  | 3       | 0            |
| 20  | M     | 406 | CDL  | 5       | 0            |
| 21  | K     | 104 | PEF  | 2       | 0            |
| 13  | F     | 103 | BCL  | 7       | 0            |
| 13  | S     | 101 | BCL  | 6       | 0            |
| 13  | Q     | 103 | BCL  | 2       | 0            |
| 13  | L     | 302 | BCL  | 2       | 0            |
| 13  | 9     | 103 | BCL  | 4       | 0            |
| 20  | H     | 305 | CDL  | 6       | 0            |
| 12  | D     | 106 | PGV  | 2       | 0            |
| 19  | A     | 104 | CRT  | 8       | 0            |
| 21  | 1     | 103 | PEF  | 2       | 0            |
| 13  | Y     | 101 | BCL  | 5       | 0            |
| 13  | 7     | 103 | BCL  | 5       | 0            |
| 8   | C     | 504 | HEC  | 2       | 0            |

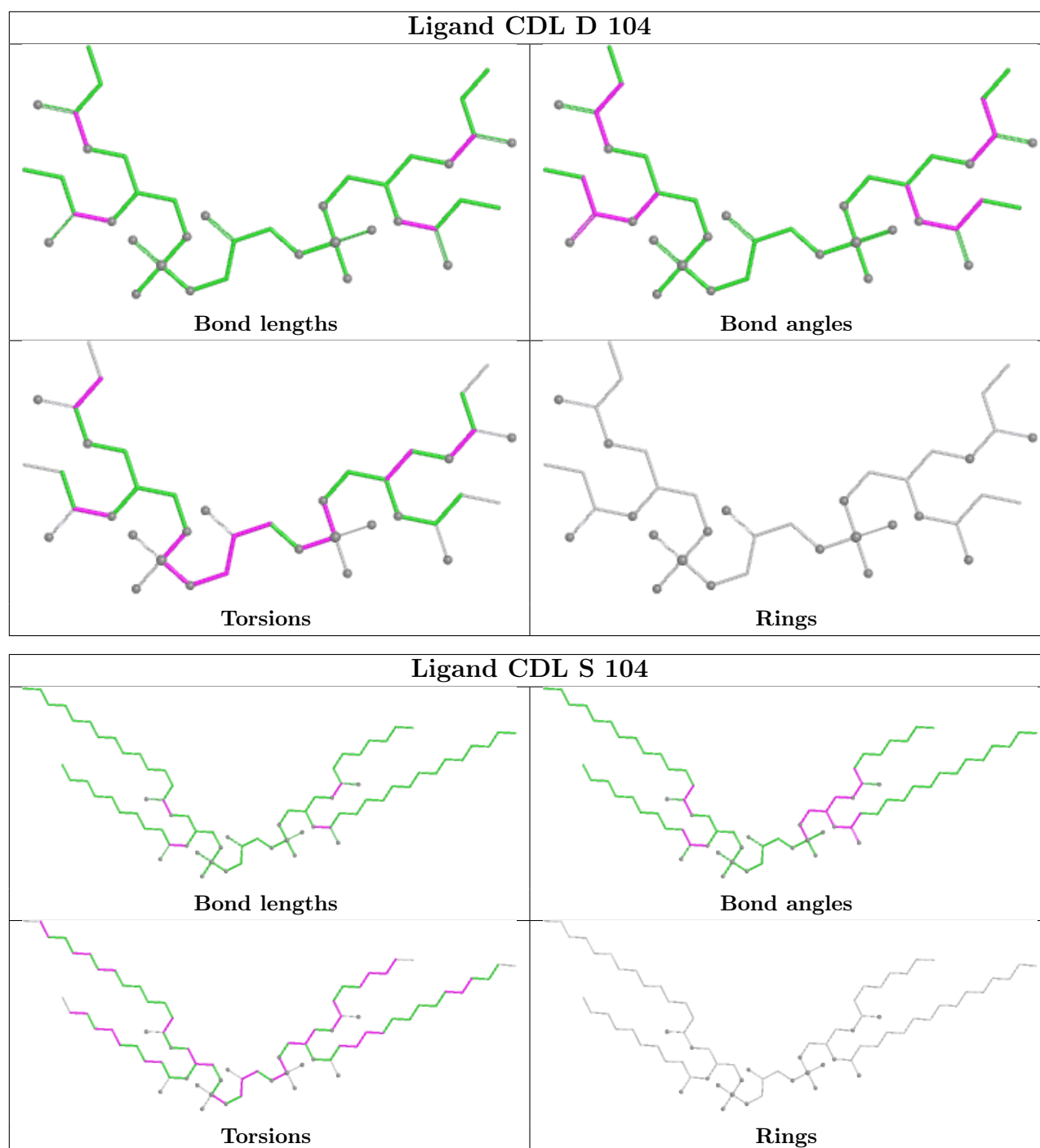
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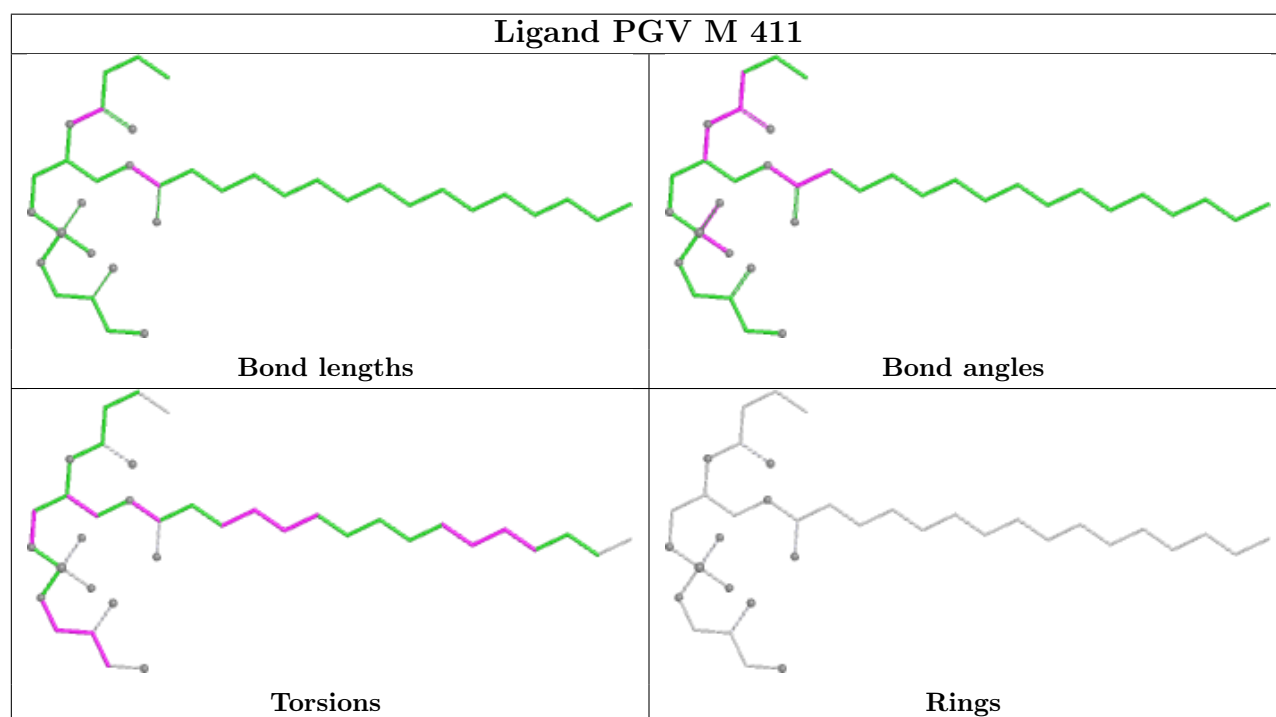
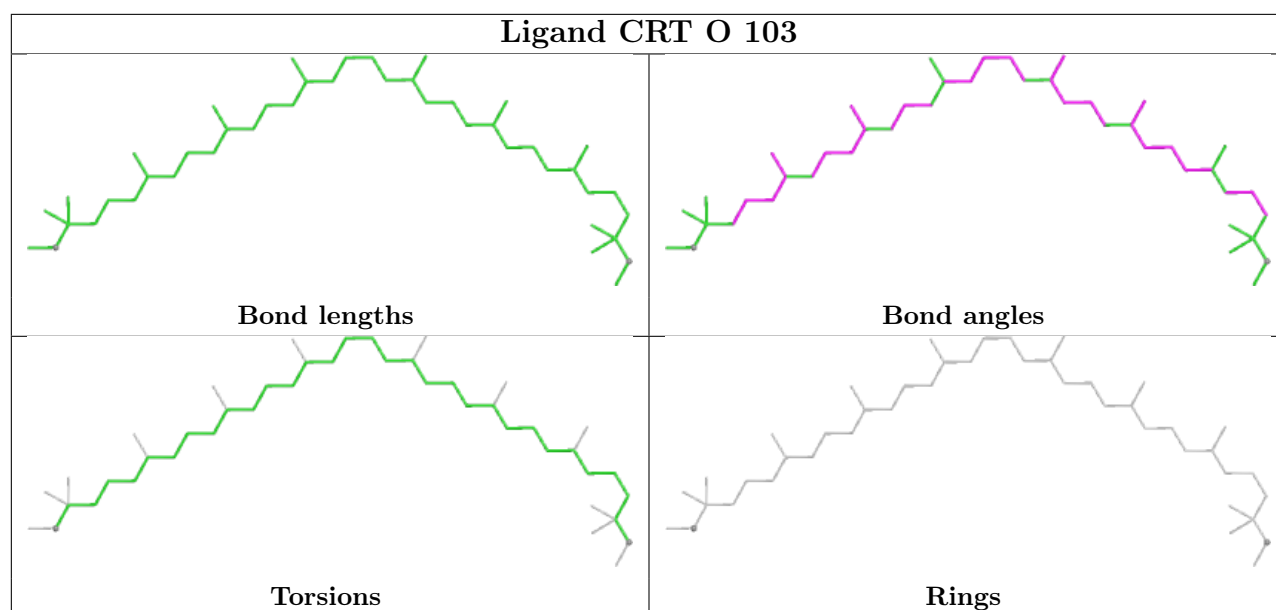
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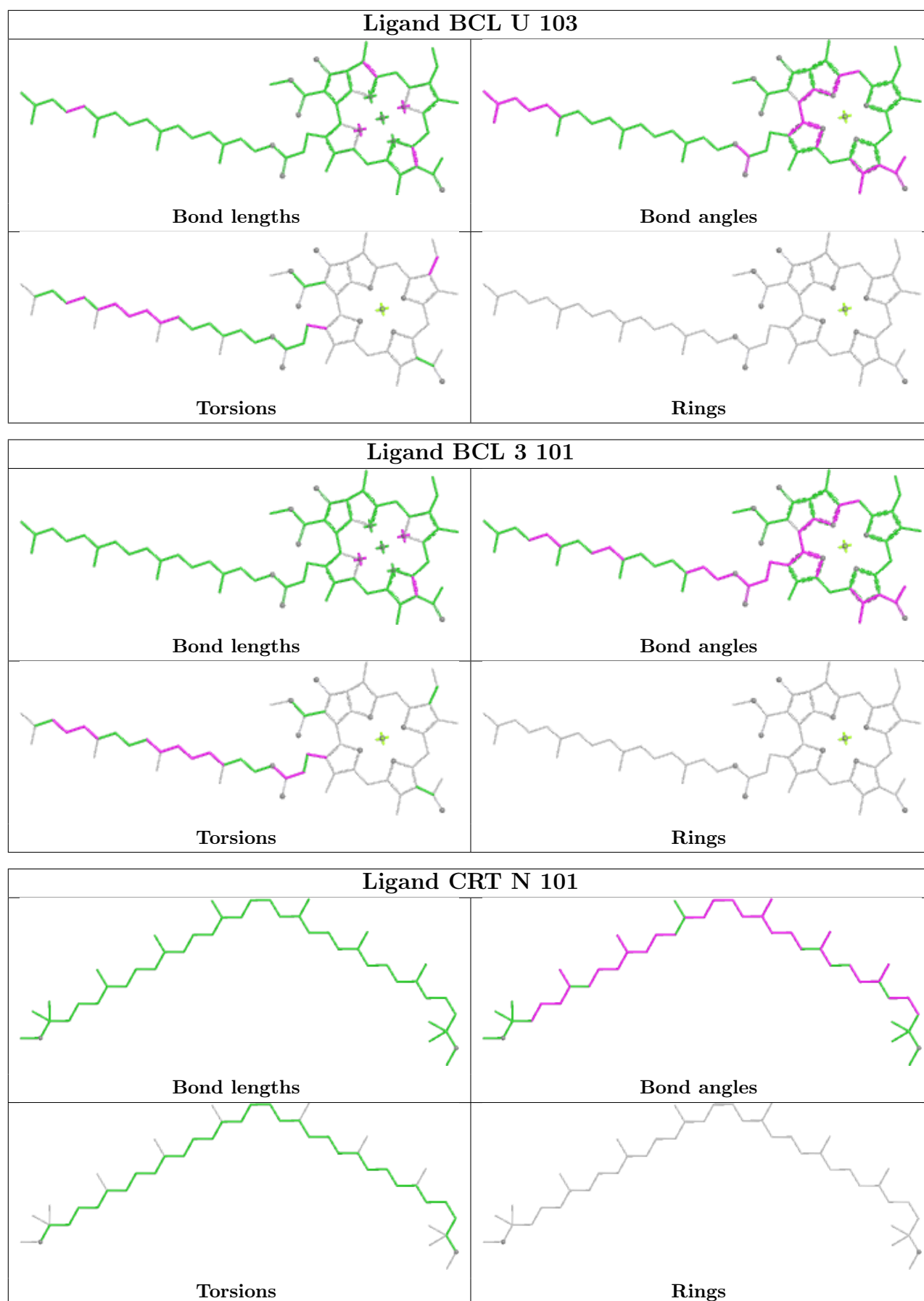
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | 3     | 105 | PGV  | 6       | 0            |
| 19  | W     | 102 | CRT  | 1       | 0            |
| 19  | B     | 101 | CRT  | 6       | 0            |
| 15  | M     | 413 | UQ8  | 1       | 0            |
| 13  | A     | 103 | BCL  | 4       | 0            |
| 13  | S     | 103 | BCL  | 4       | 0            |
| 13  | 9     | 101 | BCL  | 4       | 0            |
| 20  | Y     | 104 | CDL  | 3       | 0            |
| 19  | 3     | 103 | CRT  | 2       | 0            |
| 18  | M     | 404 | MQ8  | 5       | 0            |
| 14  | L     | 303 | BPH  | 4       | 0            |

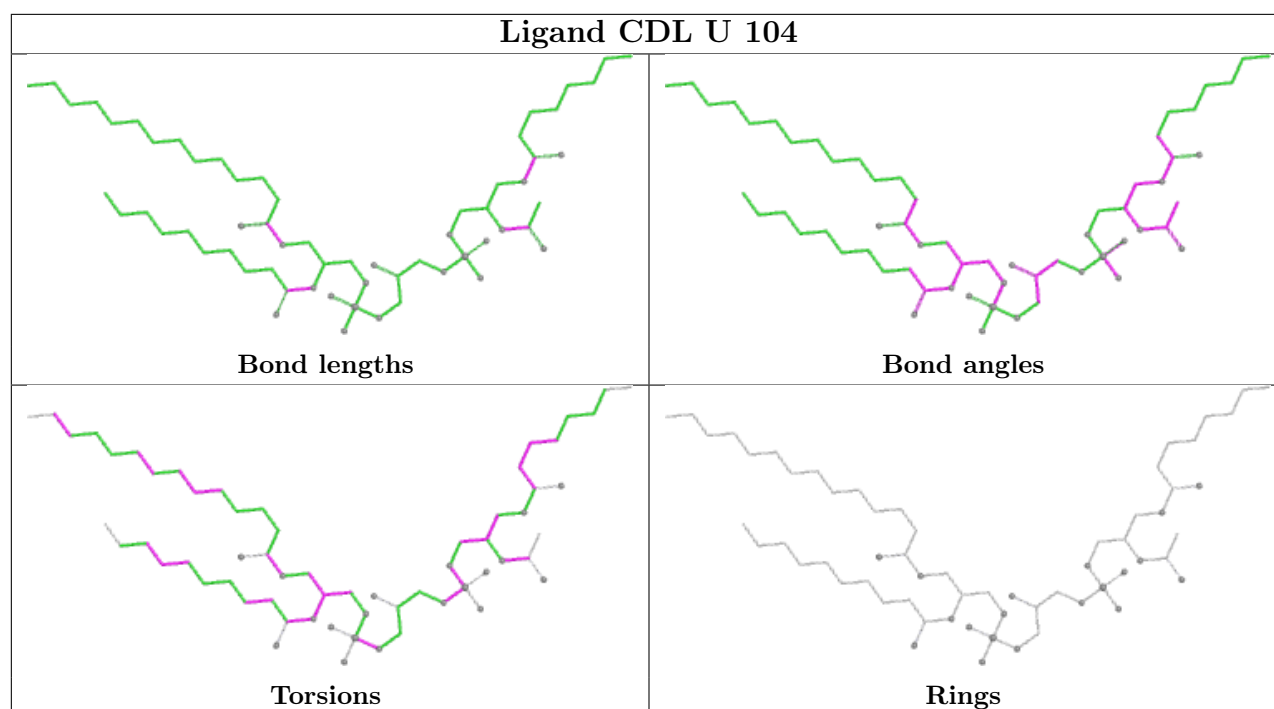
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

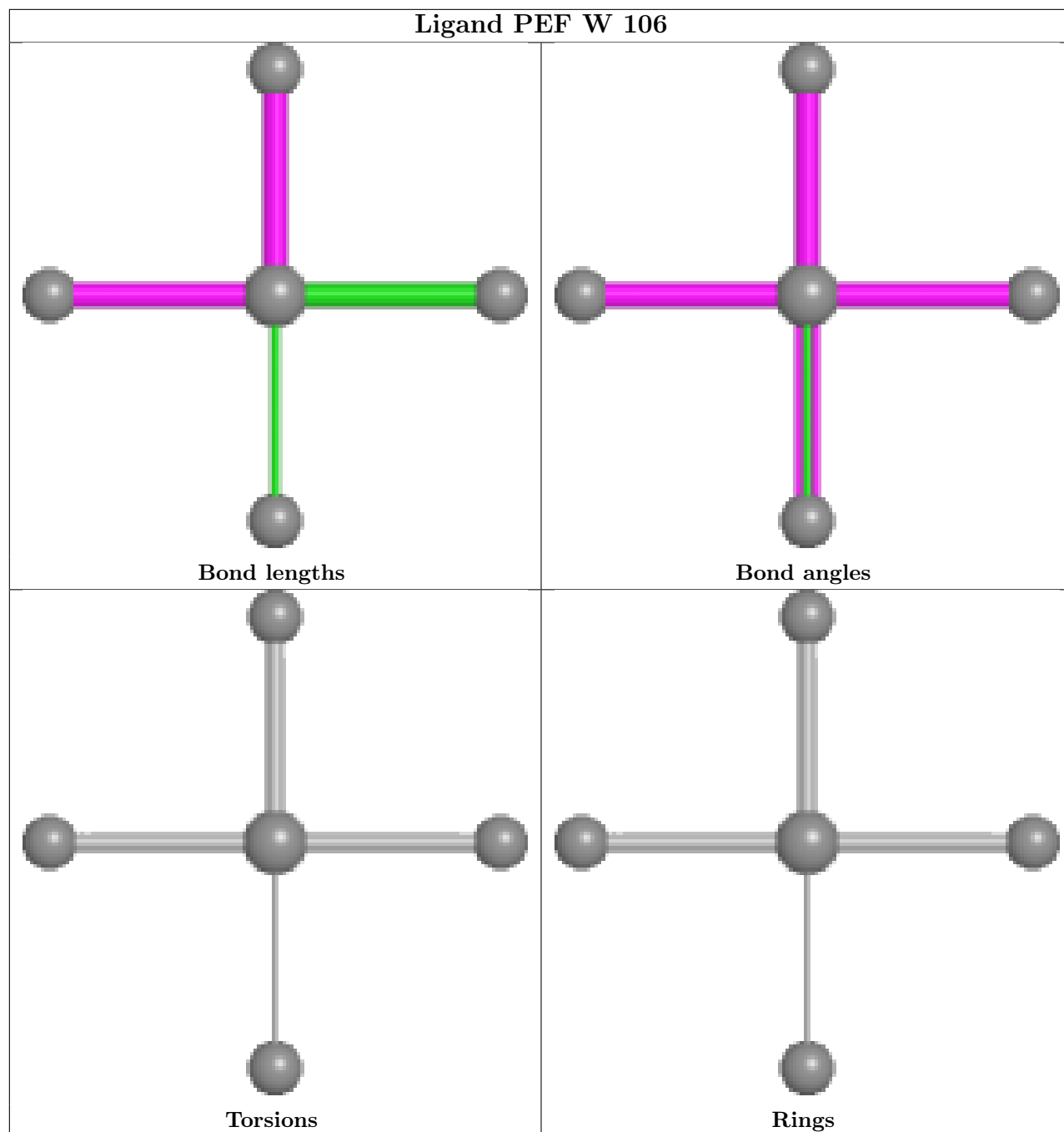


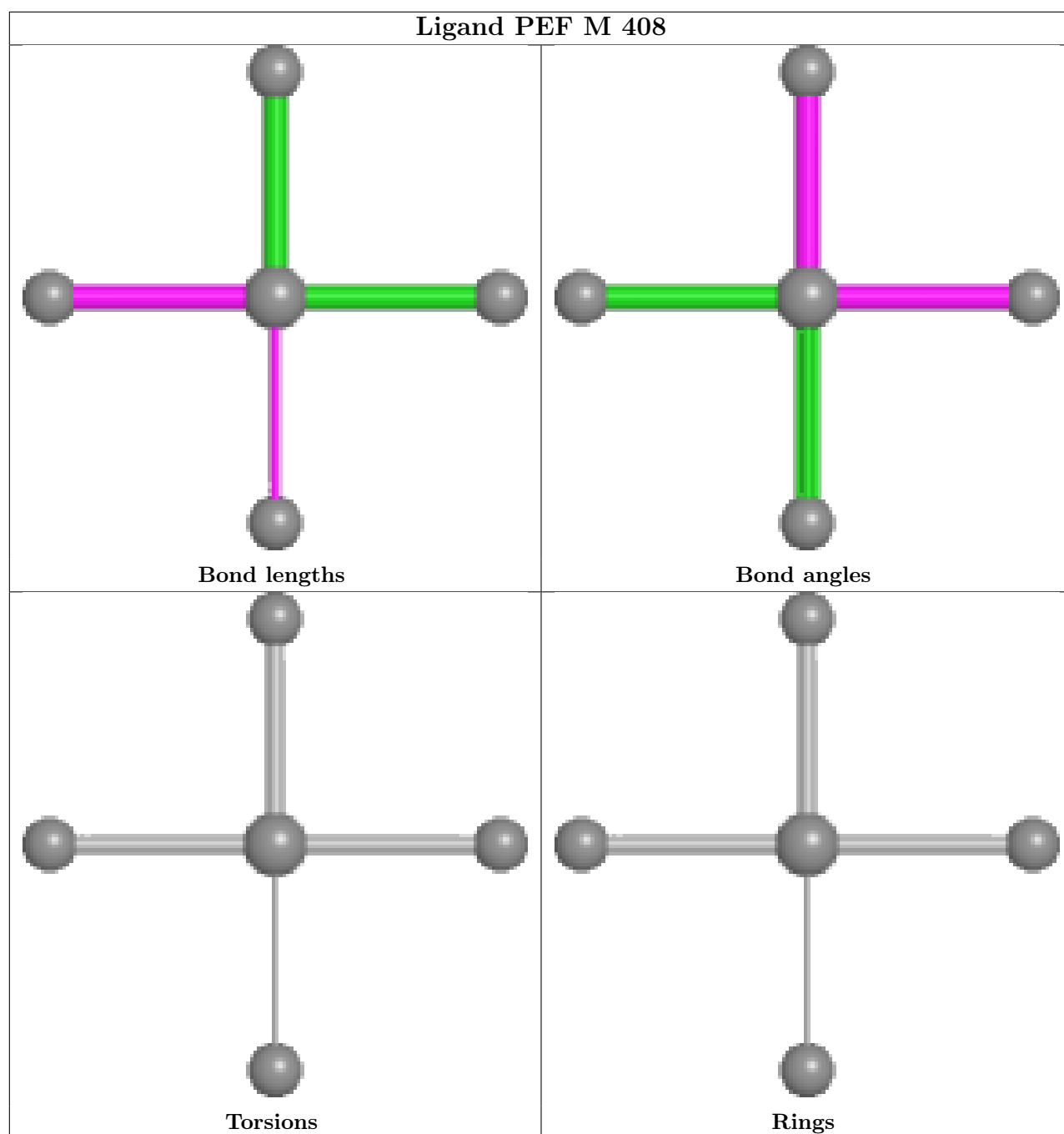


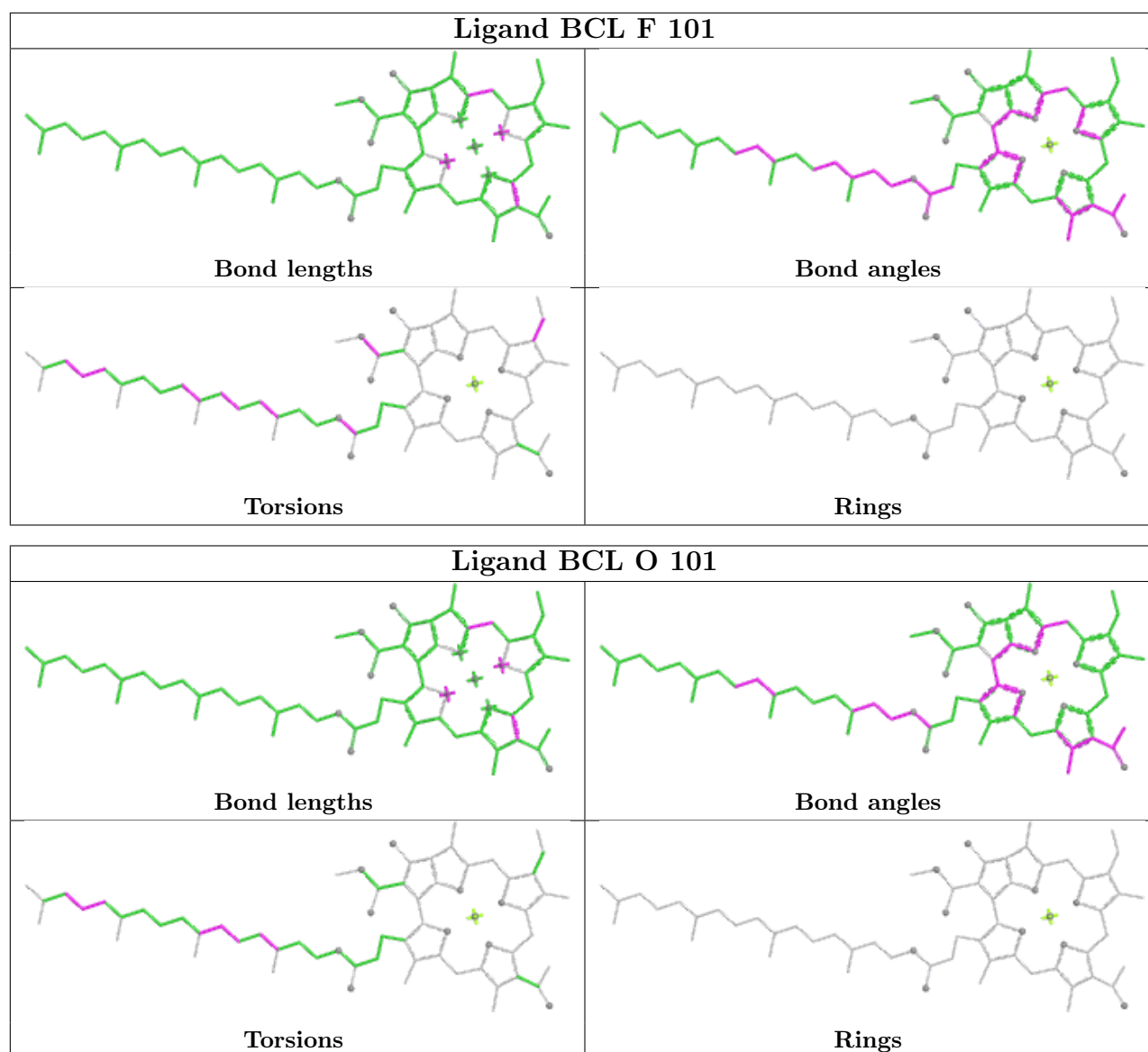




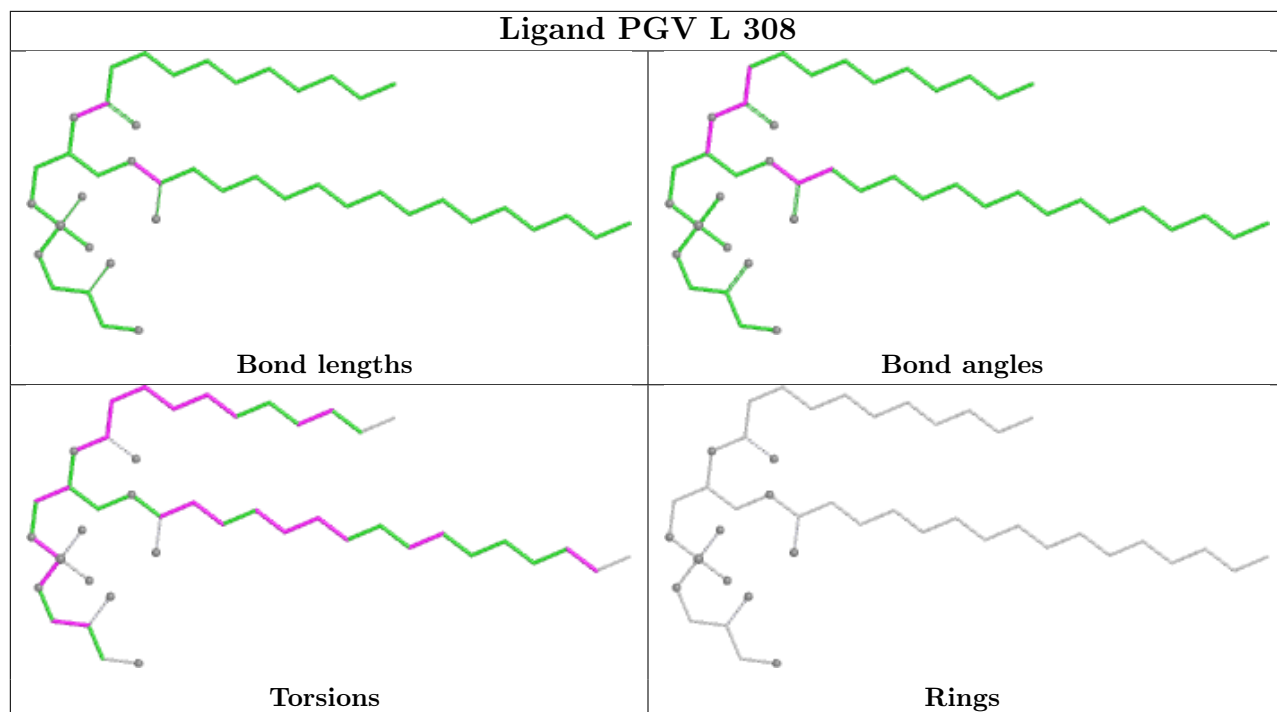




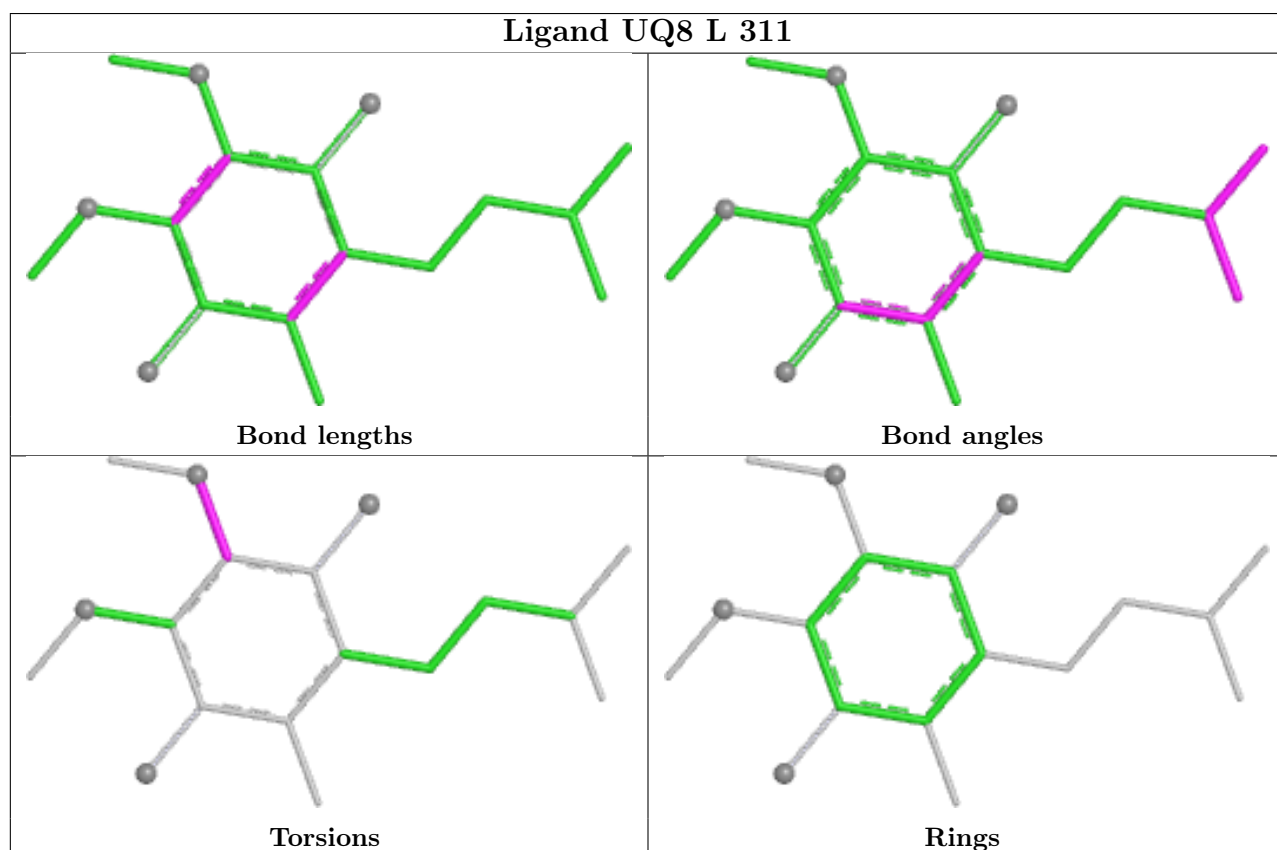


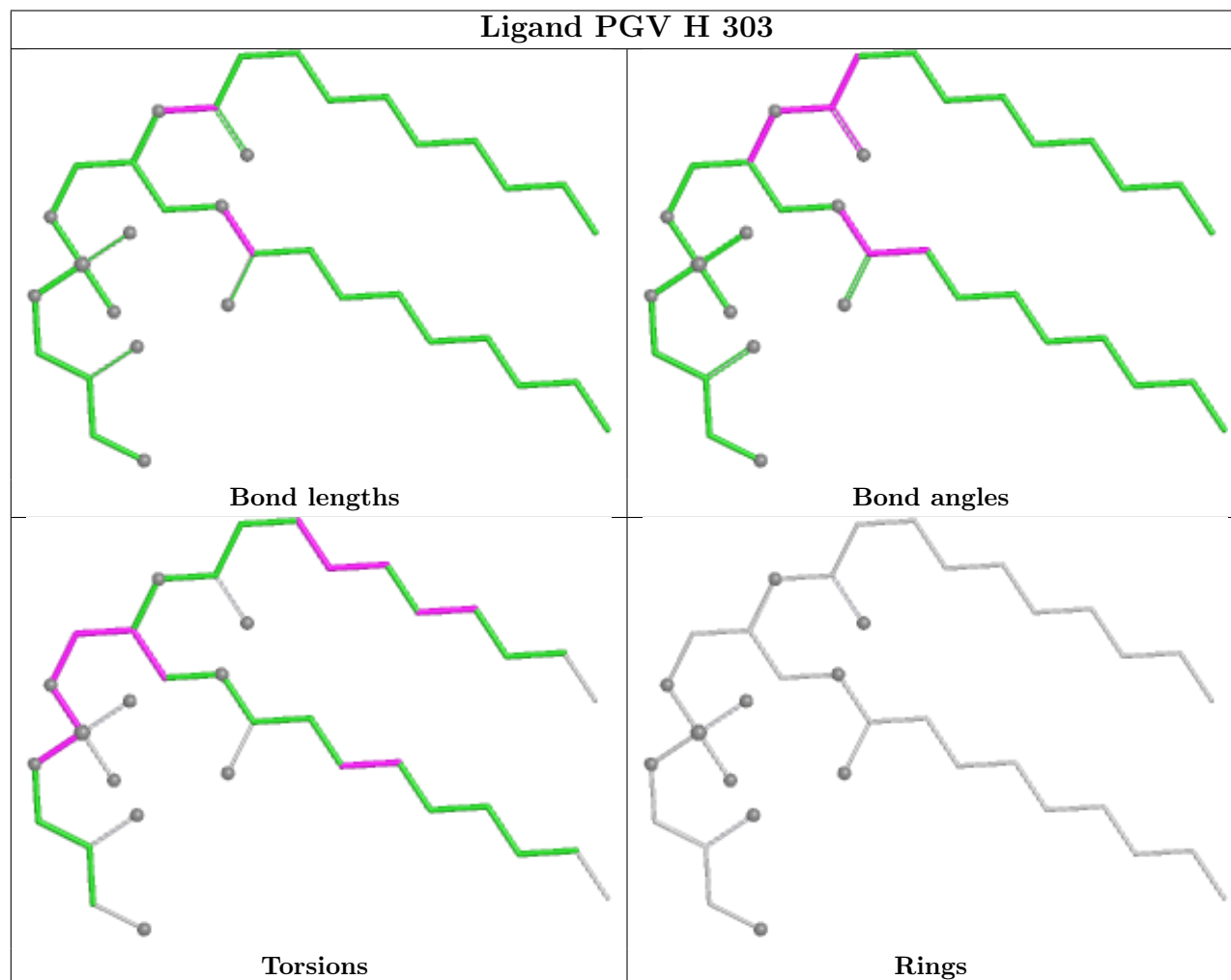
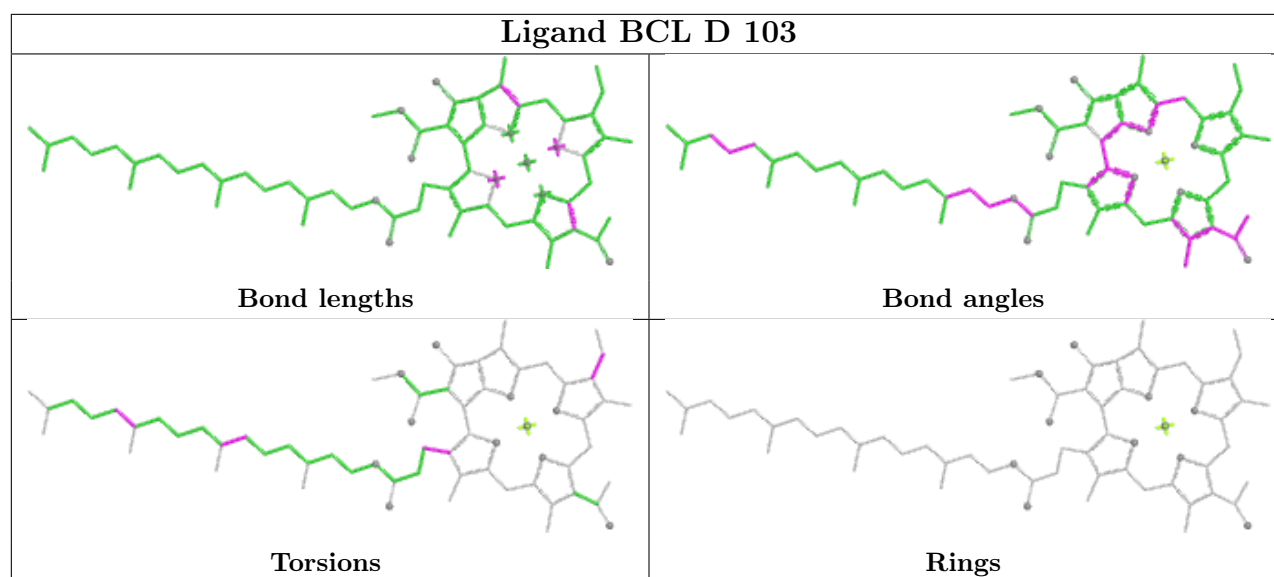


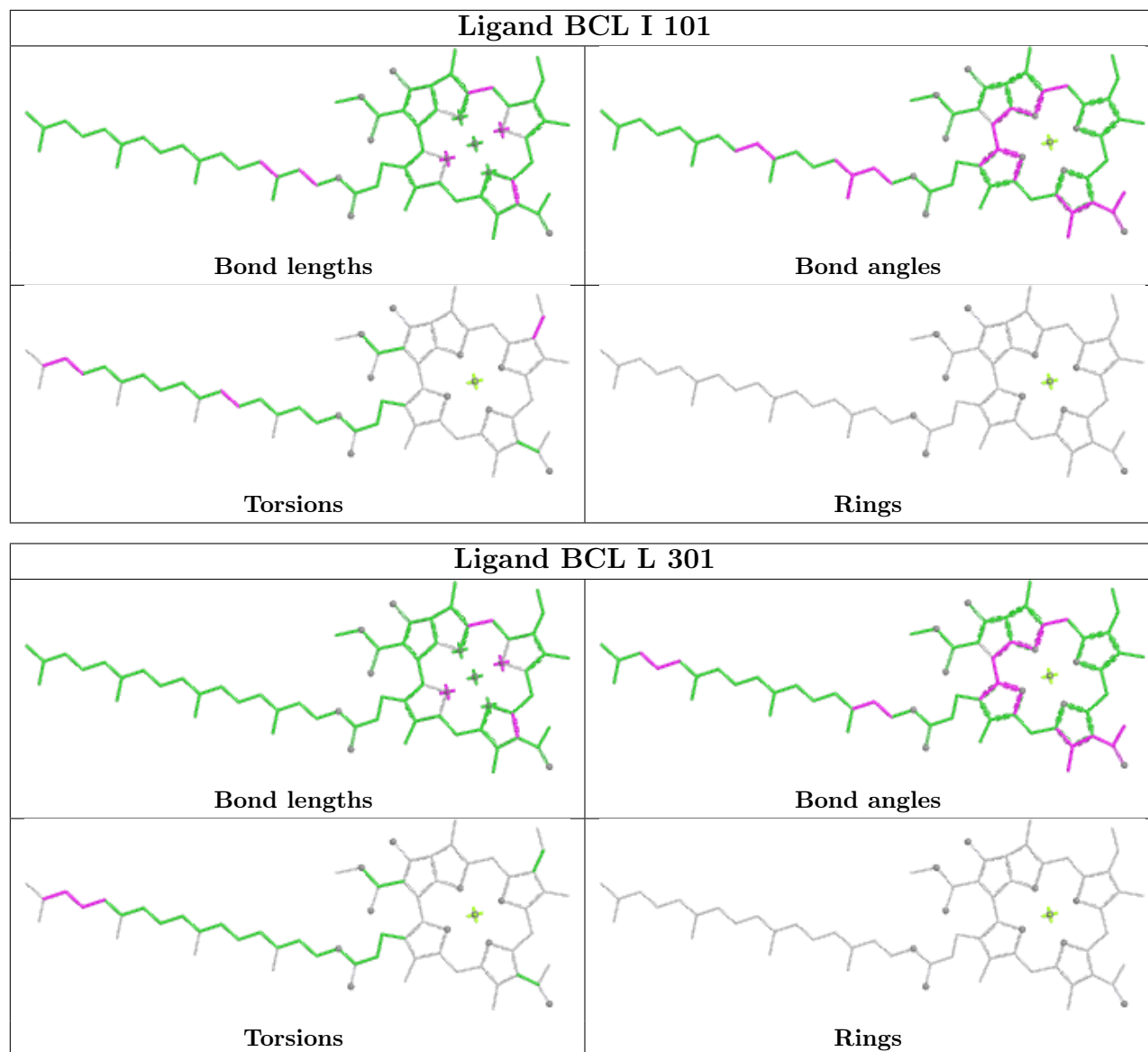
## Ligand PGV L 308



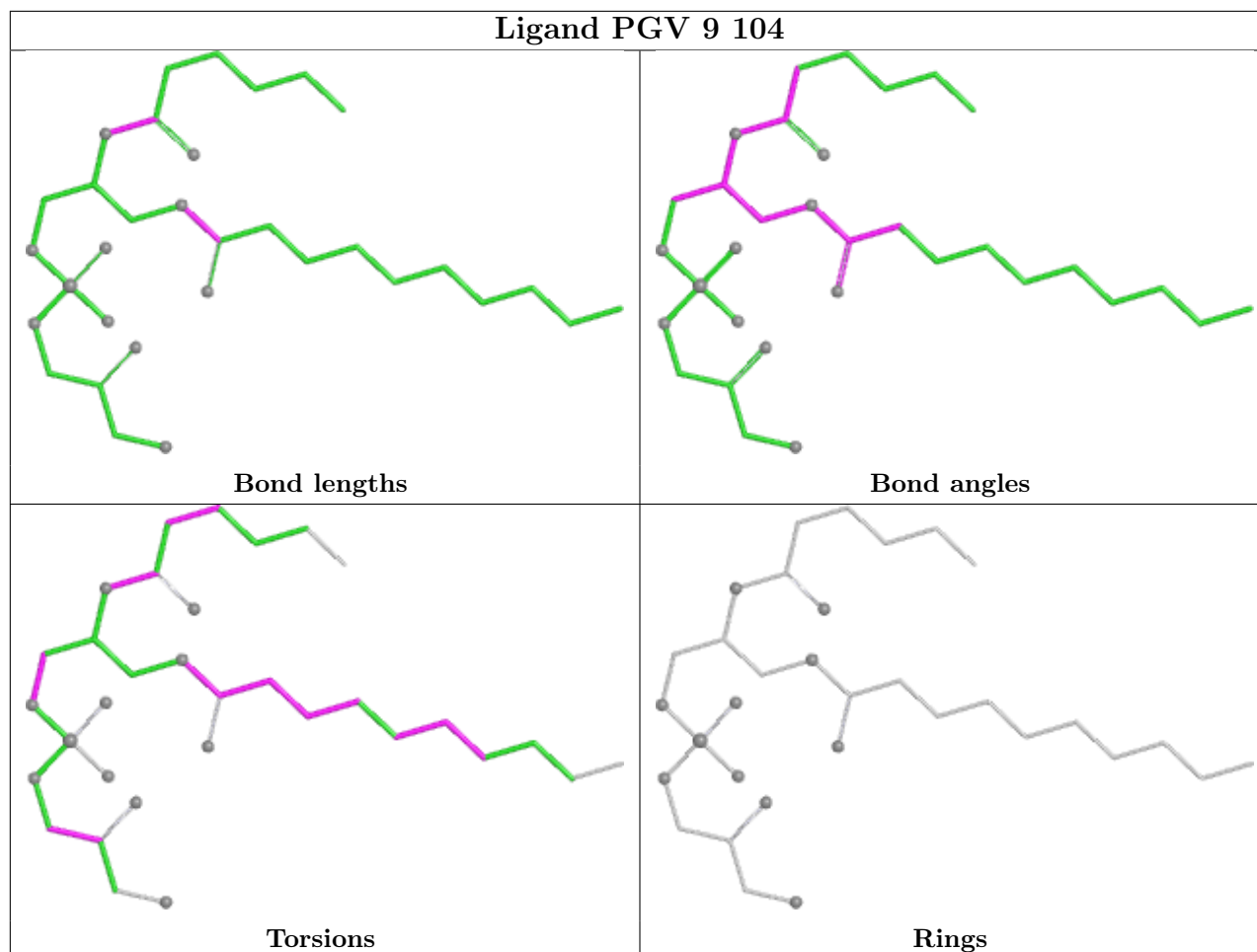
## Ligand UQ8 L 311



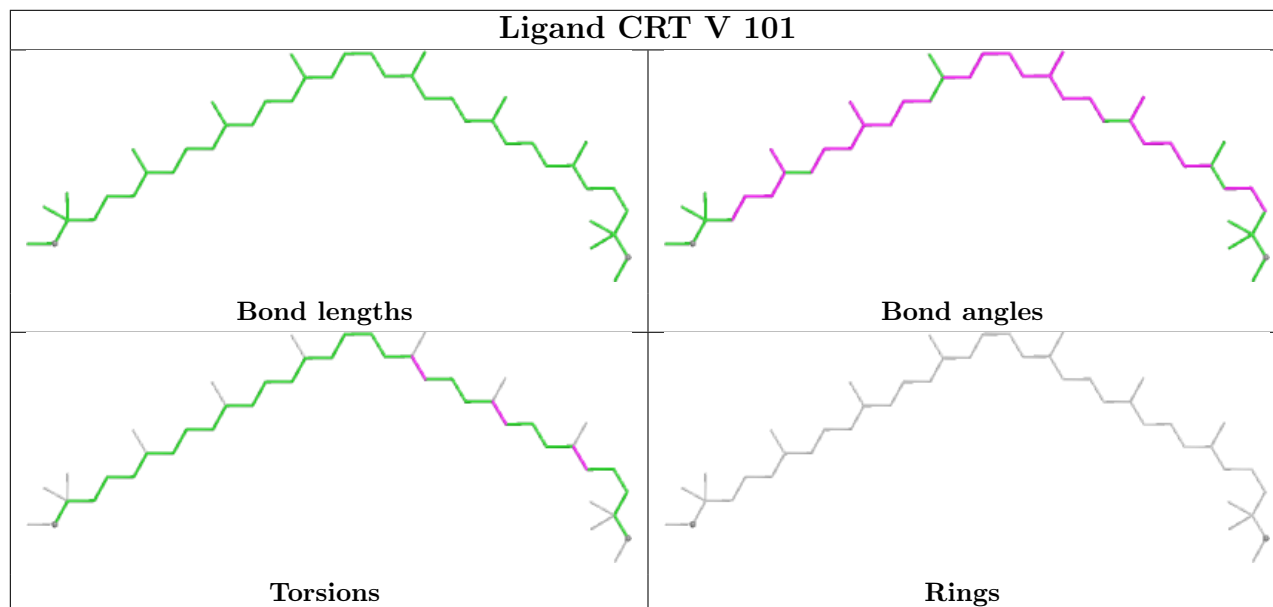




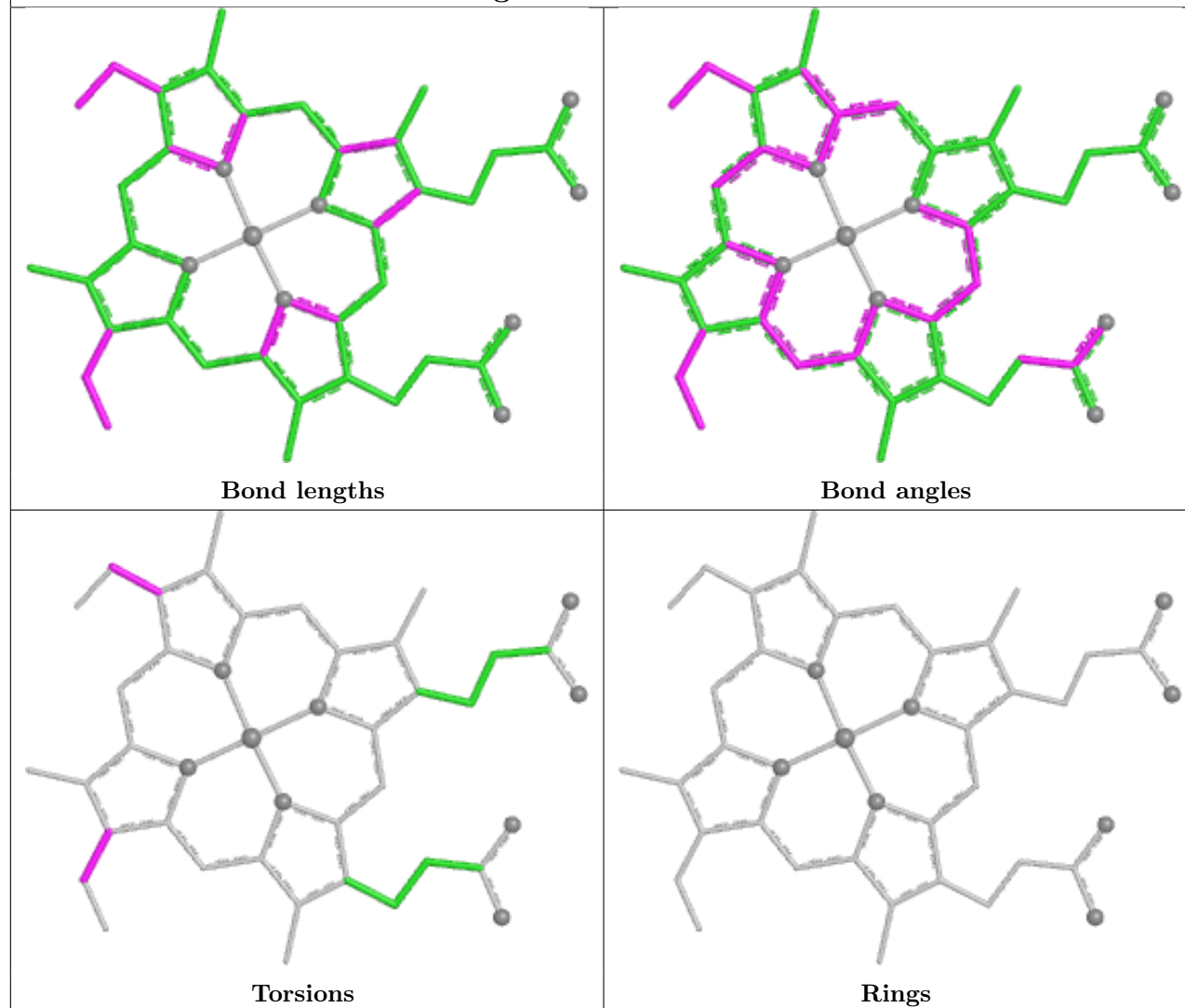
## Ligand PGV 9 104



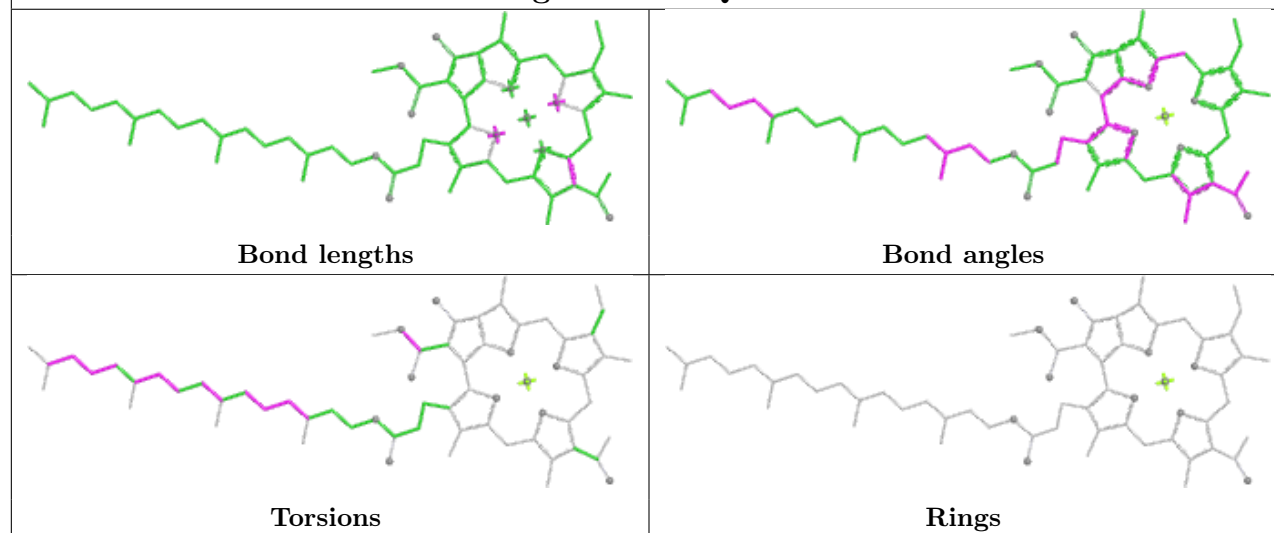
## Ligand CRT V 101

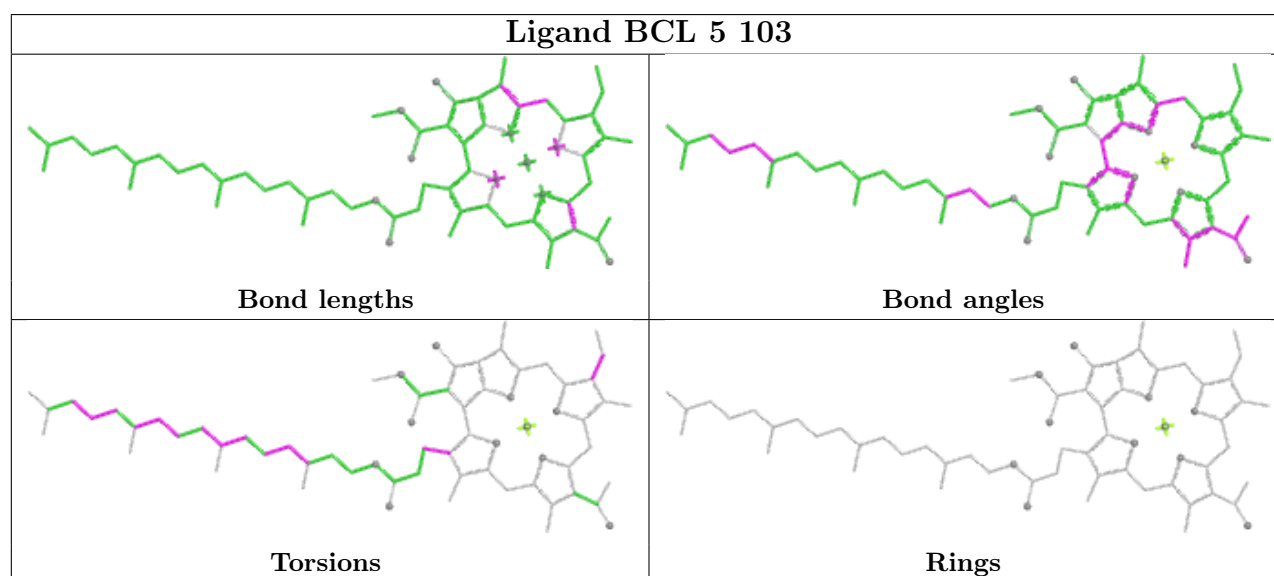
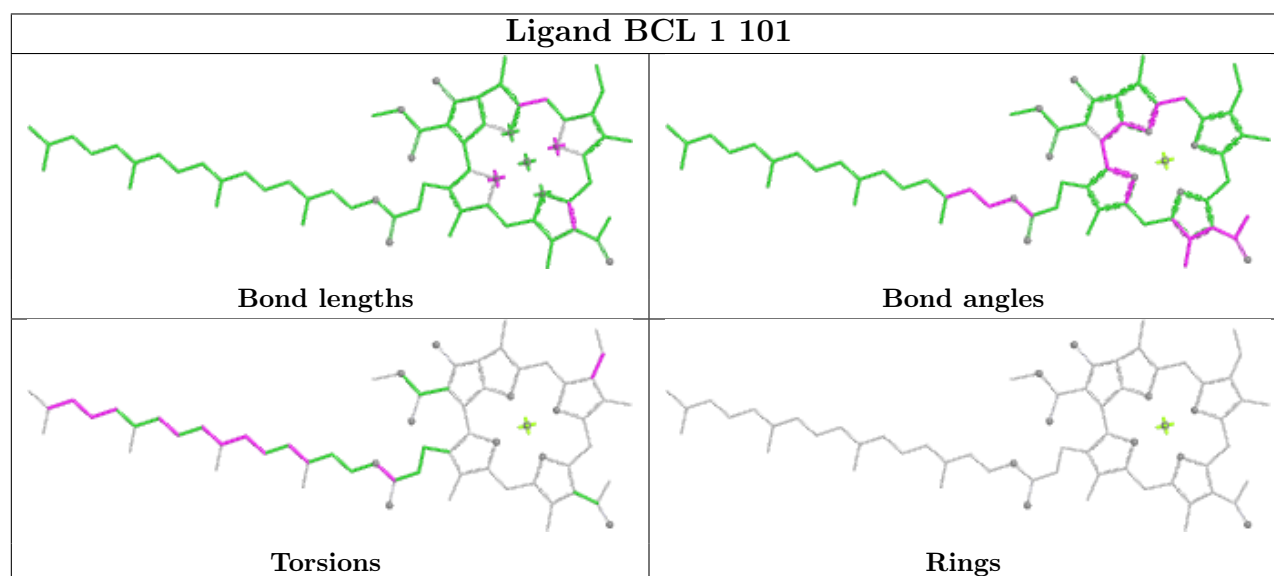
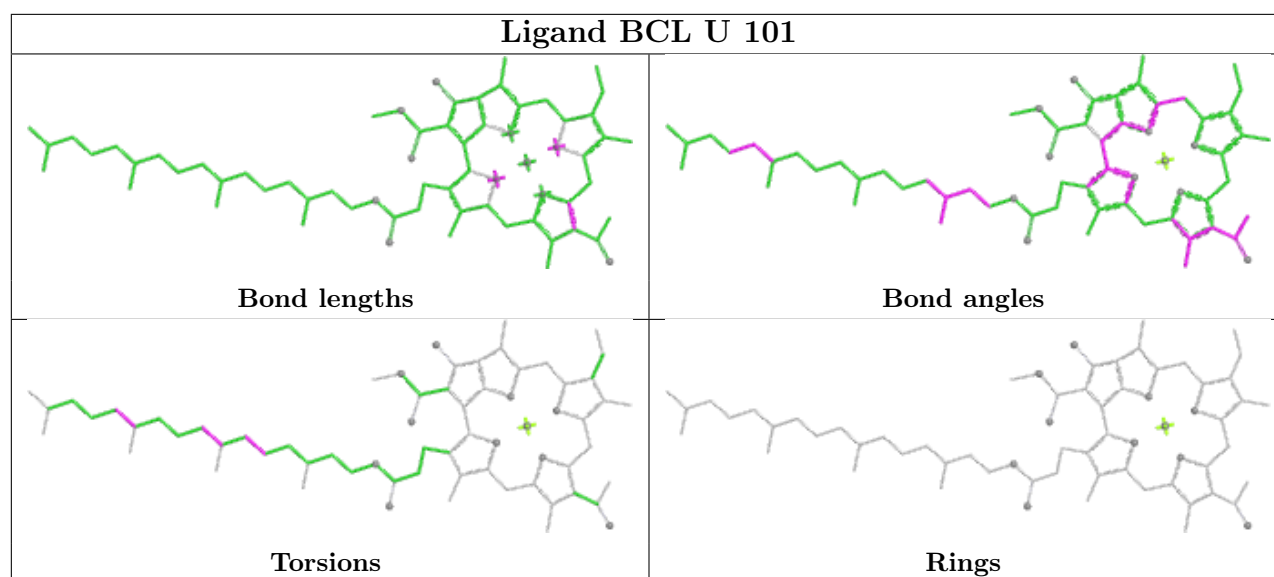


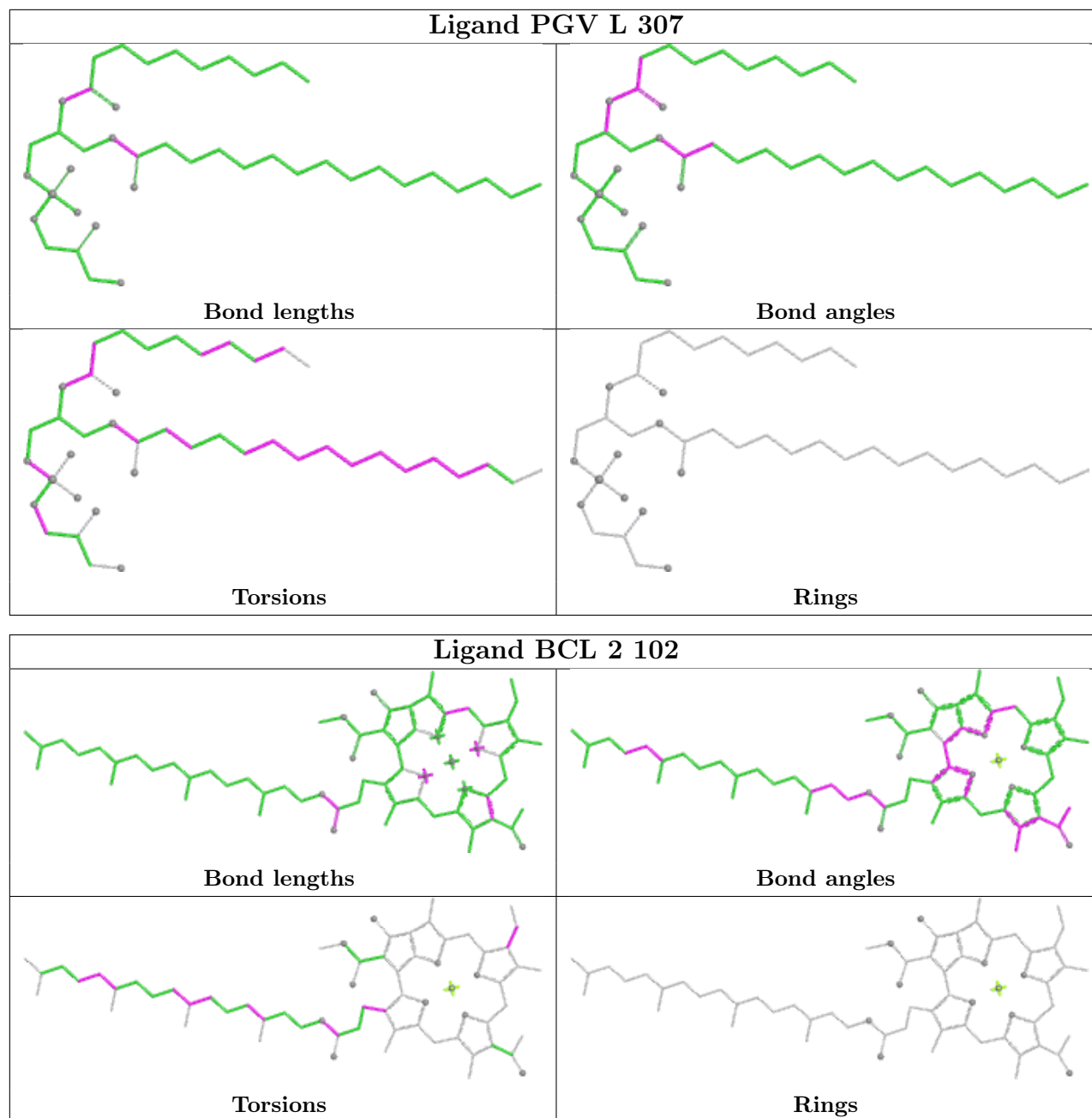
## Ligand HEC C 503

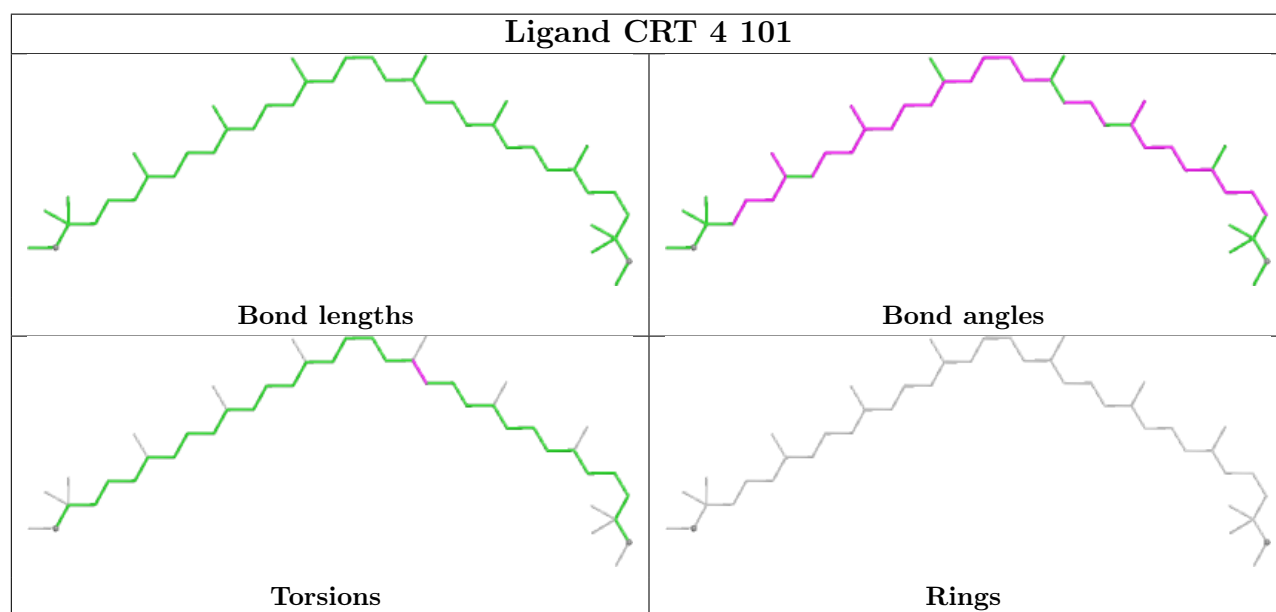
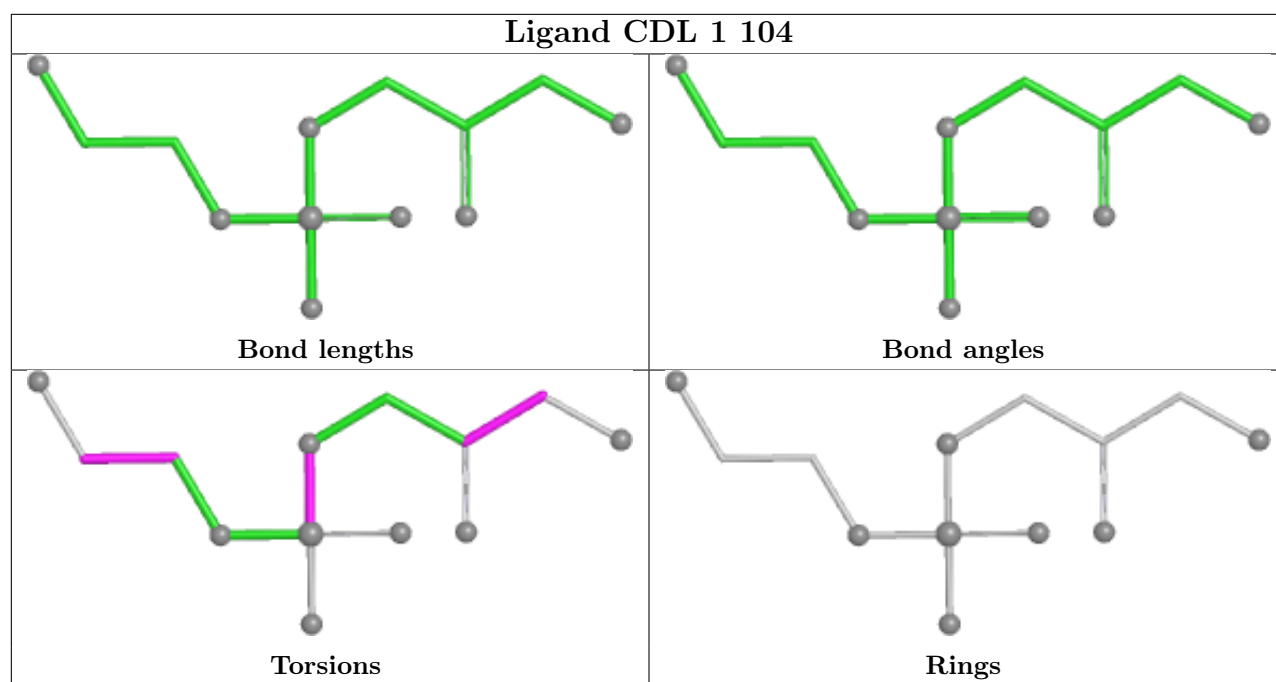


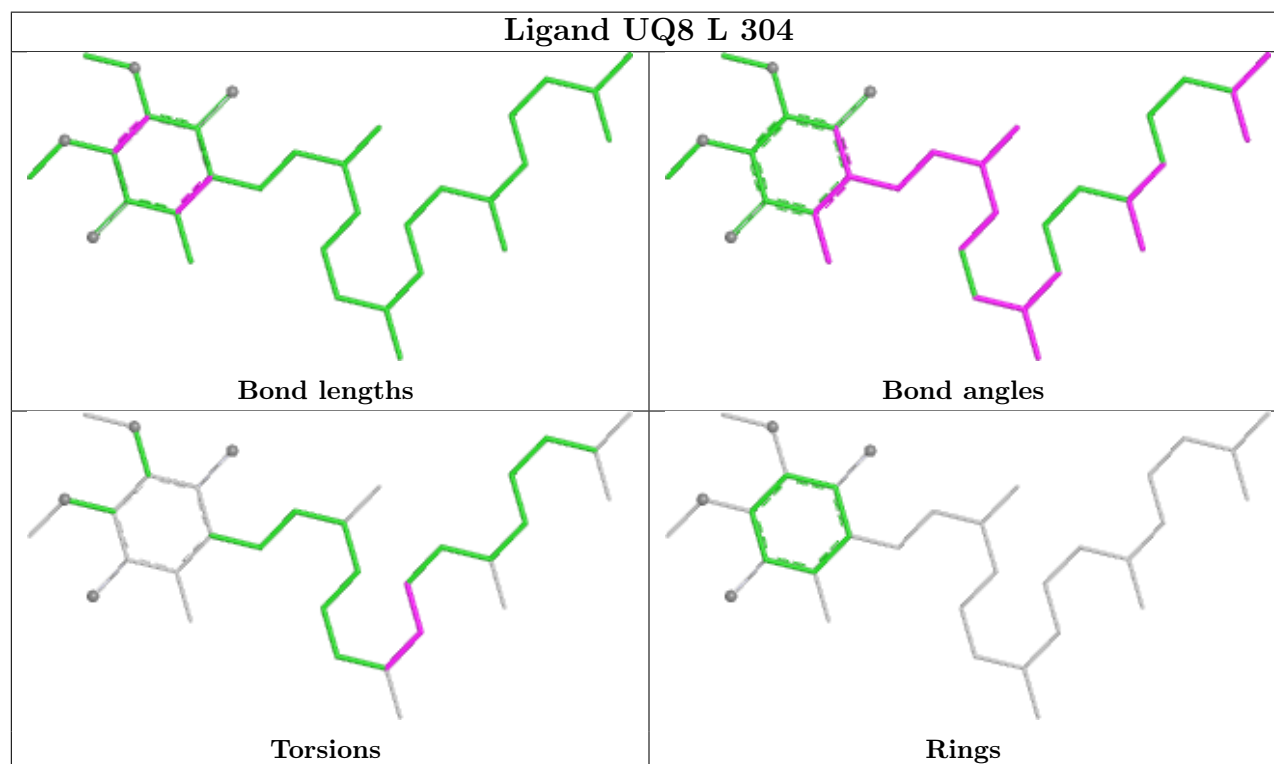
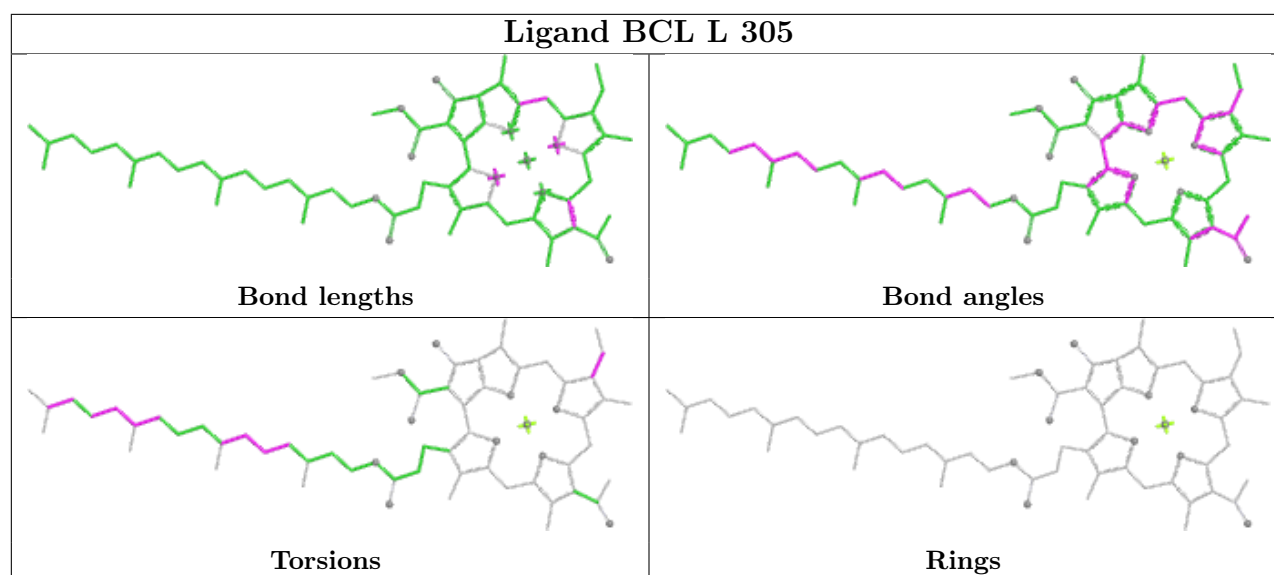
## Ligand BCL Q 101

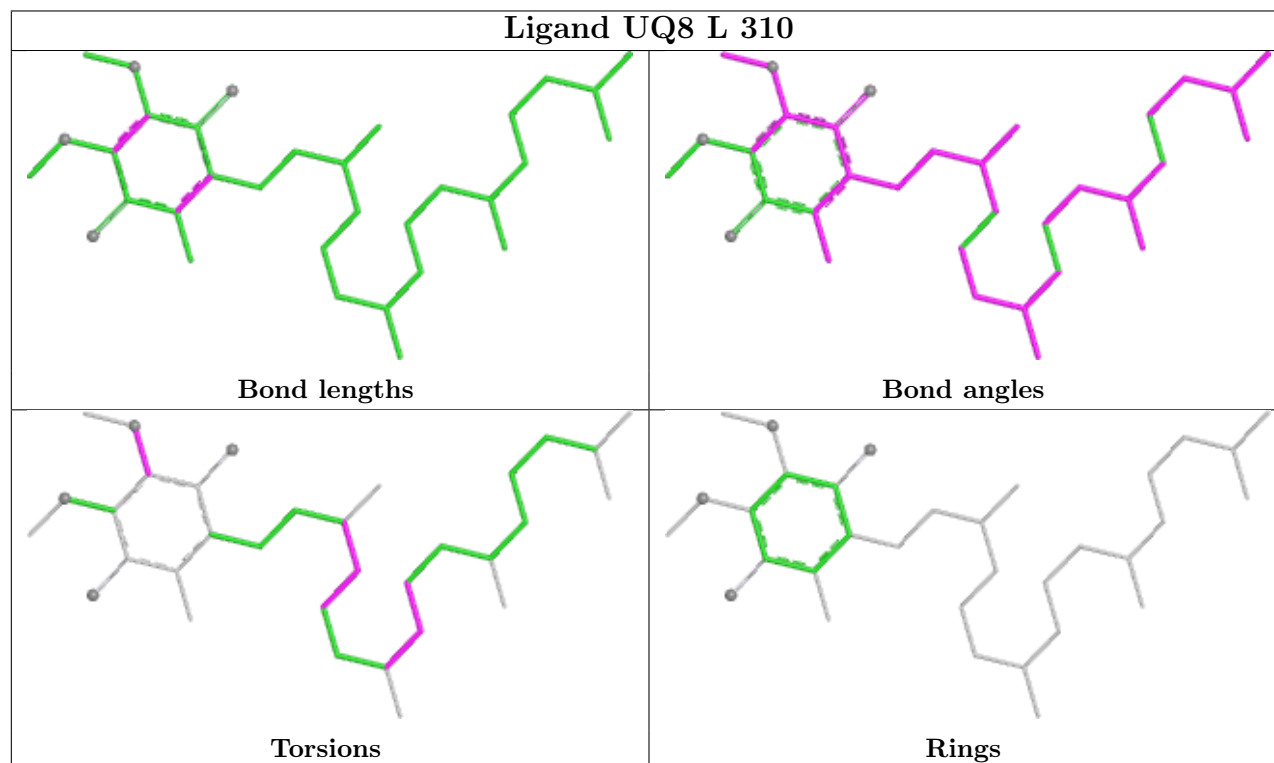
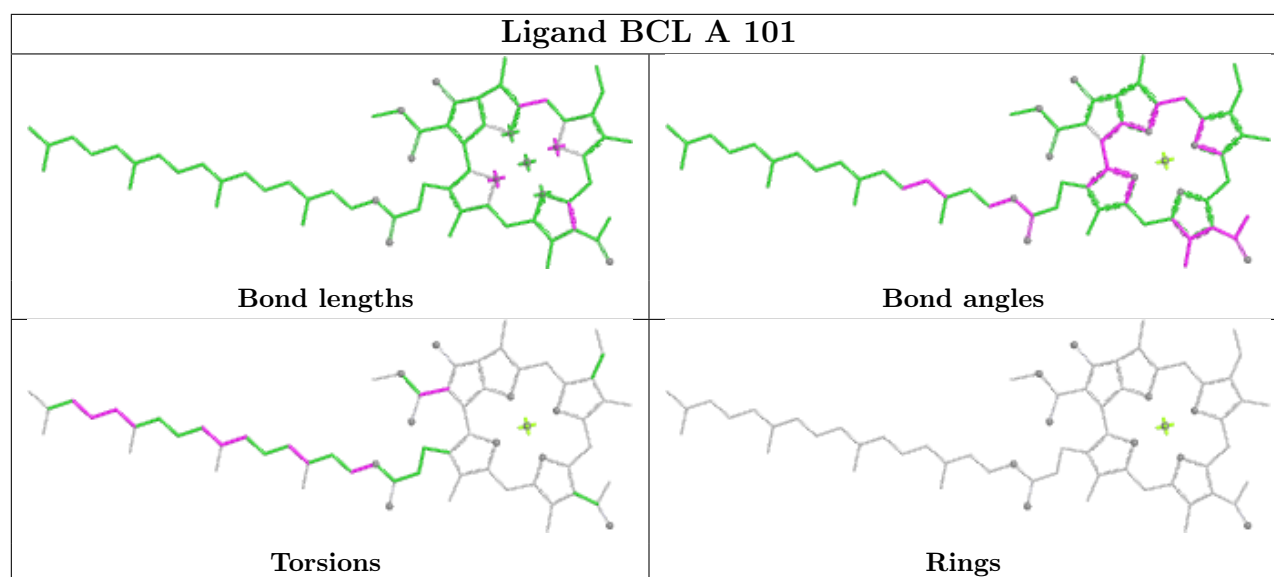


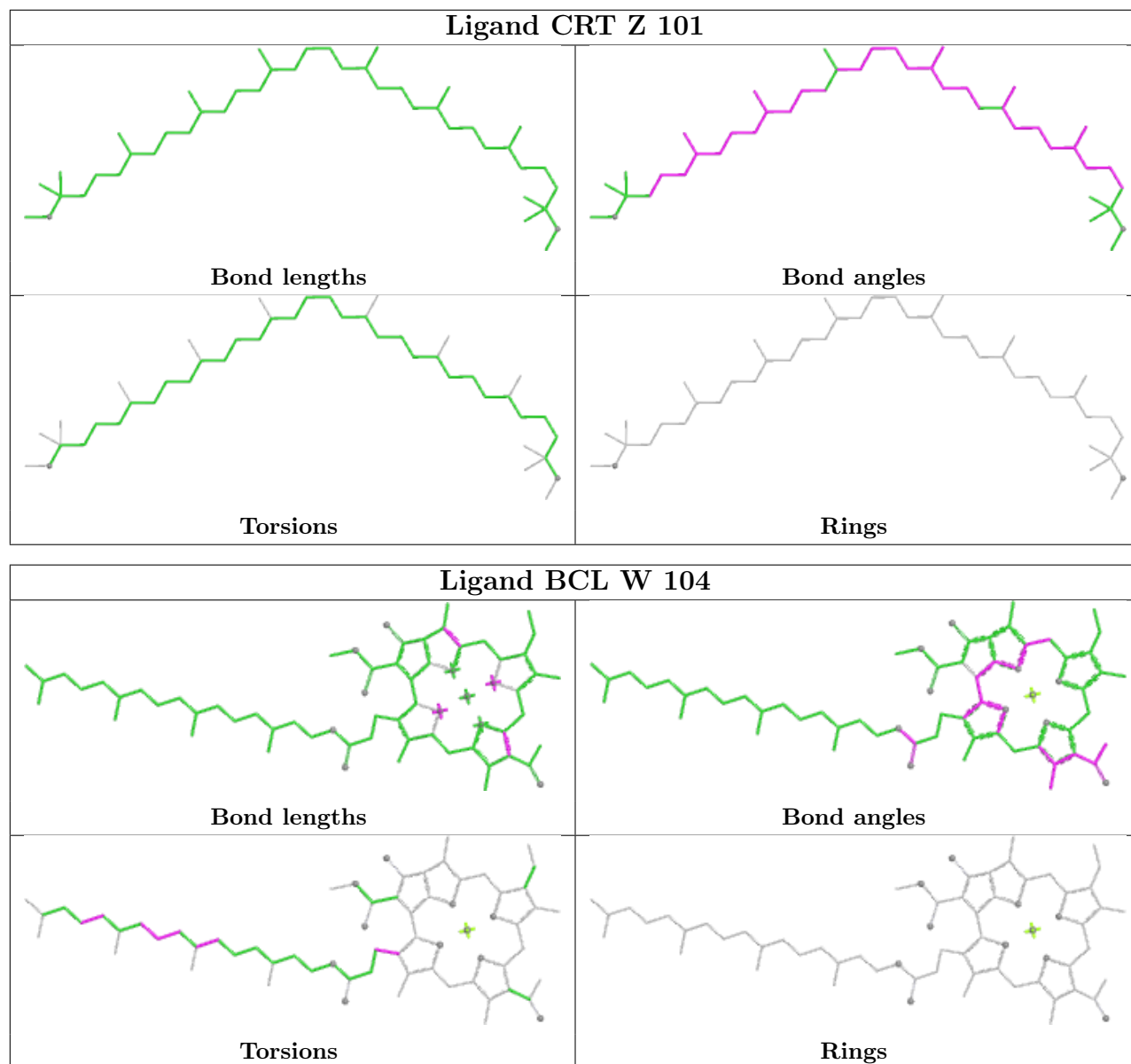


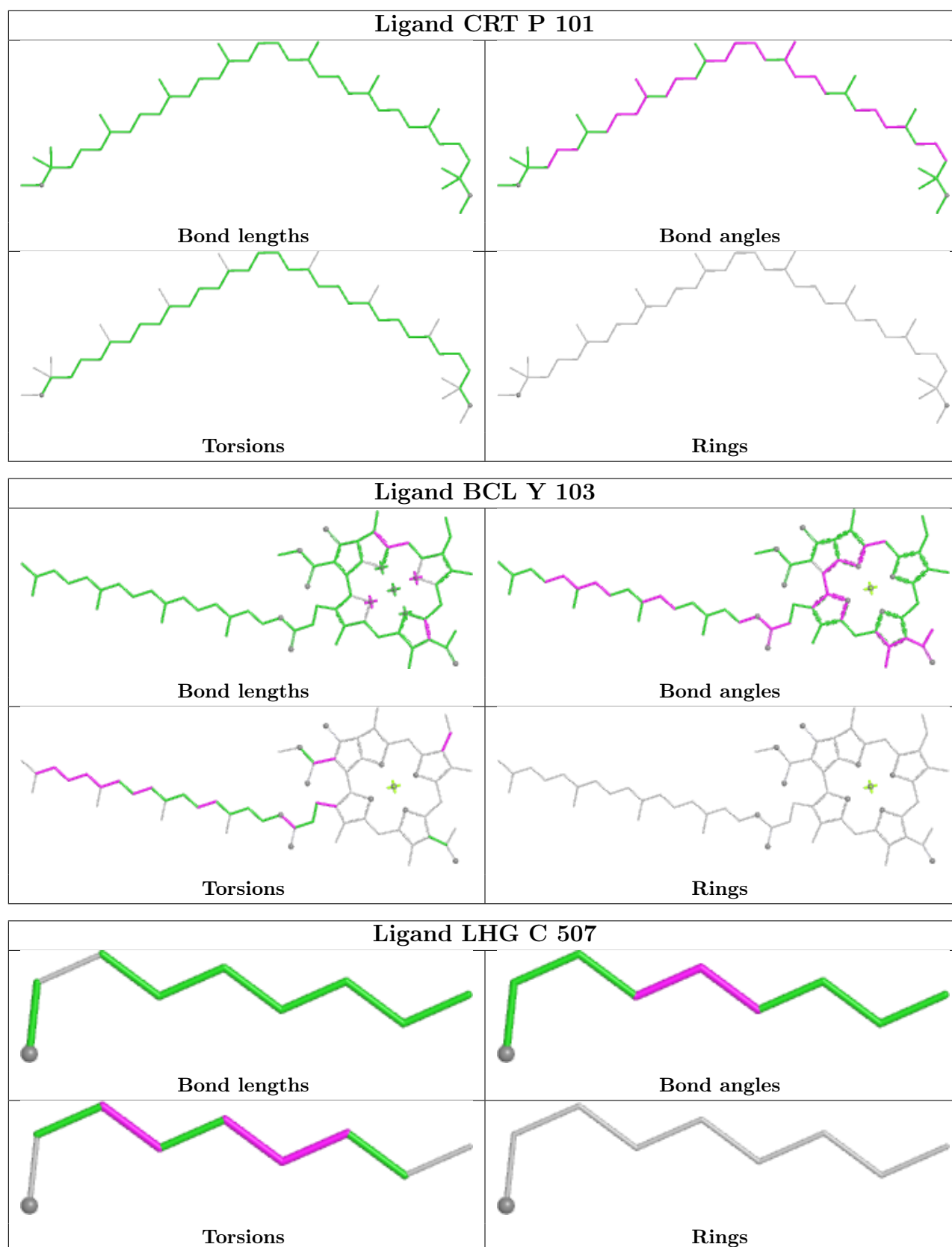


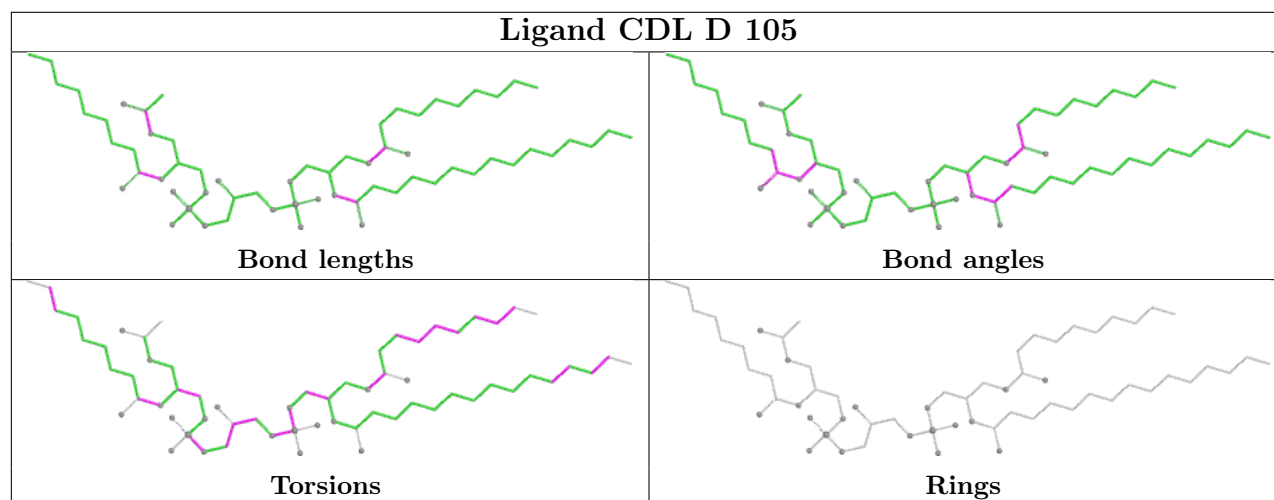
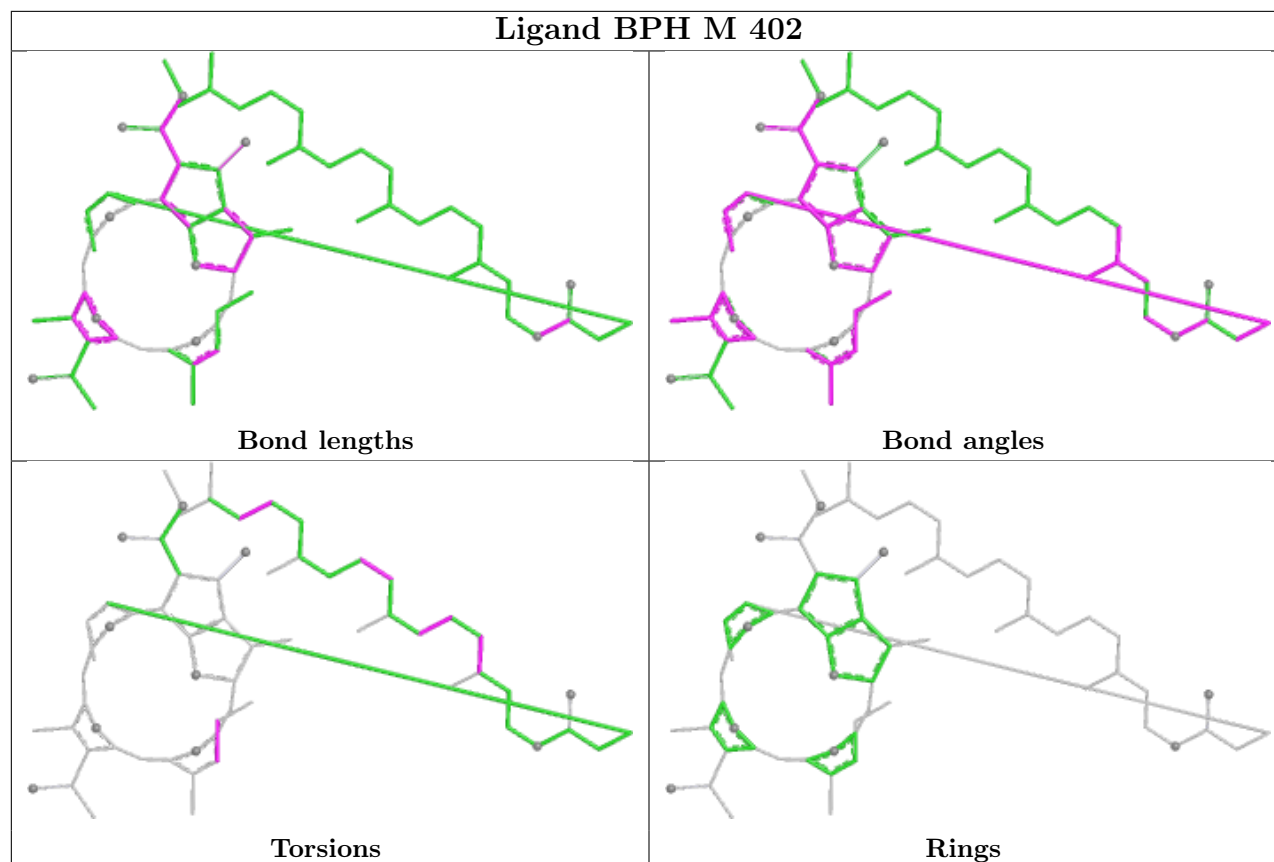


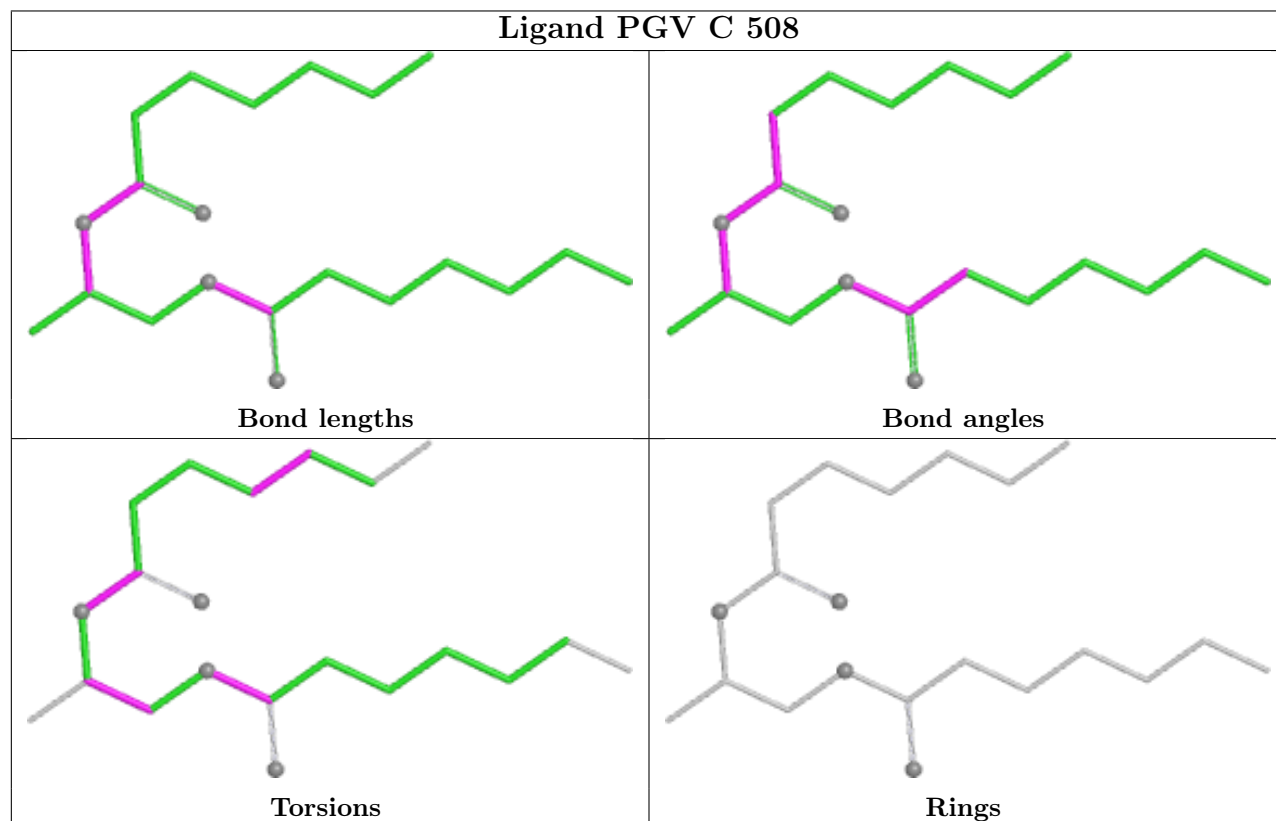
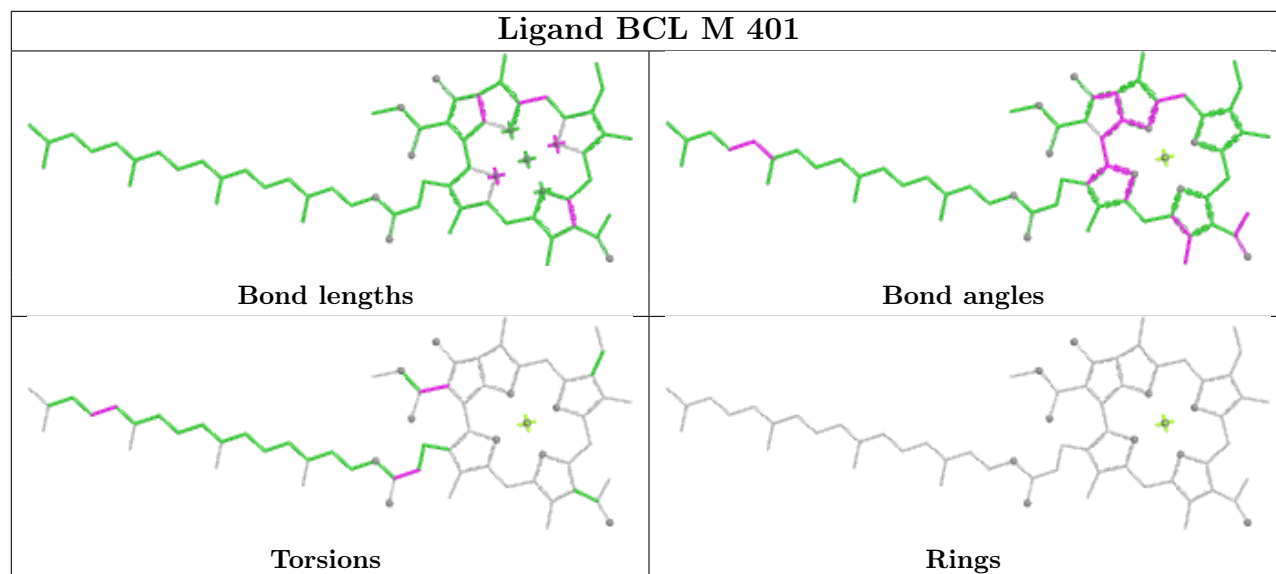


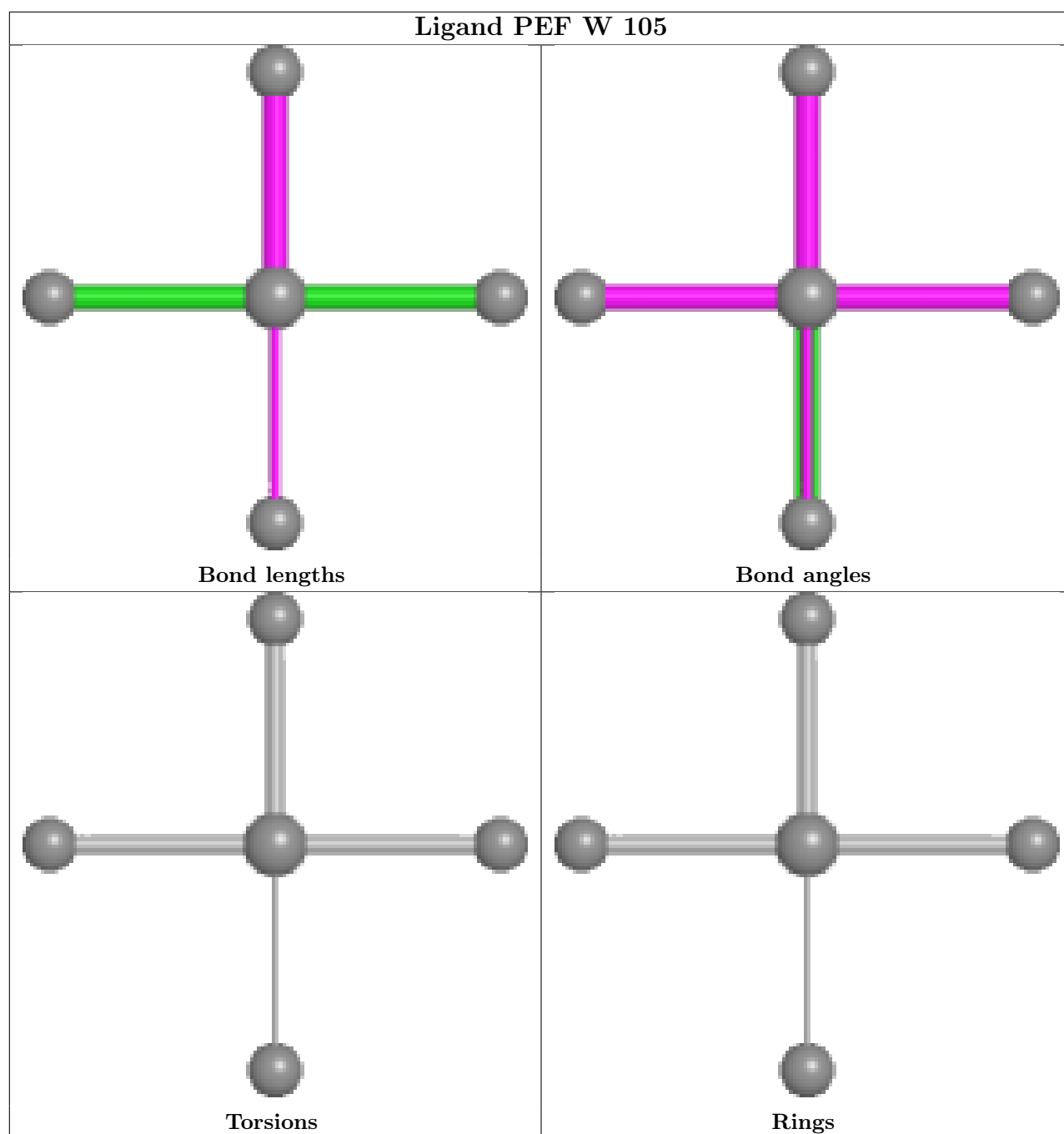


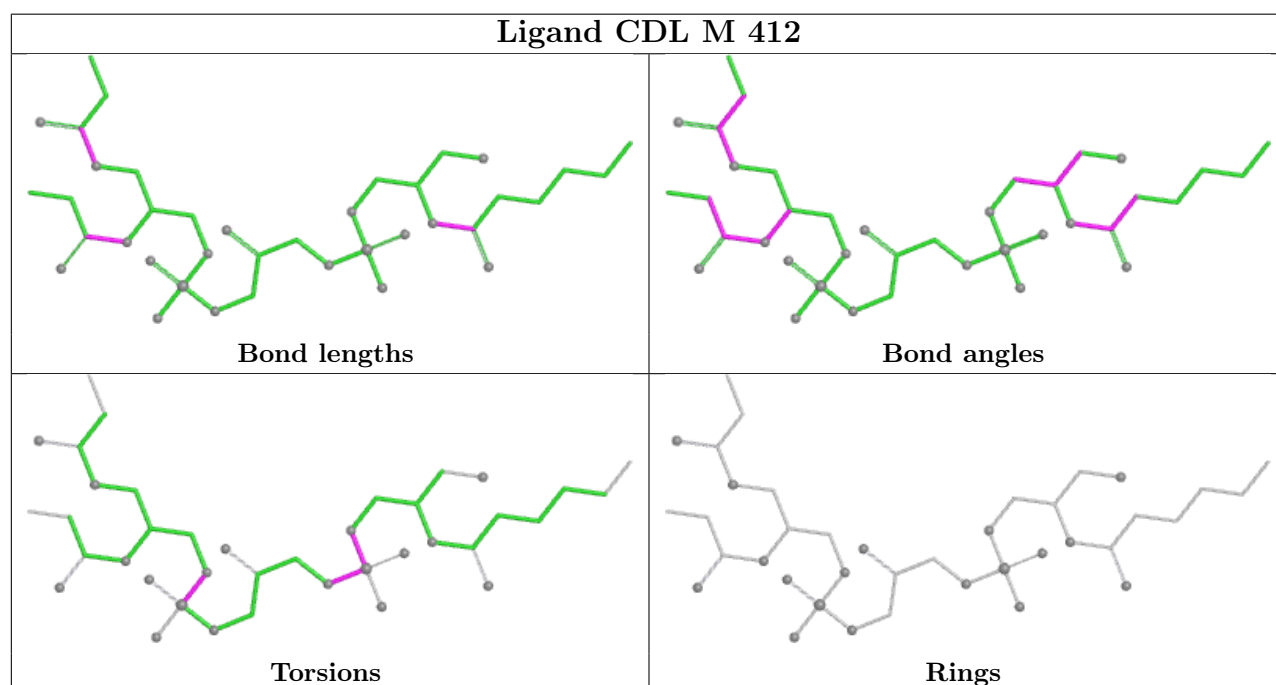
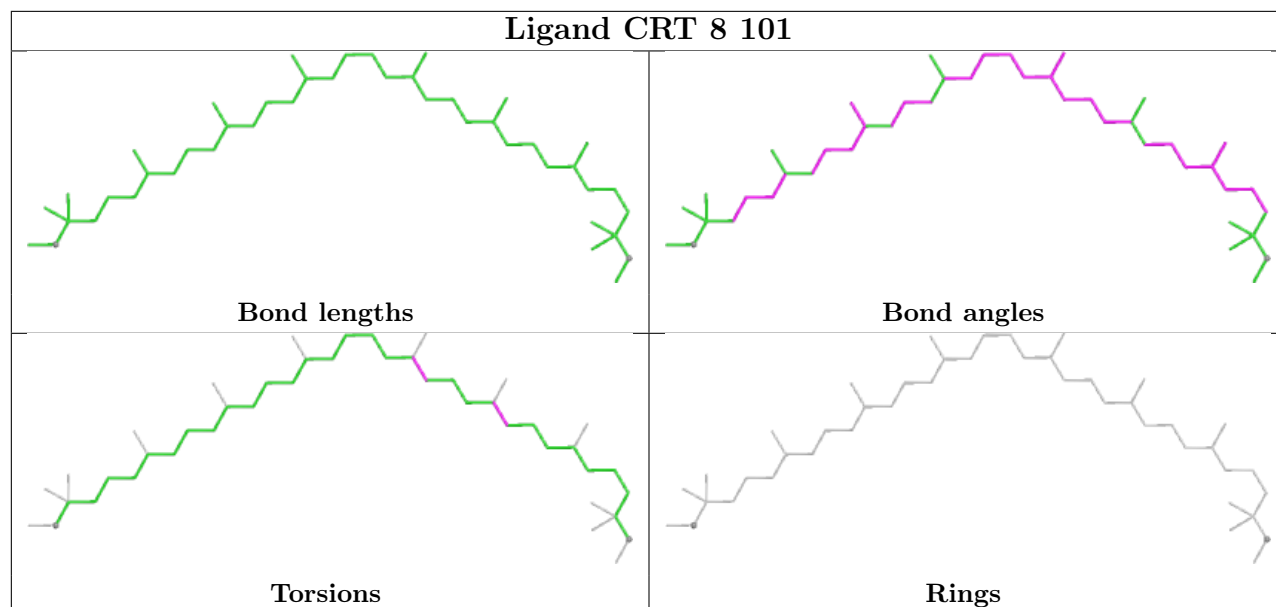


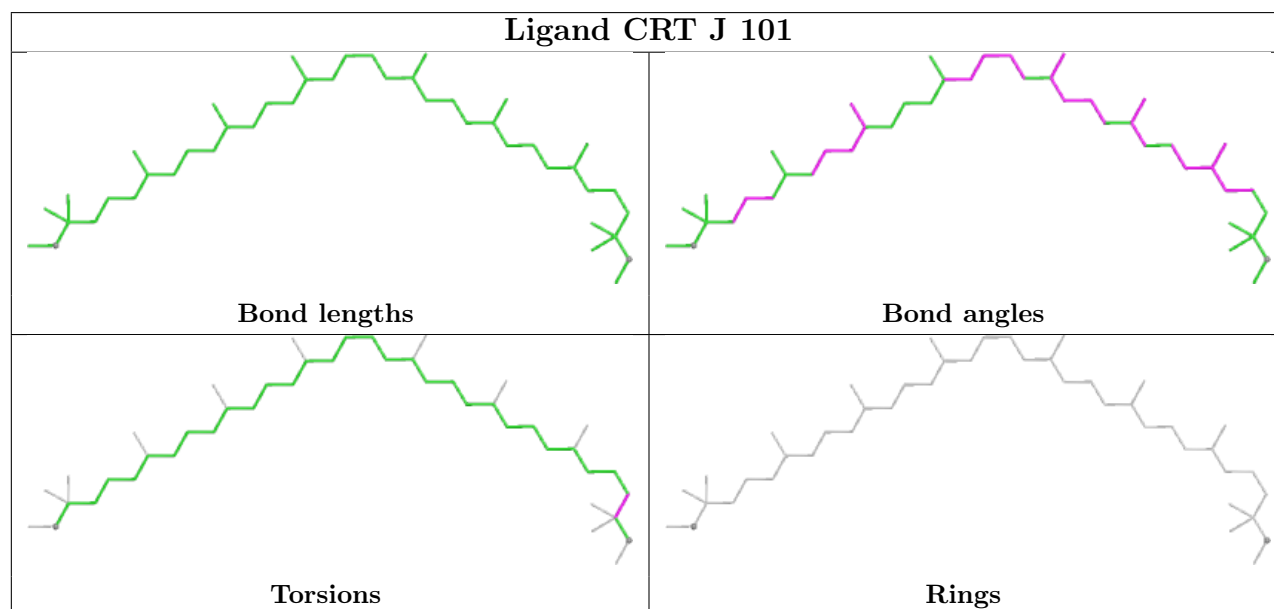
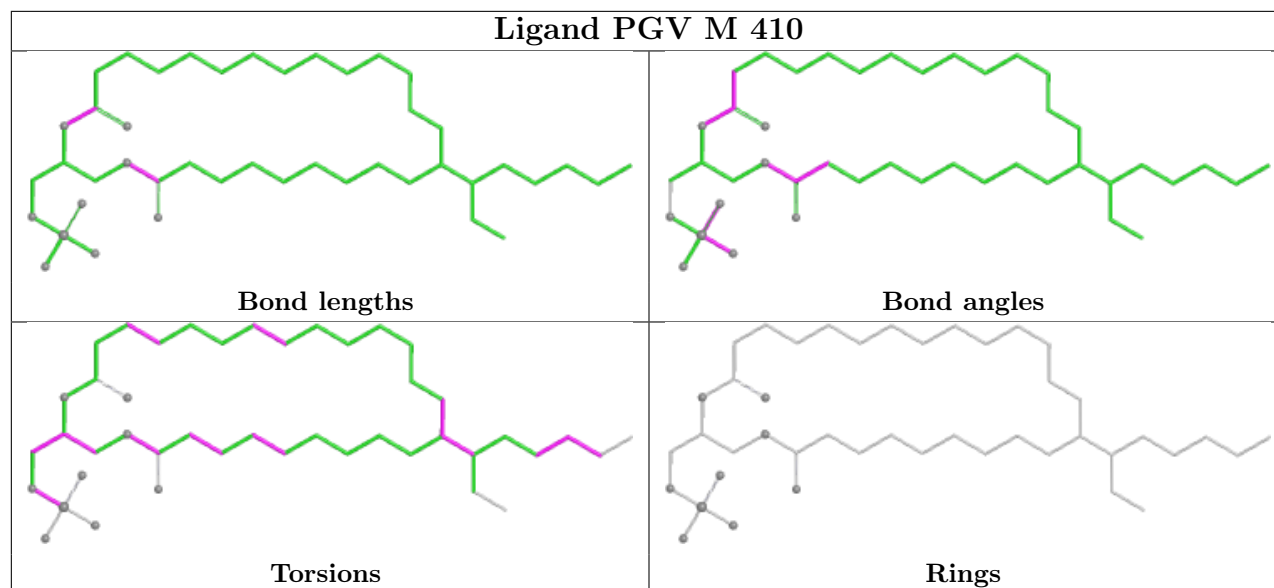


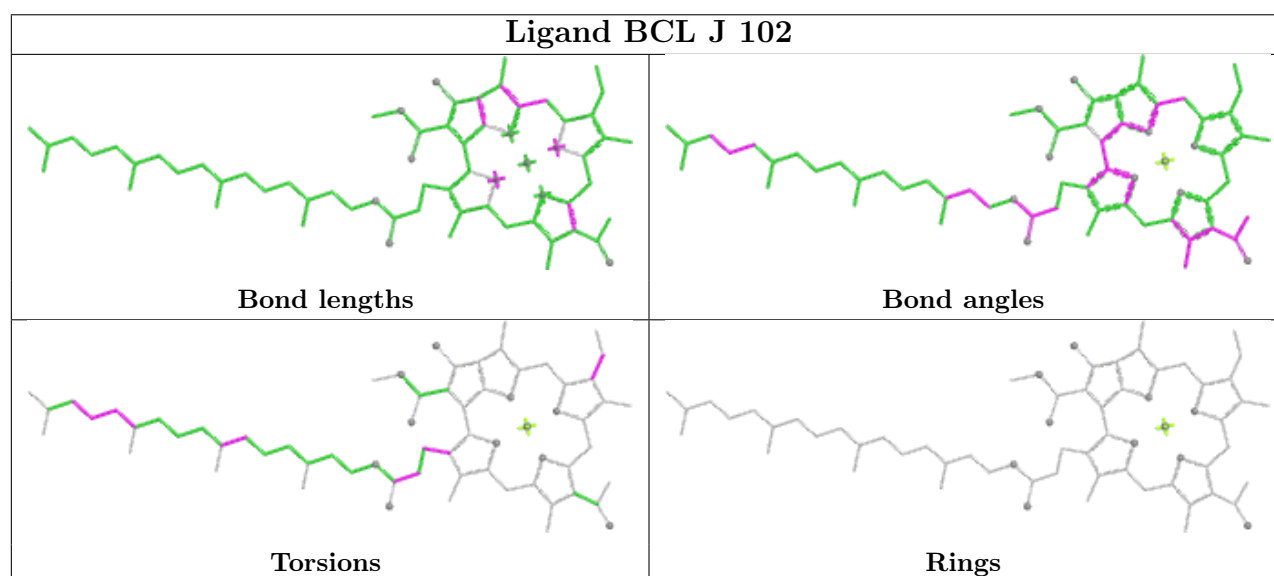
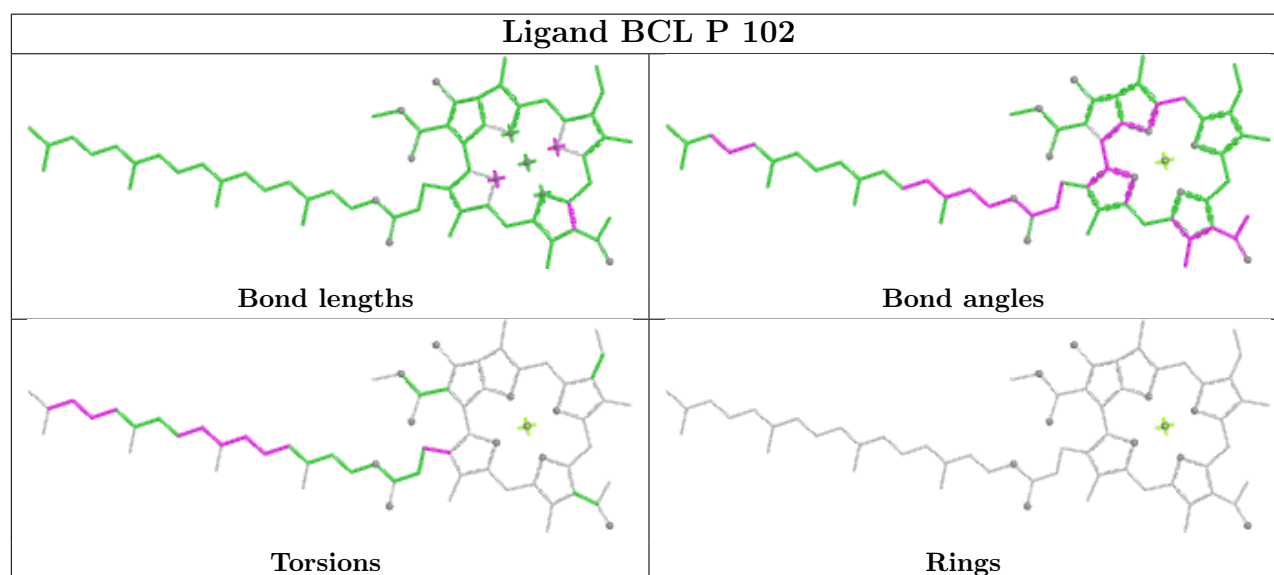
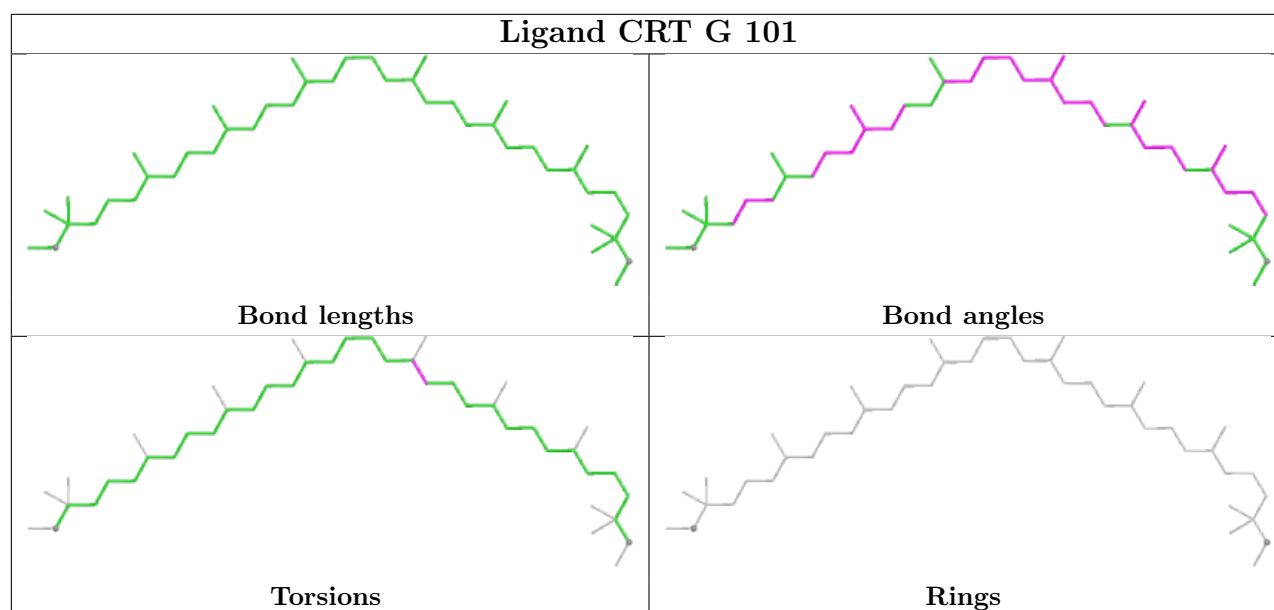


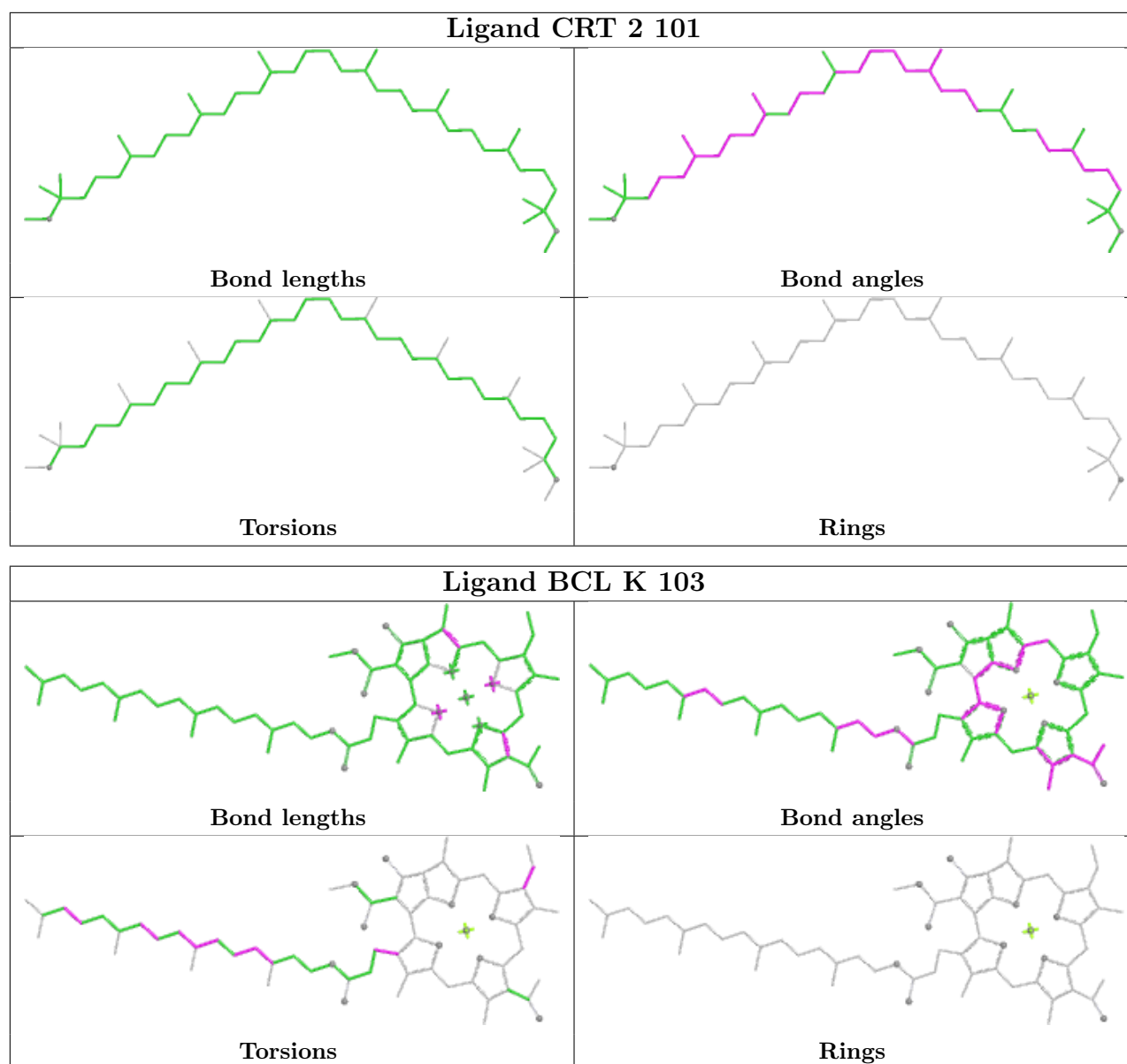


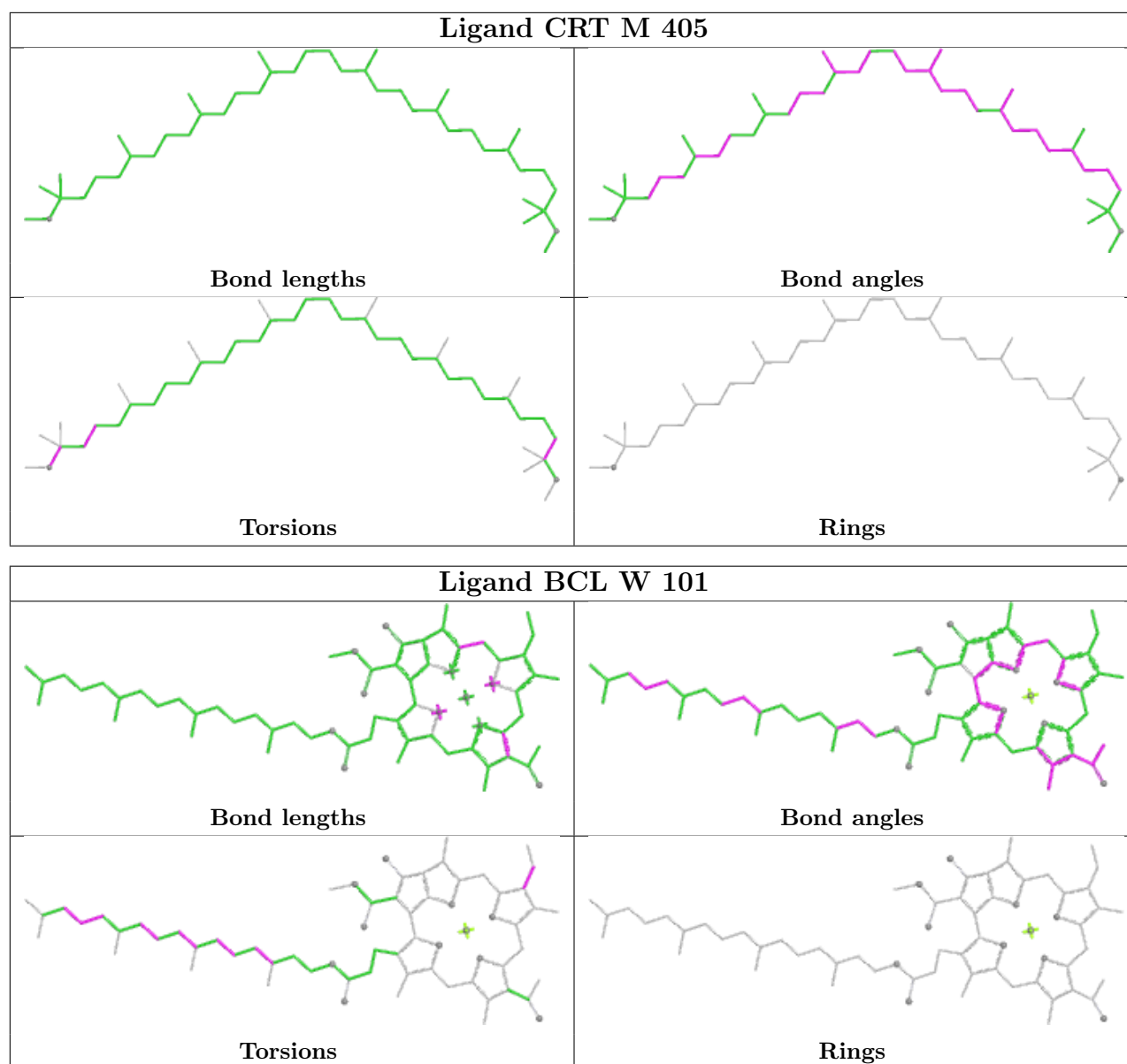


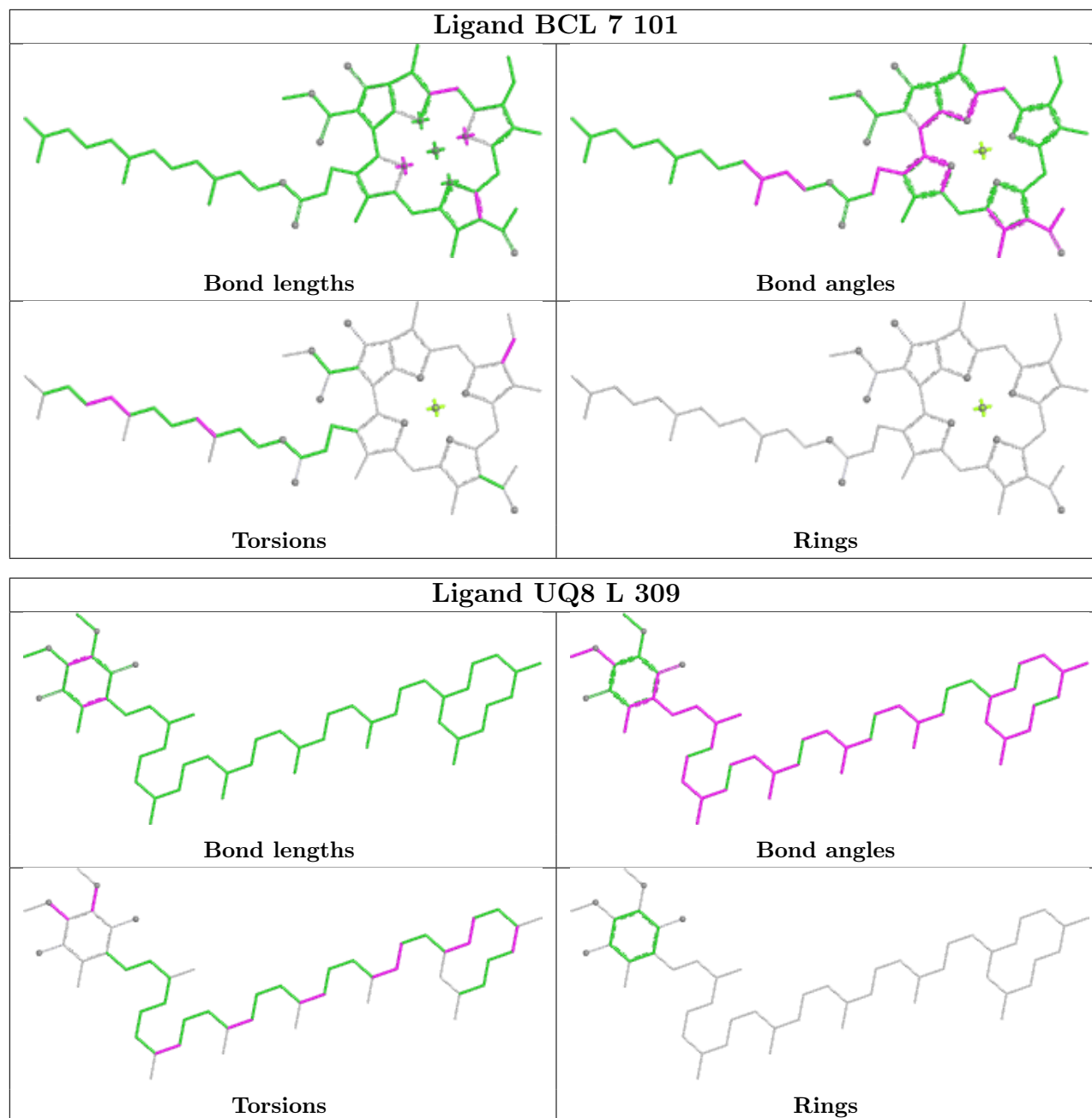


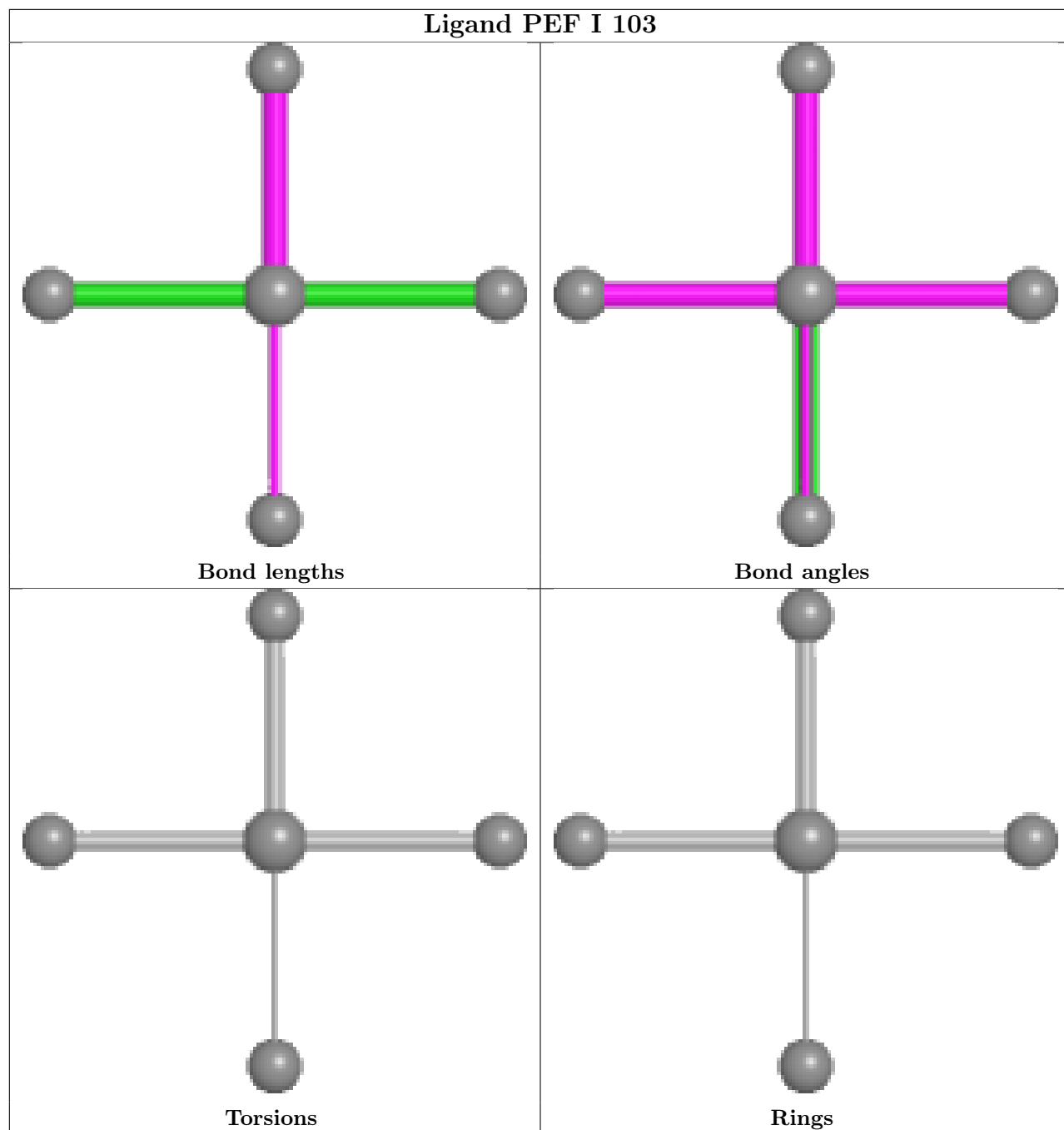


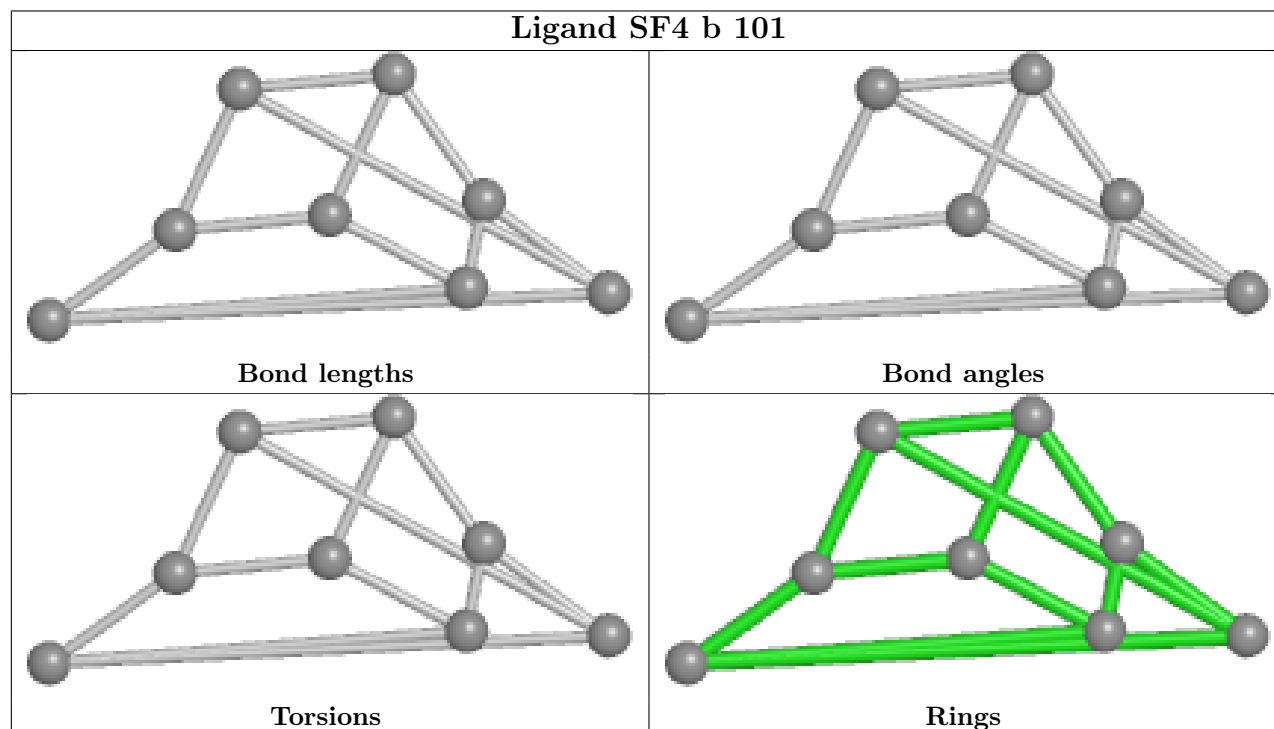
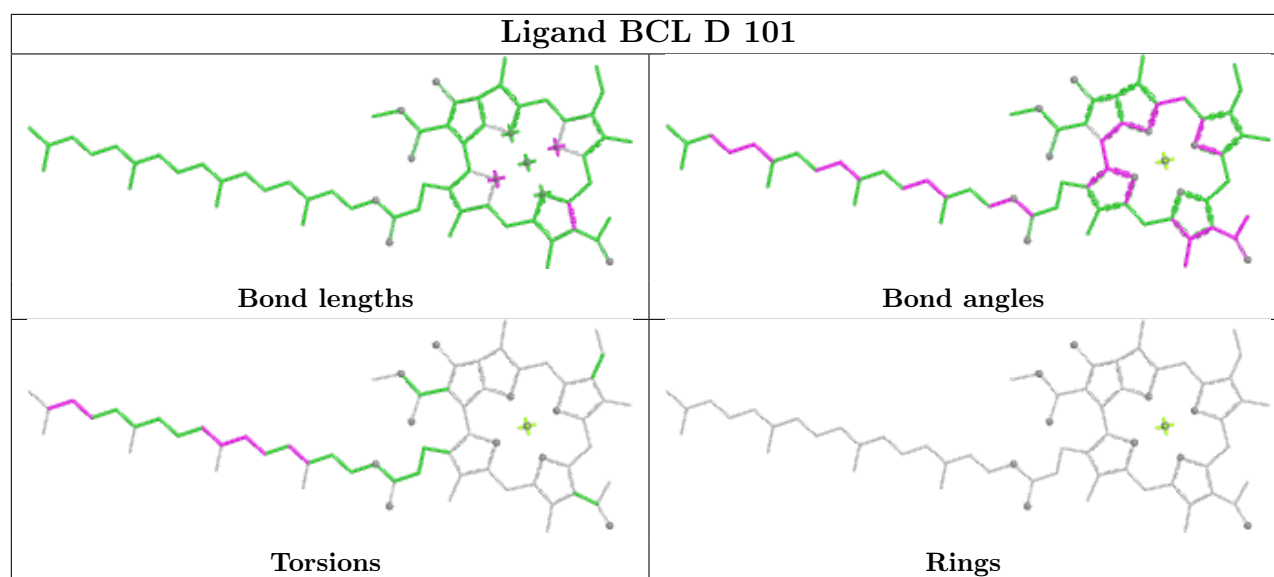


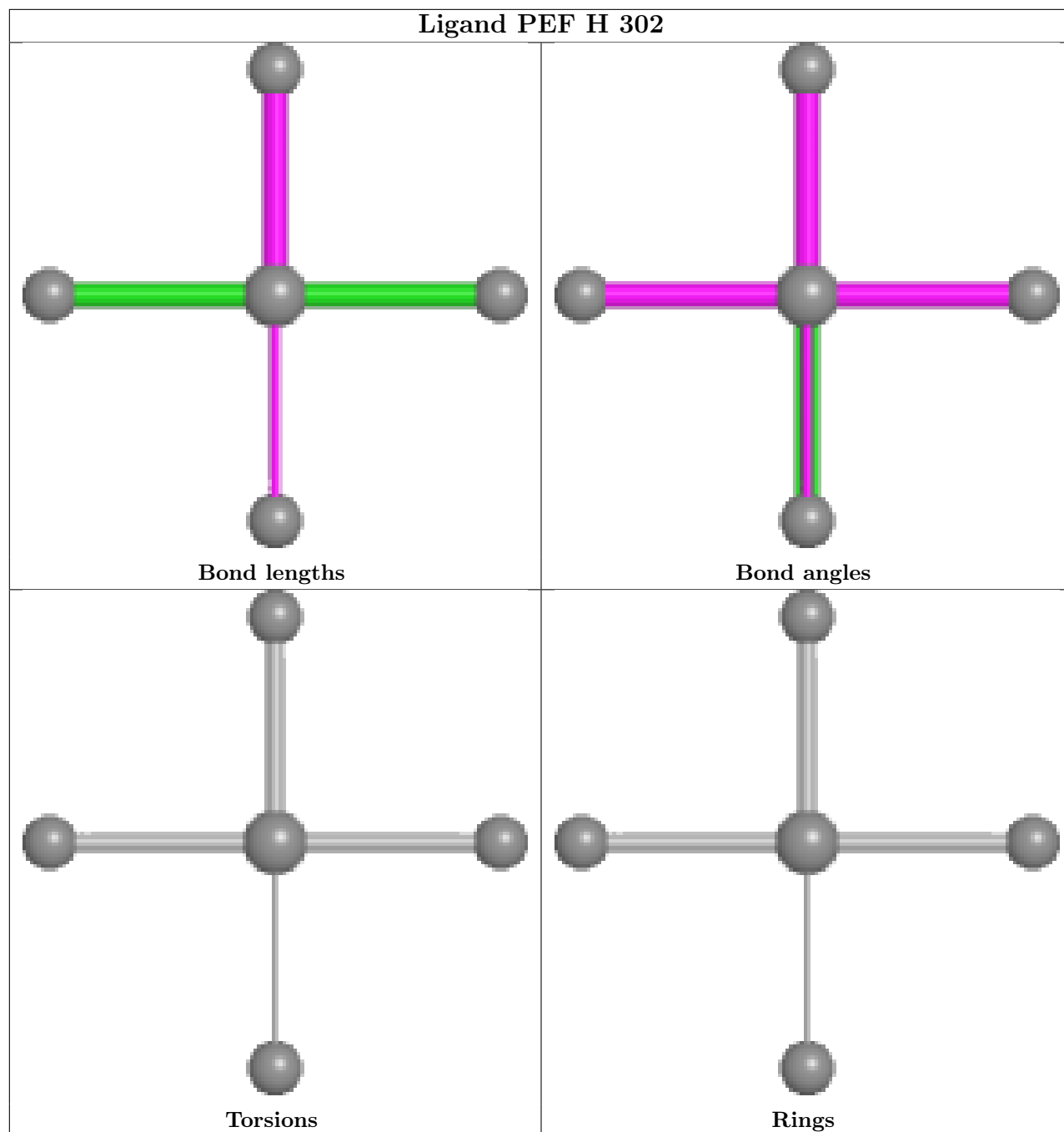




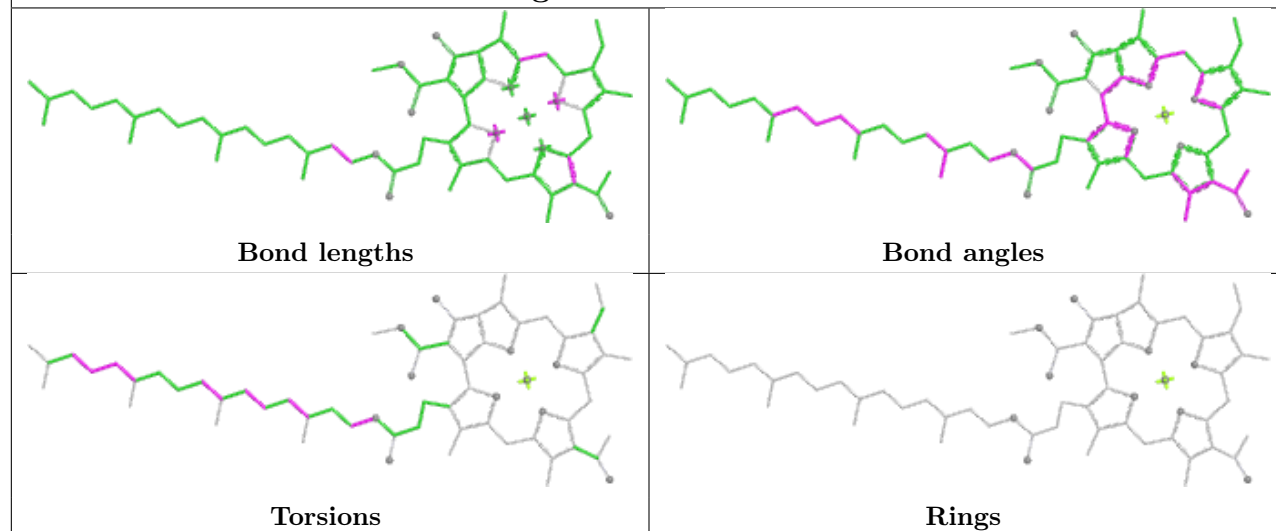




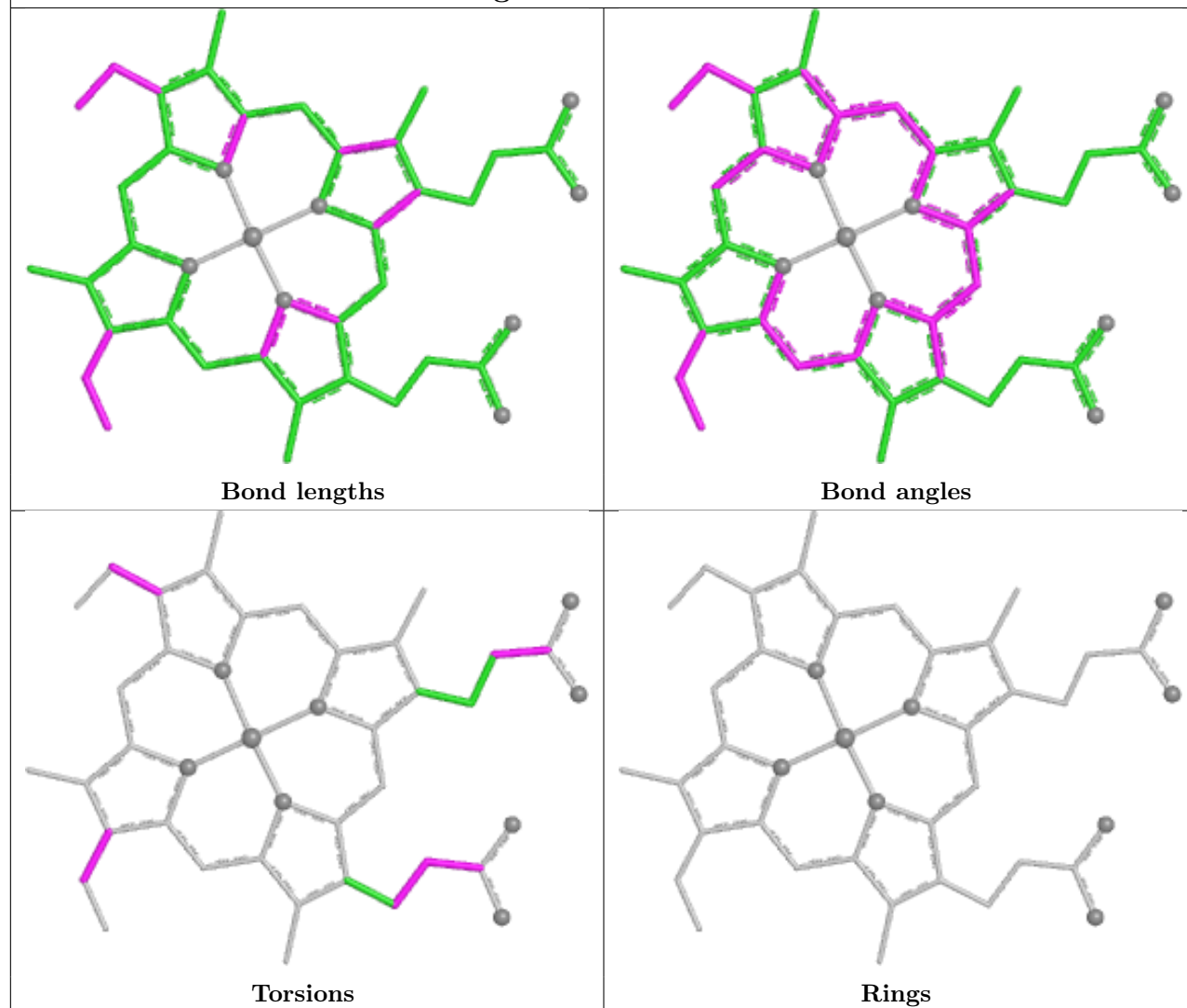


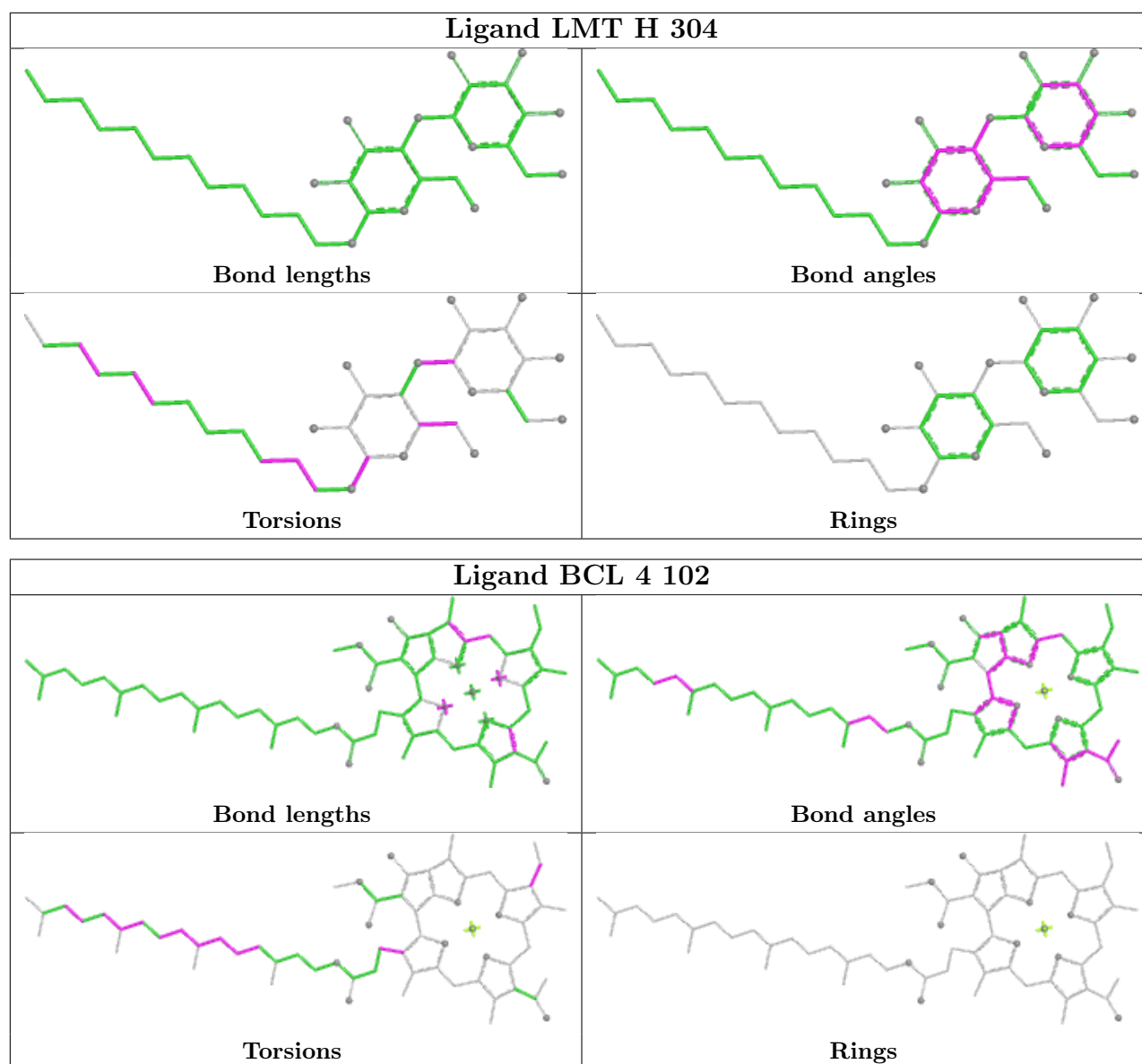


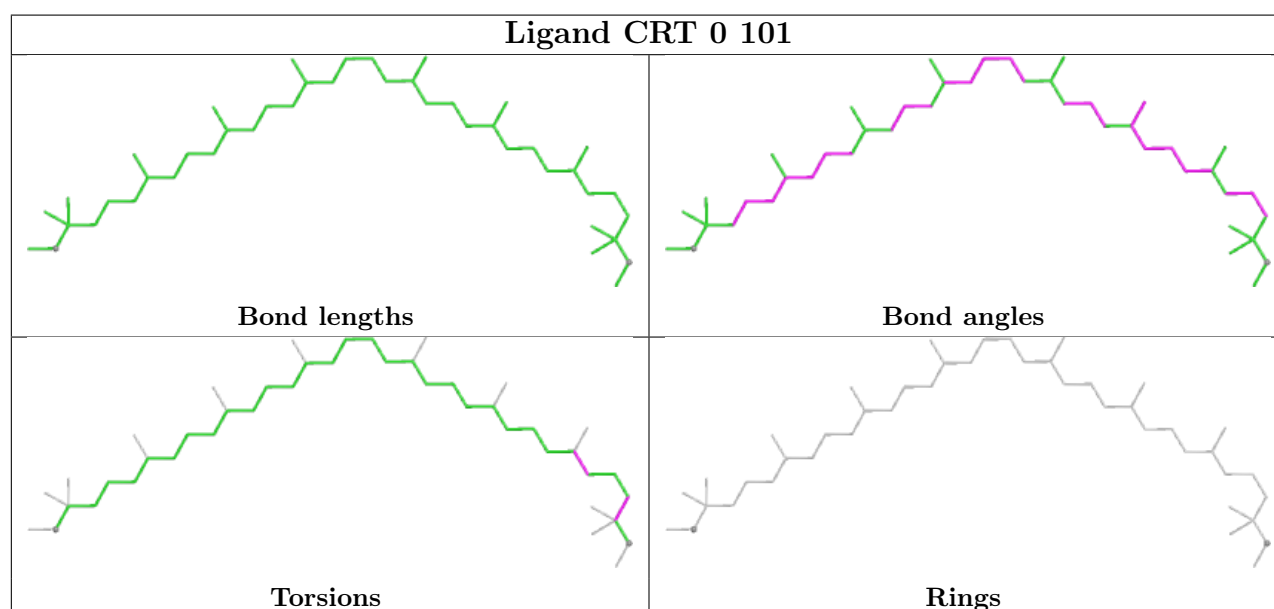
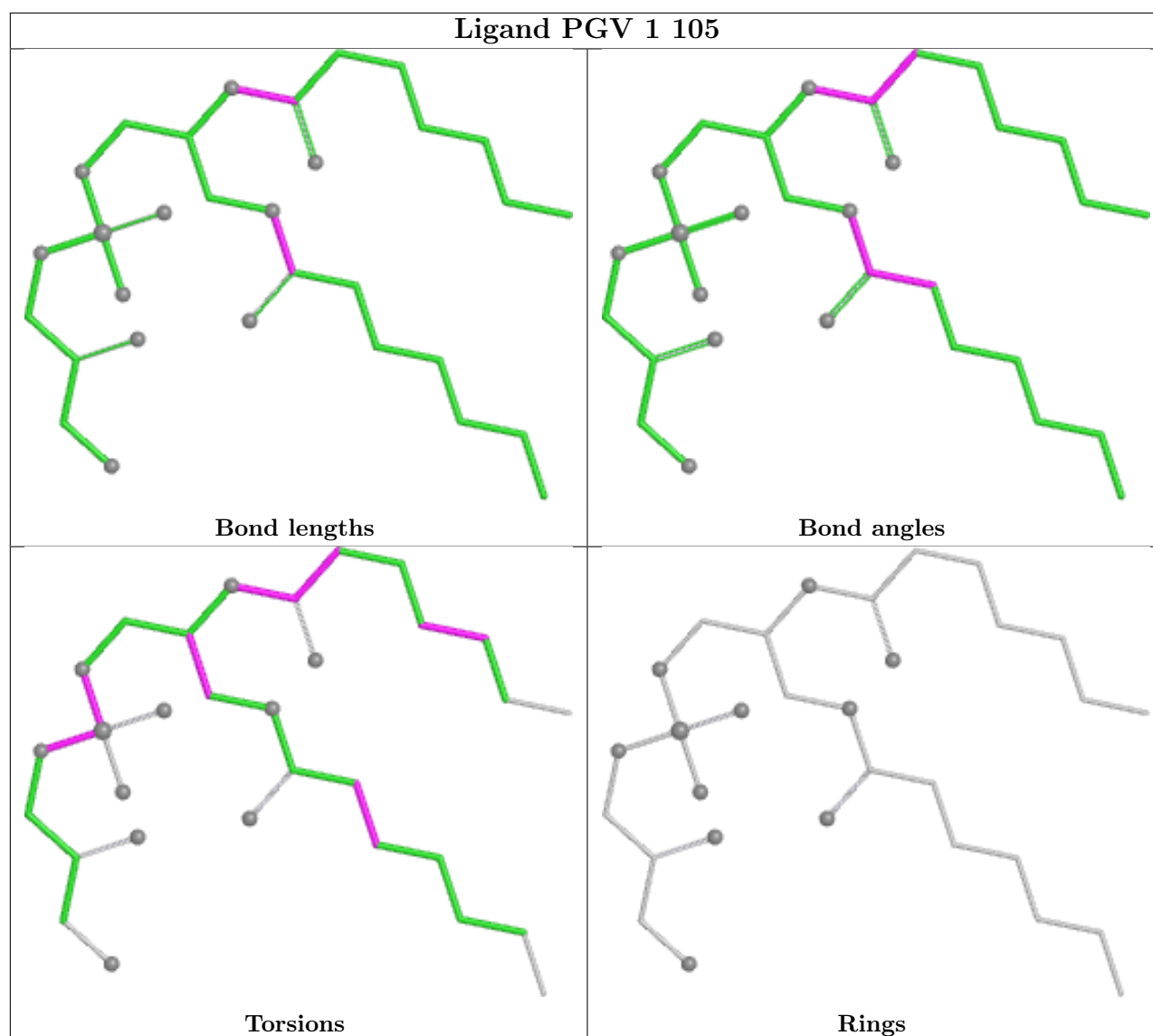
## Ligand BCL K 101

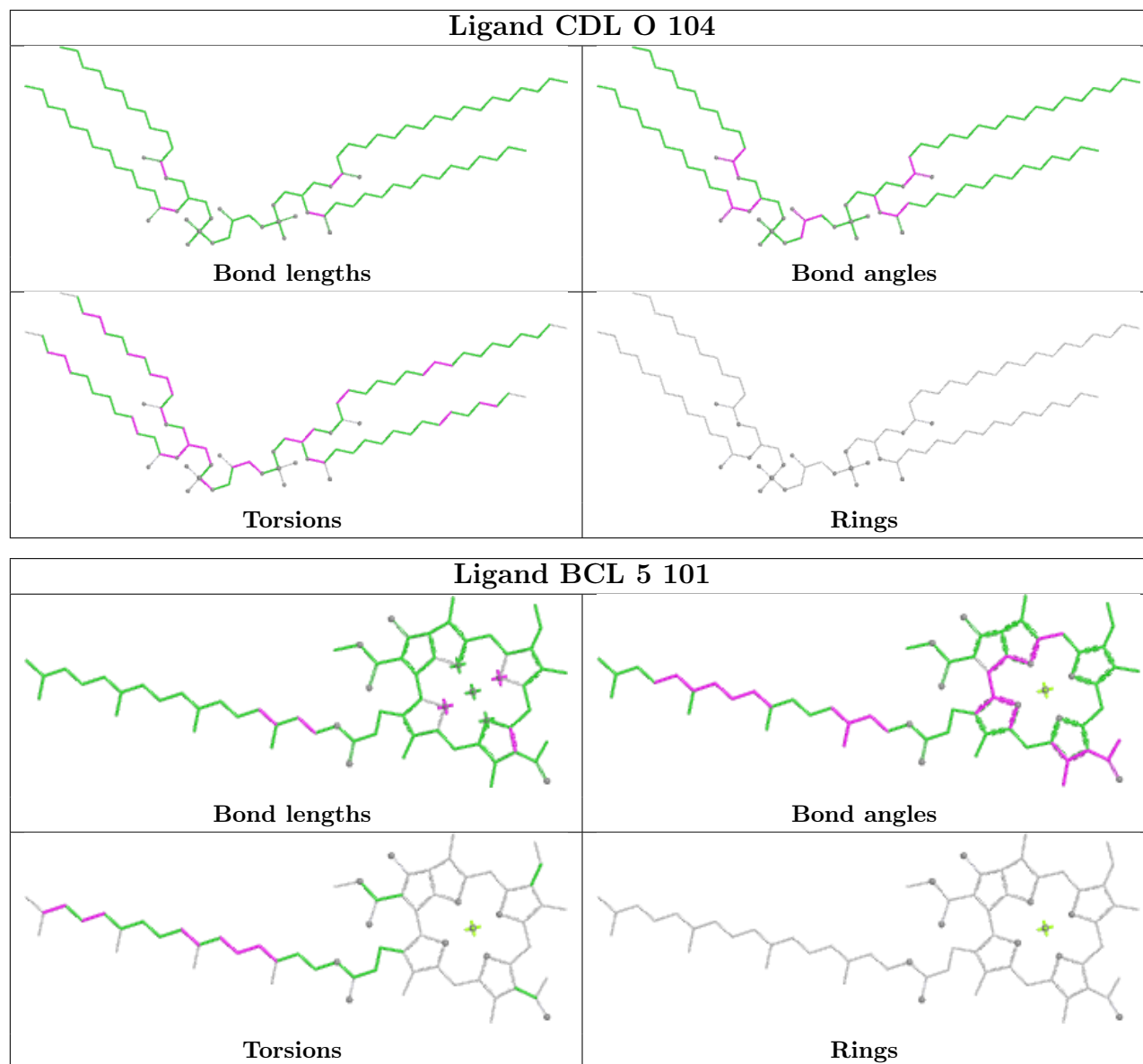


## Ligand HEC C 502

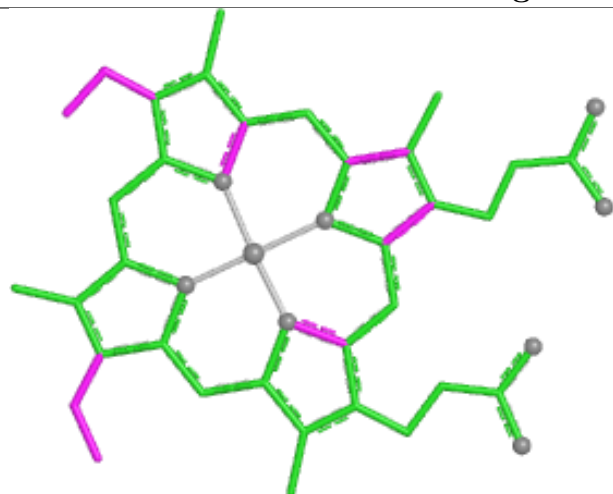




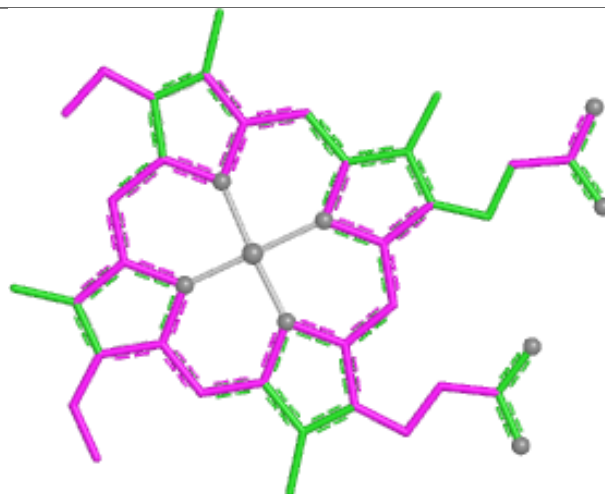




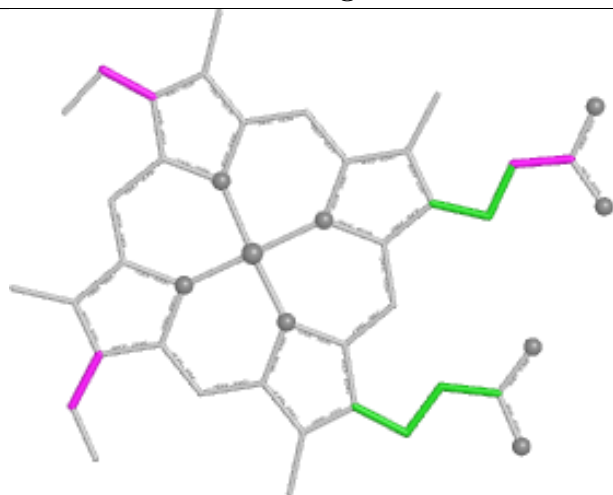
## Ligand HEC C 501



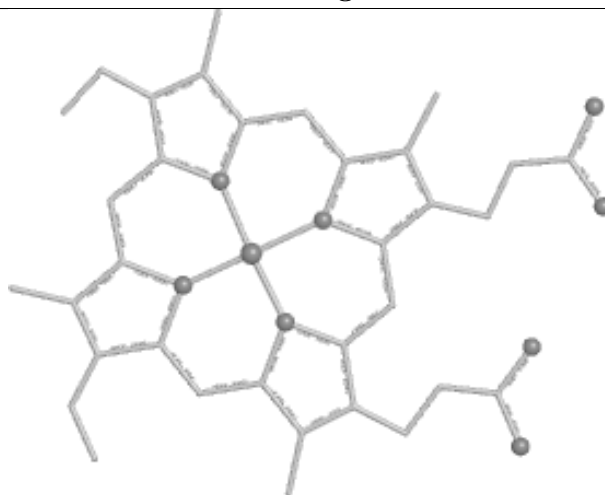
Bond lengths



Bond angles

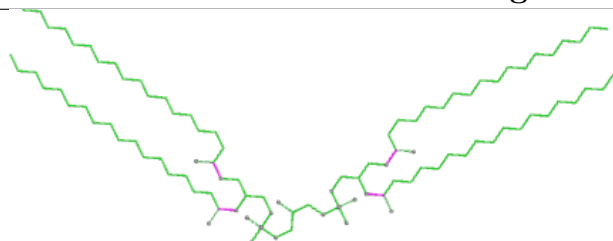


Torsions

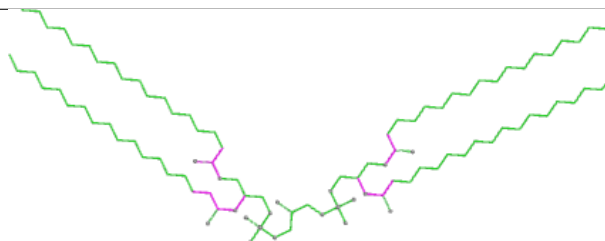


Rings

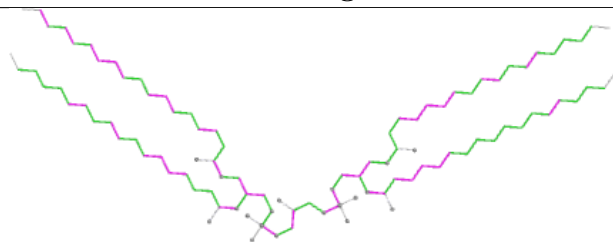
## Ligand CDL M 406



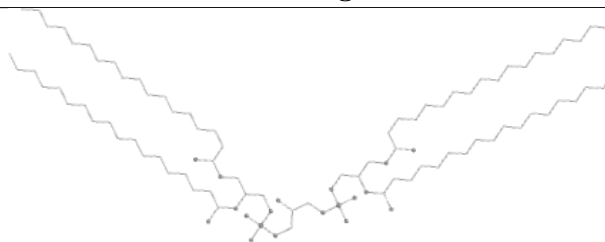
Bond lengths



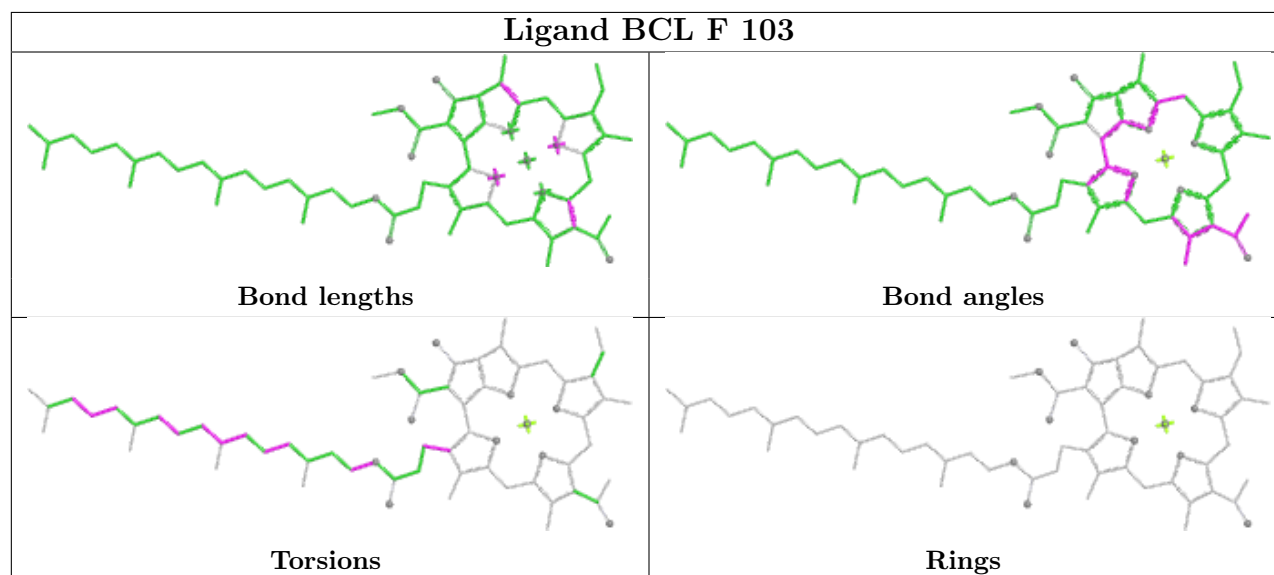
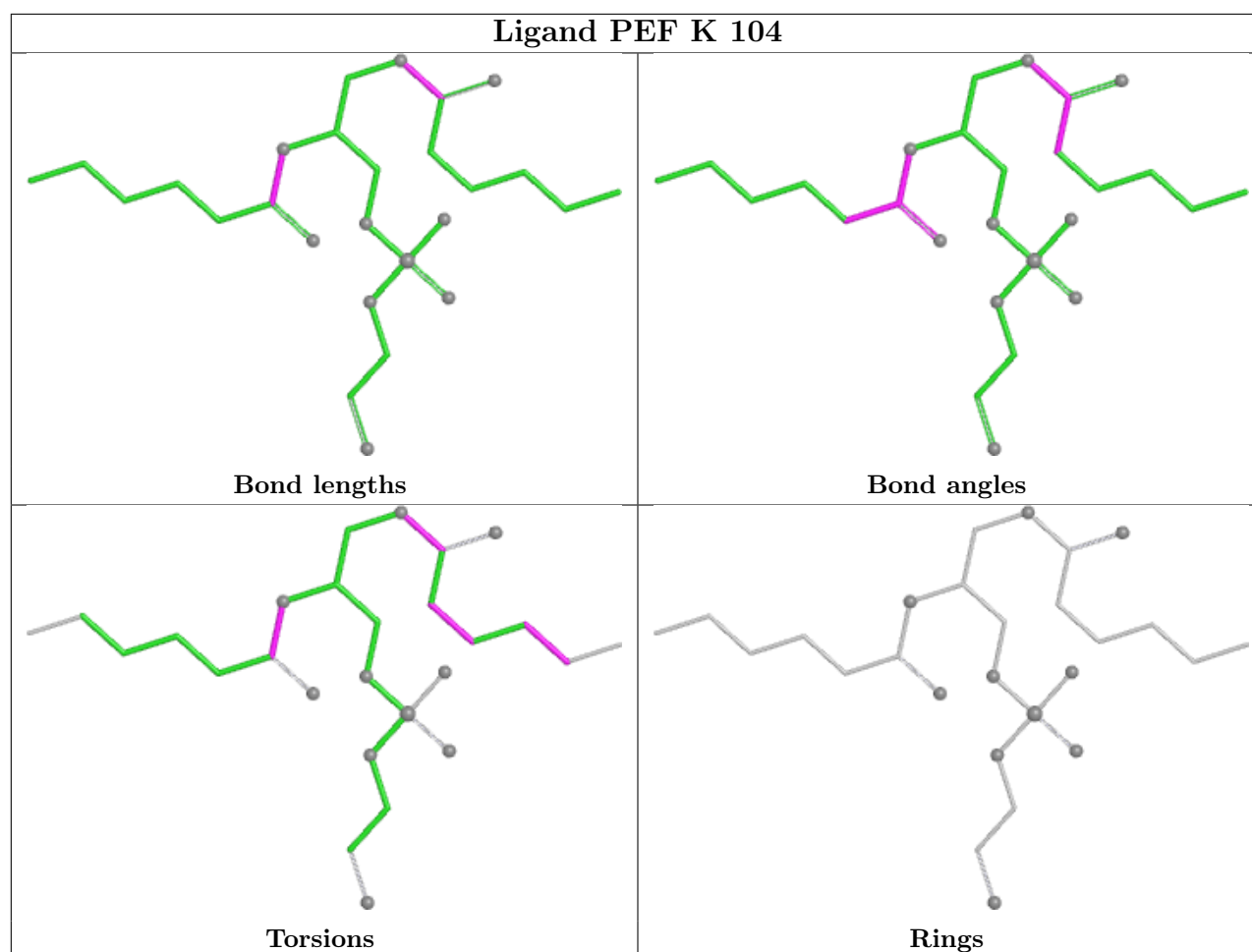
Bond angles

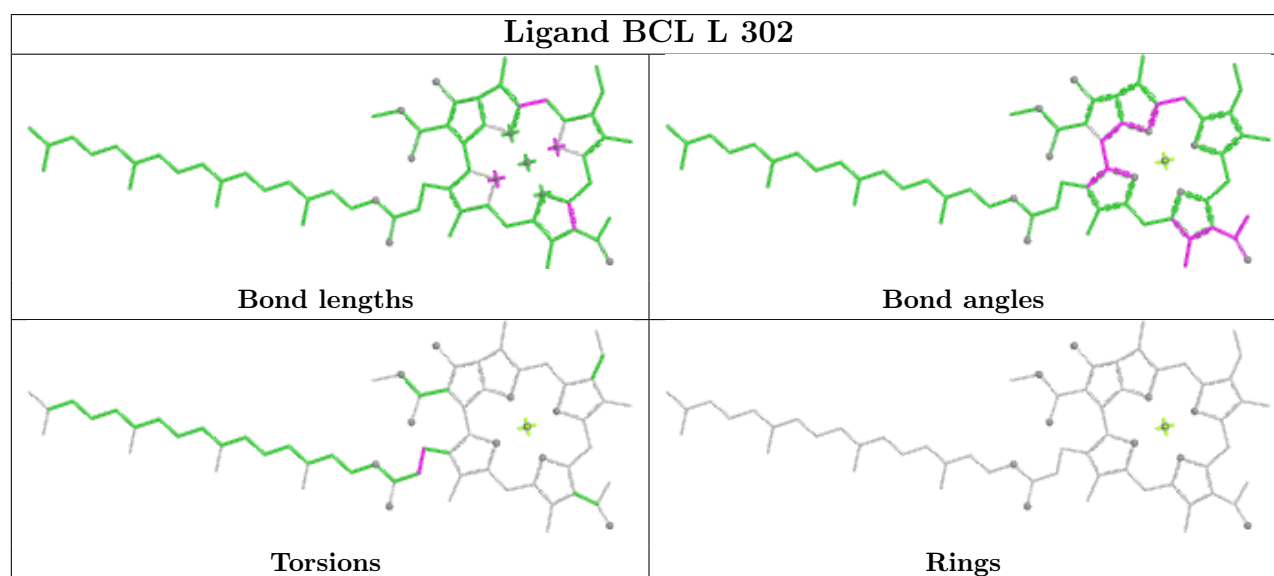
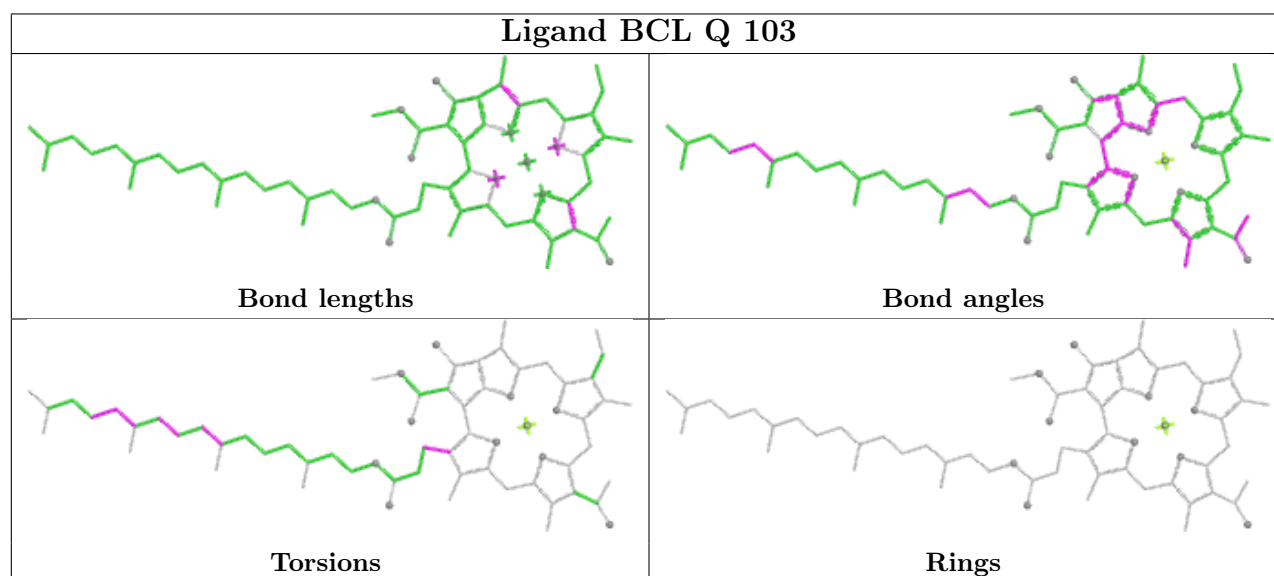
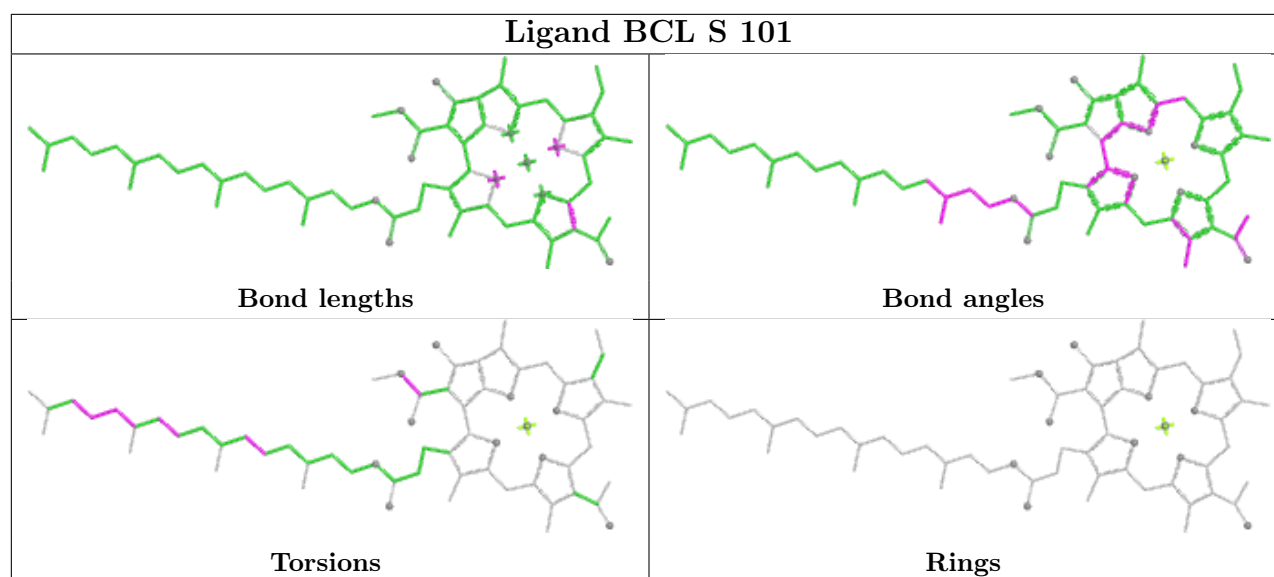


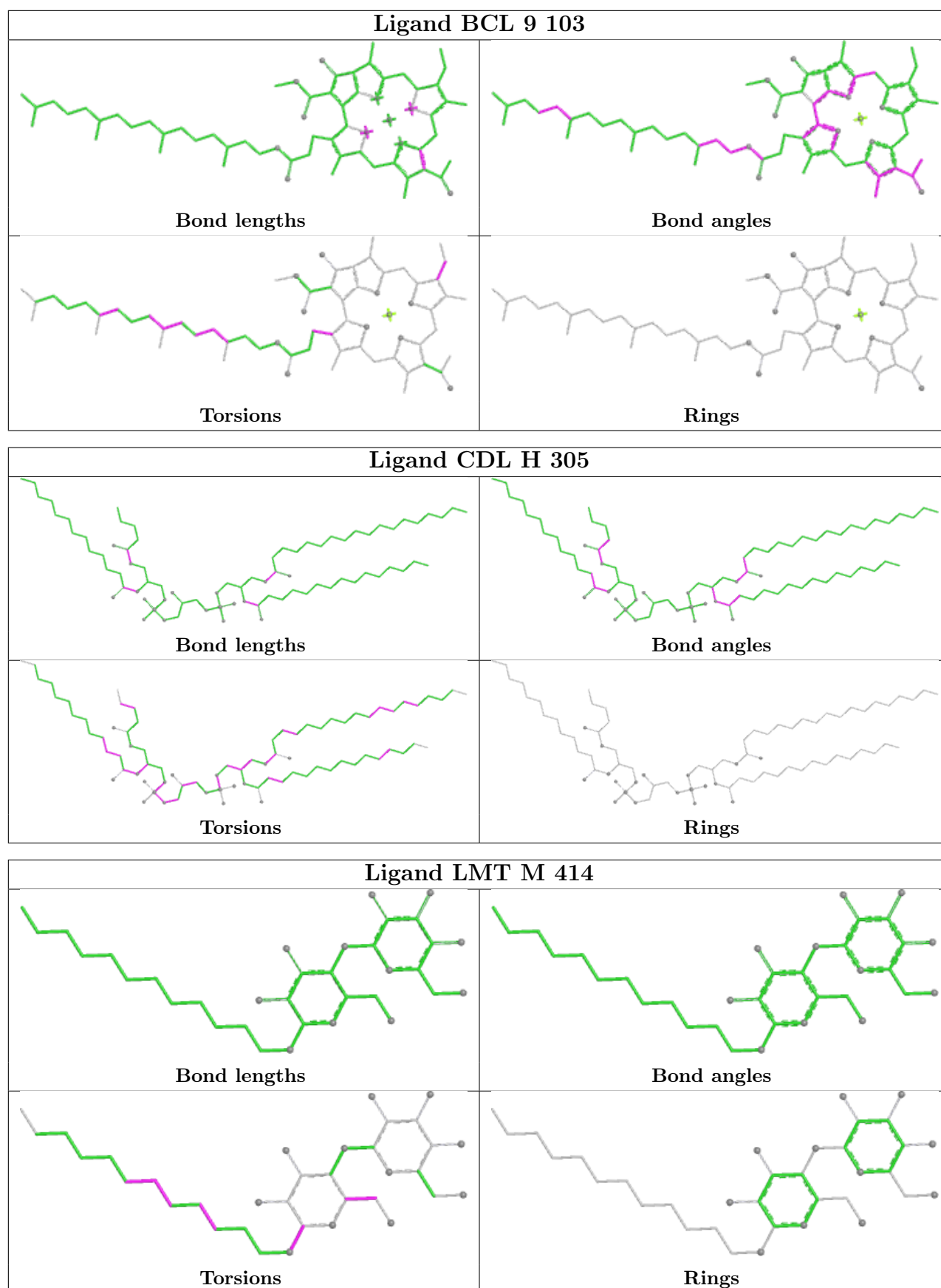
Torsions

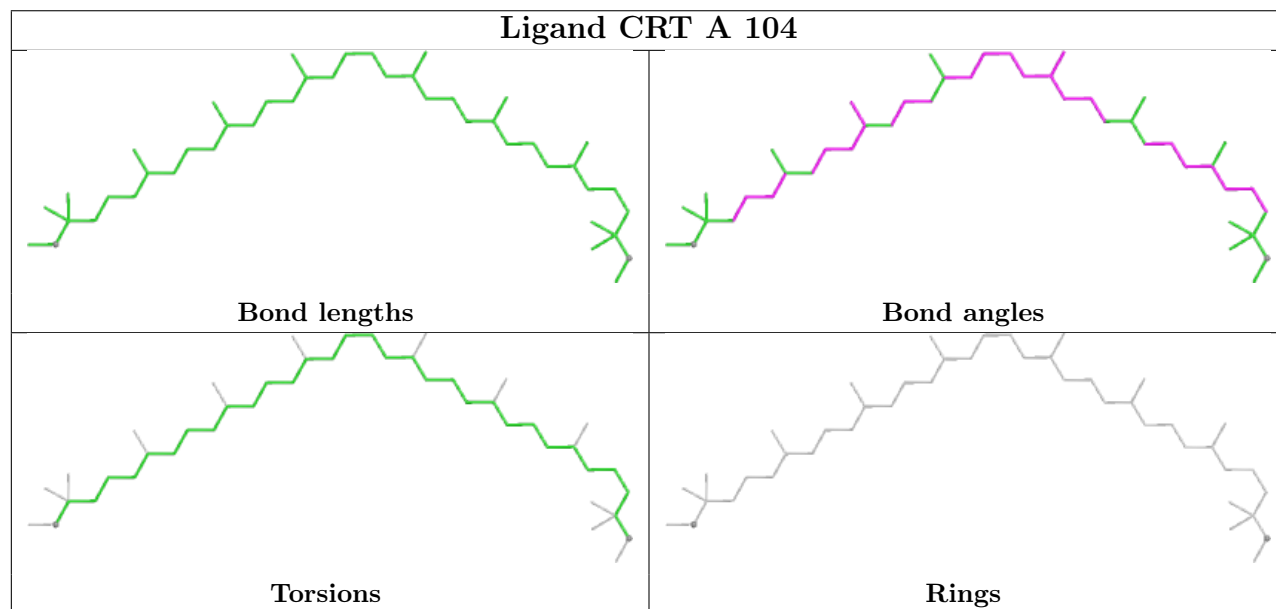
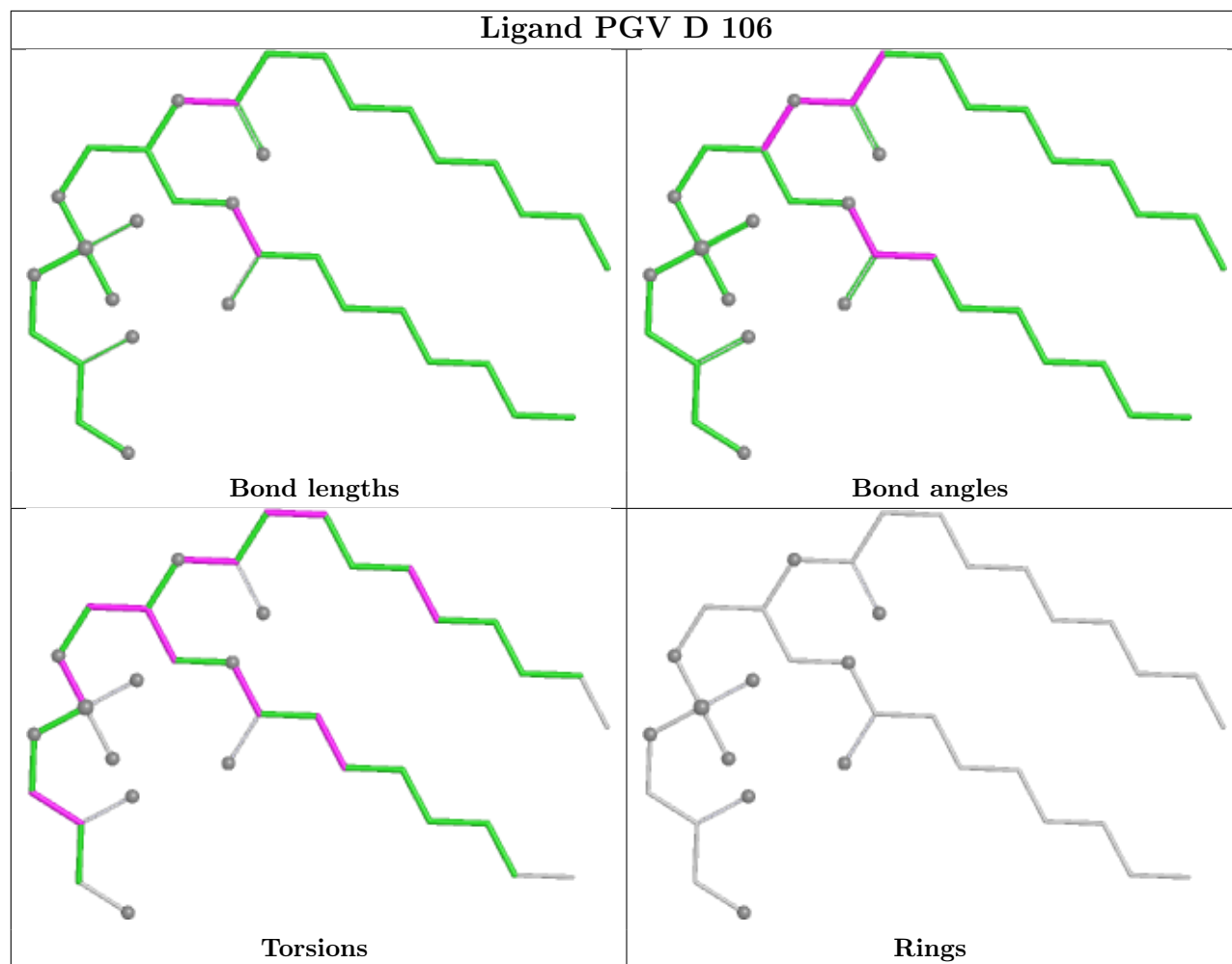


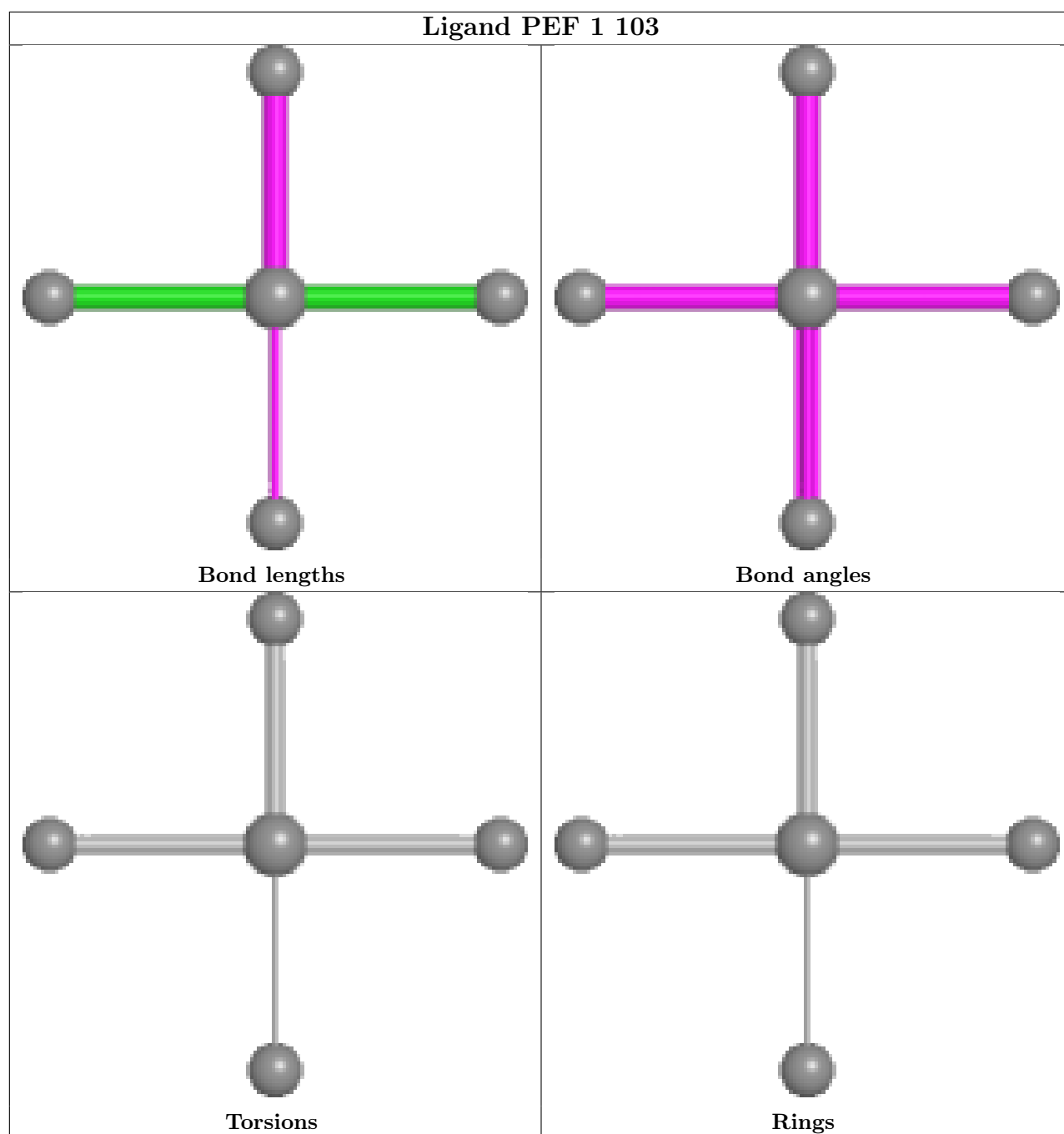
Rings

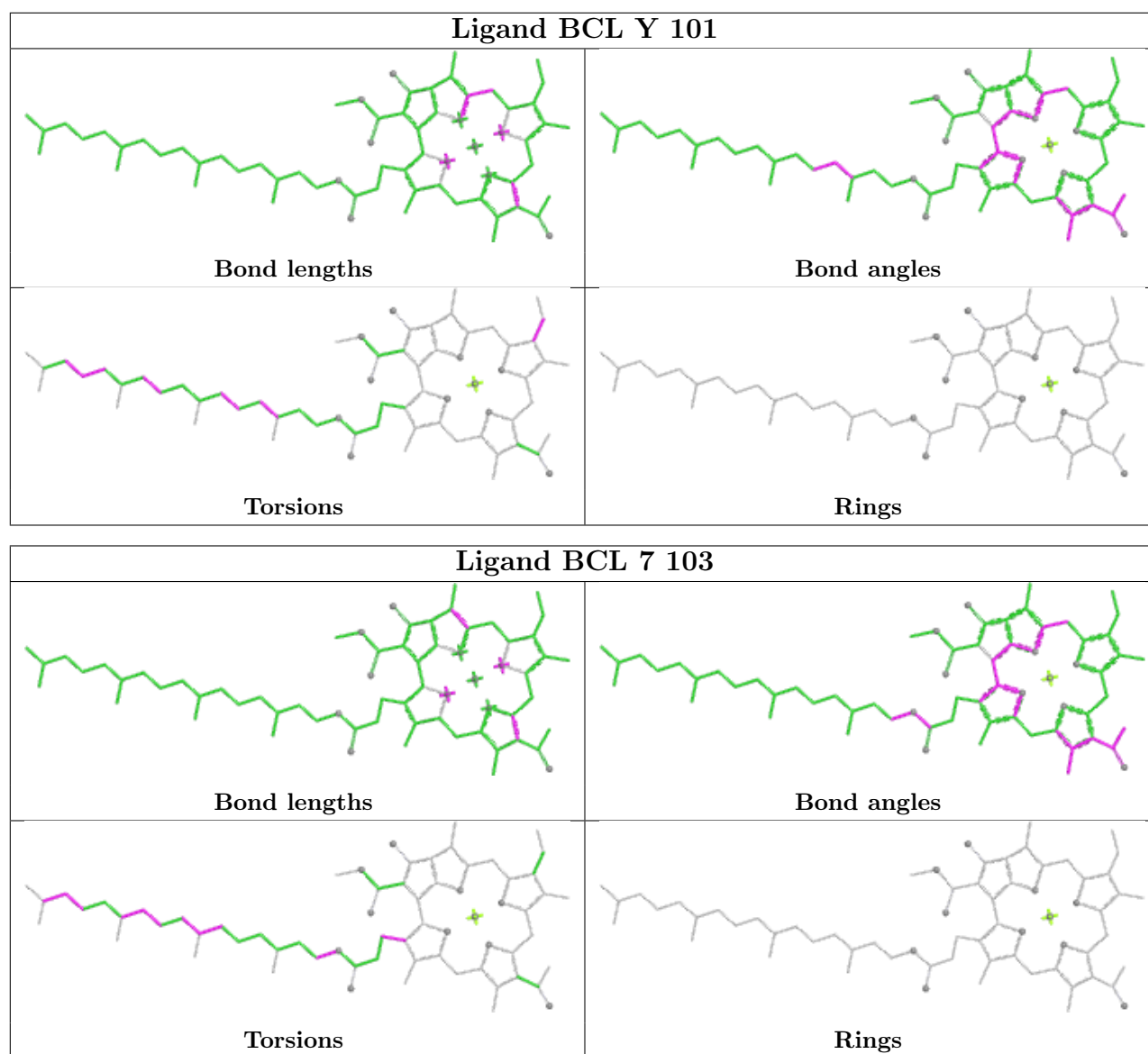


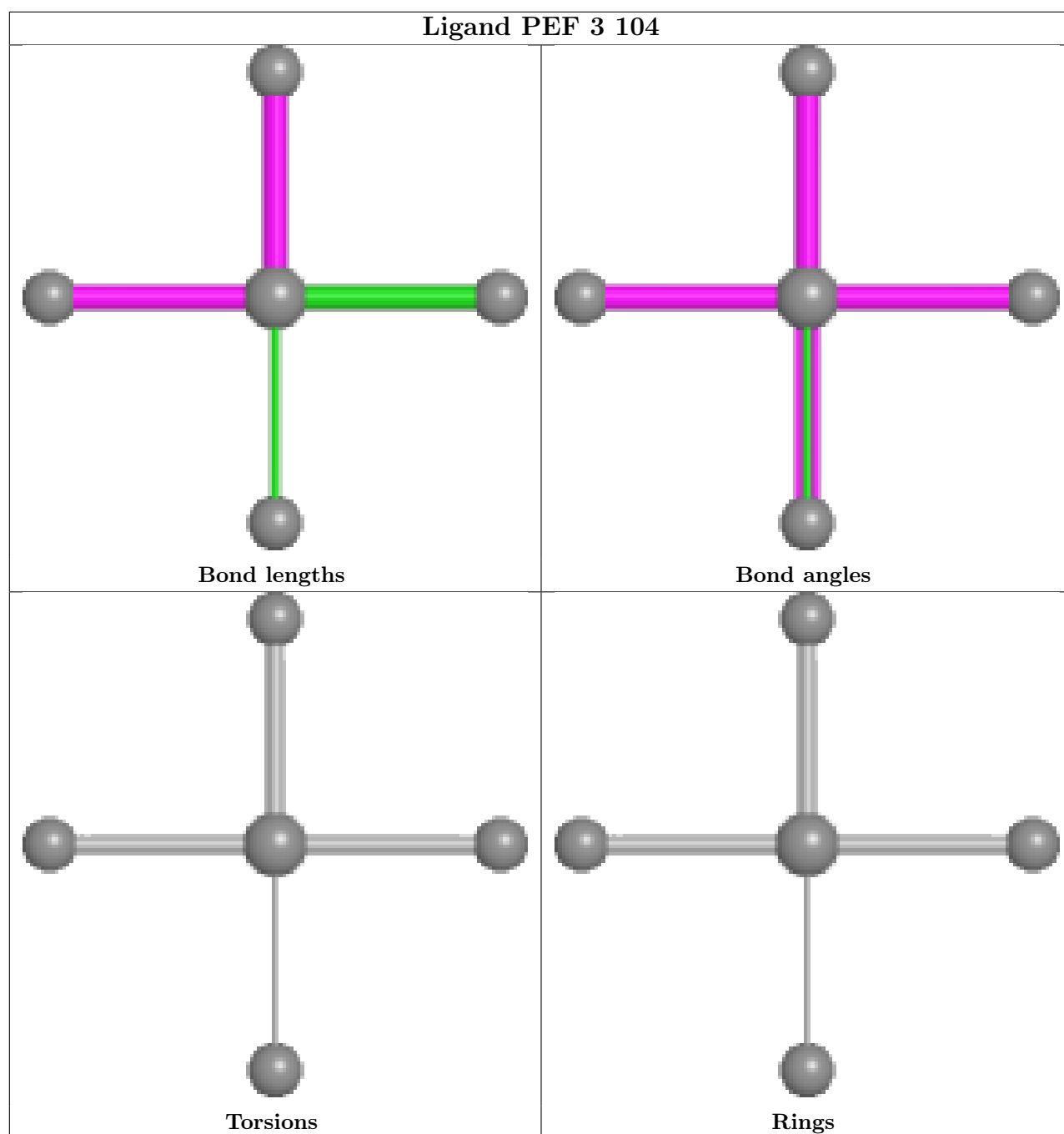




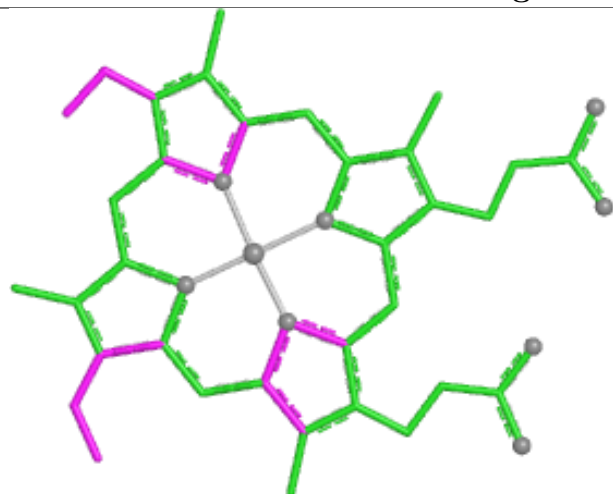




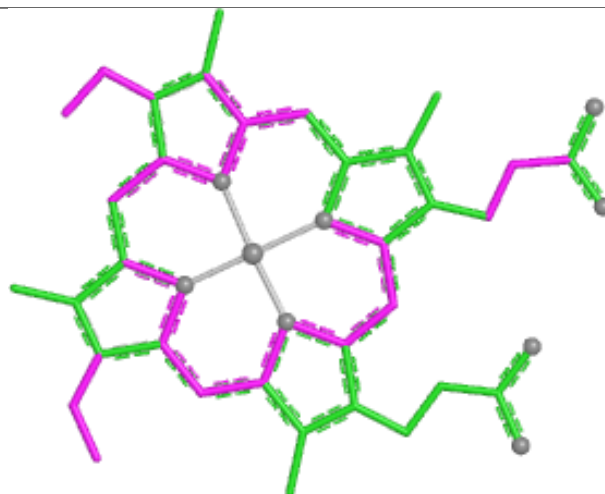




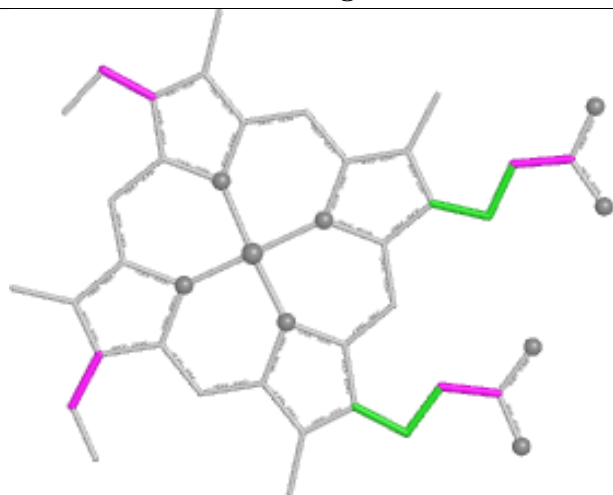
## Ligand HEC C 504



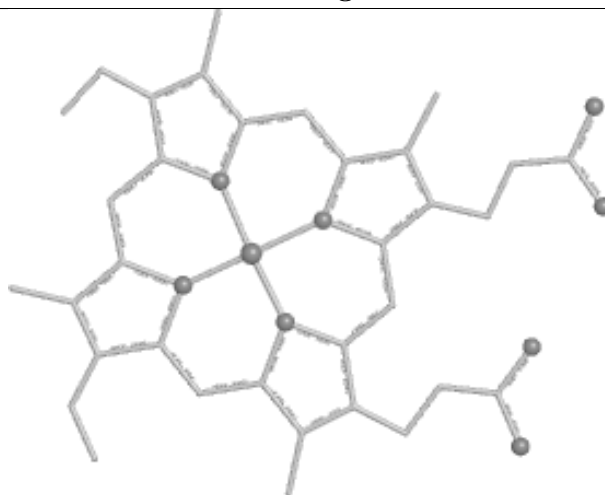
Bond lengths



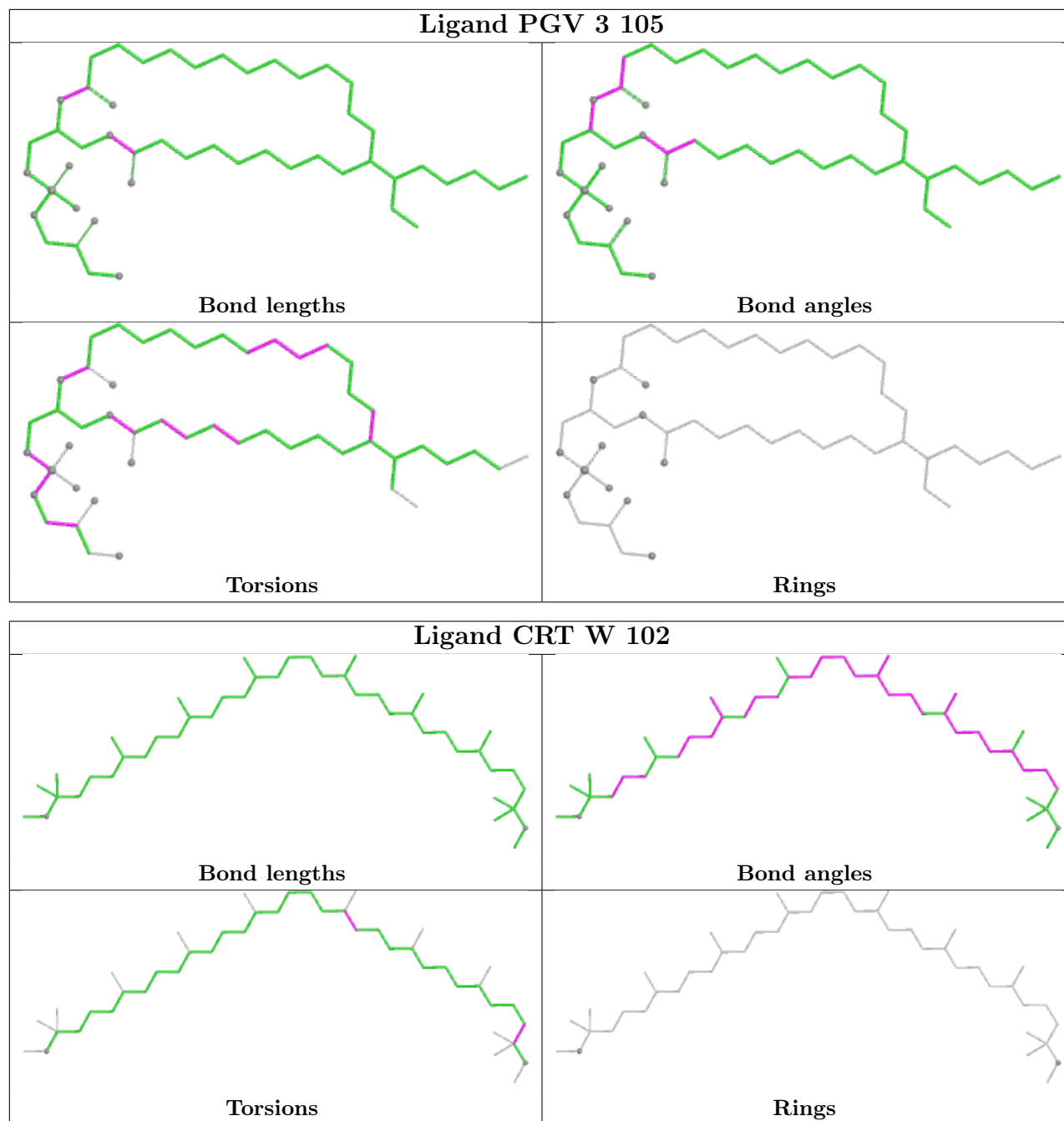
Bond angles

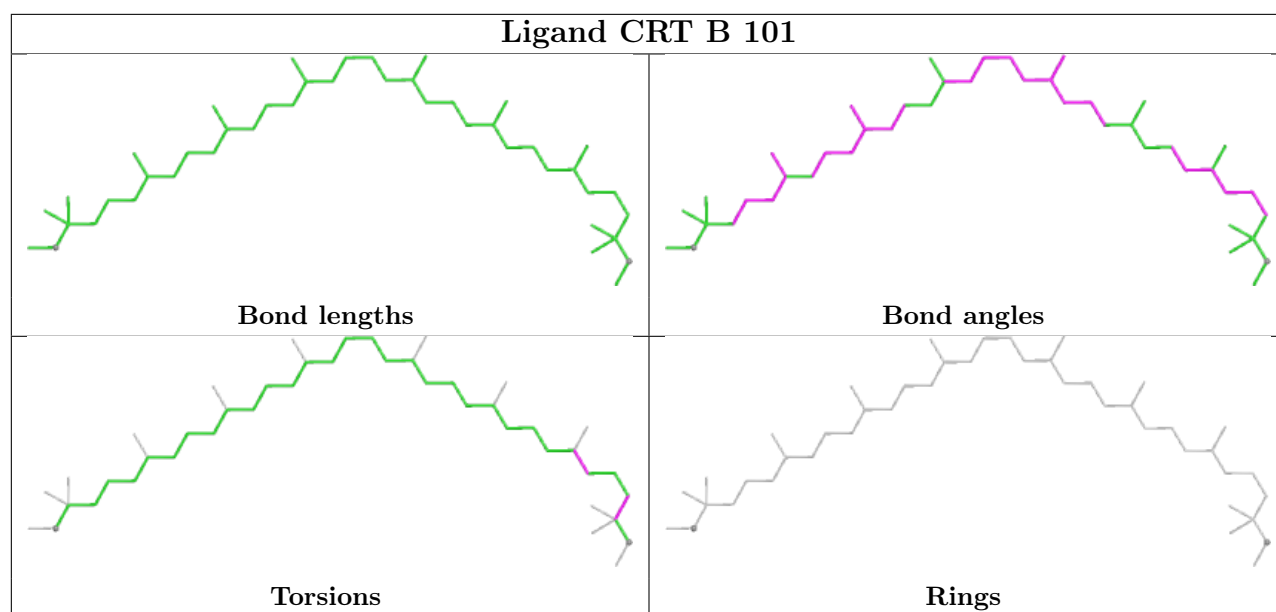


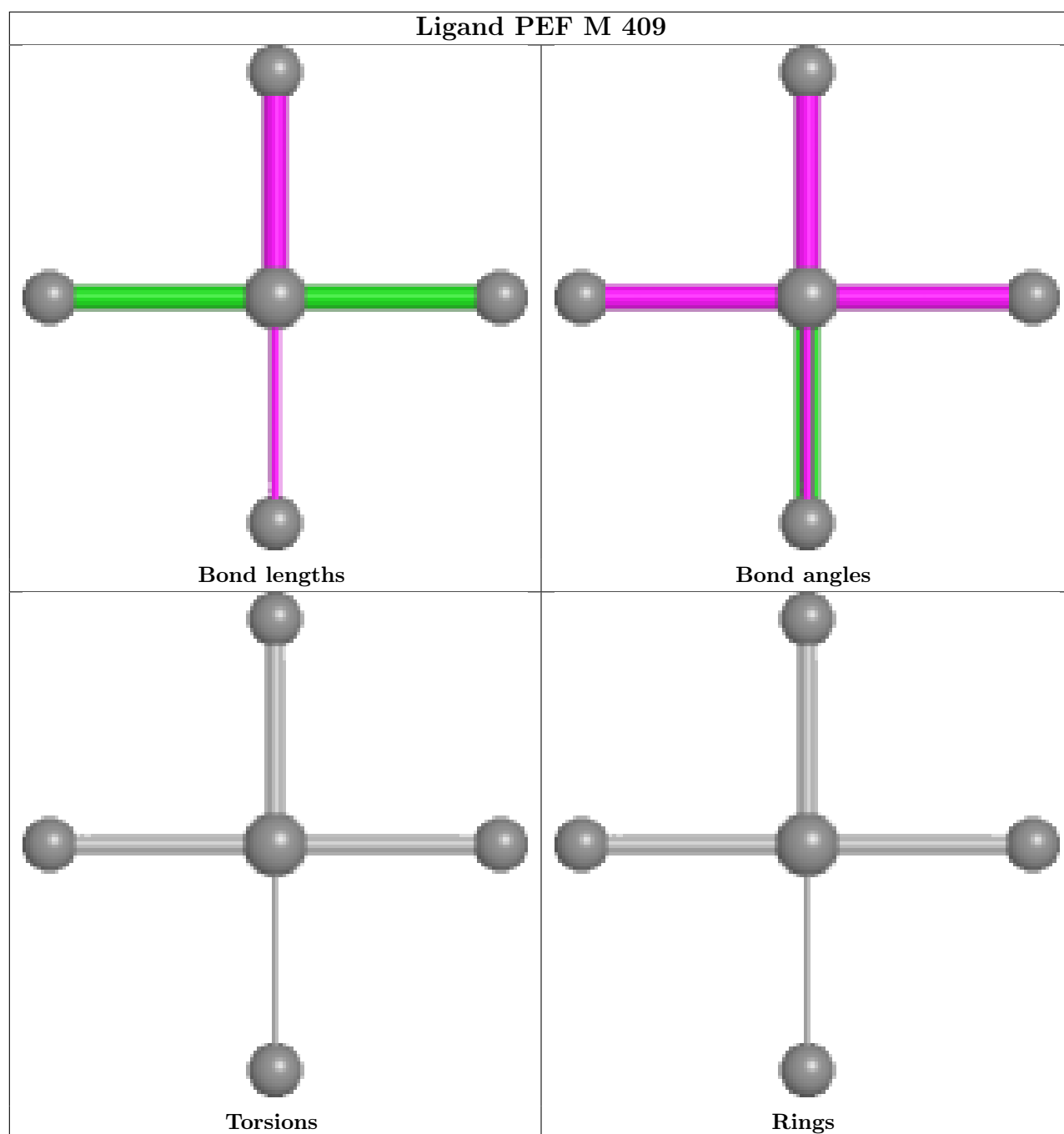
Torsions

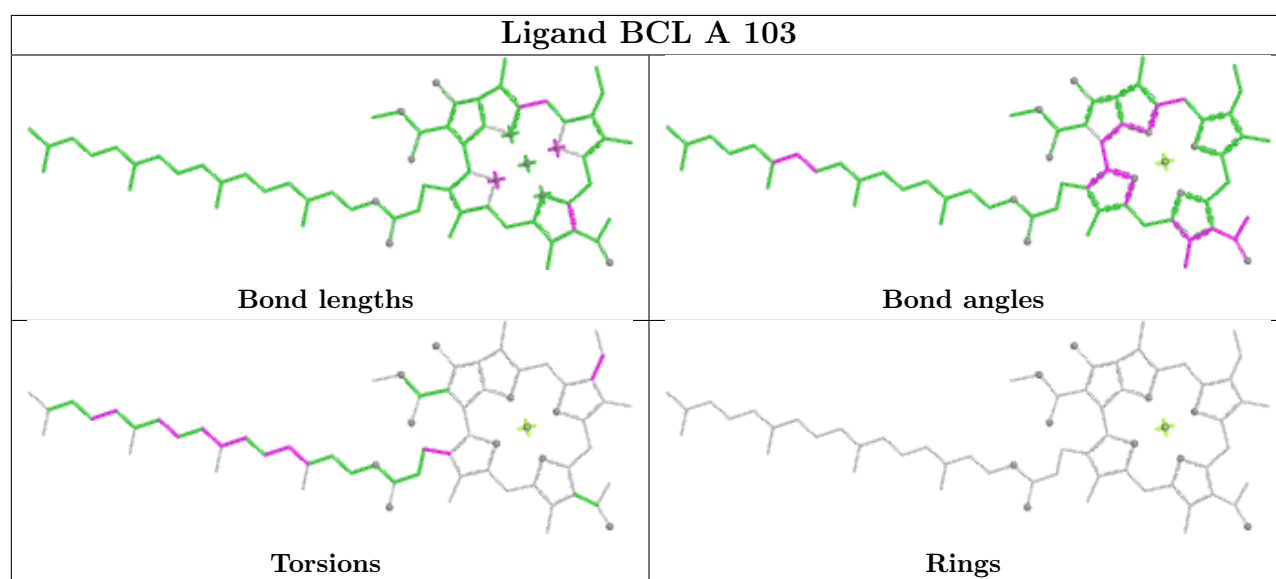
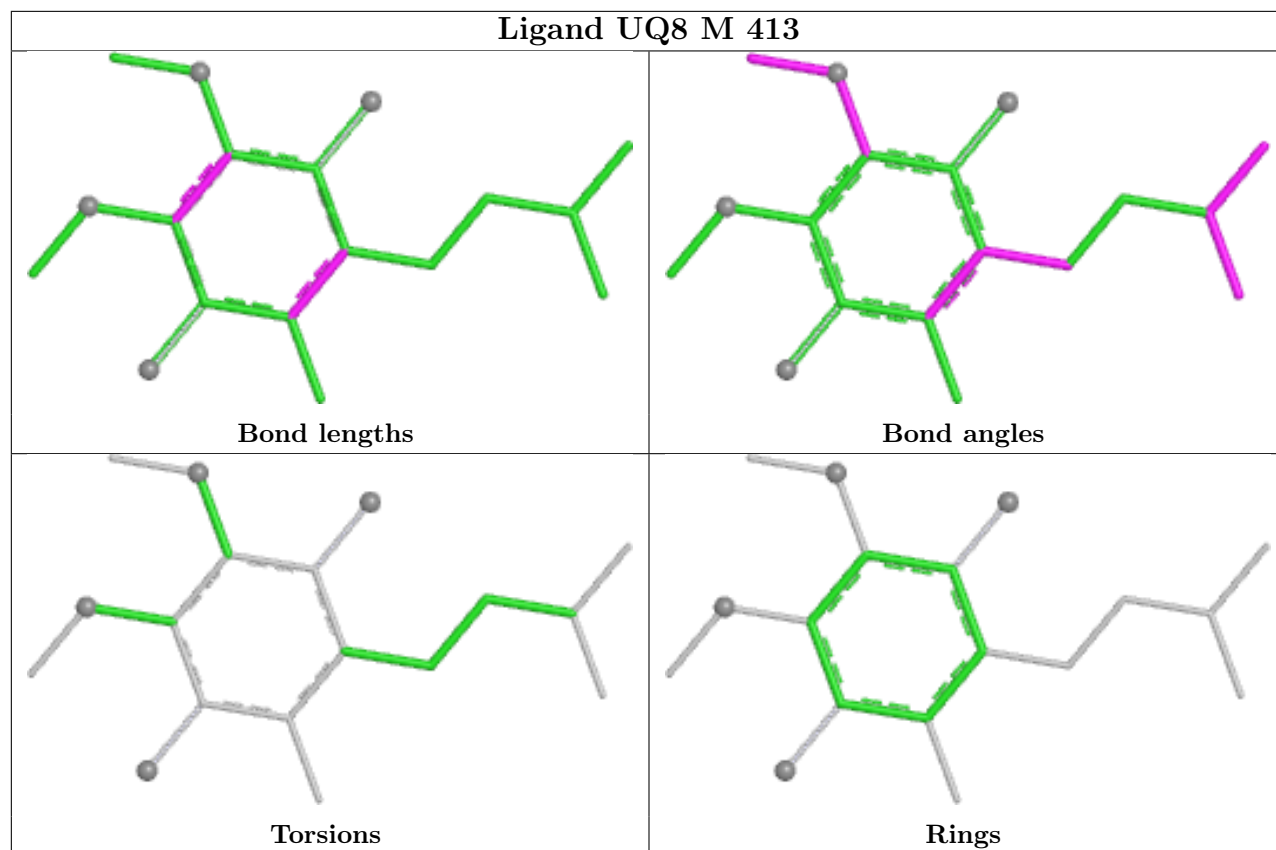


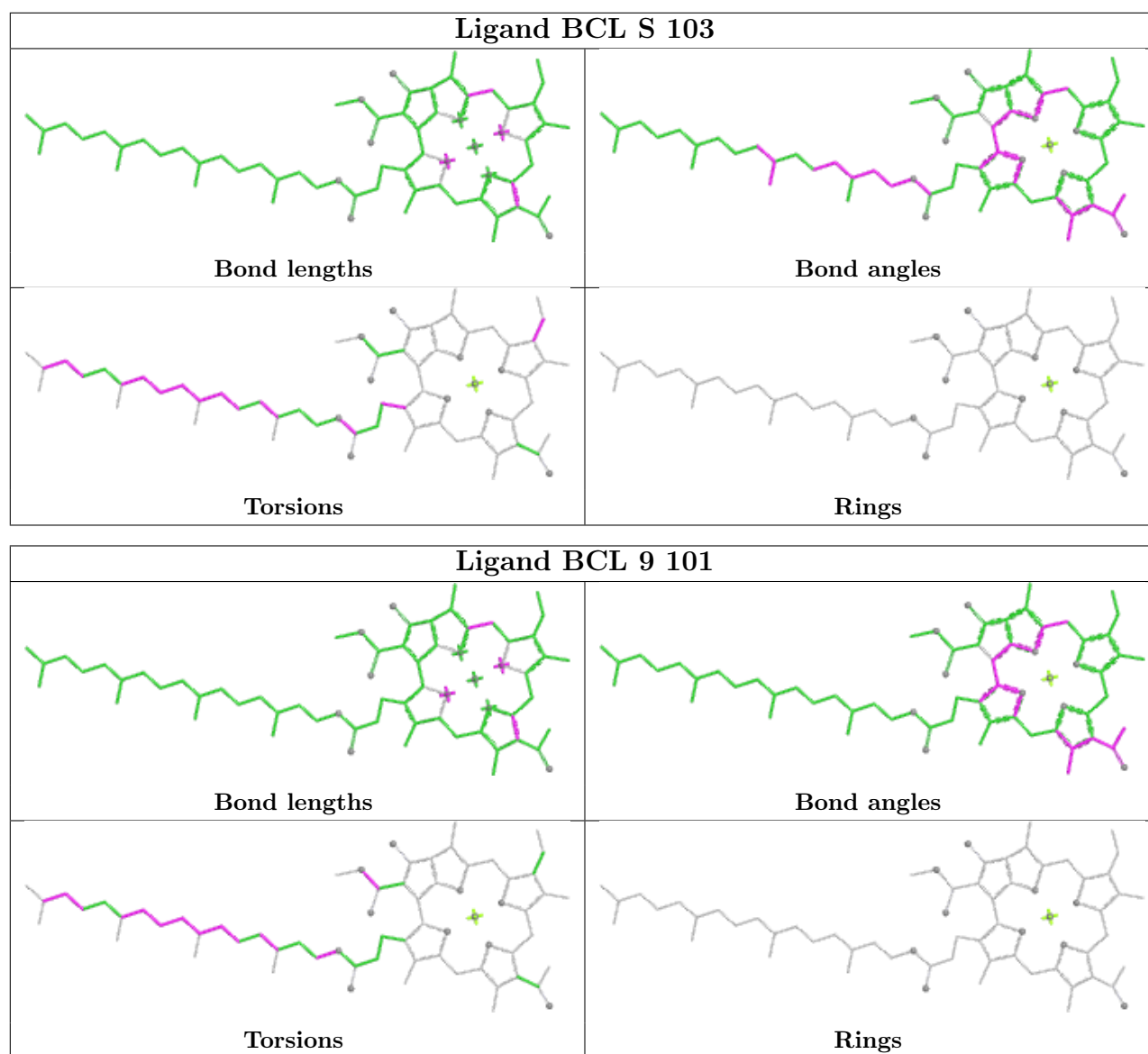
Rings

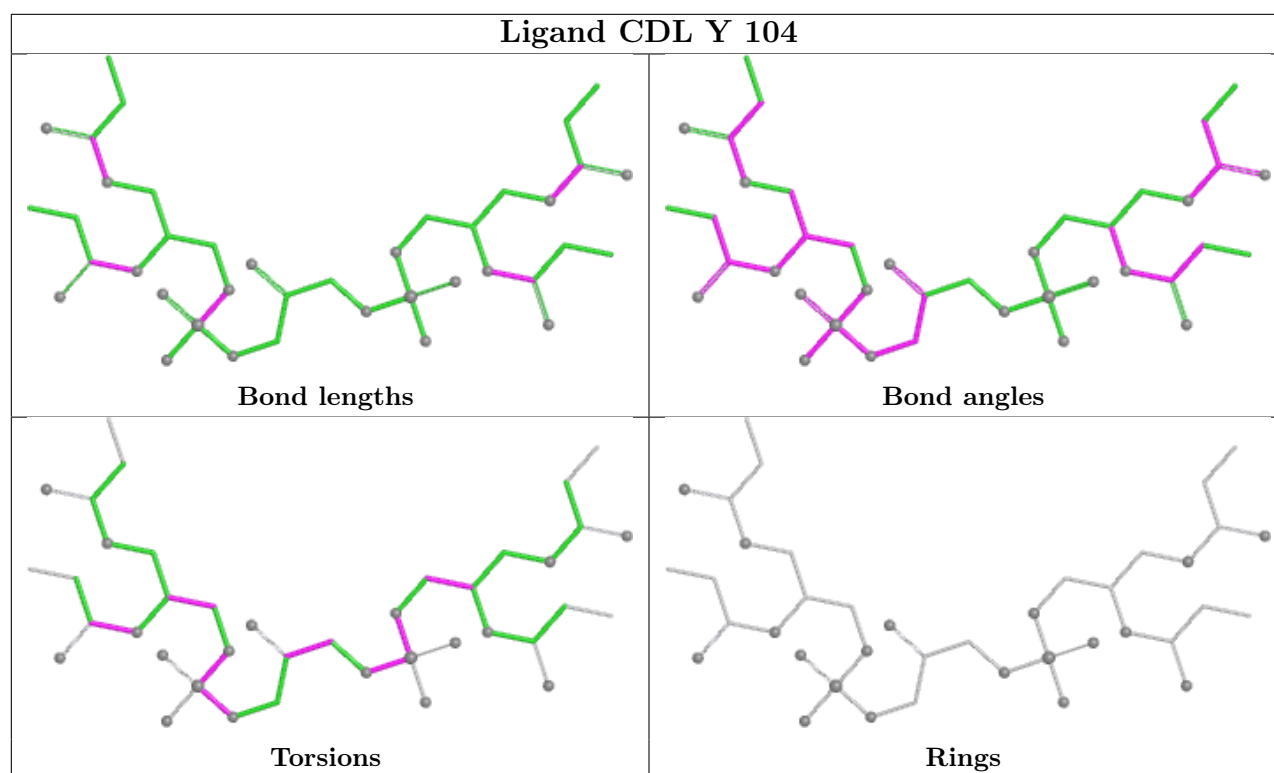


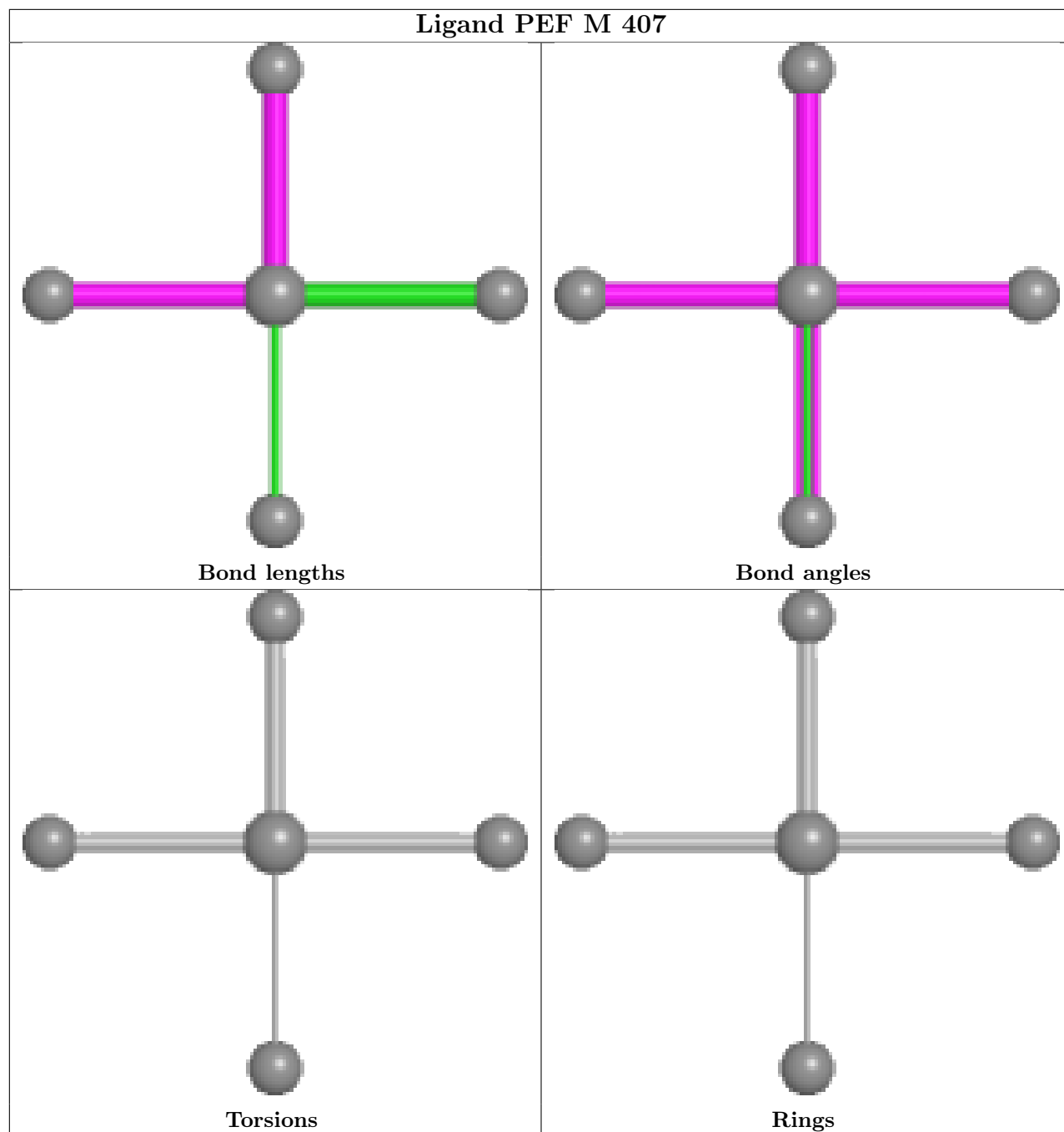


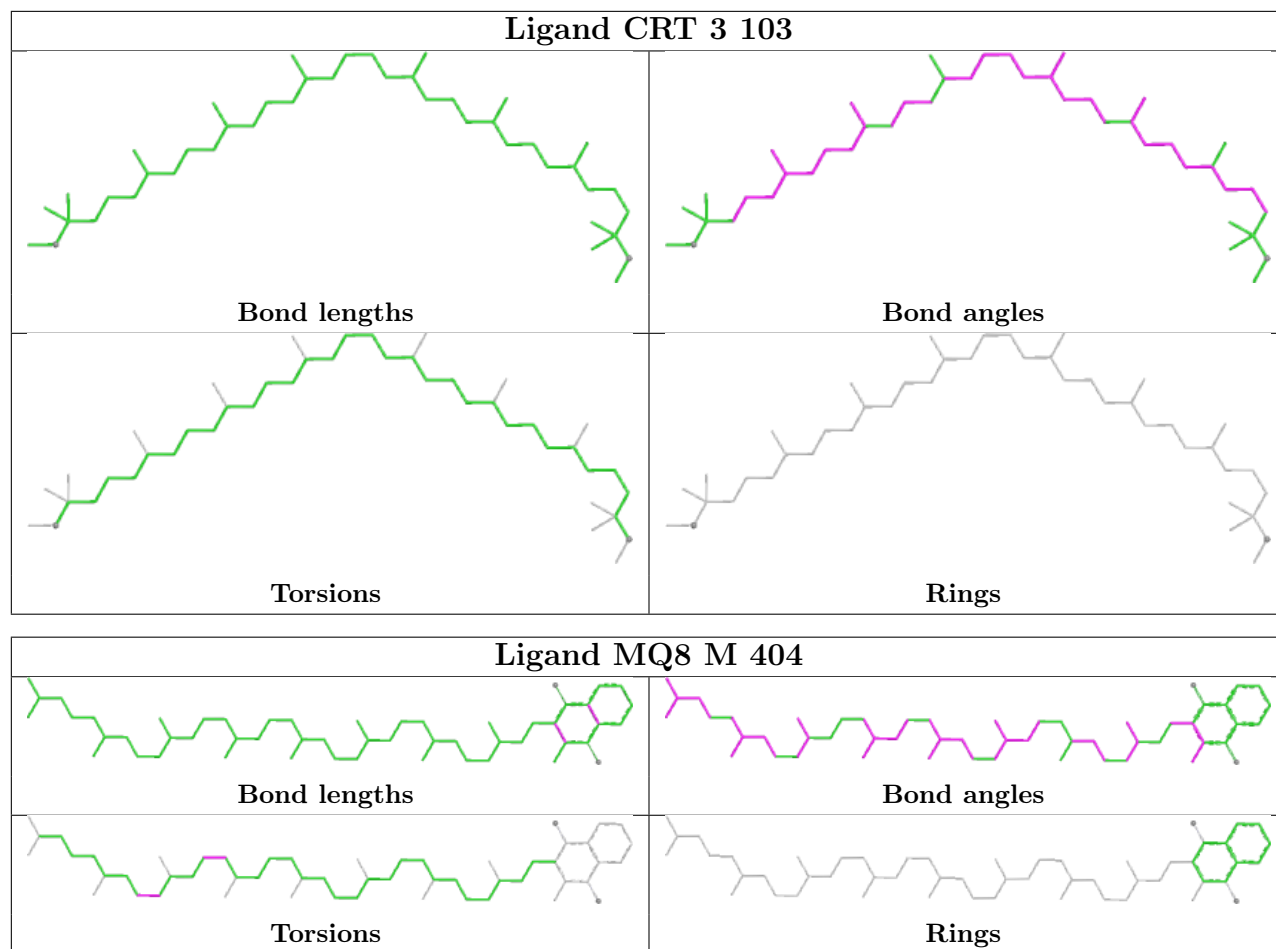


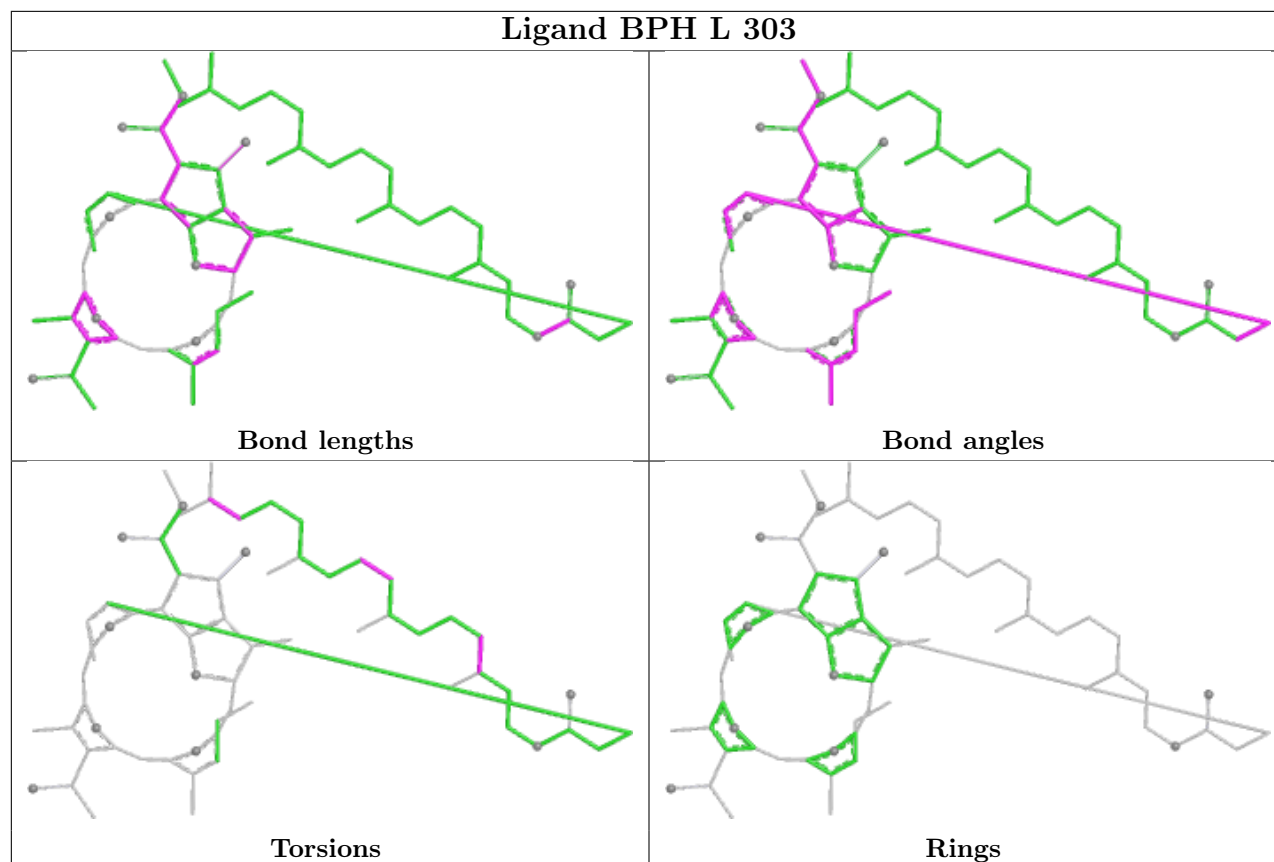












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 311/311 (100%) | -0.25  | 4 (1%) 75 67 | 71, 98, 140, 179      | 0      |
| 2   | L     | 280/281 (99%)  | -0.22  | 6 (2%) 63 54 | 64, 93, 123, 156      | 1 (0%) |
| 3   | M     | 318/325 (97%)  | -0.33  | 4 (1%) 75 67 | 57, 94, 119, 178      | 2 (0%) |
| 4   | H     | 255/259 (98%)  | -0.14  | 5 (1%) 65 56 | 62, 117, 153, 208     | 2 (0%) |
| 5   | 1     | 56/61 (91%)    | -0.29  | 2 (3%) 46 38 | 97, 126, 177, 195     | 0      |
| 5   | 3     | 56/61 (91%)    | -0.29  | 0 100 100    | 82, 128, 177, 199     | 1 (1%) |
| 5   | 5     | 54/61 (88%)    | -0.16  | 3 (5%) 30 23 | 101, 132, 199, 226    | 0      |
| 5   | 7     | 57/61 (93%)    | 0.06   | 1 (1%) 67 59 | 101, 147, 221, 254    | 0      |
| 5   | 9     | 57/61 (93%)    | -0.19  | 1 (1%) 67 59 | 108, 131, 219, 251    | 0      |
| 5   | A     | 54/61 (88%)    | -0.16  | 1 (1%) 66 58 | 110, 133, 174, 191    | 0      |
| 5   | D     | 55/61 (90%)    | -0.21  | 0 100 100    | 74, 129, 192, 206     | 1 (1%) |
| 5   | F     | 55/61 (90%)    | -0.10  | 0 100 100    | 82, 135, 180, 190     | 1 (1%) |
| 5   | I     | 57/61 (93%)    | -0.14  | 1 (1%) 67 59 | 72, 137, 191, 214     | 1 (1%) |
| 5   | K     | 57/61 (93%)    | 0.12   | 2 (3%) 47 38 | 108, 132, 181, 185    | 0      |
| 5   | O     | 56/61 (91%)    | -0.09  | 0 100 100    | 71, 136, 173, 188     | 1 (1%) |
| 5   | Q     | 57/61 (93%)    | -0.15  | 1 (1%) 67 59 | 98, 125, 196, 238     | 0      |
| 5   | S     | 56/61 (91%)    | -0.05  | 1 (1%) 67 59 | 56, 129, 205, 221     | 3 (5%) |
| 5   | U     | 58/61 (95%)    | -0.30  | 0 100 100    | 96, 126, 199, 214     | 0      |
| 5   | W     | 56/61 (91%)    | -0.30  | 2 (3%) 46 38 | 94, 131, 174, 211     | 0      |
| 5   | Y     | 57/61 (93%)    | -0.29  | 3 (5%) 32 25 | 93, 121, 215, 248     | 0      |
| 6   | 0     | 43/47 (91%)    | -0.33  | 0 100 100    | 137, 155, 181, 190    | 0      |
| 6   | 2     | 41/47 (87%)    | -0.47  | 0 100 100    | 121, 147, 174, 178    | 0      |
| 6   | 4     | 42/47 (89%)    | -0.46  | 0 100 100    | 125, 153, 188, 200    | 0      |
| 6   | 6     | 42/47 (89%)    | -0.22  | 0 100 100    | 134, 160, 235, 254    | 0      |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 6   | 8     | 41/47 (87%)     | -0.41  | 1 (2%) 59 50  | 124, 157, 227, 310    | 0       |
| 6   | B     | 42/47 (89%)     | -0.28  | 1 (2%) 59 50  | 132, 153, 177, 204    | 0       |
| 6   | E     | 38/47 (80%)     | -0.26  | 0 100 100     | 132, 150, 168, 170    | 0       |
| 6   | G     | 42/47 (89%)     | -0.38  | 0 100 100     | 132, 154, 180, 191    | 0       |
| 6   | J     | 42/47 (89%)     | -0.29  | 0 100 100     | 130, 152, 185, 201    | 0       |
| 6   | N     | 42/47 (89%)     | -0.19  | 1 (2%) 59 50  | 135, 147, 168, 180    | 0       |
| 6   | P     | 42/47 (89%)     | -0.33  | 0 100 100     | 126, 144, 170, 184    | 0       |
| 6   | R     | 41/47 (87%)     | -0.45  | 0 100 100     | 128, 141, 154, 158    | 0       |
| 6   | T     | 43/47 (91%)     | -0.26  | 1 (2%) 61 52  | 128, 151, 173, 185    | 0       |
| 6   | V     | 42/47 (89%)     | -0.35  | 0 100 100     | 122, 154, 203, 239    | 0       |
| 6   | X     | 41/47 (87%)     | -0.35  | 0 100 100     | 119, 146, 175, 186    | 0       |
| 6   | Z     | 40/47 (85%)     | -0.40  | 0 100 100     | 123, 146, 177, 192    | 0       |
| 7   | b     | 83/83 (100%)    | 0.28   | 2 (2%) 59 50  | 116, 154, 194, 233    | 0       |
| All | All   | 2809/2987 (94%) | -0.22  | 43 (1%) 72 64 | 56, 126, 182, 310     | 13 (0%) |

All (43) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | Y     | 17  | PRO  | 3.7  |
| 5   | 7     | 21  | LEU  | 3.6  |
| 1   | C     | 120 | ASP  | 3.5  |
| 4   | H     | 61  | LEU  | 3.2  |
| 5   | 5     | 47  | LEU  | 3.2  |
| 5   | Q     | 21  | LEU  | 3.1  |
| 5   | W     | 25  | VAL  | 3.0  |
| 2   | L     | 207 | THR  | 3.0  |
| 7   | b     | 14  | ALA  | 2.9  |
| 3   | M     | 55  | LEU  | 2.8  |
| 4   | H     | 138 | VAL  | 2.8  |
| 5   | Y     | 21  | LEU  | 2.8  |
| 7   | b     | 12  | PRO  | 2.8  |
| 5   | K     | 3   | THR  | 2.7  |
| 1   | C     | 140 | ASP  | 2.7  |
| 5   | I     | 47  | LEU  | 2.6  |
| 5   | 5     | 58  | LEU  | 2.6  |
| 4   | H     | 146 | GLU  | 2.6  |
| 1   | C     | 162 | PRO  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | 5     | 21  | LEU  | 2.6  |
| 5   | A     | 13  | LEU  | 2.5  |
| 2   | L     | 169 | VAL  | 2.5  |
| 6   | N     | 21  | PHE  | 2.5  |
| 2   | L     | 166 | VAL  | 2.4  |
| 1   | C     | 313 | ALA  | 2.4  |
| 2   | L     | 206 | VAL  | 2.3  |
| 6   | T     | 34  | ILE  | 2.3  |
| 5   | Y     | 59  | GLY  | 2.3  |
| 4   | H     | 12  | ALA  | 2.3  |
| 5   | 1     | 21  | LEU  | 2.3  |
| 3   | M     | 319 | THR  | 2.3  |
| 5   | K     | 30  | VAL  | 2.3  |
| 4   | H     | 194 | LEU  | 2.2  |
| 5   | S     | 39  | VAL  | 2.2  |
| 3   | M     | 23  | LEU  | 2.2  |
| 5   | 9     | 21  | LEU  | 2.2  |
| 6   | B     | 10  | THR  | 2.1  |
| 3   | M     | 81  | TRP  | 2.1  |
| 6   | 8     | 6   | LEU  | 2.1  |
| 2   | L     | 82  | TYR  | 2.0  |
| 5   | 1     | 44  | LEU  | 2.0  |
| 2   | L     | 142 | PHE  | 2.0  |
| 5   | W     | 14  | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms   | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|---------|------|------|-----------------------------|-------|
| 21  | PEF  | H     | 302 | 5/47    | 0.41 | 0.08 | 202,203,203,204             | 0     |
| 21  | PEF  | W     | 106 | 5/47    | 0.45 | 0.08 | 242,243,244,246             | 0     |
| 21  | PEF  | M     | 407 | 5/47    | 0.67 | 0.06 | 181,183,184,187             | 0     |
| 20  | CDL  | D     | 104 | 40/100  | 0.69 | 0.14 | 190,200,207,209             | 0     |
| 21  | PEF  | I     | 103 | 5/47    | 0.70 | 0.08 | 158,159,160,160             | 0     |
| 21  | PEF  | M     | 409 | 5/47    | 0.70 | 0.10 | 113,113,114,115             | 0     |
| 21  | PEF  | W     | 105 | 5/47    | 0.71 | 0.14 | 185,190,191,192             | 0     |
| 20  | CDL  | Y     | 104 | 40/100  | 0.73 | 0.13 | 187,196,210,210             | 0     |
| 12  | PGV  | 1     | 105 | 31/51   | 0.75 | 0.15 | 105,145,149,155             | 0     |
| 20  | CDL  | 1     | 104 | 13/100  | 0.75 | 0.11 | 153,157,163,166             | 0     |
| 15  | UQ8  | L     | 311 | 18/53   | 0.78 | 0.15 | 135,141,147,150             | 0     |
| 16  | SO4  | L     | 306 | 5/5     | 0.79 | 0.06 | 178,180,180,181             | 0     |
| 15  | UQ8  | M     | 413 | 18/53   | 0.81 | 0.13 | 154,157,166,170             | 0     |
| 21  | PEF  | 3     | 104 | 5/47    | 0.81 | 0.10 | 207,209,211,213             | 0     |
| 22  | LMT  | H     | 304 | 35/35   | 0.81 | 0.11 | 95,142,151,155              | 0     |
| 21  | PEF  | K     | 104 | 27/47   | 0.82 | 0.15 | 119,140,143,145             | 0     |
| 21  | PEF  | 1     | 103 | 5/47    | 0.82 | 0.07 | 175,175,177,179             | 0     |
| 10  | GOL  | C     | 506 | 6/6     | 0.83 | 0.10 | 139,143,147,148             | 0     |
| 20  | CDL  | U     | 104 | 62/100  | 0.83 | 0.13 | 146,181,209,216             | 0     |
| 12  | PGV  | 9     | 104 | 33/51   | 0.84 | 0.15 | 136,155,166,169             | 0     |
| 21  | PEF  | M     | 408 | 5/47    | 0.85 | 0.07 | 131,134,135,137             | 0     |
| 12  | PGV  | L     | 308 | 44/51   | 0.86 | 0.13 | 100,135,148,149             | 0     |
| 20  | CDL  | D     | 105 | 64/100  | 0.86 | 0.11 | 130,142,153,159             | 0     |
| 20  | CDL  | S     | 104 | 75/100  | 0.87 | 0.15 | 120,157,196,209             | 0     |
| 12  | PGV  | D     | 106 | 35/51   | 0.87 | 0.10 | 115,135,159,167             | 0     |
| 22  | LMT  | M     | 414 | 35/35   | 0.87 | 0.10 | 128,162,179,183             | 0     |
| 12  | PGV  | L     | 307 | 43/51   | 0.87 | 0.14 | 98,150,173,178              | 0     |
| 19  | CRT  | G     | 101 | 44/44   | 0.88 | 0.16 | 113,138,160,162             | 0     |
| 19  | CRT  | 0     | 101 | 44/44   | 0.88 | 0.17 | 109,135,168,170             | 0     |
| 12  | PGV  | H     | 303 | 36/51   | 0.88 | 0.10 | 86,123,130,131              | 0     |
| 12  | PGV  | 3     | 105 | 51/51   | 0.88 | 0.14 | 99,130,187,191              | 0     |
| 12  | PGV  | C     | 508 | 21/51   | 0.88 | 0.14 | 103,127,138,143             | 0     |
| 15  | UQ8  | L     | 309 | 53/53   | 0.89 | 0.15 | 113,137,188,192             | 0     |
| 20  | CDL  | M     | 406 | 100/100 | 0.89 | 0.12 | 92,119,155,158              | 0     |
| 19  | CRT  | O     | 103 | 44/44   | 0.89 | 0.14 | 107,121,149,152             | 0     |
| 19  | CRT  | 8     | 101 | 44/44   | 0.89 | 0.15 | 127,136,180,182             | 0     |
| 20  | CDL  | M     | 412 | 39/100  | 0.90 | 0.08 | 81,113,129,135              | 0     |
| 20  | CDL  | H     | 305 | 79/100  | 0.90 | 0.12 | 93,118,143,146              | 0     |
| 19  | CRT  | V     | 101 | 44/44   | 0.90 | 0.15 | 99,129,151,154              | 0     |
| 11  | LHG  | C     | 507 | 9/49    | 0.90 | 0.09 | 84,90,99,100                | 0     |
| 20  | CDL  | O     | 104 | 86/100  | 0.90 | 0.14 | 120,144,155,159             | 0     |
| 19  | CRT  | J     | 101 | 44/44   | 0.90 | 0.14 | 107,135,154,156             | 0     |
| 14  | BPH  | M     | 402 | 65/65   | 0.90 | 0.13 | 75,83,147,154               | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 19  | CRT  | T     | 101 | 44/44 | 0.91 | 0.12 | 103,122,140,142             | 0     |
| 12  | PGV  | M     | 410 | 46/51 | 0.91 | 0.13 | 101,119,128,131             | 0     |
| 19  | CRT  | W     | 102 | 44/44 | 0.91 | 0.15 | 102,126,152,153             | 0     |
| 19  | CRT  | B     | 101 | 44/44 | 0.91 | 0.13 | 116,139,157,158             | 0     |
| 9   | CA   | I     | 102 | 1/1   | 0.91 | 0.06 | 139,139,139,139             | 0     |
| 9   | CA   | F     | 102 | 1/1   | 0.91 | 0.07 | 129,129,129,129             | 0     |
| 19  | CRT  | N     | 101 | 44/44 | 0.91 | 0.13 | 104,128,137,141             | 0     |
| 13  | BCL  | S     | 103 | 66/66 | 0.91 | 0.12 | 106,120,176,189             | 0     |
| 19  | CRT  | P     | 101 | 44/44 | 0.91 | 0.13 | 100,132,147,149             | 0     |
| 15  | UQ8  | L     | 304 | 33/53 | 0.92 | 0.15 | 75,85,129,131               | 0     |
| 12  | PGV  | M     | 411 | 37/51 | 0.92 | 0.10 | 120,151,194,196             | 0     |
| 19  | CRT  | M     | 405 | 44/44 | 0.92 | 0.11 | 72,88,127,129               | 0     |
| 13  | BCL  | S     | 101 | 66/66 | 0.92 | 0.11 | 111,123,163,167             | 0     |
| 13  | BCL  | A     | 101 | 66/66 | 0.93 | 0.11 | 130,139,162,170             | 0     |
| 13  | BCL  | U     | 103 | 66/66 | 0.93 | 0.11 | 113,131,174,185             | 0     |
| 13  | BCL  | 5     | 103 | 66/66 | 0.93 | 0.11 | 116,136,163,167             | 0     |
| 13  | BCL  | 9     | 103 | 66/66 | 0.93 | 0.09 | 113,129,177,186             | 0     |
| 9   | CA   | Y     | 102 | 1/1   | 0.93 | 0.06 | 115,115,115,115             | 0     |
| 19  | CRT  | 2     | 101 | 44/44 | 0.93 | 0.13 | 113,129,154,157             | 0     |
| 19  | CRT  | 3     | 103 | 44/44 | 0.93 | 0.13 | 116,127,160,162             | 0     |
| 19  | CRT  | 4     | 101 | 44/44 | 0.93 | 0.12 | 101,131,161,164             | 0     |
| 13  | BCL  | F     | 101 | 66/66 | 0.94 | 0.10 | 119,131,162,173             | 0     |
| 13  | BCL  | 9     | 101 | 66/66 | 0.94 | 0.10 | 126,133,177,179             | 0     |
| 13  | BCL  | Q     | 103 | 66/66 | 0.94 | 0.10 | 105,123,170,181             | 0     |
| 9   | CA   | 9     | 102 | 1/1   | 0.94 | 0.09 | 120,120,120,120             | 0     |
| 9   | CA   | 1     | 102 | 1/1   | 0.94 | 0.05 | 107,107,107,107             | 0     |
| 13  | BCL  | U     | 101 | 66/66 | 0.94 | 0.09 | 102,122,167,172             | 0     |
| 19  | CRT  | Z     | 101 | 44/44 | 0.94 | 0.13 | 91,133,166,169              | 0     |
| 15  | UQ8  | L     | 310 | 33/53 | 0.94 | 0.10 | 118,126,138,139             | 0     |
| 13  | BCL  | A     | 103 | 66/66 | 0.94 | 0.11 | 114,124,178,185             | 0     |
| 13  | BCL  | W     | 101 | 66/66 | 0.94 | 0.11 | 105,127,170,178             | 0     |
| 13  | BCL  | W     | 104 | 66/66 | 0.94 | 0.09 | 112,123,162,167             | 0     |
| 18  | MQ8  | M     | 404 | 53/53 | 0.94 | 0.11 | 84,88,161,163               | 0     |
| 13  | BCL  | Y     | 101 | 66/66 | 0.94 | 0.10 | 101,118,165,167             | 0     |
| 19  | CRT  | A     | 104 | 44/44 | 0.94 | 0.10 | 110,126,154,156             | 0     |
| 13  | BCL  | 1     | 101 | 66/66 | 0.94 | 0.10 | 106,118,161,165             | 0     |
| 13  | BCL  | 2     | 102 | 66/66 | 0.94 | 0.12 | 104,125,164,174             | 0     |
| 13  | BCL  | 3     | 101 | 66/66 | 0.94 | 0.12 | 108,131,180,185             | 0     |
| 9   | CA   | 3     | 102 | 1/1   | 0.95 | 0.05 | 121,121,121,121             | 0     |
| 13  | BCL  | M     | 401 | 66/66 | 0.95 | 0.10 | 61,80,89,92                 | 0     |
| 9   | CA   | 5     | 102 | 1/1   | 0.95 | 0.06 | 118,118,118,118             | 0     |
| 9   | CA   | Q     | 102 | 1/1   | 0.95 | 0.07 | 116,116,116,116             | 0     |

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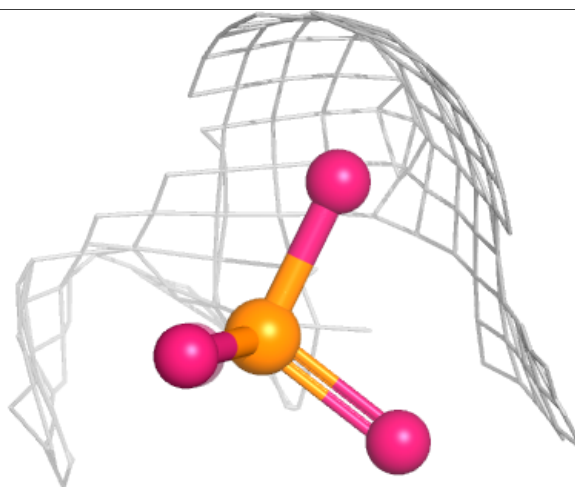
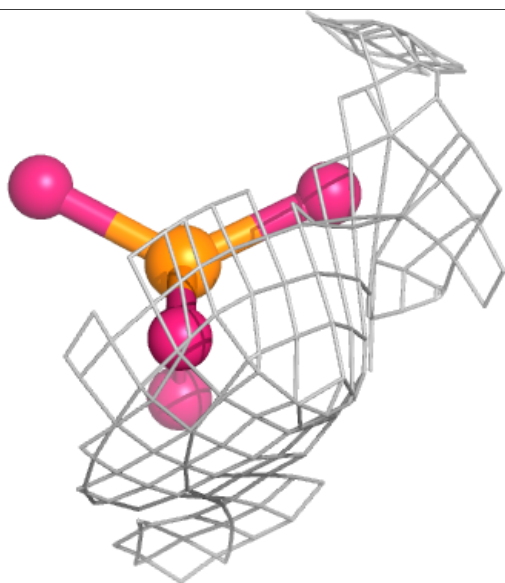
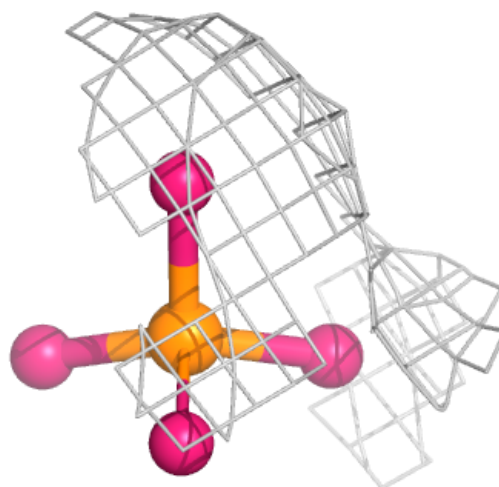
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 13  | BCL  | D     | 101 | 66/66 | 0.95 | 0.10 | 109,130,160,165            | 0     |
| 13  | BCL  | Y     | 103 | 66/66 | 0.95 | 0.09 | 109,120,159,166            | 0     |
| 9   | CA   | U     | 102 | 1/1   | 0.95 | 0.05 | 112,112,112,112            | 0     |
| 13  | BCL  | I     | 101 | 66/66 | 0.95 | 0.12 | 121,136,176,182            | 0     |
| 13  | BCL  | J     | 102 | 66/66 | 0.95 | 0.10 | 121,137,160,166            | 0     |
| 13  | BCL  | 4     | 102 | 66/66 | 0.95 | 0.09 | 110,131,169,182            | 0     |
| 13  | BCL  | 5     | 101 | 66/66 | 0.95 | 0.10 | 109,128,163,169            | 0     |
| 13  | BCL  | K     | 101 | 66/66 | 0.95 | 0.10 | 123,132,162,174            | 0     |
| 13  | BCL  | 7     | 101 | 61/66 | 0.95 | 0.13 | 121,135,185,188            | 0     |
| 13  | BCL  | K     | 103 | 66/66 | 0.95 | 0.10 | 119,137,170,181            | 0     |
| 13  | BCL  | O     | 101 | 66/66 | 0.95 | 0.10 | 128,137,170,177            | 0     |
| 14  | BPH  | L     | 303 | 65/65 | 0.95 | 0.09 | 68,82,100,103              | 0     |
| 13  | BCL  | P     | 102 | 66/66 | 0.95 | 0.09 | 123,140,185,197            | 0     |
| 13  | BCL  | Q     | 101 | 66/66 | 0.95 | 0.10 | 110,128,174,181            | 0     |
| 9   | CA   | W     | 103 | 1/1   | 0.95 | 0.05 | 105,105,105,105            | 0     |
| 9   | CA   | C     | 505 | 1/1   | 0.95 | 0.14 | 103,103,103,103            | 0     |
| 9   | CA   | A     | 102 | 1/1   | 0.95 | 0.05 | 123,123,123,123            | 0     |
| 9   | CA   | D     | 102 | 1/1   | 0.96 | 0.05 | 127,127,127,127            | 0     |
| 13  | BCL  | D     | 103 | 66/66 | 0.96 | 0.09 | 118,126,164,173            | 0     |
| 13  | BCL  | L     | 301 | 66/66 | 0.96 | 0.08 | 64,80,101,108              | 0     |
| 13  | BCL  | F     | 103 | 66/66 | 0.96 | 0.10 | 123,135,177,188            | 0     |
| 13  | BCL  | L     | 302 | 66/66 | 0.96 | 0.07 | 59,68,90,98                | 0     |
| 13  | BCL  | L     | 305 | 66/66 | 0.96 | 0.09 | 69,80,135,143              | 0     |
| 10  | GOL  | H     | 301 | 6/6   | 0.96 | 0.14 | 107,113,116,117            | 0     |
| 9   | CA   | S     | 102 | 1/1   | 0.96 | 0.07 | 111,111,111,111            | 0     |
| 9   | CA   | K     | 102 | 1/1   | 0.96 | 0.04 | 120,120,120,120            | 0     |
| 13  | BCL  | 7     | 103 | 66/66 | 0.96 | 0.10 | 124,136,182,184            | 0     |
| 9   | CA   | O     | 102 | 1/1   | 0.97 | 0.07 | 121,121,121,121            | 0     |
| 9   | CA   | 7     | 102 | 1/1   | 0.97 | 0.04 | 115,115,115,115            | 0     |
| 23  | SF4  | b     | 101 | 8/8   | 0.97 | 0.04 | 123,152,192,194            | 0     |
| 8   | HEC  | C     | 504 | 43/43 | 0.98 | 0.08 | 74,79,89,92                | 0     |
| 8   | HEC  | C     | 501 | 43/43 | 0.98 | 0.07 | 97,107,117,120             | 0     |
| 8   | HEC  | C     | 502 | 43/43 | 0.98 | 0.09 | 71,88,104,106              | 0     |
| 17  | FE   | M     | 403 | 1/1   | 0.98 | 0.05 | 75,75,75,75                | 0     |
| 8   | HEC  | C     | 503 | 43/43 | 0.98 | 0.09 | 70,80,95,100               | 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.

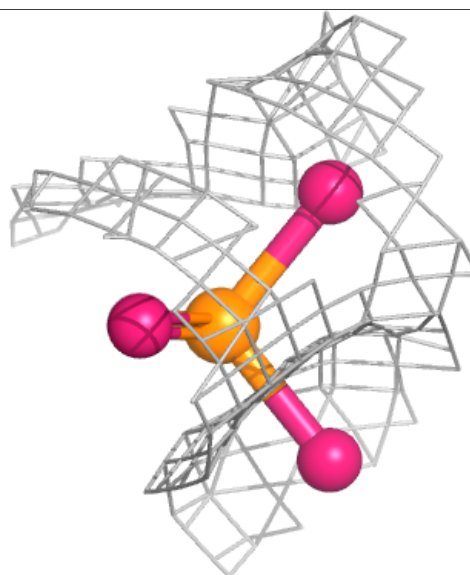
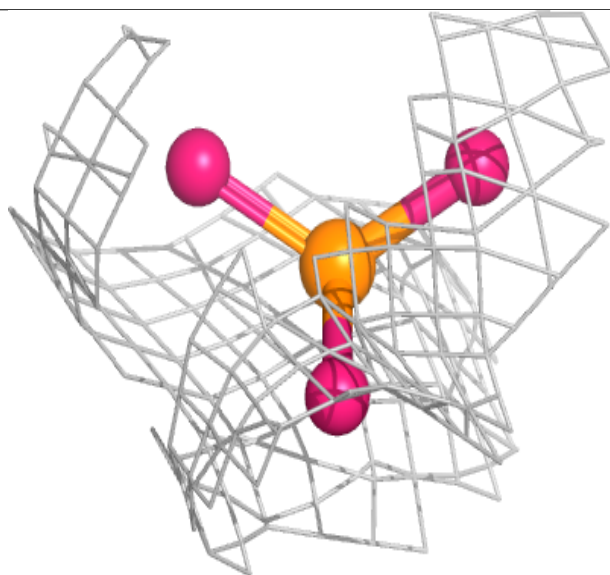
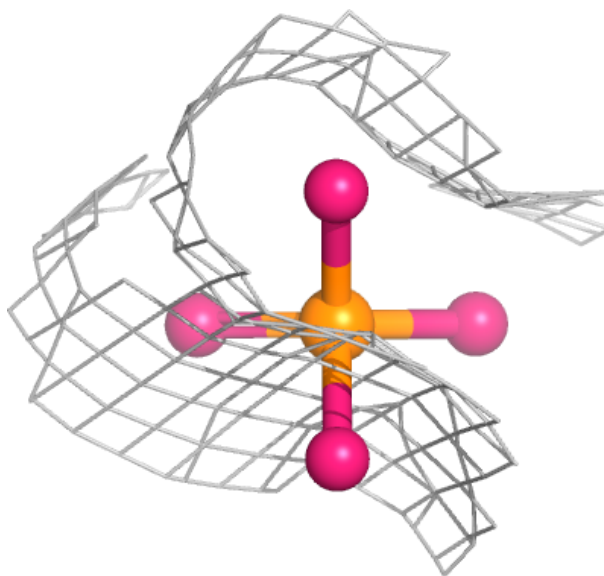
**Electron density around PEF H 302:**

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



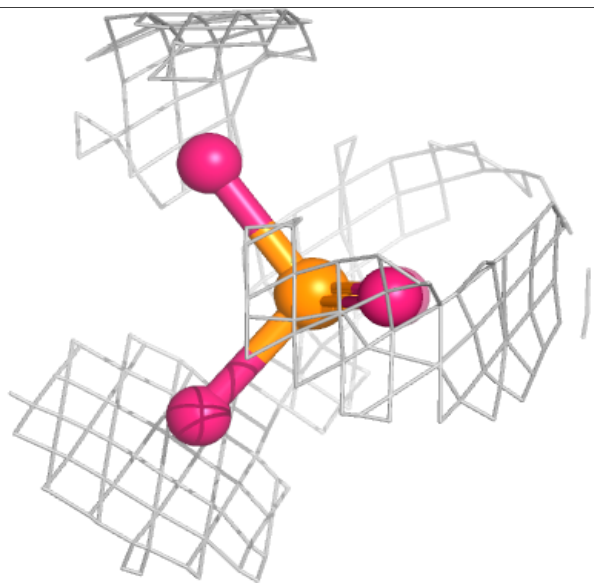
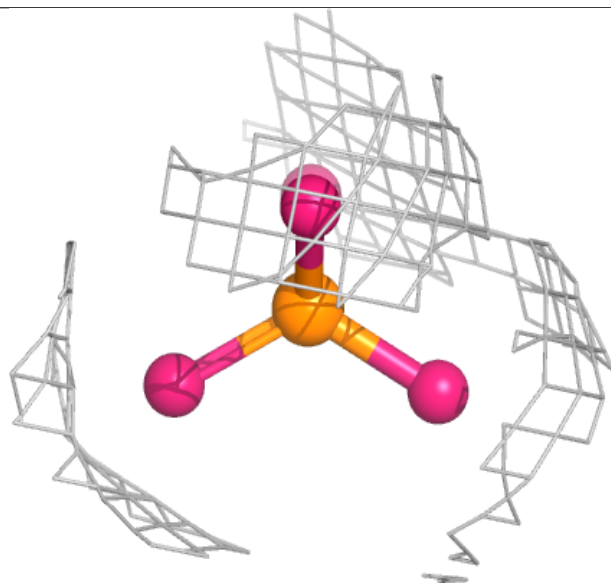
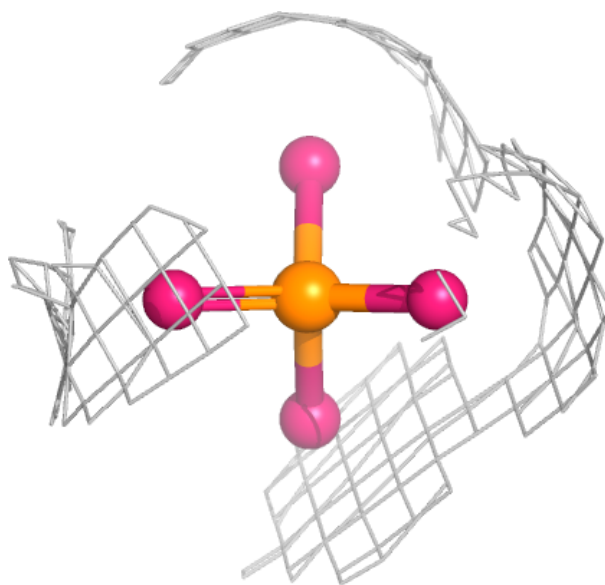
**Electron density around PEF W 106:**

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



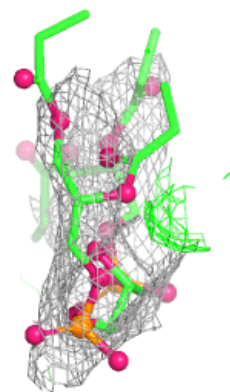
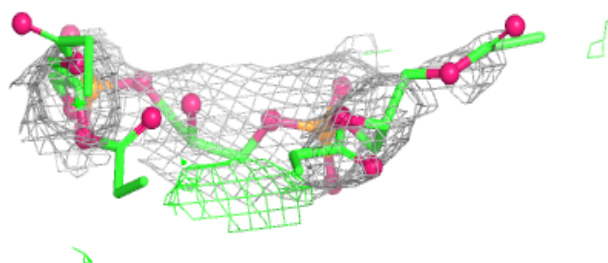
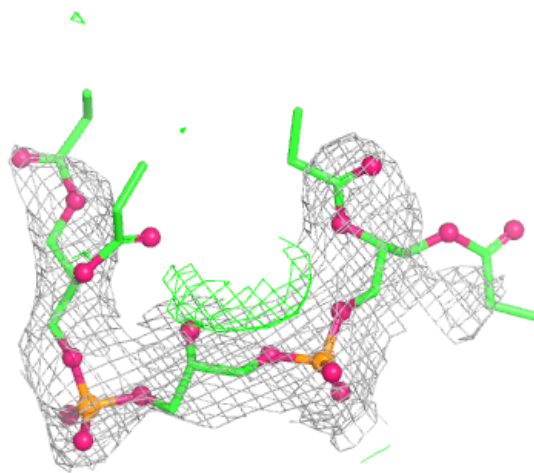
**Electron density around PEF M 407:**

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



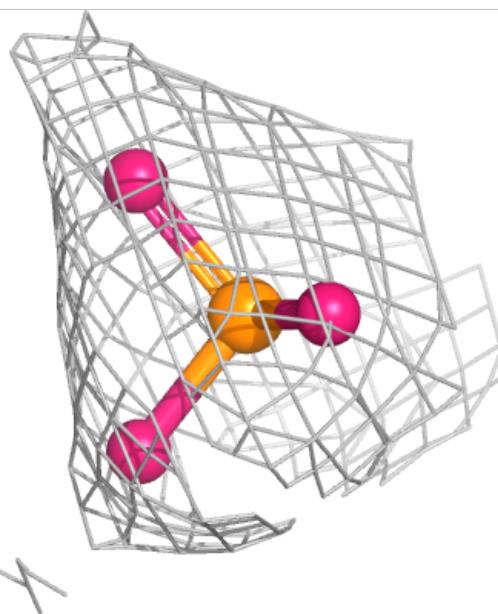
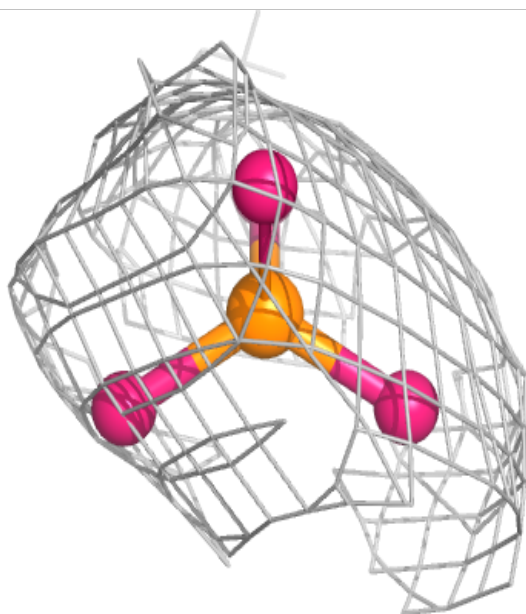
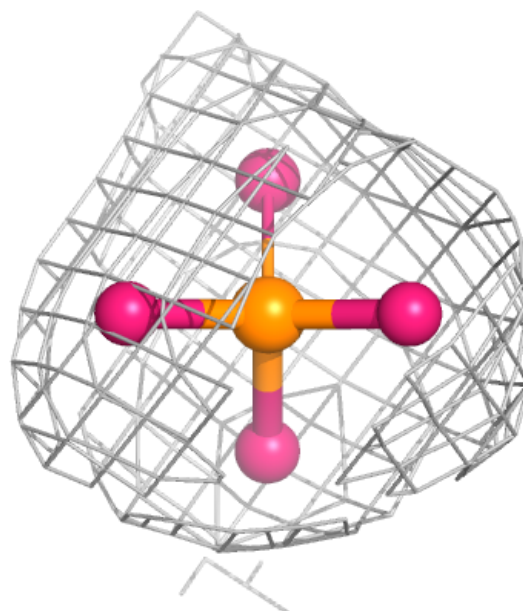
**Electron density around CDL D 104:**

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



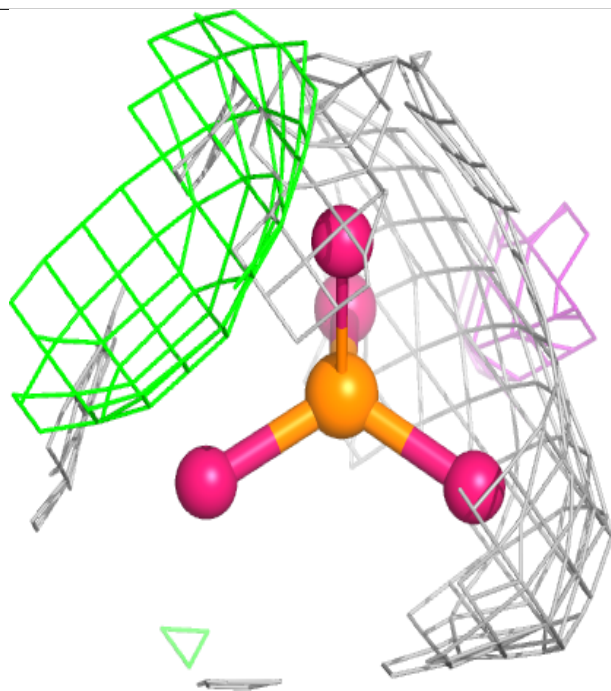
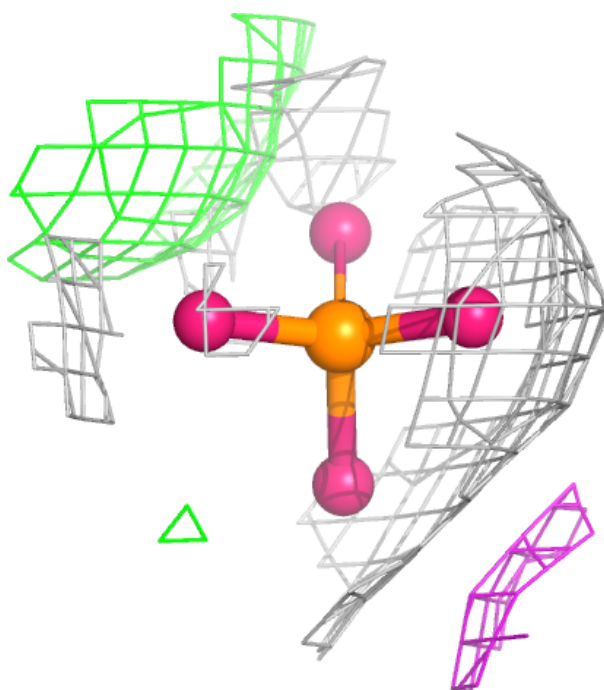
**Electron density around PEF I 103:**

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



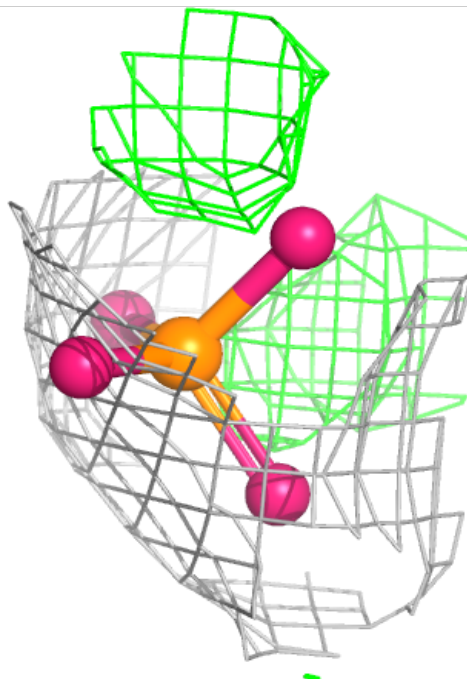
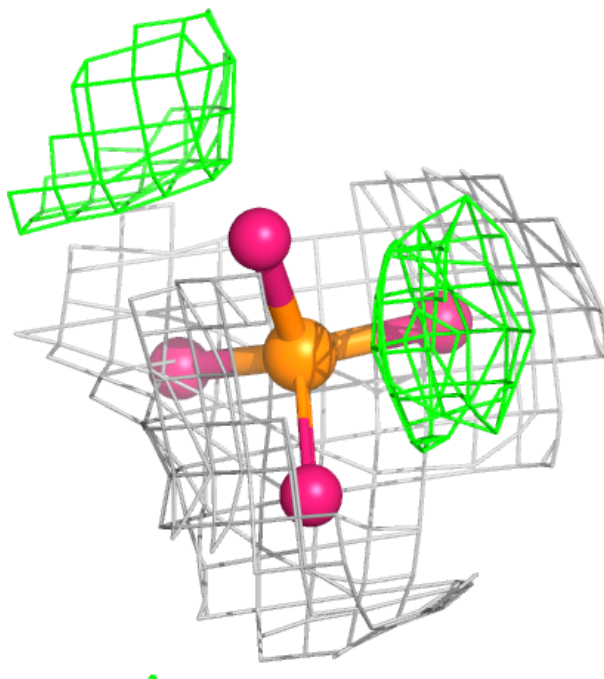
**Electron density around PEF M 409:**

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



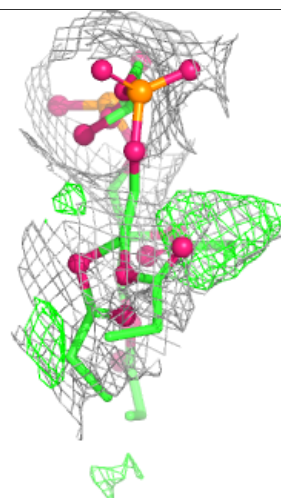
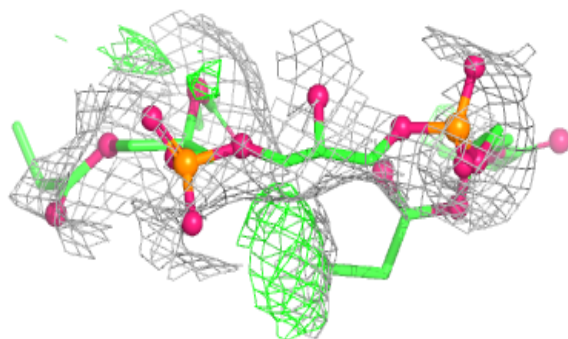
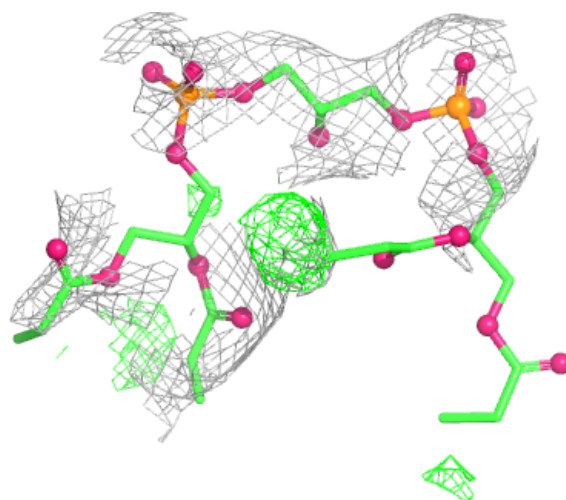
**Electron density around PEF W 105:**

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



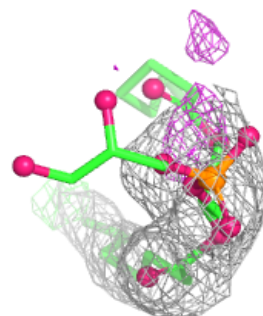
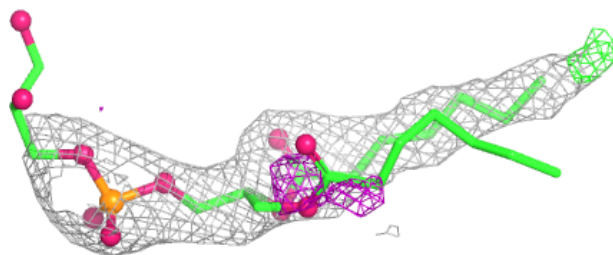
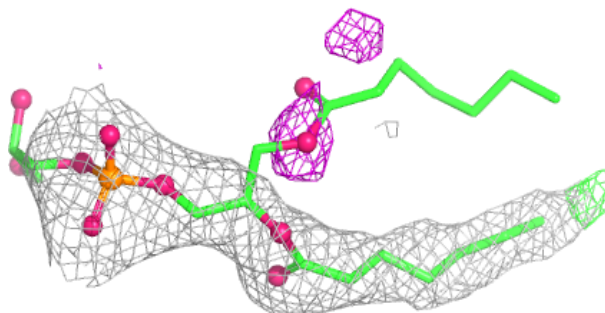
**Electron density around CDL Y 104:**

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



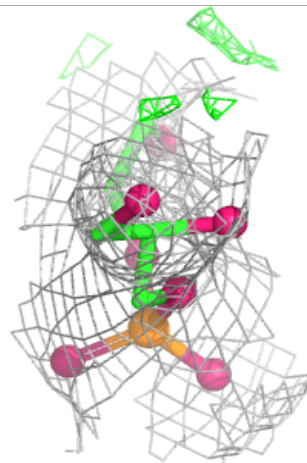
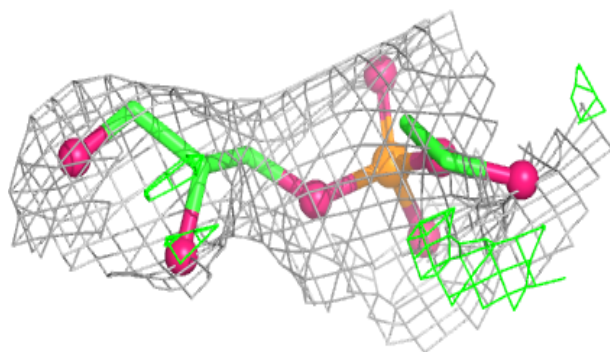
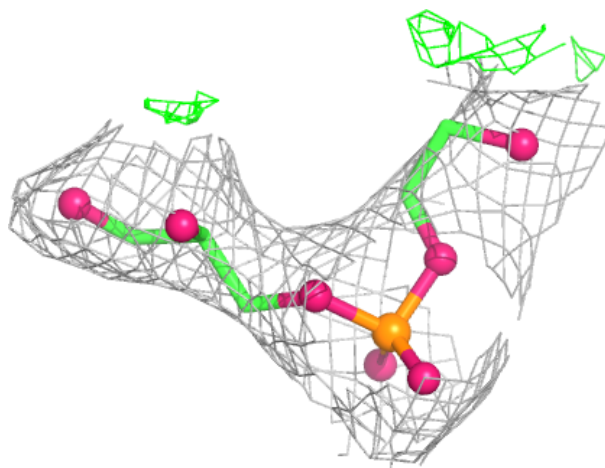
**Electron density around PGV 1 105:**

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



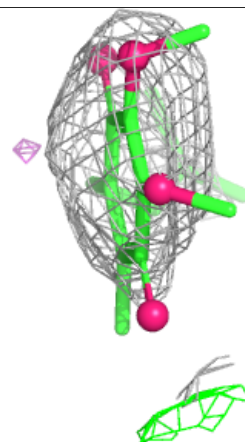
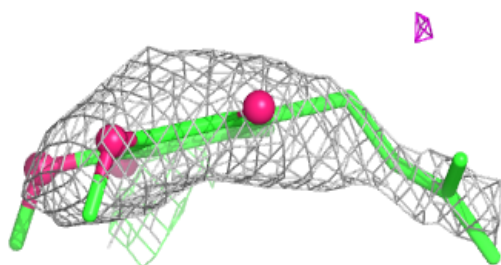
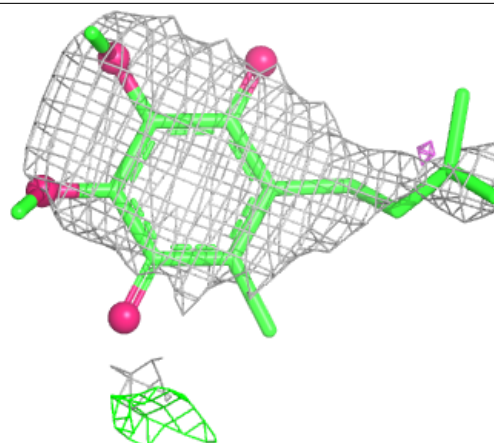
**Electron density around CDL 1 104:**

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



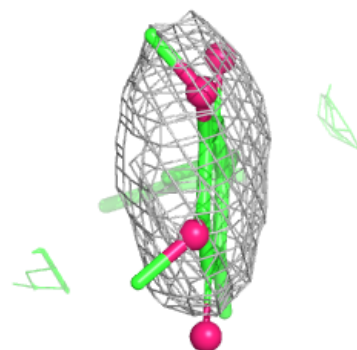
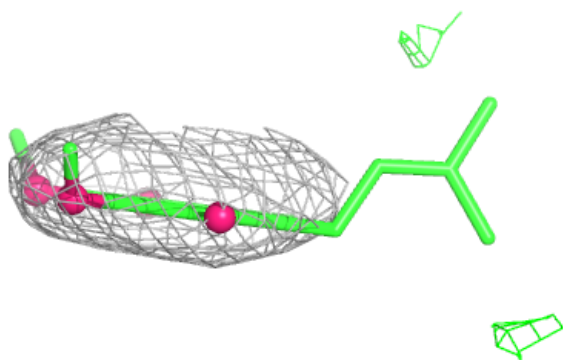
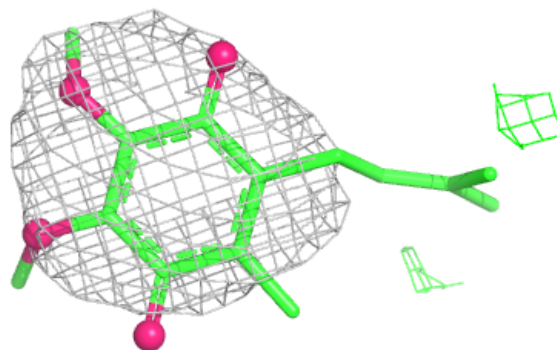
**Electron density around UQ8 L 311:**

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

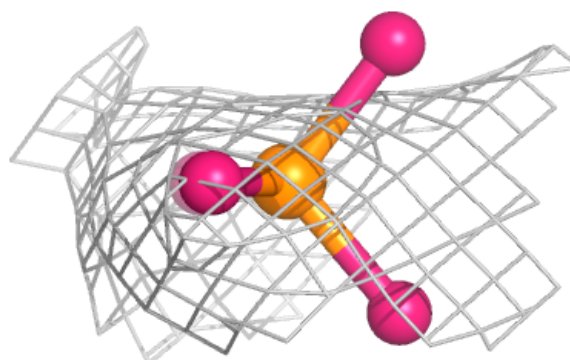
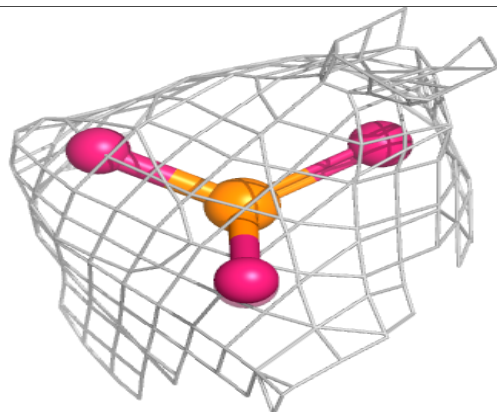
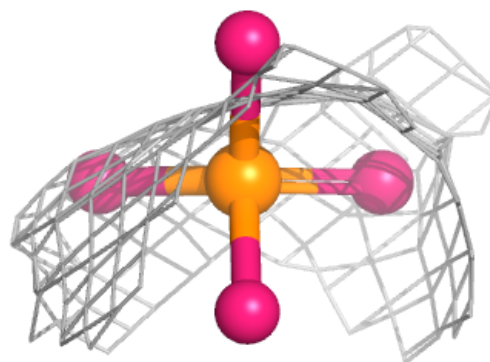


**Electron density around UQ8 M 413:**

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

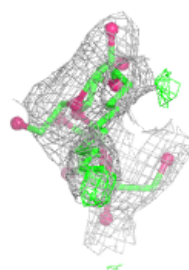
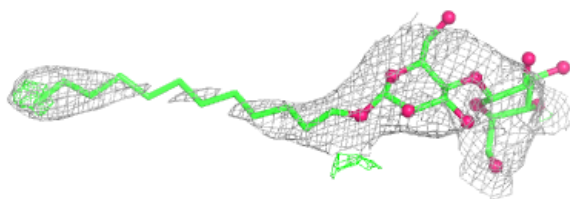
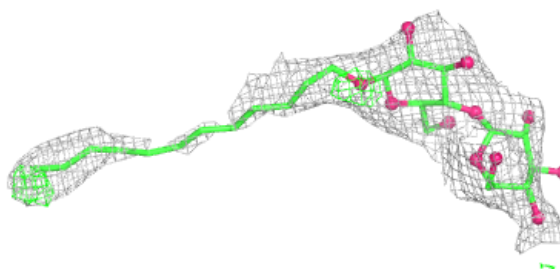
**Electron density around PEF 3 104:**

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

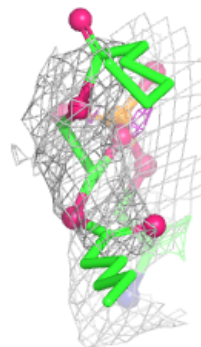
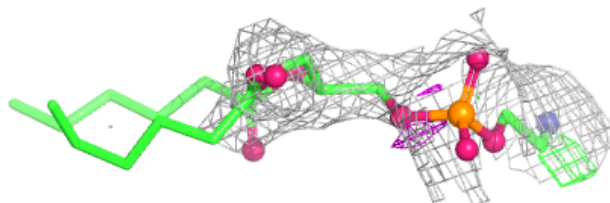
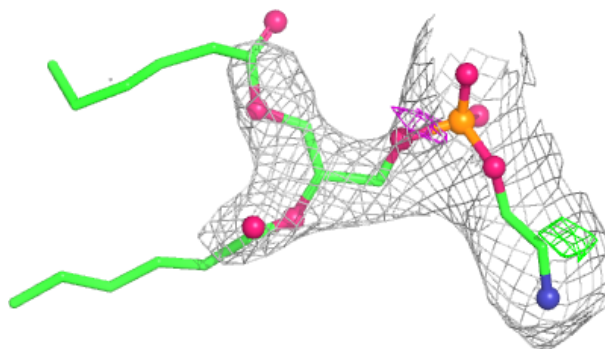


**Electron density around LMT H 304:**

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

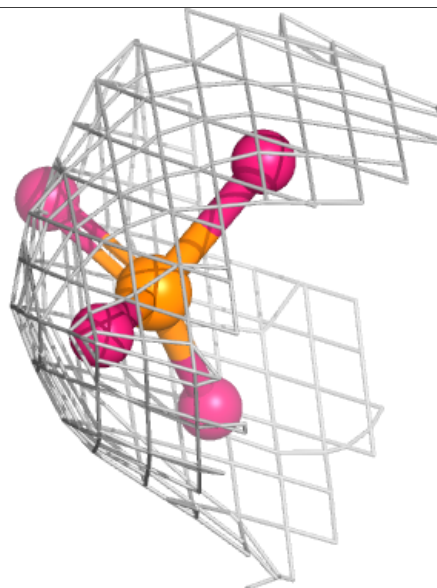
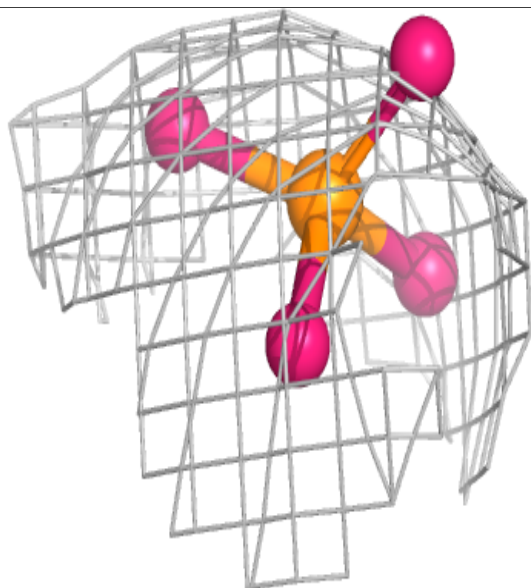
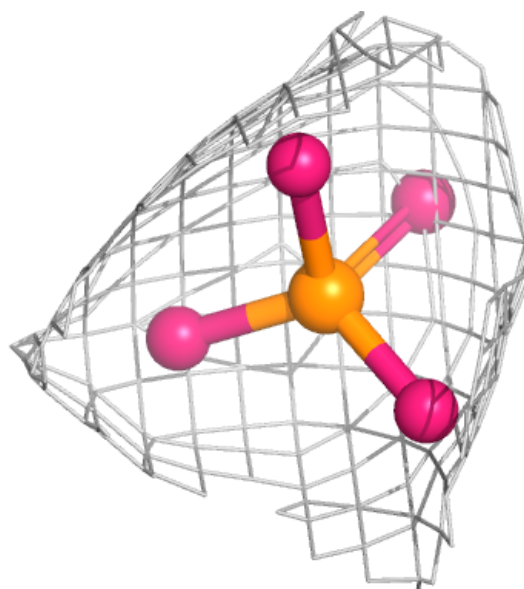
**Electron density around PEF K 104:**

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



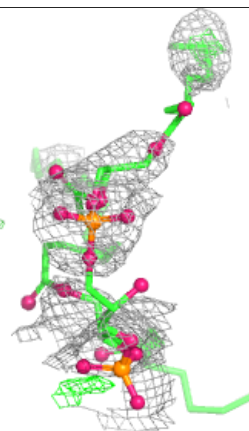
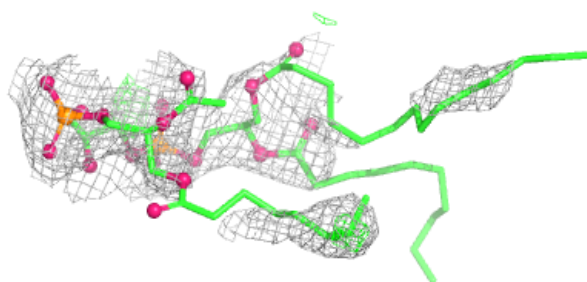
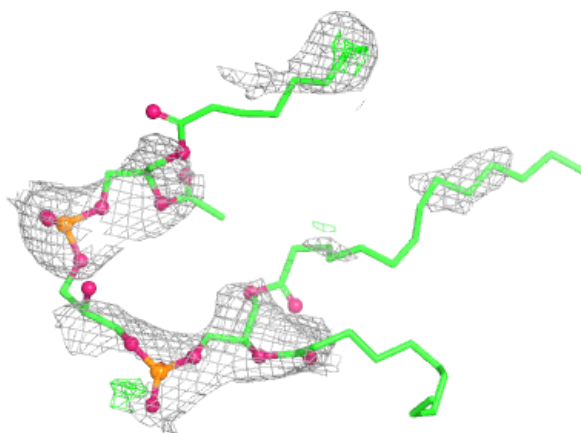
**Electron density around PEF 1 103:**

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

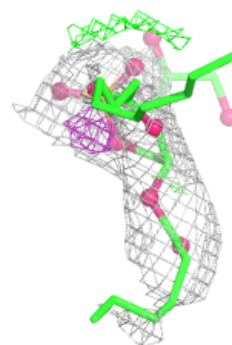
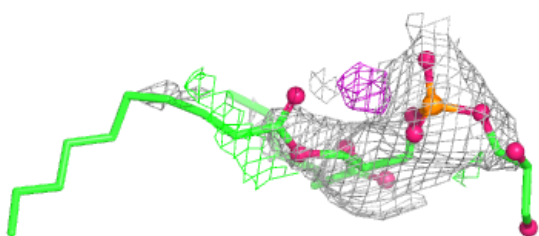
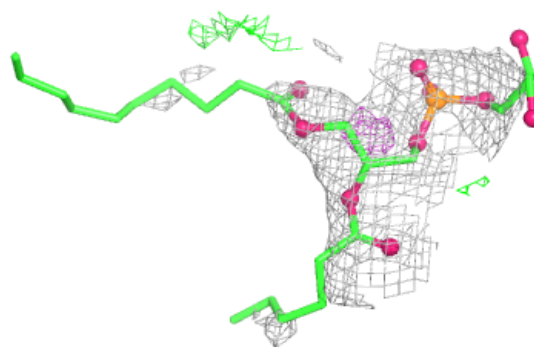


**Electron density around CDL U 104:**

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

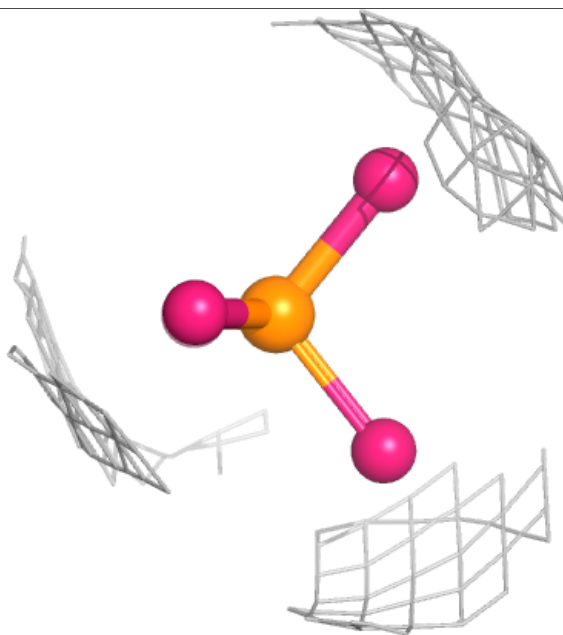
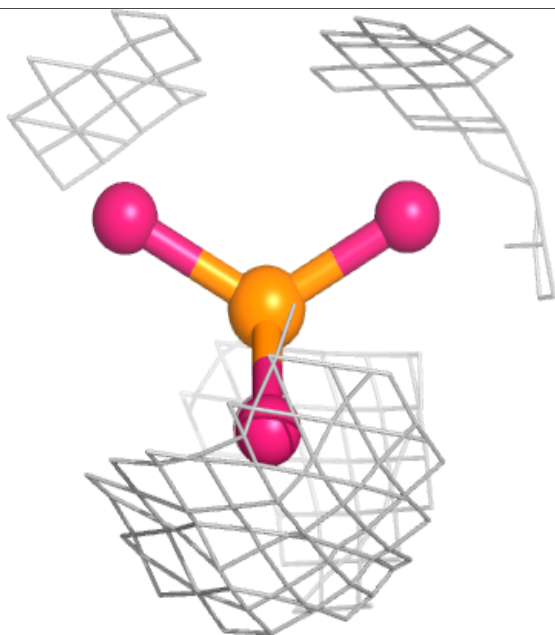
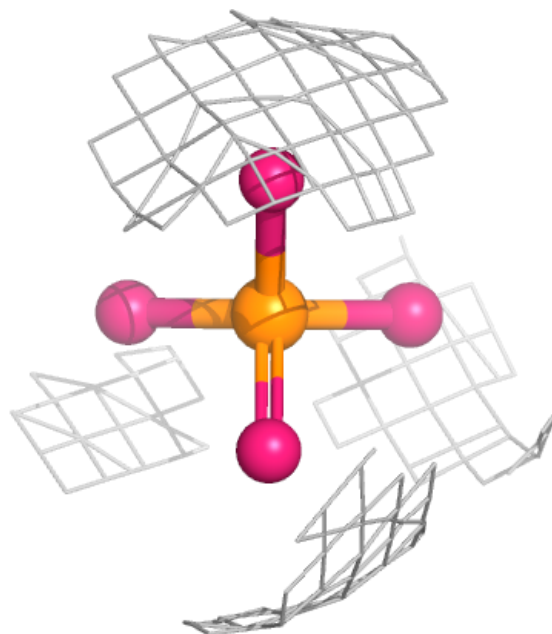
**Electron density around PGV 9 104:**

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



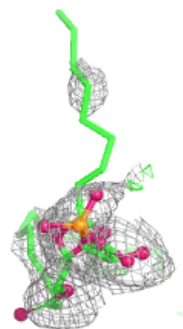
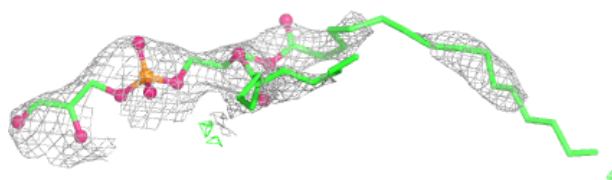
**Electron density around PEF M 408:**

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



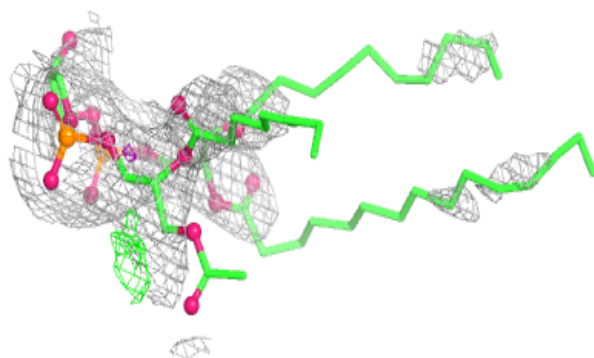
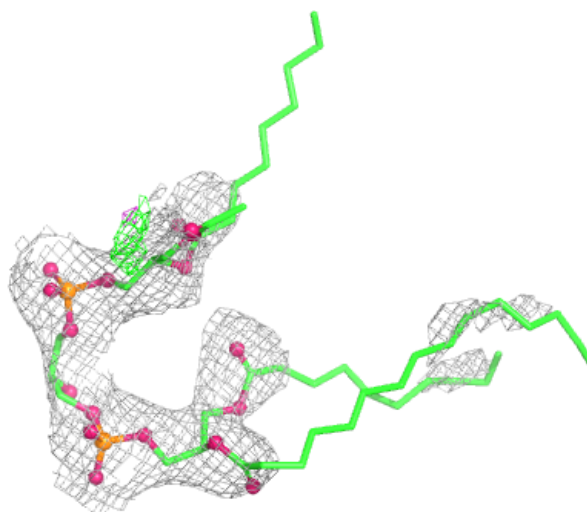
**Electron density around PGV L 308:**

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



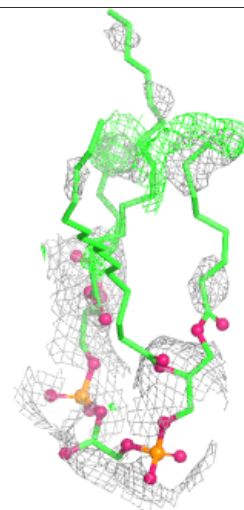
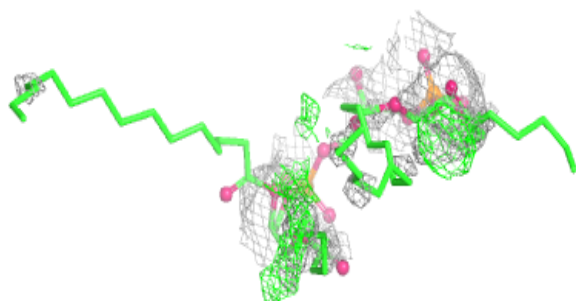
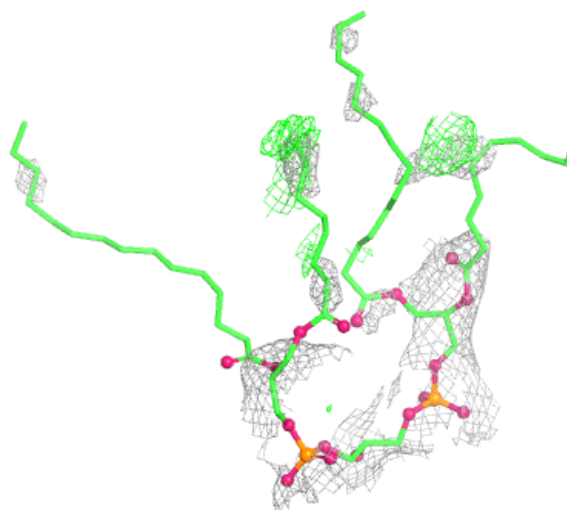
**Electron density around CDL D 105:**

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



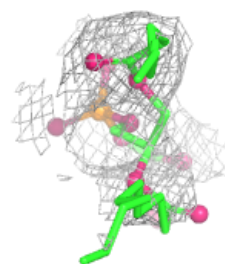
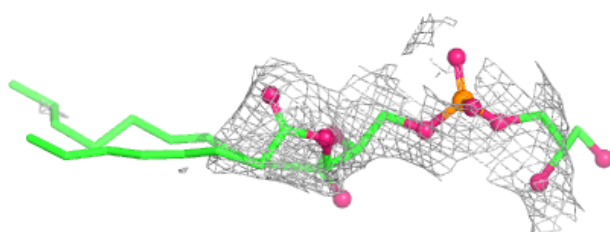
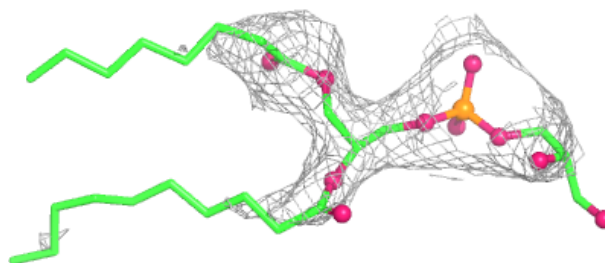
**Electron density around CDL S 104:**

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

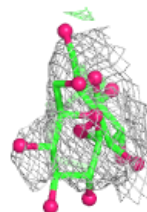
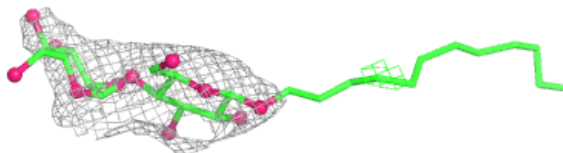
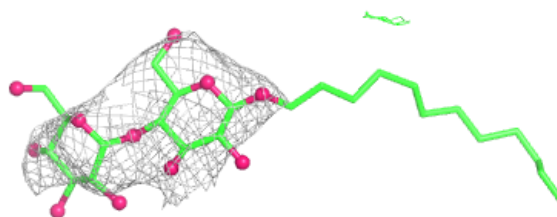


**Electron density around PGV D 106:**

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

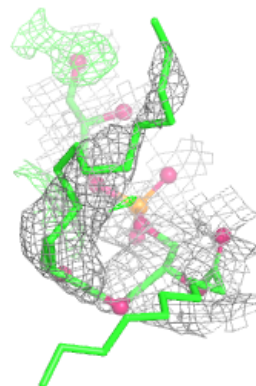
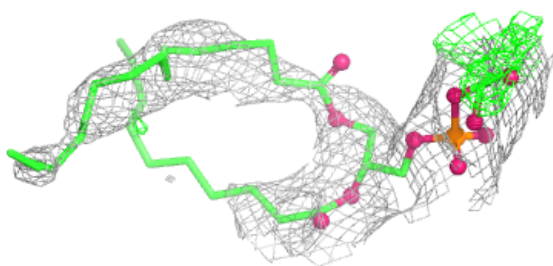
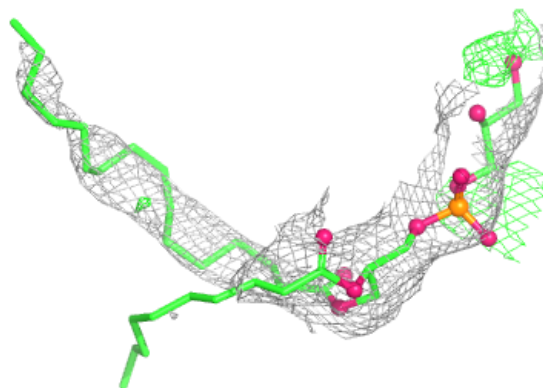
**Electron density around LMT M 414:**

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

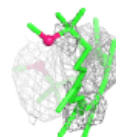
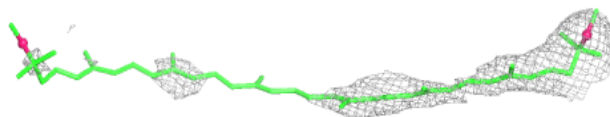
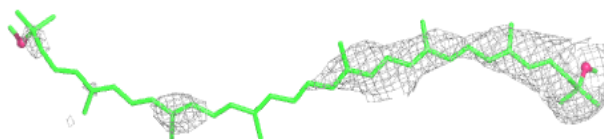


**Electron density around PGV L 307:**

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

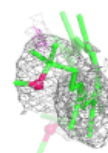
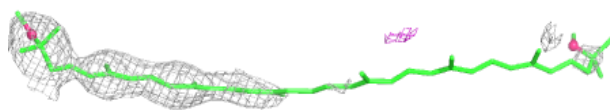
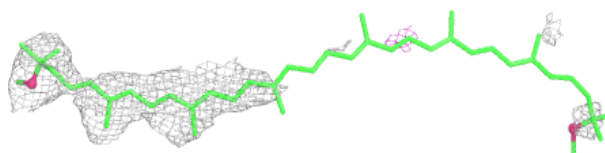
**Electron density around CRT G 101:**

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

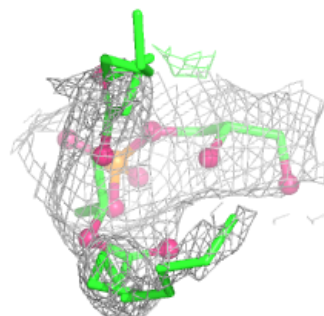
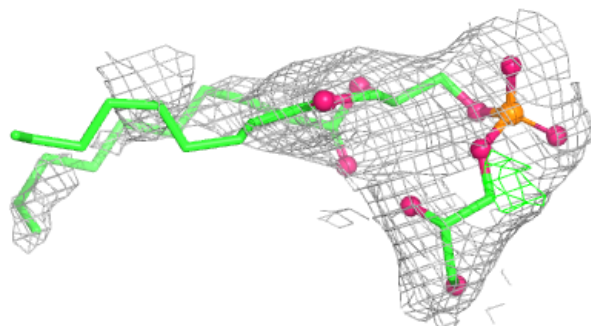
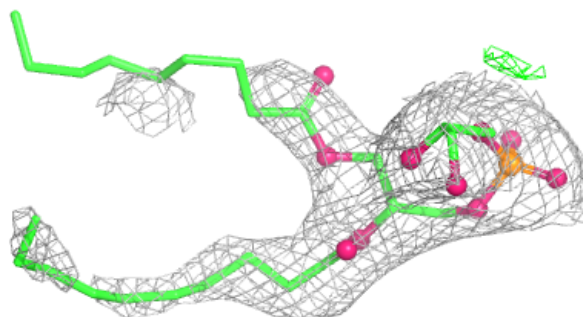


**Electron density around CRT 0 101:**

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

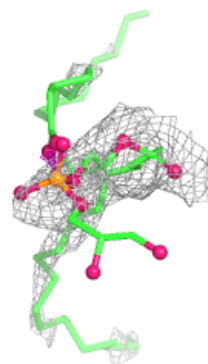
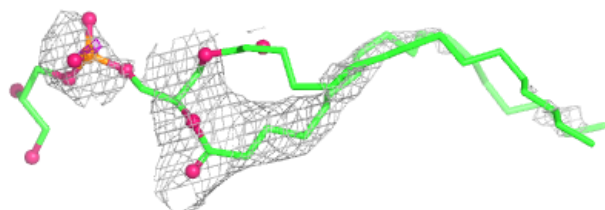
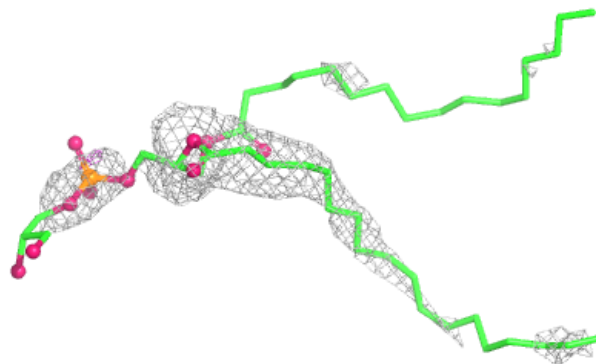
**Electron density around PGV H 303:**

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



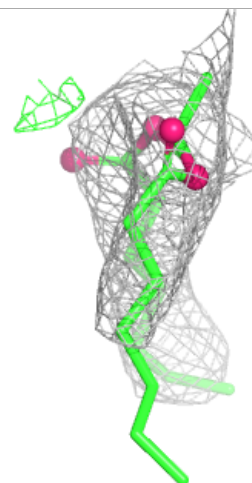
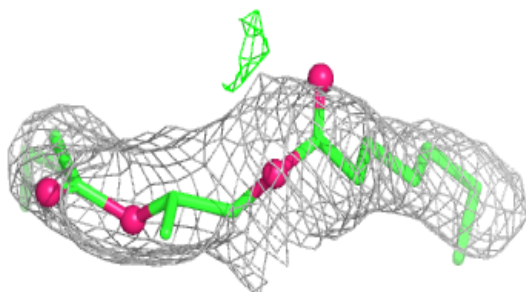
**Electron density around PGV 3 105:**

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



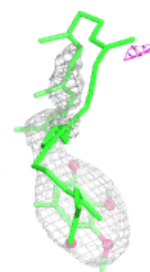
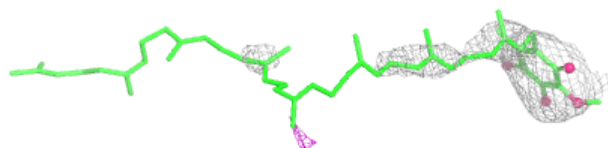
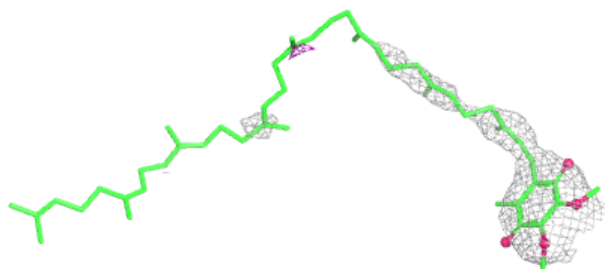
**Electron density around PGV C 508:**

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



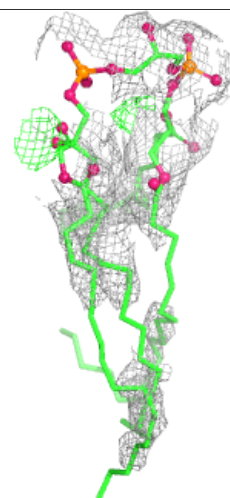
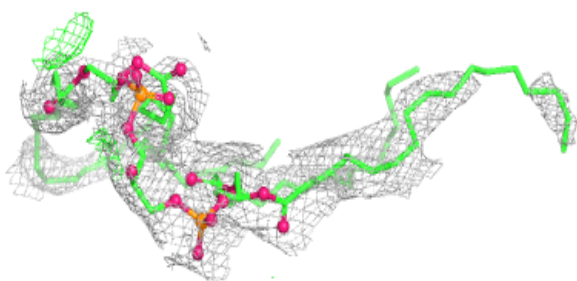
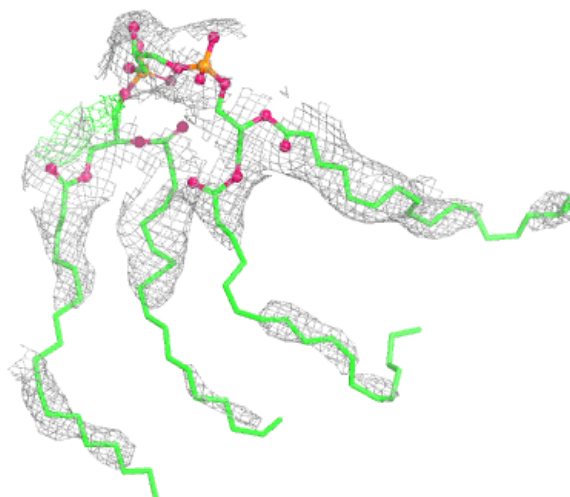
**Electron density around UQ8 L 309:**

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



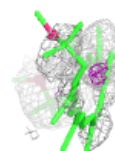
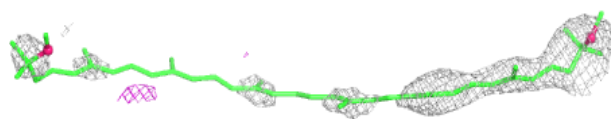
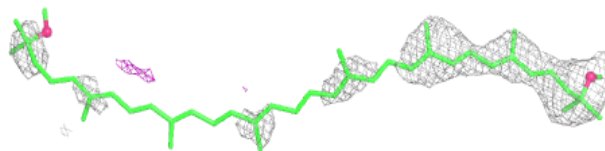
**Electron density around CDL M 406:**

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

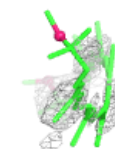
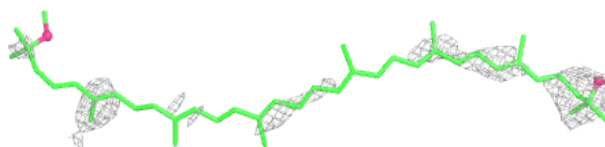


**Electron density around CRT O 103:**

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

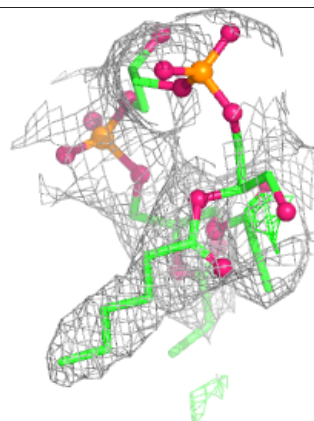
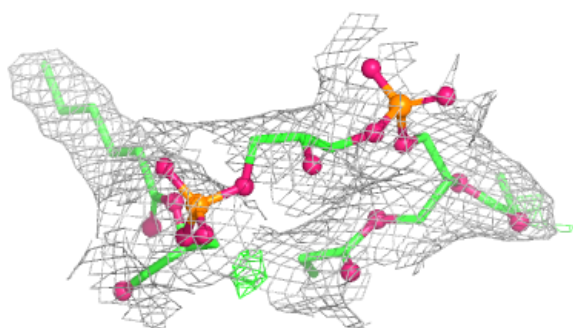
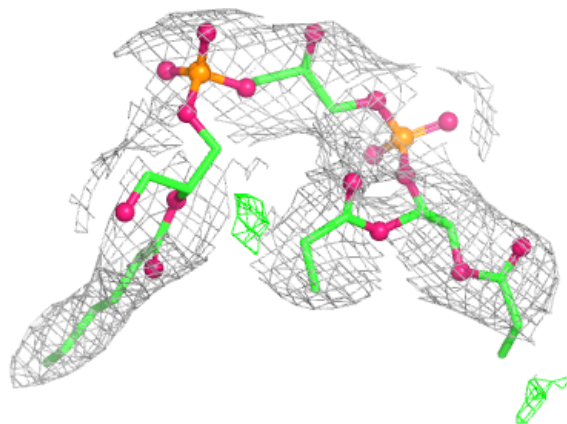
**Electron density around CRT 8 101:**

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



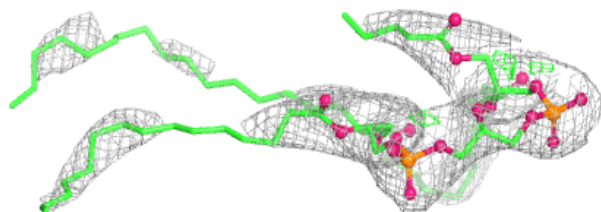
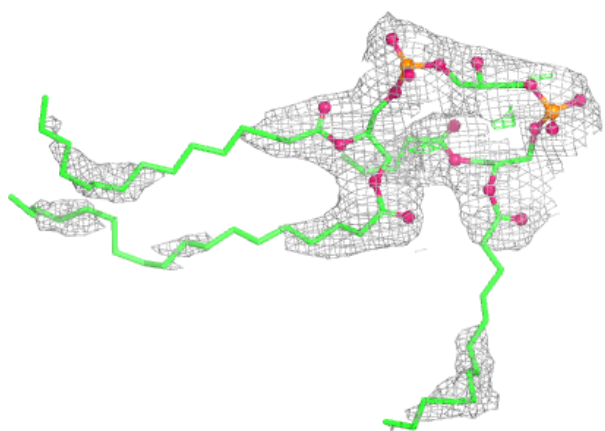
**Electron density around CDL M 412:**

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

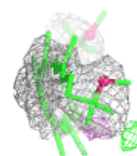
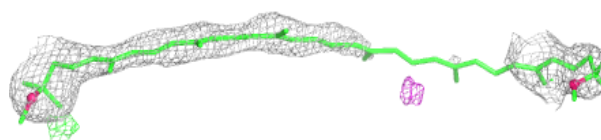
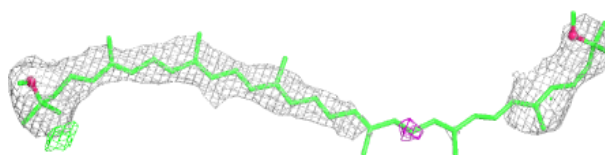


**Electron density around CDL H 305:**

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

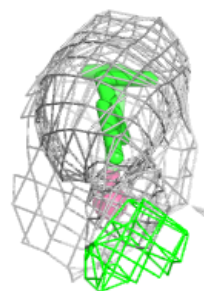
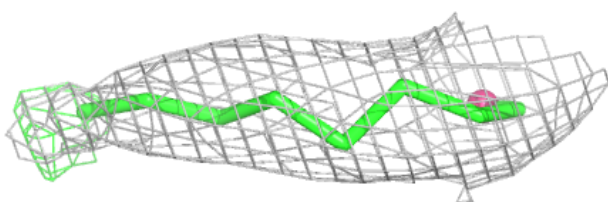
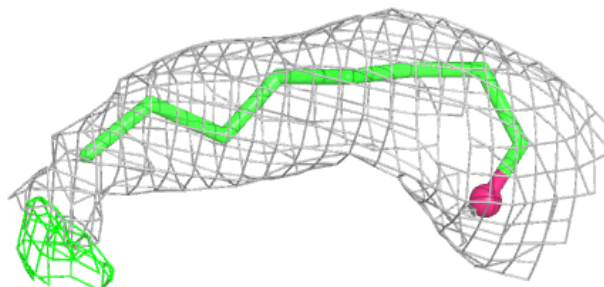
**Electron density around CRT V 101:**

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

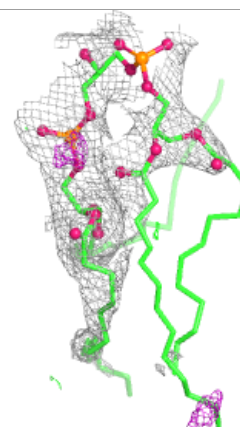
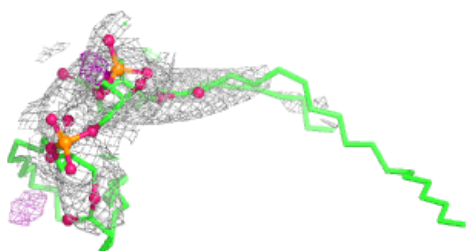


**Electron density around LHG C 507:**

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

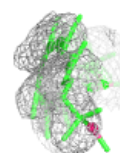
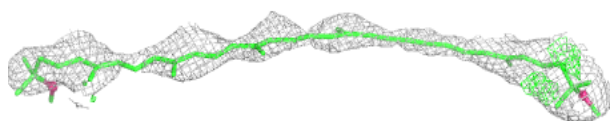
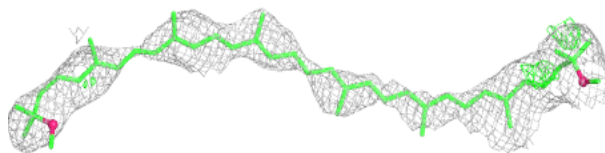
**Electron density around CDL O 104:**

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

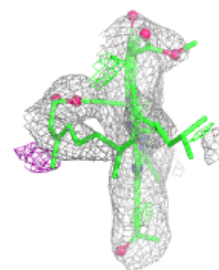
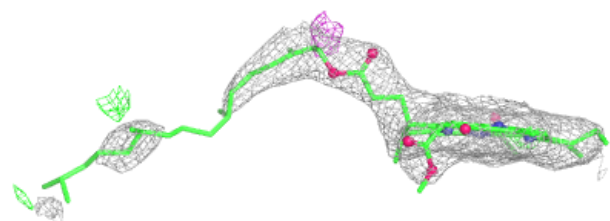
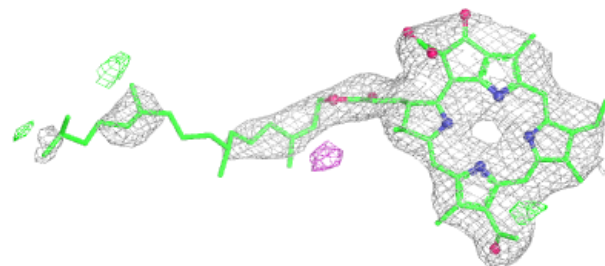


**Electron density around CRT J 101:**

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

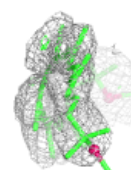
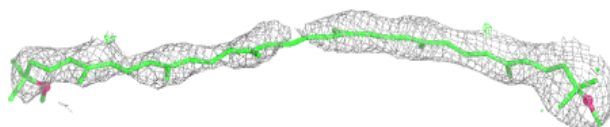
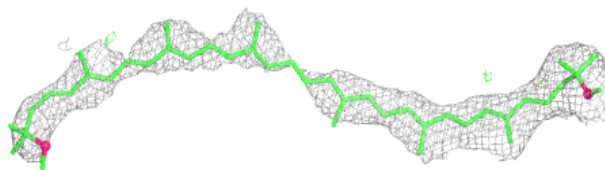
**Electron density around BPH M 402:**

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



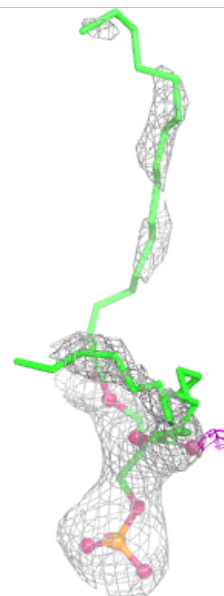
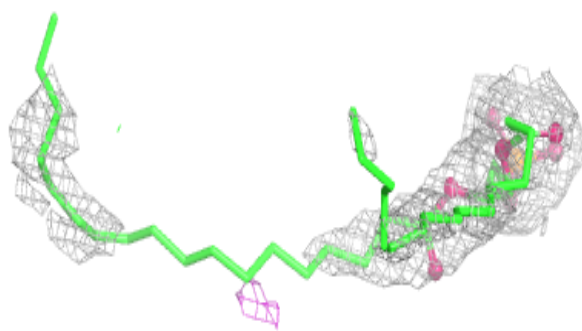
**Electron density around CRT T 101:**

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



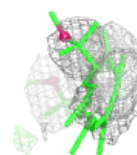
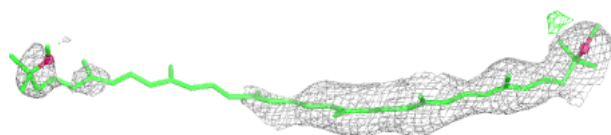
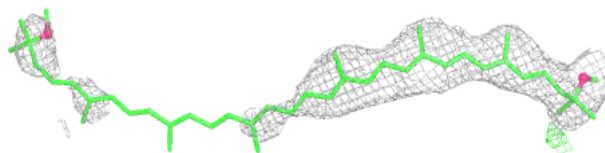
**Electron density around PGV M 410:**

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

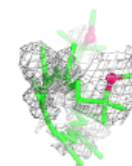
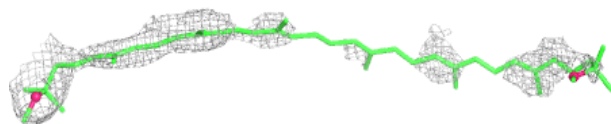
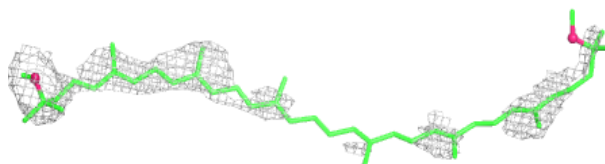


**Electron density around CRT W 102:**

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

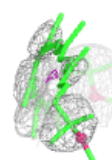
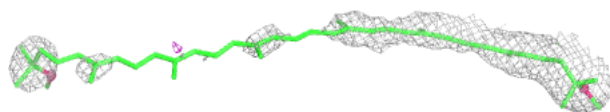
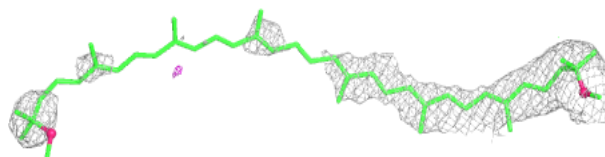
**Electron density around CRT B 101:**

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

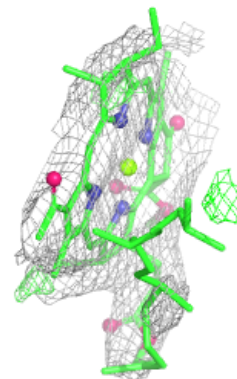
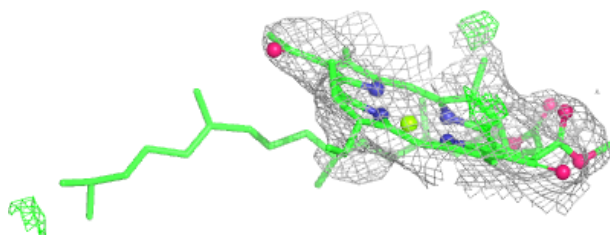
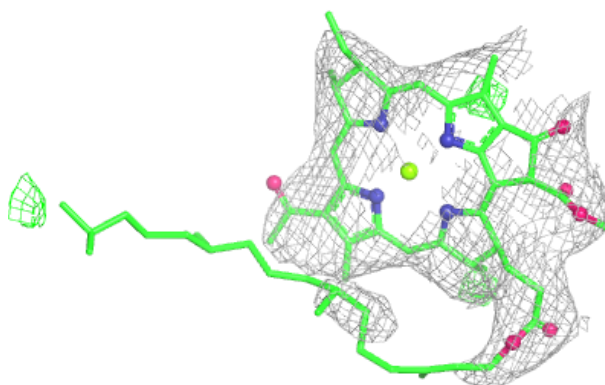


**Electron density around CRT N 101:**

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

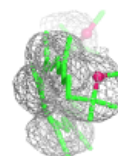
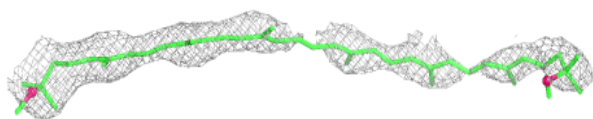
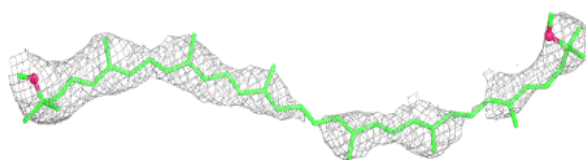
**Electron density around BCL S 103:**

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

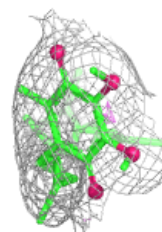
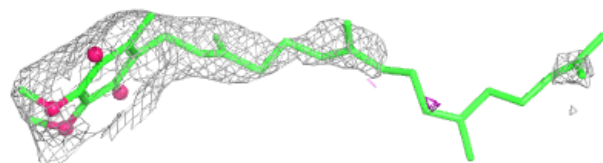
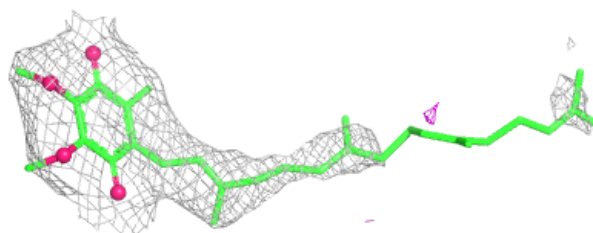


**Electron density around CRT P 101:**

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

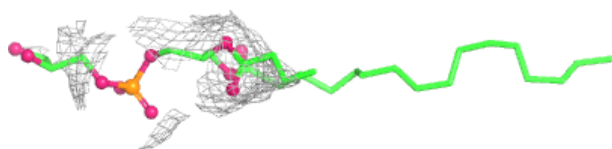
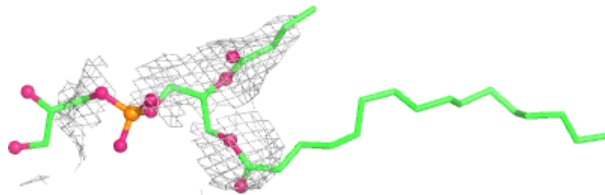
**Electron density around UQ8 L 304:**

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

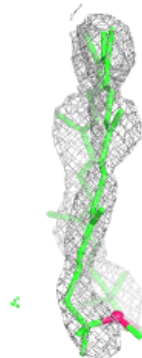
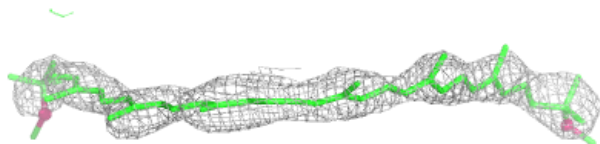
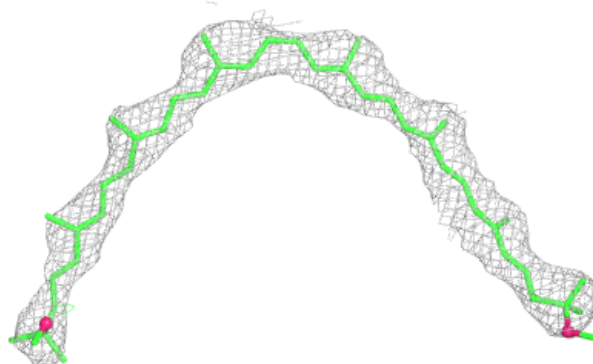


**Electron density around PGV M 411:**

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

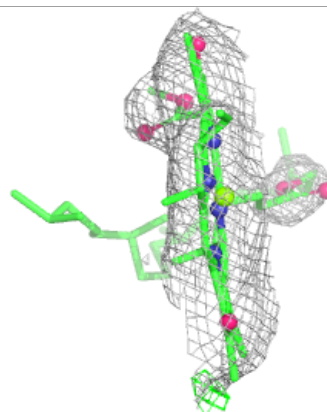
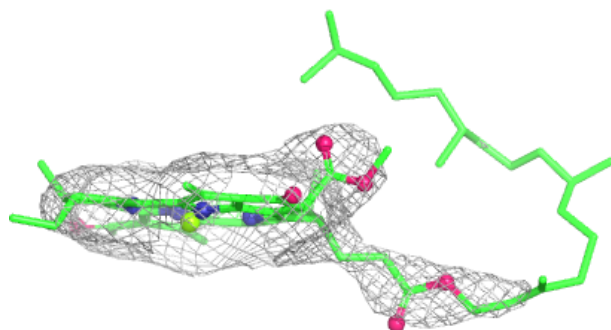
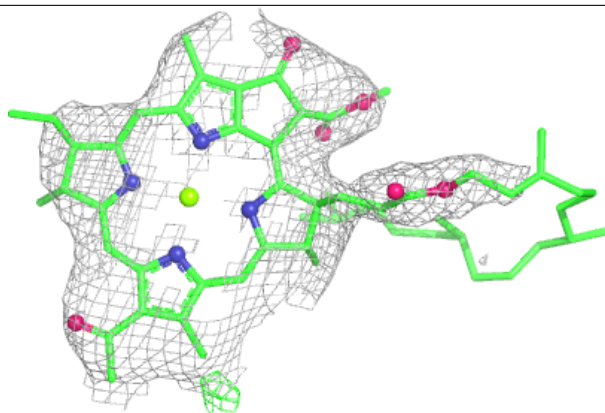
**Electron density around CRT M 405:**

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

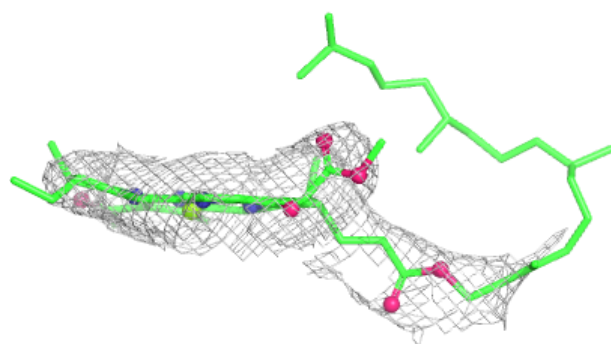
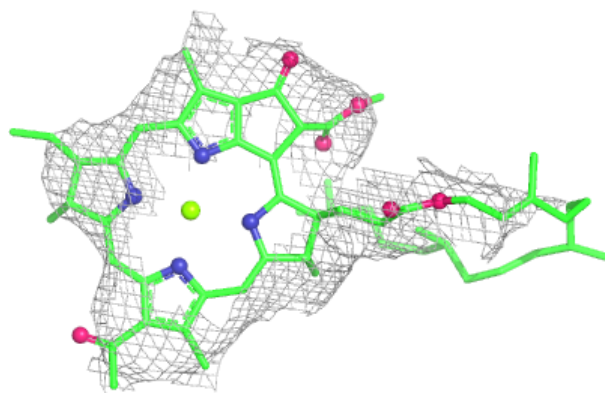


**Electron density around BCL S 101:**

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

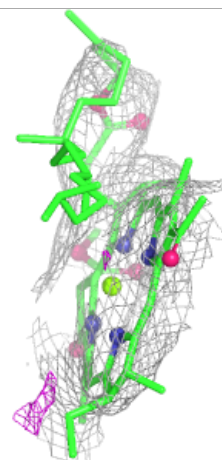
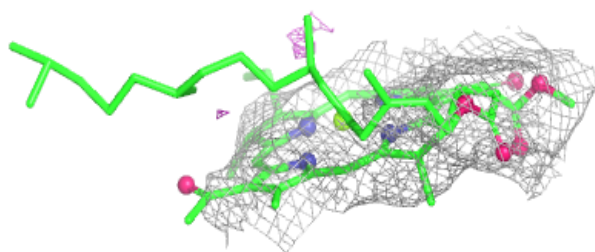
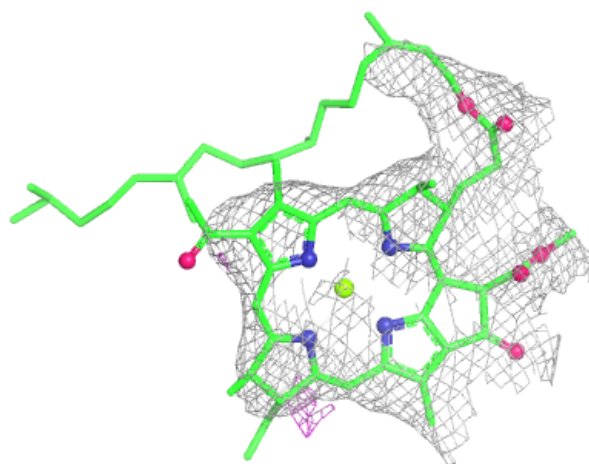
**Electron density around BCL A 101:**

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



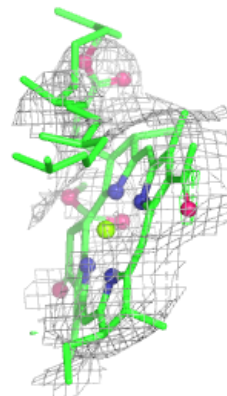
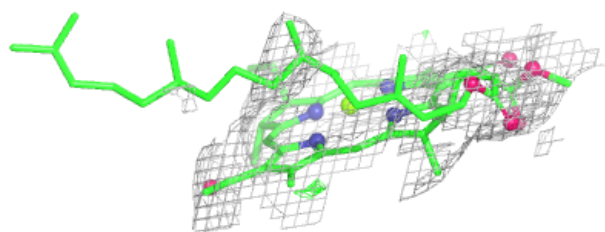
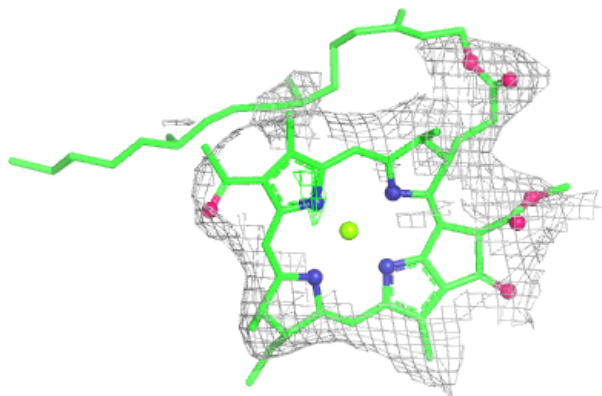
**Electron density around BCL U 103:**

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



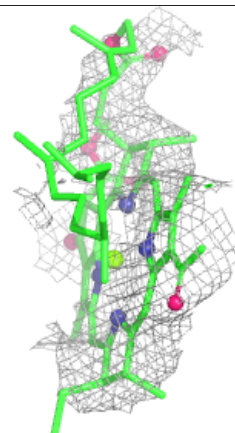
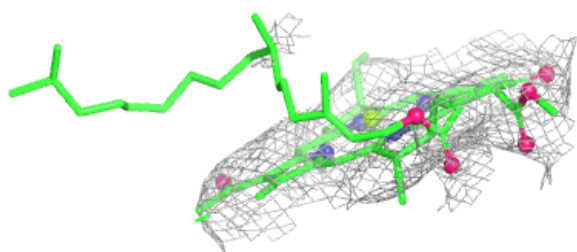
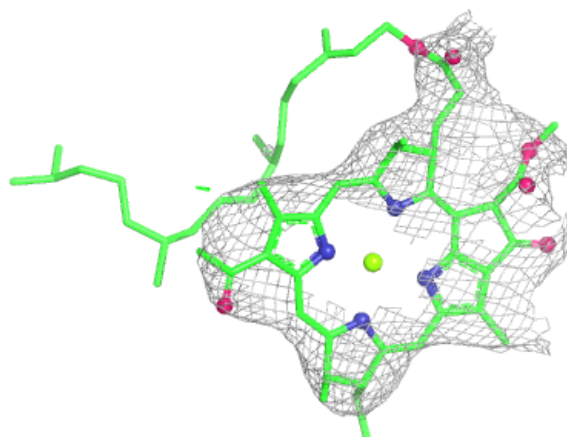
**Electron density around BCL 5 103:**

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

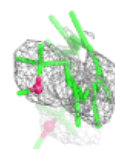
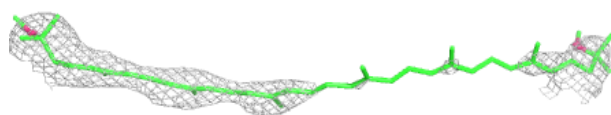
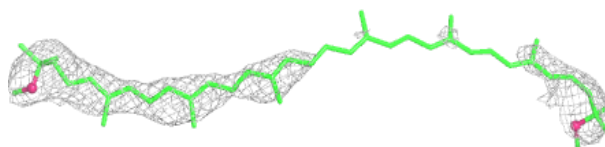


**Electron density around BCL 9 103:**

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

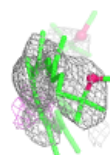
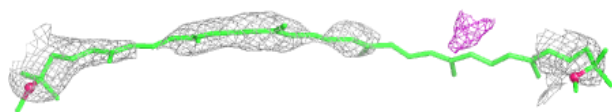
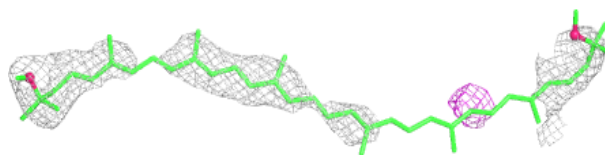
**Electron density around CRT 2 101:**

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

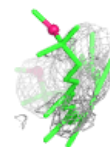
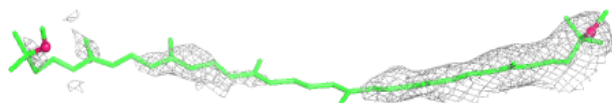
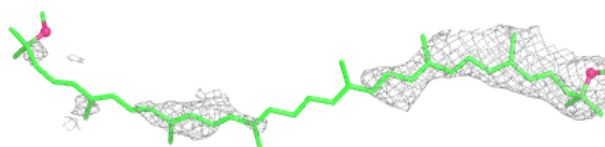


**Electron density around CRT 3 103:**

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

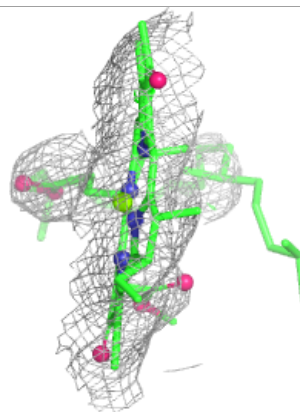
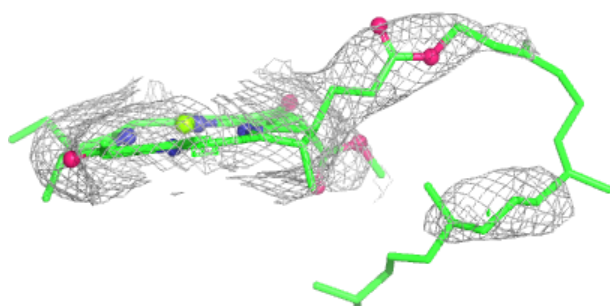
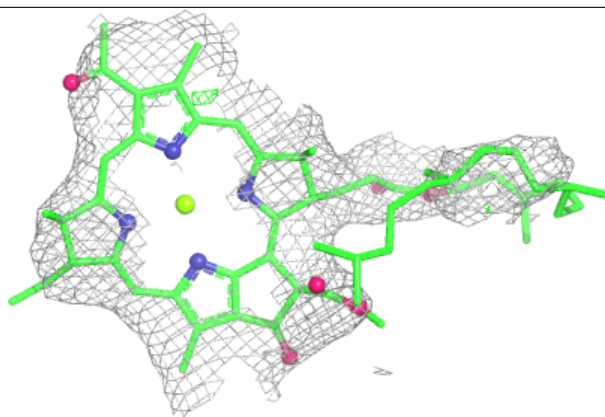
**Electron density around CRT 4 101:**

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

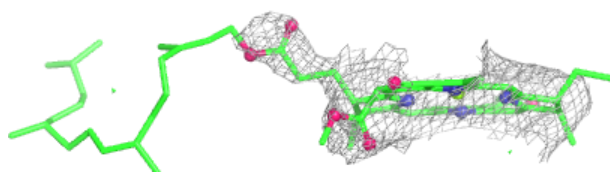
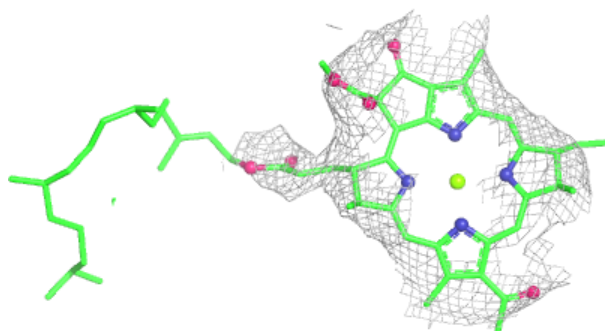


**Electron density around BCL F 101:**

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

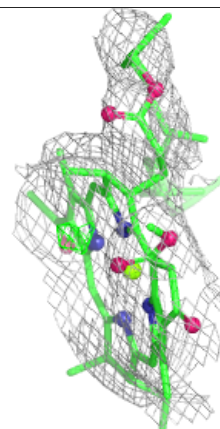
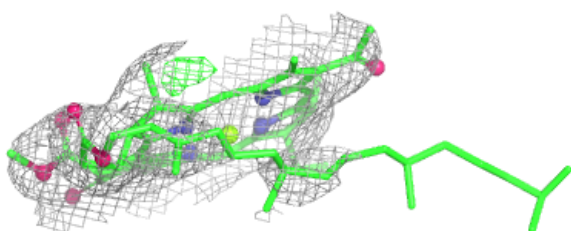
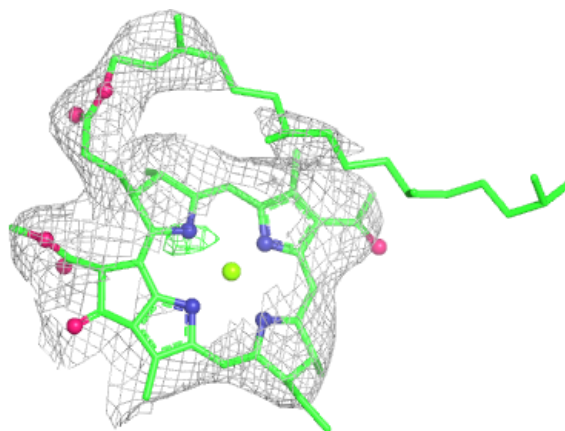
**Electron density around BCL 9 101:**

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

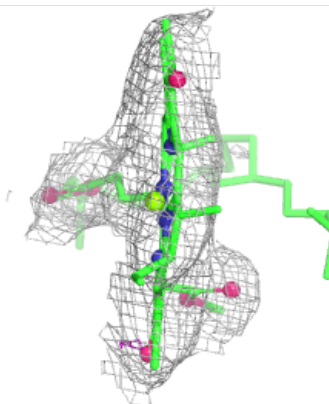
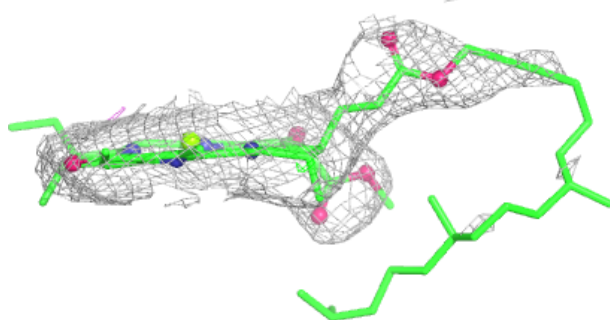
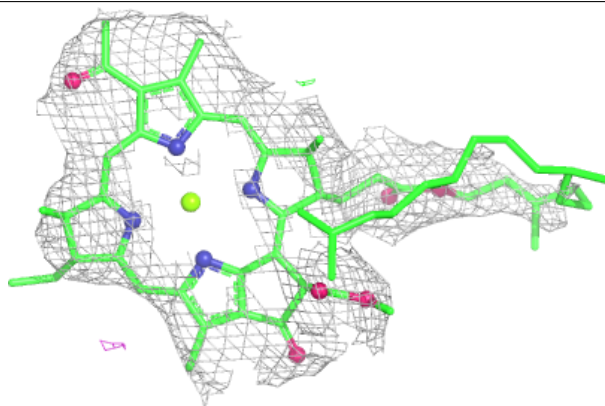


**Electron density around BCL Q 103:**

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

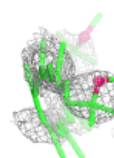
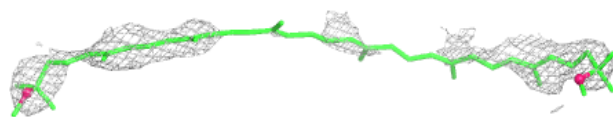
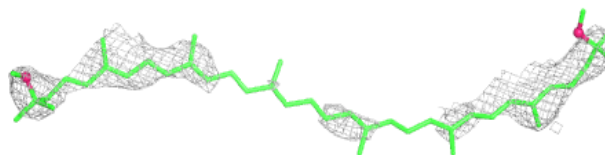
**Electron density around BCL U 101:**

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

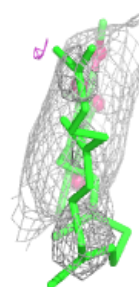
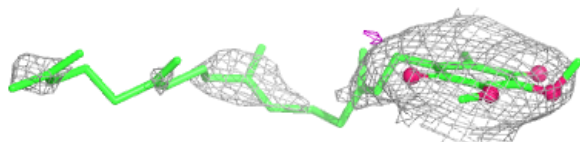


**Electron density around CRT Z 101:**

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

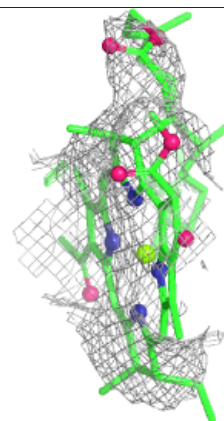
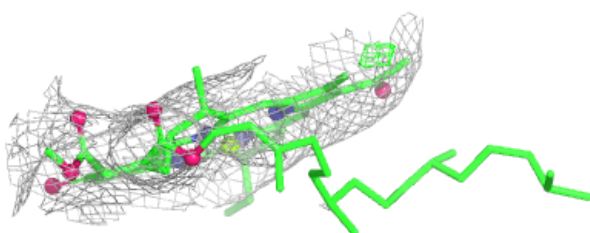
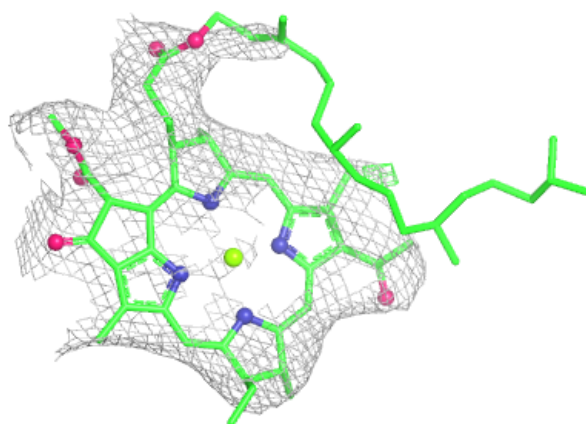
**Electron density around UQ8 L 310:**

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

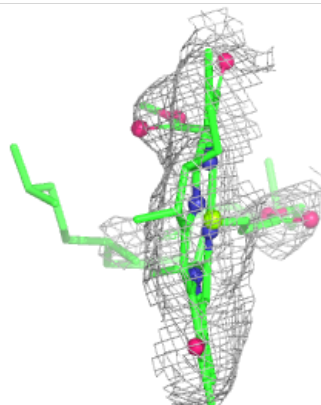
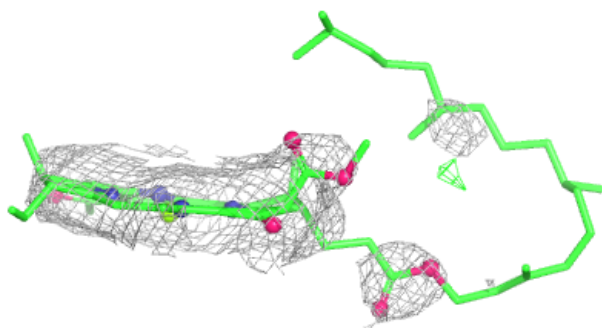
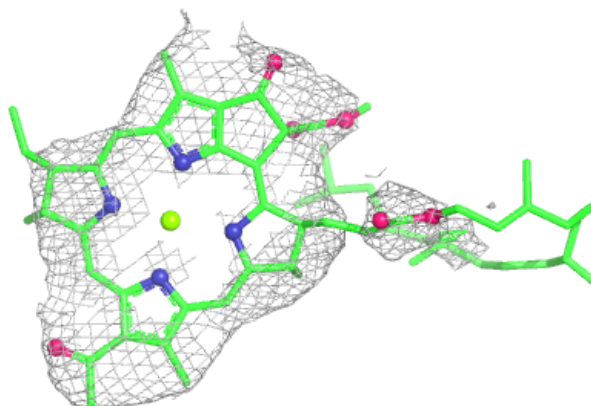


**Electron density around BCL A 103:**

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

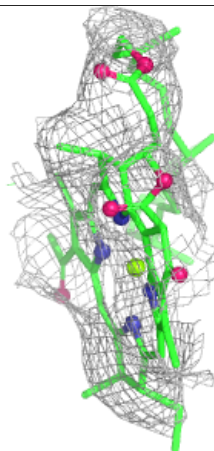
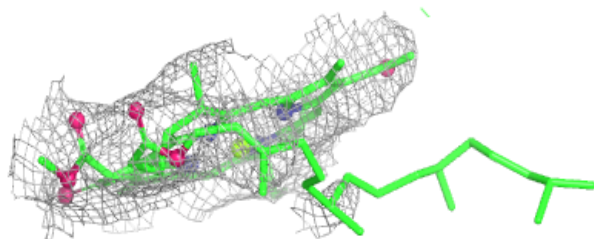
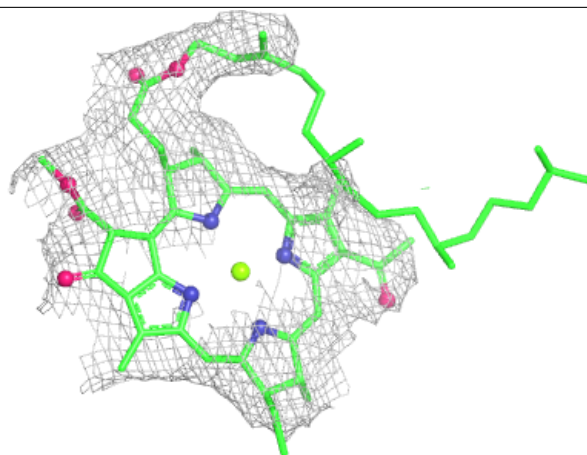
**Electron density around BCL W 101:**

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

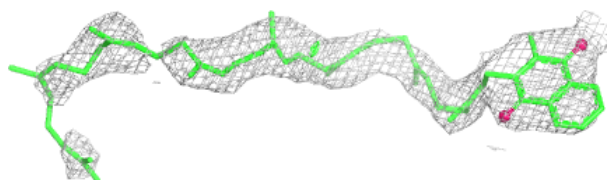
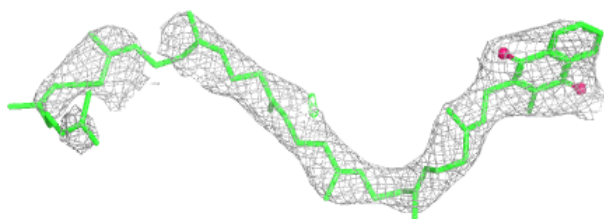


**Electron density around BCL W 104:**

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

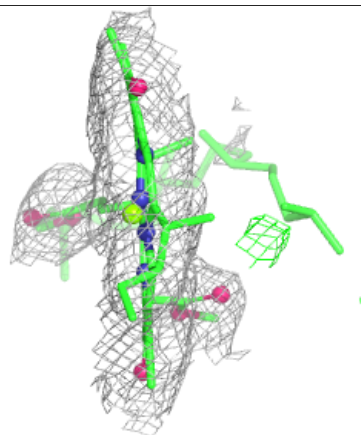
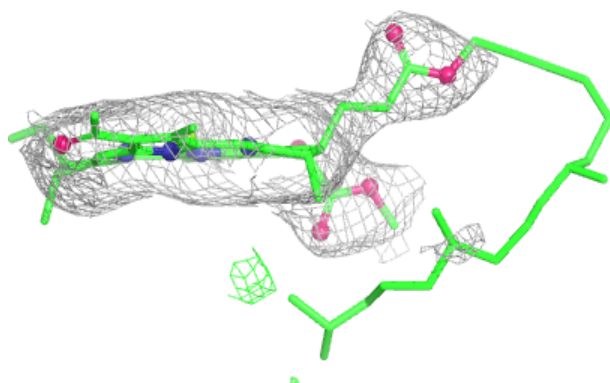
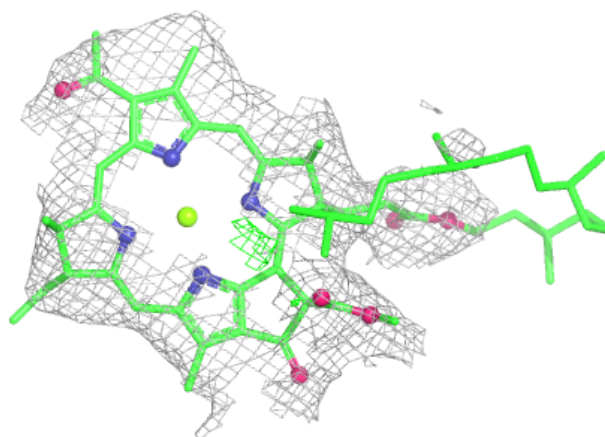
**Electron density around MQ8 M 404:**

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

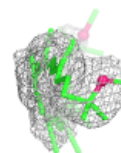
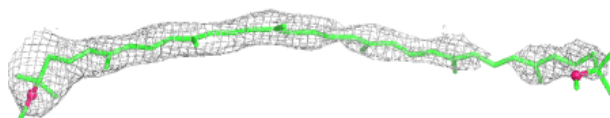
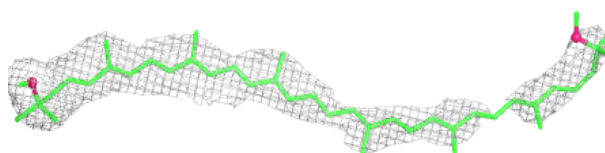


**Electron density around BCL Y 101:**

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

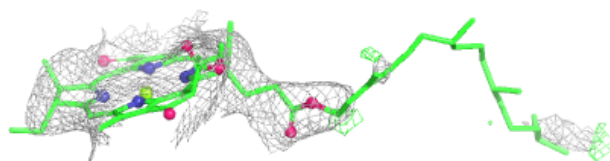
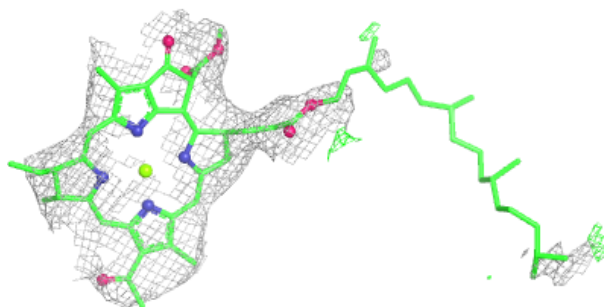
**Electron density around CRT A 104:**

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

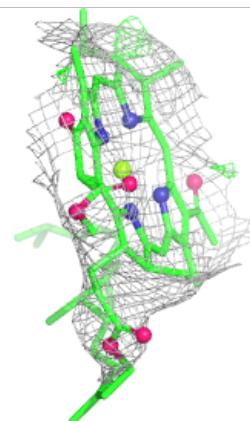
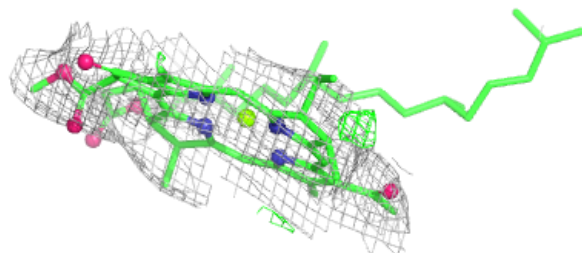
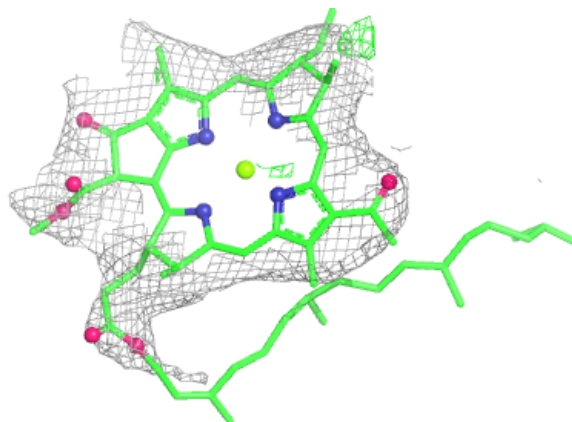


**Electron density around BCL 1 101:**

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

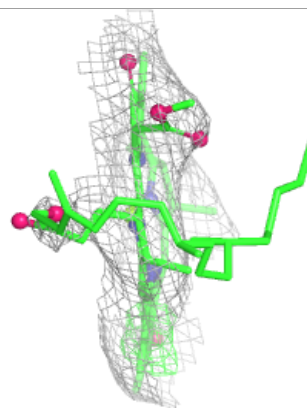
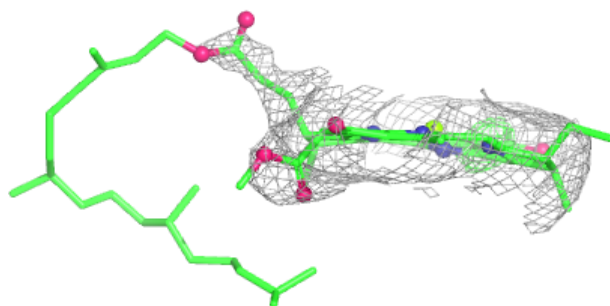
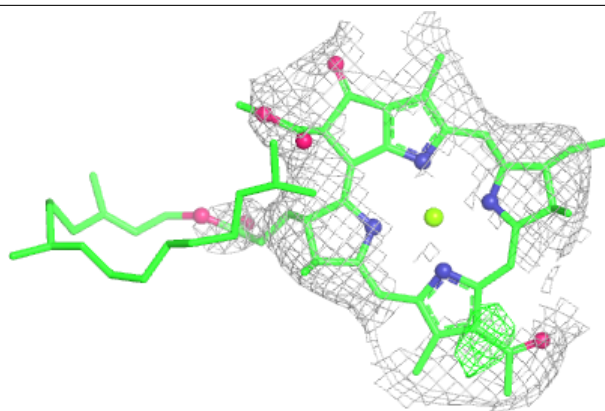
**Electron density around BCL 2 102:**

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

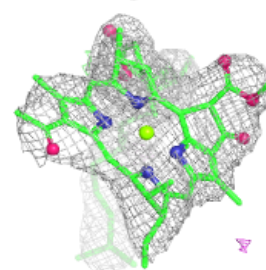
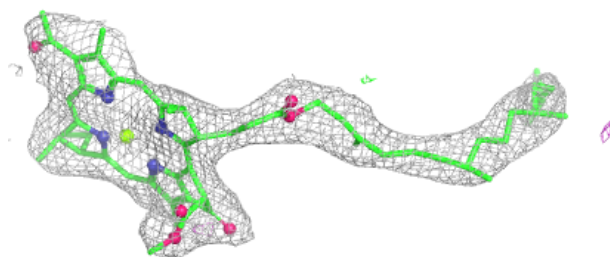
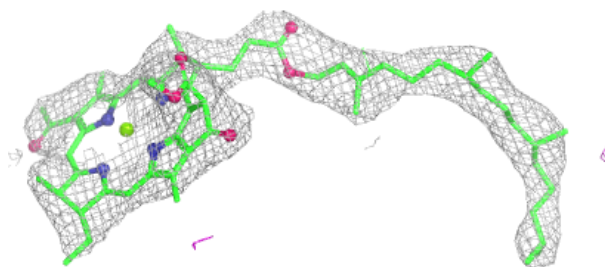


**Electron density around BCL 3 101:**

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

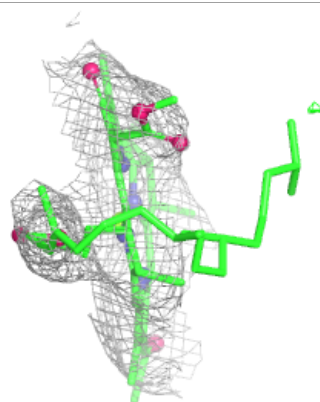
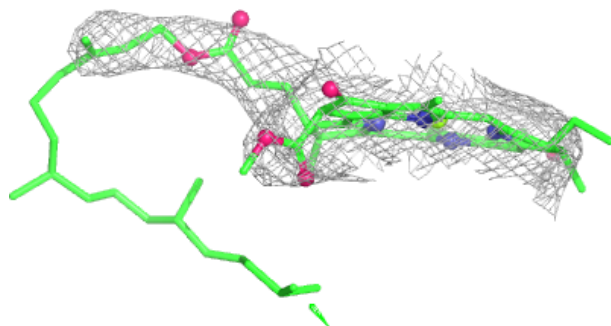
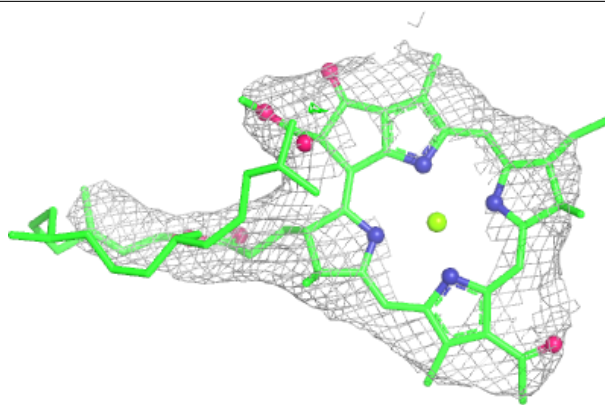
**Electron density around BCL M 401:**

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



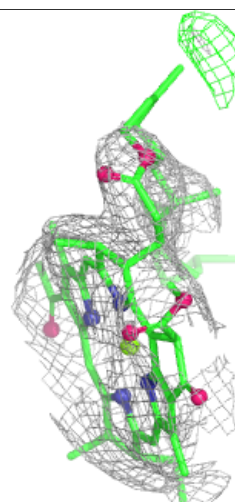
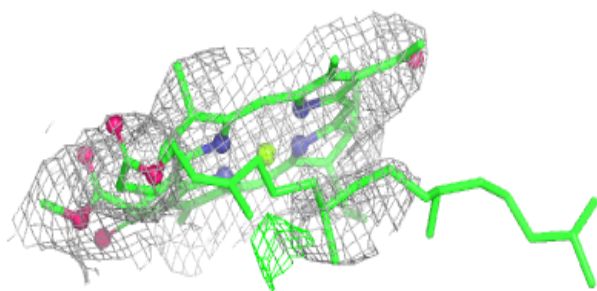
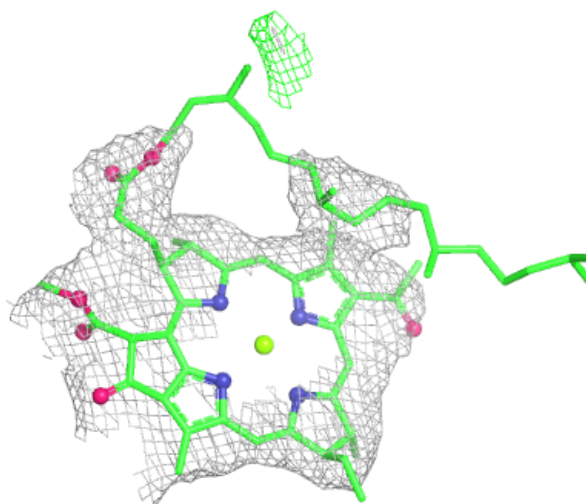
**Electron density around BCL D 101:**

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



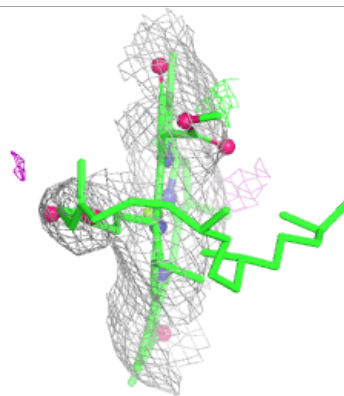
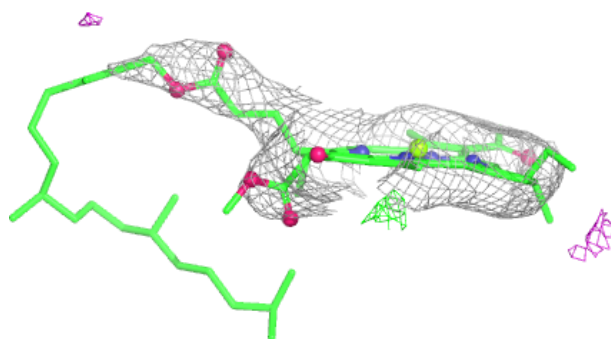
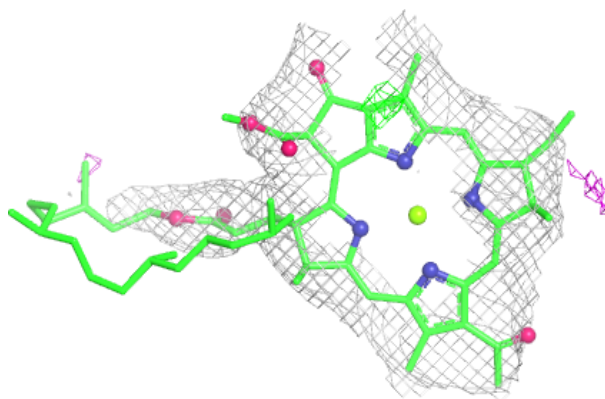
**Electron density around BCL Y 103:**

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

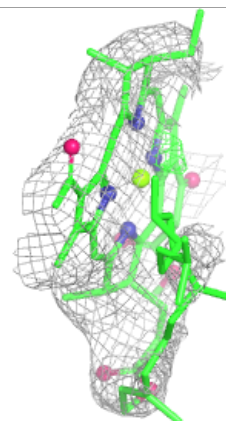
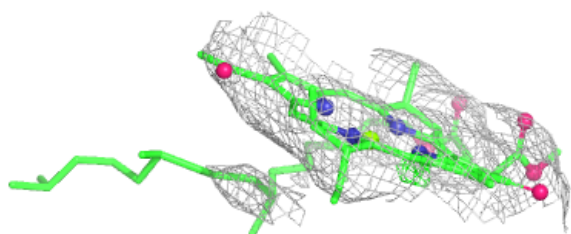
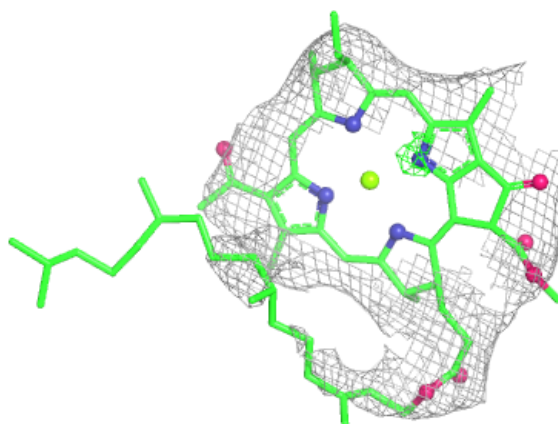


**Electron density around BCL I 101:**

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

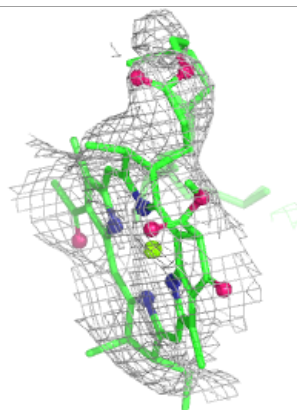
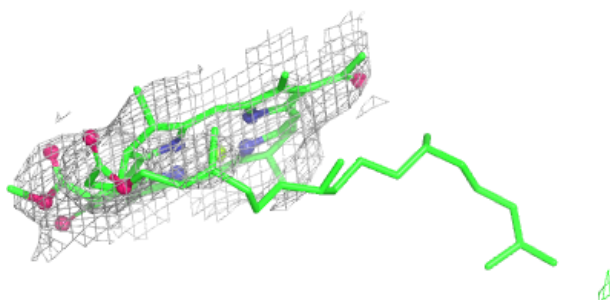
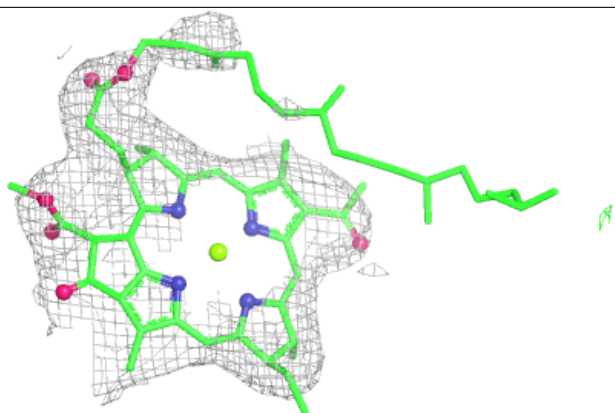
**Electron density around BCL J 102:**

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

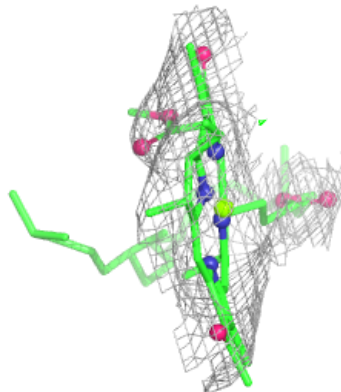
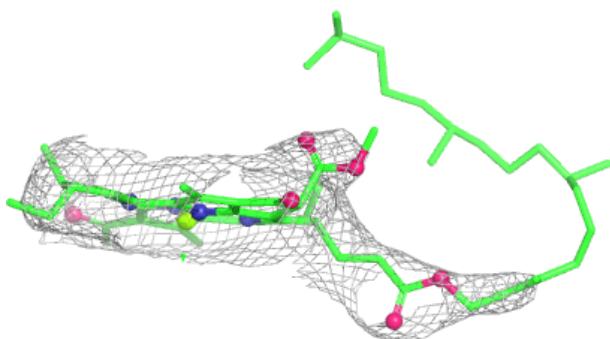
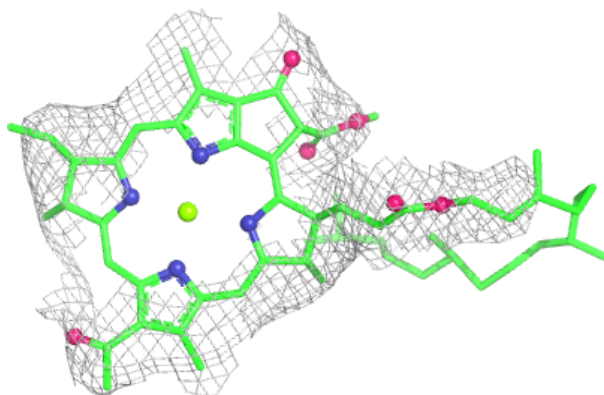


**Electron density around BCL 4 102:**

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

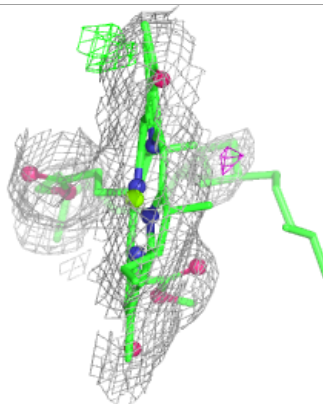
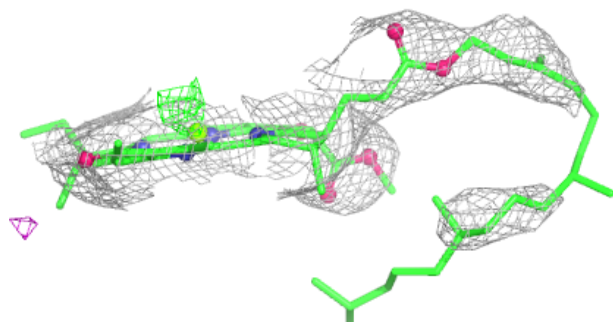
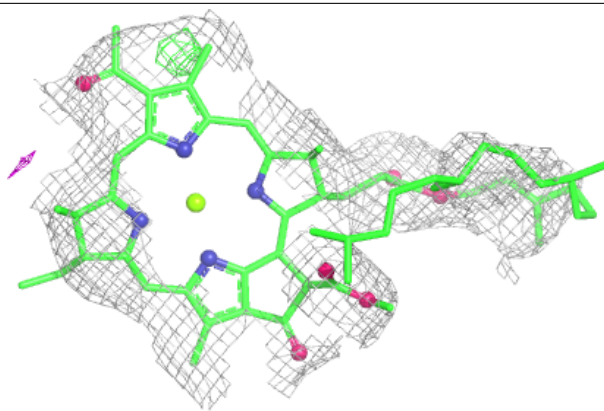
**Electron density around BCL 5 101:**

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

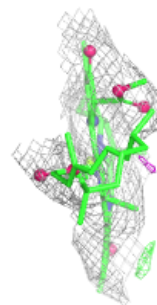
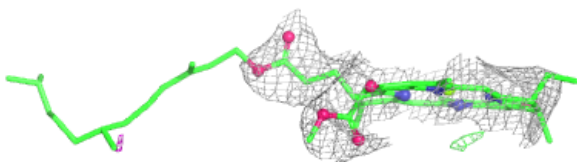
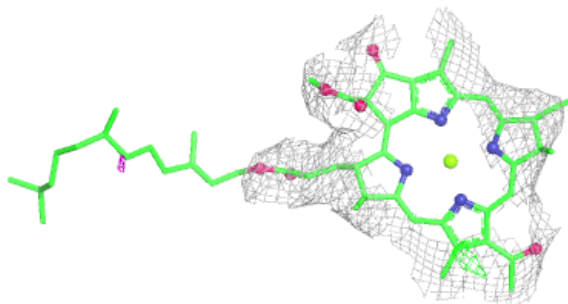


**Electron density around BCL K 101:**

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

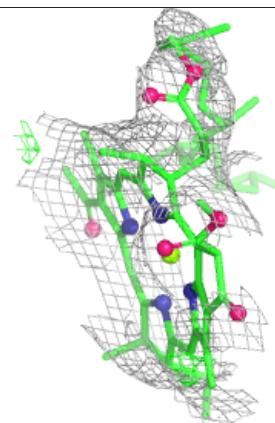
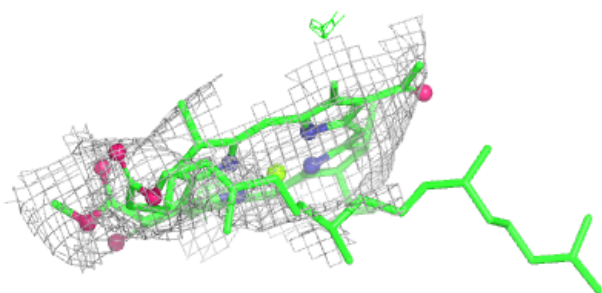
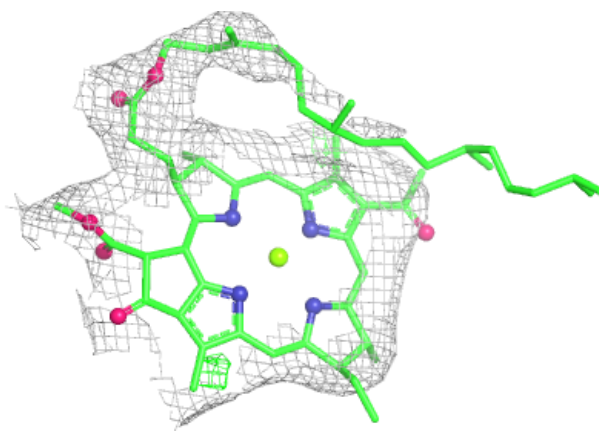
**Electron density around BCL 7 101:**

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

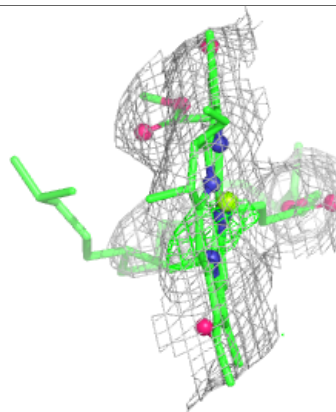
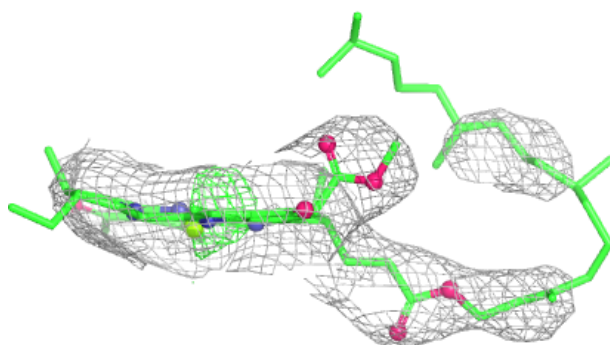
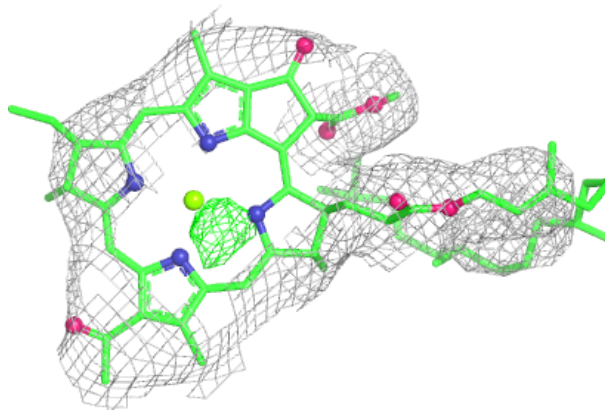


**Electron density around BCL K 103:**

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

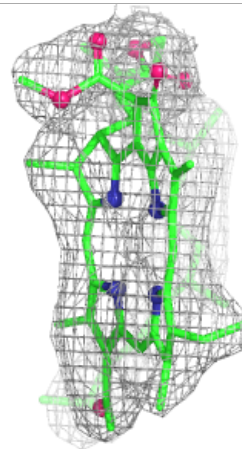
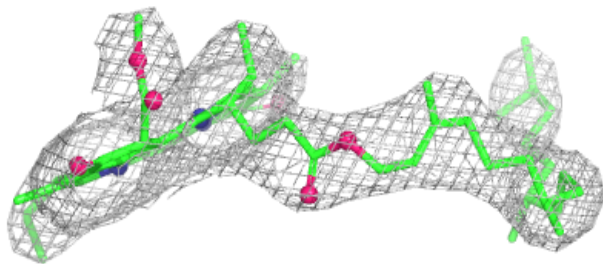
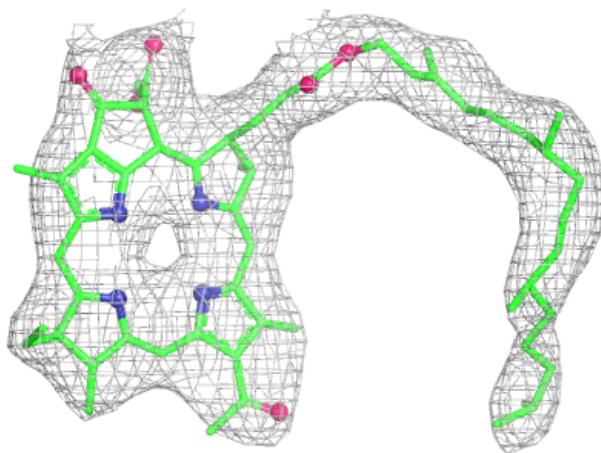
**Electron density around BCL O 101:**

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



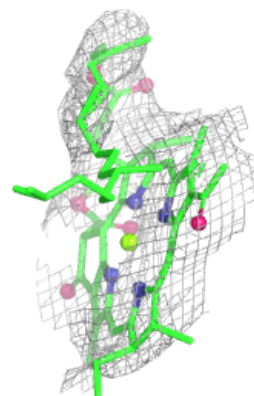
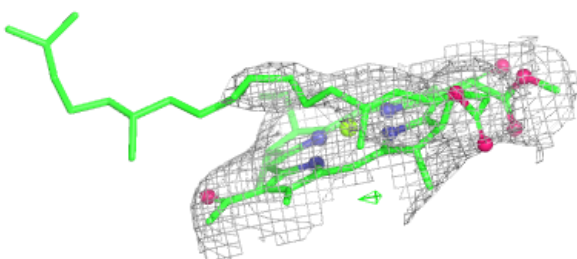
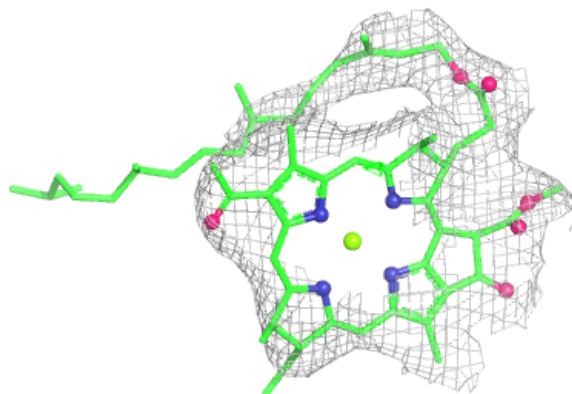
**Electron density around BPH L 303:**

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

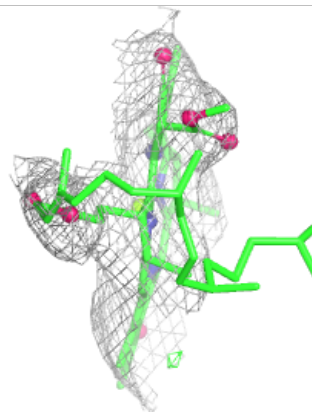
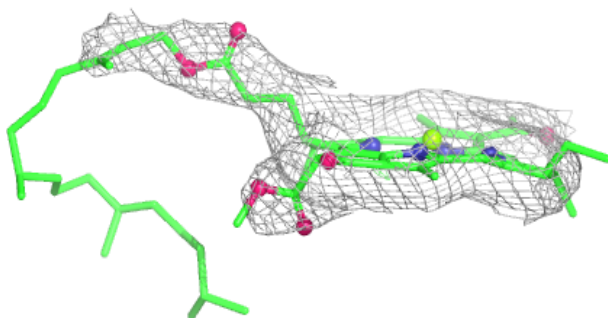
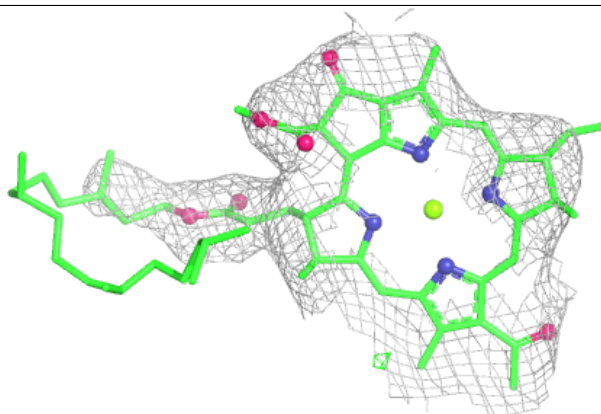


**Electron density around BCL P 102:**

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

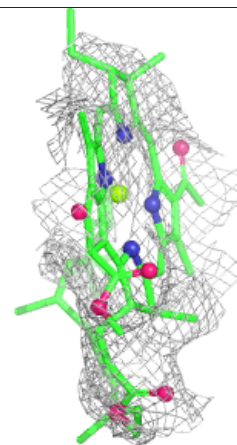
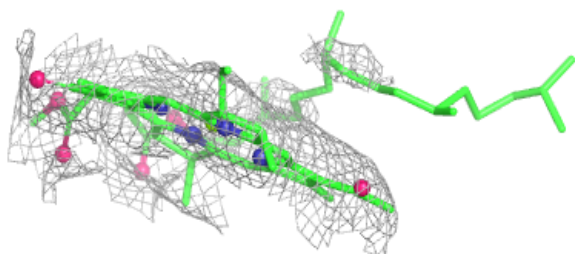
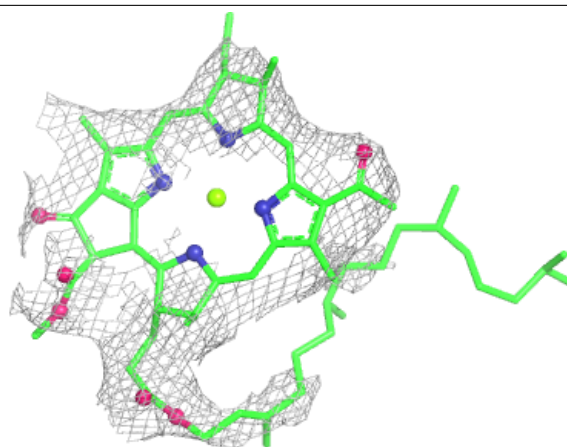
**Electron density around BCL Q 101:**

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



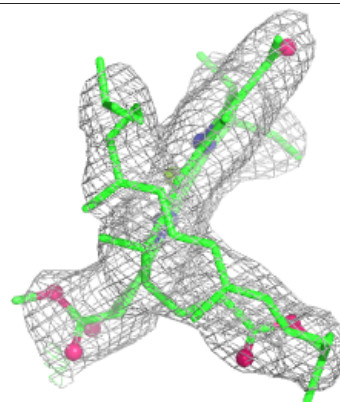
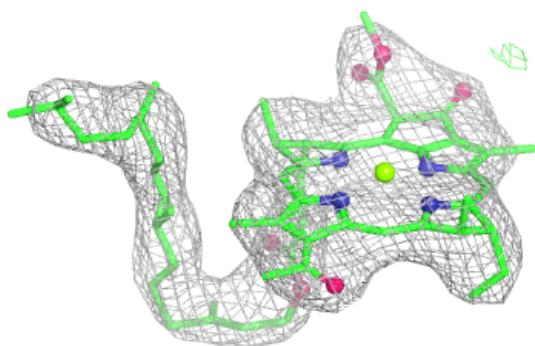
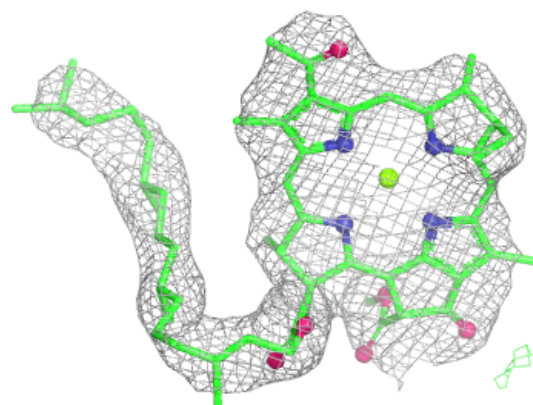
**Electron density around BCL D 103:**

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



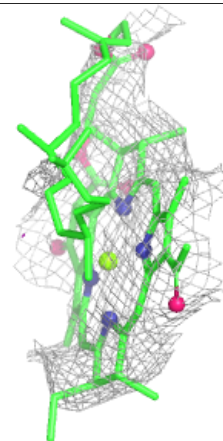
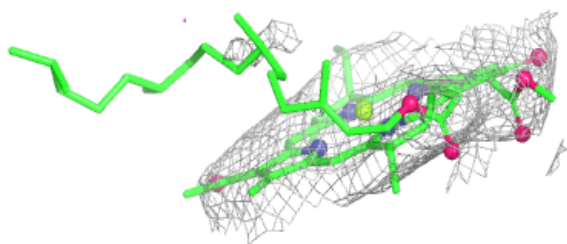
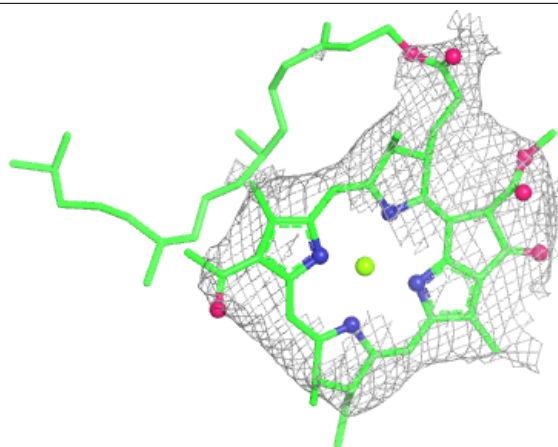
**Electron density around BCL L 301:**

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



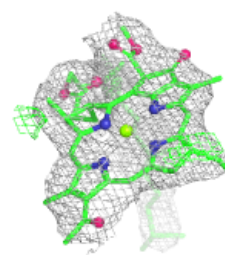
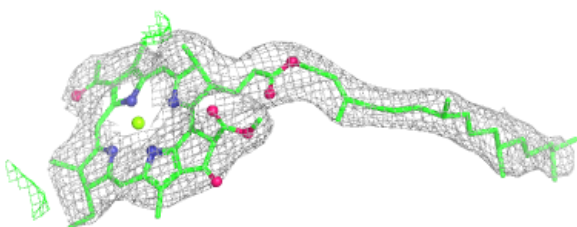
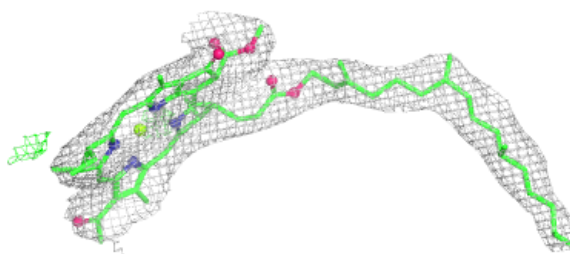
**Electron density around BCL F 103:**

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



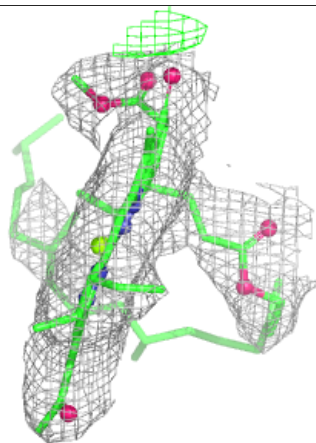
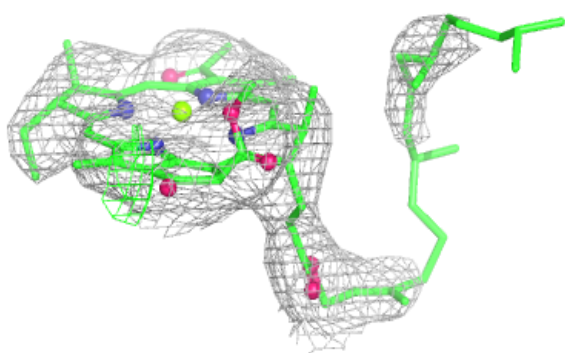
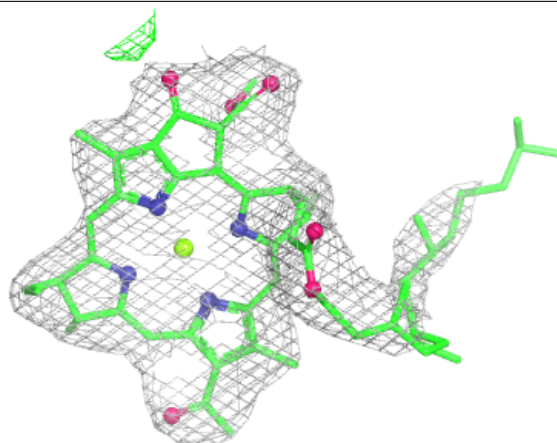
**Electron density around BCL L 302:**

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



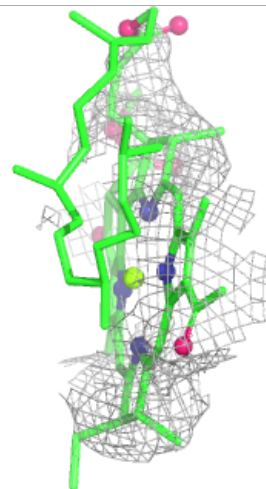
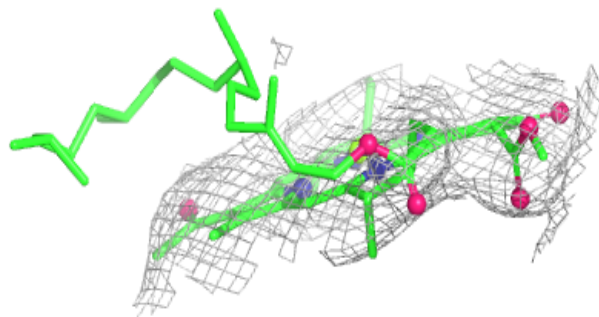
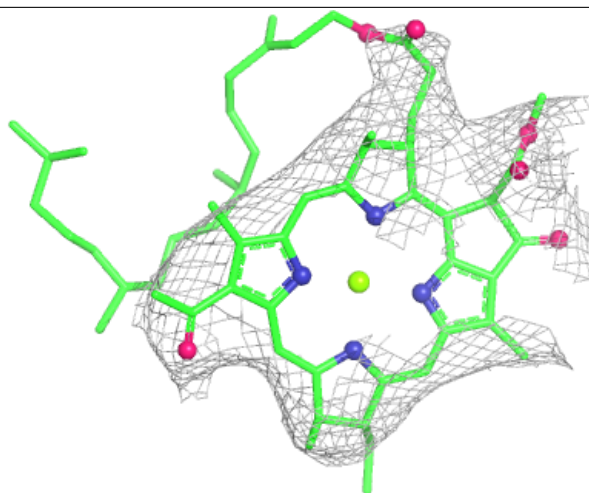
**Electron density around BCL L 305:**

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



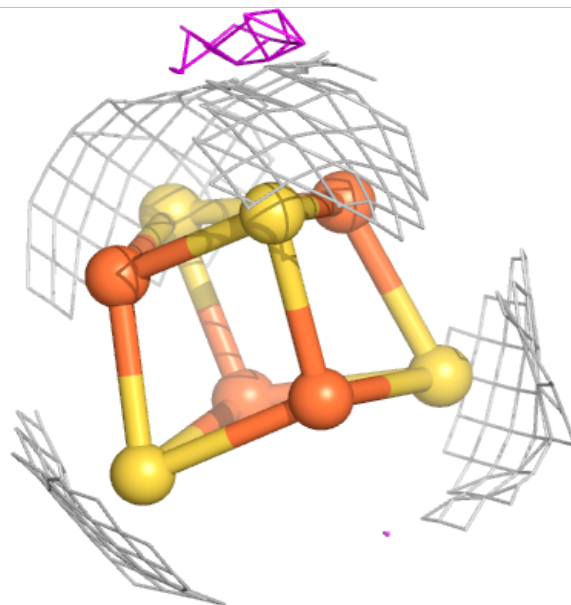
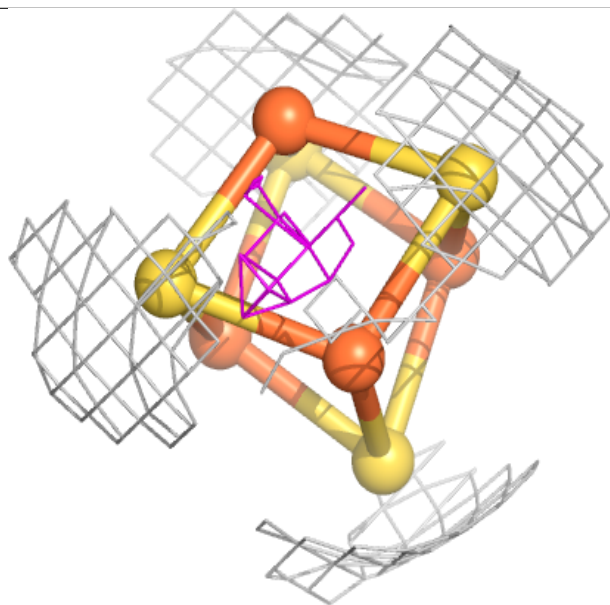
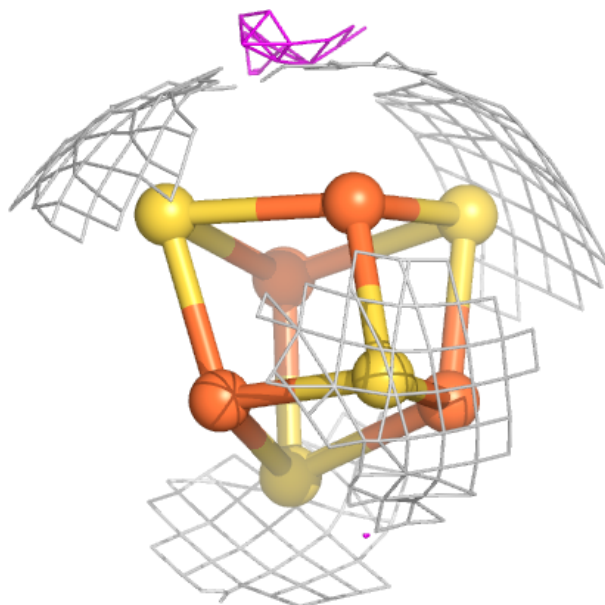
**Electron density around BCL 7 103:**

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



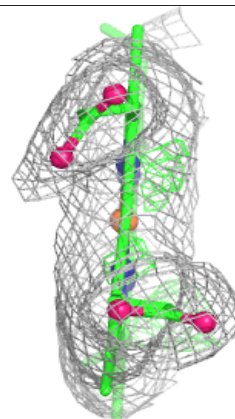
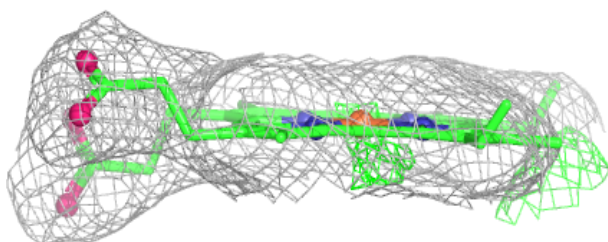
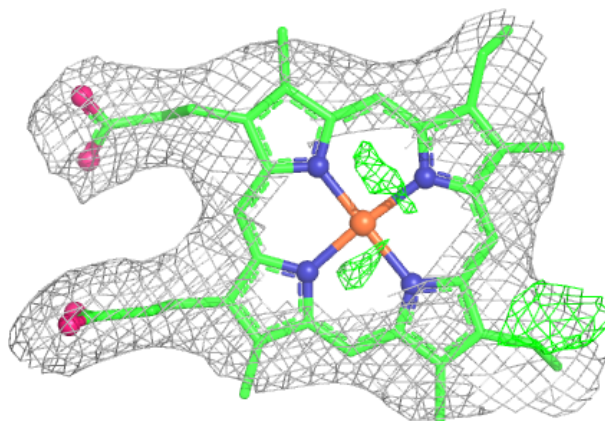
**Electron density around SF4 b 101:**

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



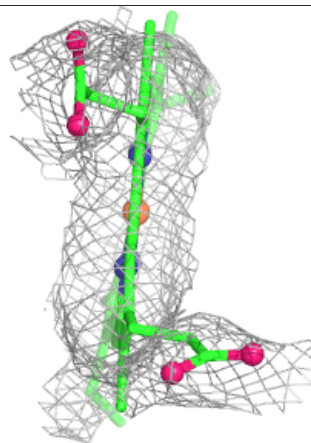
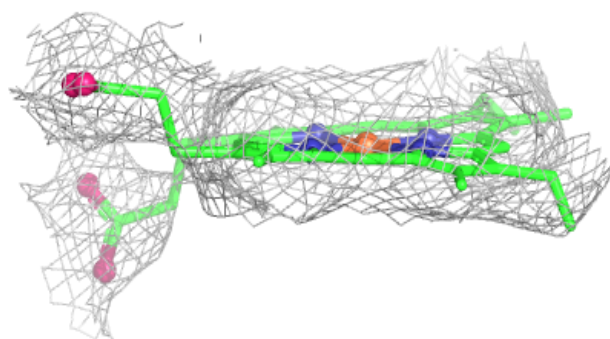
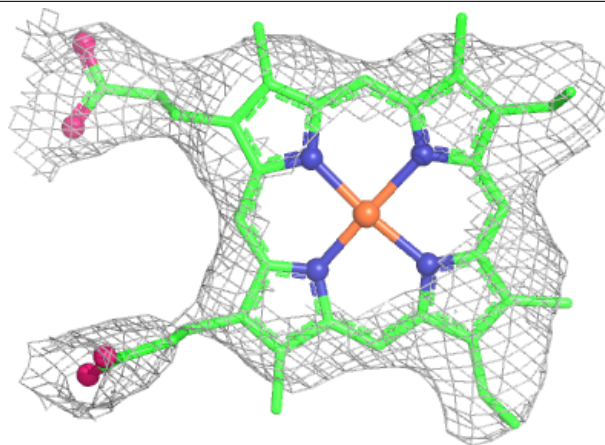
**Electron density around HEC C 504:**

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



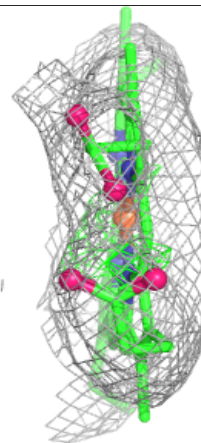
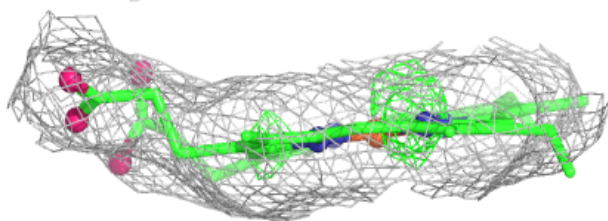
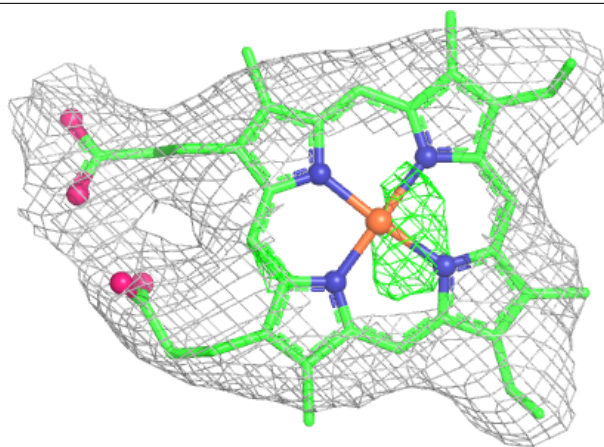
**Electron density around HEC C 501:**

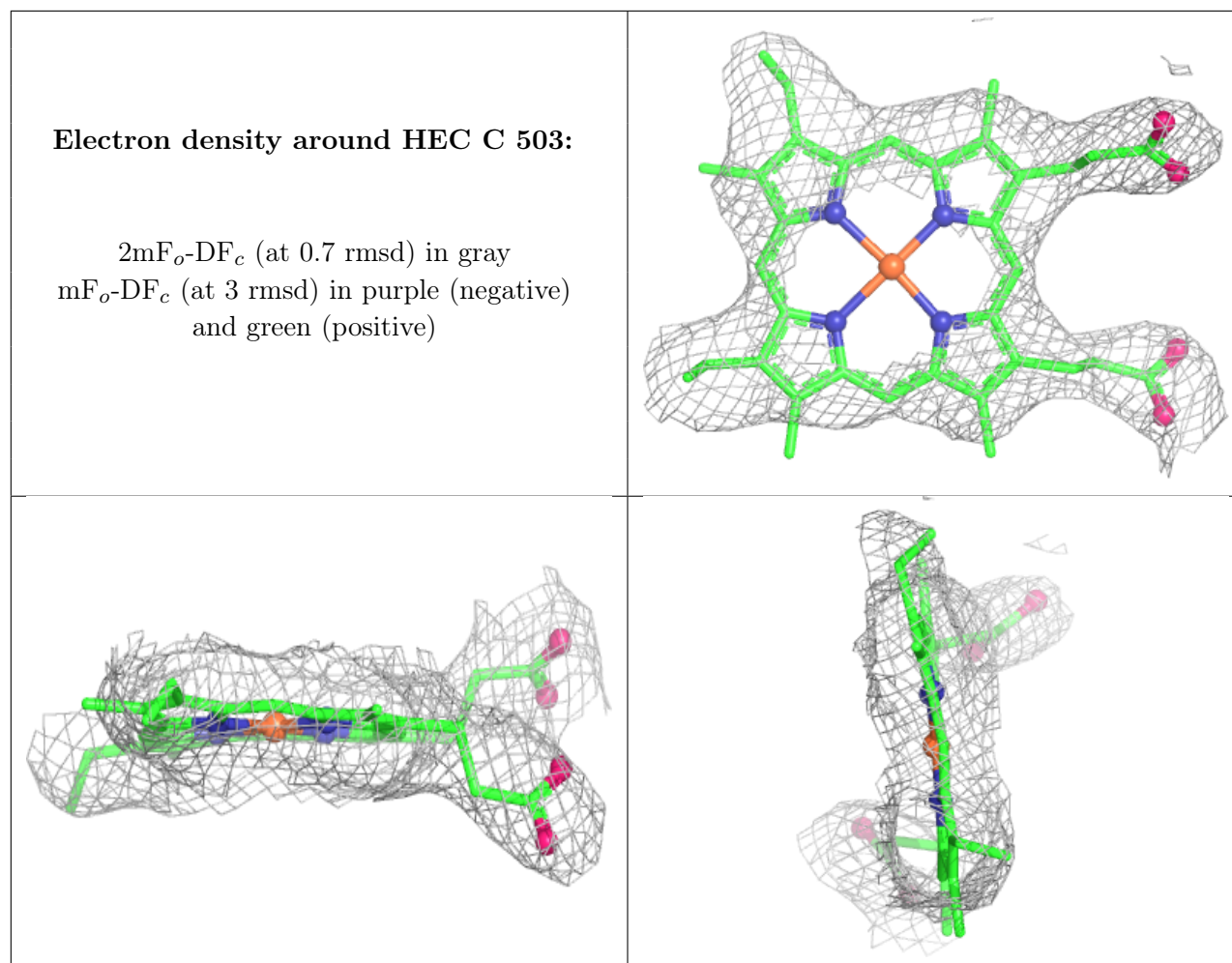
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC C 502:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.