



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:17 AM UTC

PDB ID : 2FKW / pdb\_00002fkw  
Title : Structure of LH2 from Rps. acidophila crystallized in lipidic mesophases  
Authors : Papiz, M.Z.; Cherezov, V.; Clogston, J.; Caffrey, M.  
Deposited on : 2006-01-05  
Resolution : 2.45 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                                                             |

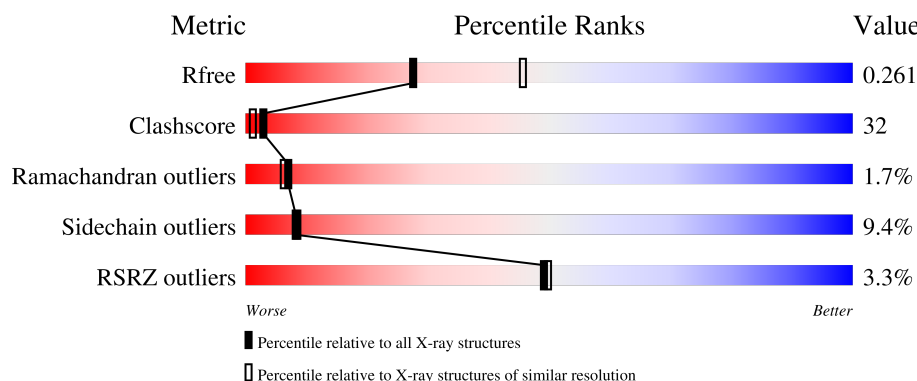
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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                      | 1190 (2.46-2.46)                                      |
| Clashscore            | 190562                      | 1229 (2.46-2.46)                                      |
| Ramachandran outliers | 187476                      | 1218 (2.46-2.46)                                      |
| Sidechain outliers    | 187428                      | 1218 (2.46-2.46)                                      |
| RSRZ outliers         | 180081                      | 1190 (2.46-2.46)                                      |

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

| Mol | Chain | Length | Quality of chain                                  |
|-----|-------|--------|---------------------------------------------------|
| 1   | A     | 53     | <div> <div>4%</div> <div>53% 36% 11%</div> </div> |
| 1   | C     | 53     | <div> <div>6%</div> <div>58% 28% 11%</div> </div> |
| 1   | E     | 53     | <div> <div>6%</div> <div>62% 25% 9%</div> </div>  |
| 1   | G     | 53     | <div> <div>8%</div> <div>64% 26% 9%</div> </div>  |
| 1   | I     | 53     | <div> <div>6%</div> <div>60% 32%</div> </div>     |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 53     |                  |
| 1   | M     | 53     |                  |
| 1   | O     | 53     |                  |
| 1   | R     | 53     |                  |
| 2   | B     | 41     |                  |
| 2   | D     | 41     |                  |
| 2   | F     | 41     |                  |
| 2   | H     | 41     |                  |
| 2   | J     | 41     |                  |
| 2   | L     | 41     |                  |
| 2   | N     | 41     |                  |
| 2   | P     | 41     |                  |
| 2   | S     | 41     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | BCL  | A     | 1501 | X         | -        | -       | -                |
| 3   | BCL  | A     | 1701 | X         | -        | -       | -                |
| 3   | BCL  | B     | 1601 | X         | -        | -       | -                |
| 3   | BCL  | C     | 1502 | X         | -        | -       | -                |
| 3   | BCL  | C     | 1702 | X         | -        | -       | -                |
| 3   | BCL  | G     | 1704 | X         | -        | -       | -                |
| 3   | BCL  | H     | 1604 | X         | -        | -       | -                |
| 3   | BCL  | J     | 1605 | X         | -        | -       | -                |
| 3   | BCL  | K     | 1506 | X         | -        | -       | -                |
| 3   | BCL  | K     | 1706 | X         | -        | -       | -                |
| 3   | BCL  | L     | 1606 | X         | -        | X       | -                |
| 3   | BCL  | M     | 1707 | X         | -        | -       | -                |
| 3   | BCL  | N     | 1607 | X         | -        | -       | -                |
| 3   | BCL  | O     | 1508 | X         | -        | -       | -                |
| 3   | BCL  | O     | 1708 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | BCL  | P     | 1608 | X         | -        | -       | -                |
| 3   | BCL  | R     | 1509 | X         | -        | -       | -                |
| 3   | BCL  | R     | 1709 | X         | -        | X       | -                |
| 3   | BCL  | S     | 1609 | X         | -        | -       | -                |
| 4   | LDA  | G     | 1824 | -         | -        | X       | -                |
| 4   | LDA  | R     | 1818 | -         | -        | X       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9829 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 Light-harvesting protein B-800/850, alpha chain.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 1   | A     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | C     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | E     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | G     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | I     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | K     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | M     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | O     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |
| 1   | R     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 403   | 269 | 67 | 66 | 1 |         |         |       |

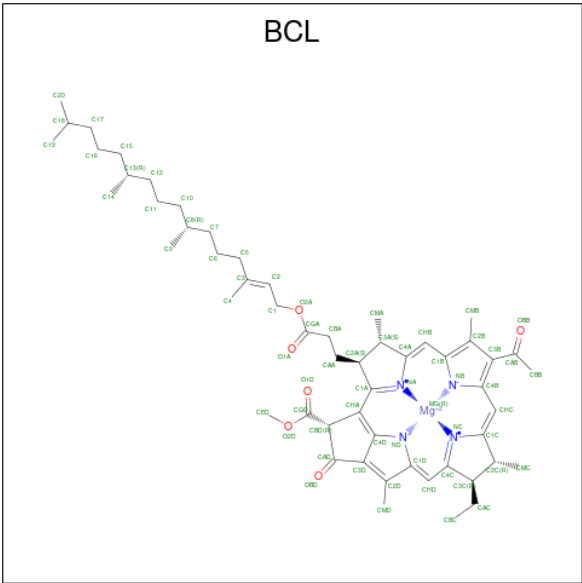
There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| C     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| E     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| G     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| I     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| K     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| M     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| O     | 1       | CXM      | MET    | modified residue | UNP P26789 |
| R     | 1       | CXM      | MET    | modified residue | UNP P26789 |

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 2   | B     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | D     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | F     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | H     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | J     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | L     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | N     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | P     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |
| 2   | S     | 41       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 323   | 213 | 53 | 57 |         |         |       |

- Molecule 3 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 |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 3   | A     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |
| 3   | B     | 1        | Total | C  | Mg | N | O | 0       | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |         |

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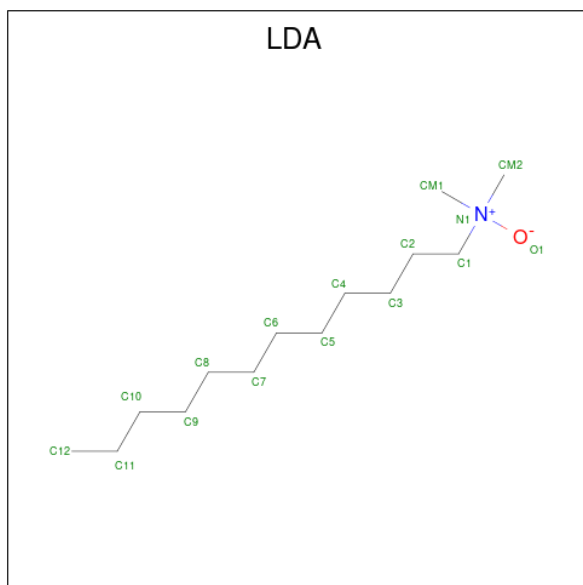
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | C     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | C     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | D     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | E     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | E     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | F     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | G     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | H     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | I     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | I     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | J     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | K     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | L     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | M     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | N     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | O     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | O     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | P     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | R     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 3   | S     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       | 0       |

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

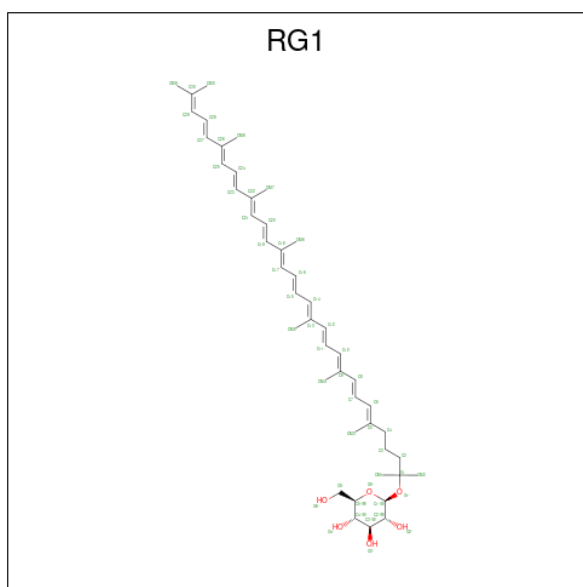
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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | O     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | R     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | R     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |
| 4   | R     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

- Molecule 5 is Rhodopin b-D-glucoside (CCD ID: RG1) (formula:  $C_{46}H_{66}O_6$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 5   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | F     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | H     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | L     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | R     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |
| 5   | S     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 52    | 46 | 6 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 33       | Total | O  | 0       | 0       |
|     |       |          | 33    | 33 |         |         |
| 6   | B     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 6   | C     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 6   | D     | 27       | Total<br>27 | O<br>27 | 0       | 0       |
| 6   | E     | 40       | Total<br>40 | O<br>40 | 0       | 0       |
| 6   | F     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 6   | G     | 41       | Total<br>41 | O<br>41 | 0       | 0       |
| 6   | H     | 37       | Total<br>37 | O<br>37 | 2       | 0       |
| 6   | I     | 38       | Total<br>38 | O<br>38 | 0       | 0       |
| 6   | J     | 39       | Total<br>39 | O<br>39 | 1       | 0       |
| 6   | K     | 47       | Total<br>47 | O<br>47 | 0       | 0       |
| 6   | L     | 29       | Total<br>29 | O<br>29 | 0       | 0       |
| 6   | M     | 36       | Total<br>36 | O<br>36 | 0       | 0       |
| 6   | N     | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 6   | O     | 33       | Total<br>33 | O<br>33 | 1       | 0       |
| 6   | P     | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 6   | R     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 6   | S     | 34       | Total<br>34 | O<br>34 | 0       | 0       |

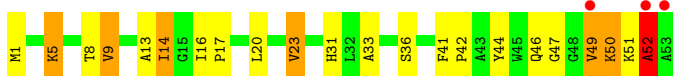
### 3 Residue-property plots

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

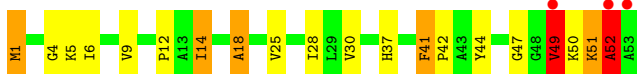
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



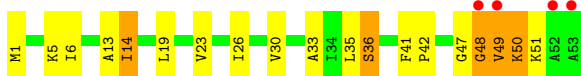
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



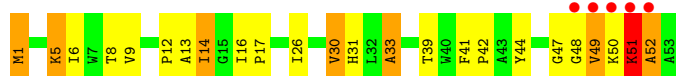
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



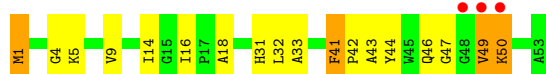
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain

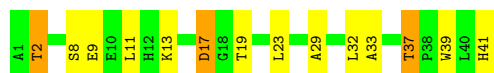


- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain H:  66% 27% 7%



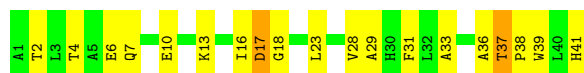
- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain J:  68% 27% 5%



- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain L:  54% 41% 5%



- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain N:  49% 46% 5%



- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain P:  54% 24% 22%



- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain S:  71% 27% 0%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 81.44Å 126.38Å 129.71Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 10.00 – 2.45<br>10.00 – 2.45                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (10.00-2.45)<br>98.1 (10.00-2.45)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.62 (at 2.45Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.183 , 0.254<br>0.203 , 0.261                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2531 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 43.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.620                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.44 , 89.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 9829                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 48.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: CXM, RG1, LDA, BCL

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

| Mol | Chain | Bond lengths |                | Bond angles |               |
|-----|-------|--------------|----------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5       |
| 1   | A     | 1.75         | 6/404 (1.5%)   | 0.71        | 0/556         |
| 1   | C     | 1.94         | 7/404 (1.7%)   | 0.75        | 1/556 (0.2%)  |
| 1   | E     | 1.89         | 9/404 (2.2%)   | 0.81        | 0/556         |
| 1   | G     | 1.83         | 8/404 (2.0%)   | 0.86        | 1/556 (0.2%)  |
| 1   | I     | 1.78         | 4/404 (1.0%)   | 0.77        | 0/556         |
| 1   | K     | 1.99         | 14/404 (3.5%)  | 0.78        | 0/556         |
| 1   | M     | 1.73         | 5/404 (1.2%)   | 0.82        | 1/556 (0.2%)  |
| 1   | O     | 1.78         | 5/404 (1.2%)   | 0.76        | 0/556         |
| 1   | R     | 1.79         | 5/404 (1.2%)   | 0.77        | 0/556         |
| 2   | B     | 1.71         | 3/332 (0.9%)   | 0.71        | 0/453         |
| 2   | D     | 1.53         | 0/332          | 0.65        | 0/453         |
| 2   | F     | 1.75         | 5/332 (1.5%)   | 0.69        | 0/453         |
| 2   | H     | 1.69         | 2/332 (0.6%)   | 0.71        | 0/453         |
| 2   | J     | 1.57         | 3/332 (0.9%)   | 0.70        | 0/453         |
| 2   | L     | 1.89         | 7/332 (2.1%)   | 0.67        | 0/453         |
| 2   | N     | 1.56         | 3/332 (0.9%)   | 0.70        | 0/453         |
| 2   | P     | 1.75         | 7/332 (2.1%)   | 0.69        | 0/453         |
| 2   | S     | 1.56         | 1/332 (0.3%)   | 0.69        | 0/453         |
| All | All   | 1.76         | 94/6624 (1.4%) | 0.74        | 3/9081 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | C     | 2                   | 1                   |
| 1   | E     | 1                   | 0                   |
| 1   | G     | 1                   | 0                   |
| 1   | I     | 2                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | K     | 1                   | 1                   |
| 1   | M     | 3                   | 1                   |
| 1   | O     | 0                   | 1                   |
| 1   | R     | 2                   | 0                   |
| All | All   | 12                  | 7                   |

All (94) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 49  | VAL  | CA-CB  | 11.67 | 1.70        | 1.54     |
| 1   | G     | 36  | SER  | C-O    | -9.64 | 1.11        | 1.24     |
| 1   | E     | 49  | VAL  | N-CA   | 8.41  | 1.56        | 1.46     |
| 1   | C     | 52  | ALA  | CA-C   | 8.24  | 1.63        | 1.52     |
| 1   | R     | 49  | VAL  | CA-CB  | 8.15  | 1.65        | 1.54     |
| 2   | L     | 28  | VAL  | CA-CB  | -7.91 | 1.45        | 1.54     |
| 1   | A     | 14  | ILE  | C-O    | 7.76  | 1.31        | 1.23     |
| 1   | C     | 52  | ALA  | CA-CB  | -7.75 | 1.40        | 1.53     |
| 2   | L     | 17  | ASP  | CG-OD1 | 7.74  | 1.40        | 1.25     |
| 1   | G     | 49  | VAL  | CA-CB  | 7.70  | 1.64        | 1.53     |
| 1   | R     | 49  | VAL  | N-CA   | 7.69  | 1.55        | 1.46     |
| 1   | M     | 33  | ALA  | N-CA   | -7.50 | 1.37        | 1.46     |
| 1   | C     | 49  | VAL  | CA-CB  | 7.35  | 1.64        | 1.54     |
| 1   | K     | 49  | VAL  | CA-CB  | 7.23  | 1.64        | 1.54     |
| 2   | P     | 21  | VAL  | CA-CB  | -7.11 | 1.45        | 1.54     |
| 2   | P     | 6   | GLU  | CG-CD  | 6.98  | 1.69        | 1.52     |
| 1   | E     | 6   | ILE  | CA-CB  | 6.93  | 1.63        | 1.54     |
| 1   | G     | 49  | VAL  | CA-C   | 6.93  | 1.58        | 1.52     |
| 1   | K     | 30  | VAL  | N-CA   | -6.88 | 1.38        | 1.46     |
| 1   | C     | 49  | VAL  | N-CA   | 6.88  | 1.54        | 1.46     |
| 2   | F     | 26  | ALA  | CA-CB  | -6.82 | 1.42        | 1.53     |
| 1   | K     | 15  | GLY  | C-O    | -6.76 | 1.15        | 1.23     |
| 2   | L     | 10  | GLU  | CG-CD  | 6.73  | 1.68        | 1.52     |
| 1   | G     | 30  | VAL  | CA-C   | 6.71  | 1.61        | 1.52     |
| 1   | O     | 49  | VAL  | CA-C   | 6.71  | 1.61        | 1.52     |
| 1   | E     | 49  | VAL  | CA-CB  | 6.64  | 1.63        | 1.54     |
| 1   | O     | 49  | VAL  | N-CA   | 6.64  | 1.54        | 1.46     |
| 1   | E     | 28  | ILE  | CA-CB  | -6.57 | 1.46        | 1.54     |
| 1   | R     | 24  | THR  | CA-CB  | -6.54 | 1.43        | 1.53     |
| 1   | K     | 11  | ASN  | CA-C   | -6.54 | 1.45        | 1.52     |
| 2   | L     | 29  | ALA  | CA-CB  | 6.42  | 1.63        | 1.53     |
| 2   | J     | 2   | THR  | N-CA   | -6.33 | 1.38        | 1.46     |
| 2   | B     | 21  | VAL  | C-O    | 6.22  | 1.31        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | L     | 17  | ASP  | CB-CG | 6.17  | 1.67        | 1.52     |
| 1   | K     | 49  | VAL  | CA-C  | 6.16  | 1.60        | 1.52     |
| 2   | N     | 22  | PHE  | C-O   | -6.16 | 1.17        | 1.24     |
| 1   | K     | 27  | ALA  | C-O   | 6.09  | 1.31        | 1.24     |
| 1   | E     | 30  | VAL  | C-O   | -6.04 | 1.17        | 1.24     |
| 1   | A     | 49  | VAL  | N-CA  | 6.01  | 1.53        | 1.46     |
| 1   | G     | 13  | ALA  | C-N   | 5.98  | 1.39        | 1.33     |
| 2   | L     | 16  | ILE  | N-CA  | -5.95 | 1.39        | 1.46     |
| 1   | E     | 52  | ALA  | CA-C  | 5.92  | 1.60        | 1.52     |
| 1   | K     | 45  | TRP  | C-O   | -5.90 | 1.17        | 1.24     |
| 1   | G     | 48  | GLY  | CA-C  | 5.89  | 1.59        | 1.51     |
| 1   | K     | 10  | VAL  | CA-C  | -5.85 | 1.45        | 1.52     |
| 1   | M     | 26  | ILE  | C-O   | 5.84  | 1.30        | 1.24     |
| 1   | K     | 27  | ALA  | CA-C  | 5.81  | 1.60        | 1.52     |
| 1   | C     | 33  | ALA  | N-CA  | -5.80 | 1.39        | 1.46     |
| 2   | H     | 8   | SER  | C-O   | -5.78 | 1.17        | 1.24     |
| 1   | O     | 18  | ALA  | CA-CB | -5.75 | 1.44        | 1.53     |
| 1   | G     | 6   | ILE  | CA-CB | 5.74  | 1.62        | 1.54     |
| 1   | A     | 33  | ALA  | CA-CB | -5.71 | 1.44        | 1.53     |
| 2   | F     | 4   | THR  | CA-CB | 5.70  | 1.62        | 1.53     |
| 2   | F     | 15  | VAL  | C-O   | -5.69 | 1.17        | 1.24     |
| 2   | N     | 15  | VAL  | CA-CB | 5.66  | 1.61        | 1.54     |
| 1   | I     | 15  | GLY  | C-O   | -5.57 | 1.17        | 1.23     |
| 1   | R     | 51  | LYS  | N-CA  | 5.56  | 1.53        | 1.46     |
| 2   | P     | 2   | THR  | N-CA  | -5.56 | 1.39        | 1.46     |
| 2   | N     | 3   | LEU  | C-O   | -5.54 | 1.16        | 1.23     |
| 1   | E     | 41  | PHE  | C-O   | -5.54 | 1.19        | 1.24     |
| 1   | K     | 16  | ILE  | CA-CB | -5.52 | 1.47        | 1.54     |
| 2   | J     | 2   | THR  | CA-C  | 5.52  | 1.59        | 1.52     |
| 2   | F     | 10  | GLU  | CG-CD | 5.51  | 1.65        | 1.52     |
| 2   | B     | 17  | ASP  | CA-C  | -5.50 | 1.45        | 1.52     |
| 1   | G     | 33  | ALA  | N-CA  | -5.49 | 1.39        | 1.46     |
| 1   | I     | 5   | LYS  | CD-CE | 5.48  | 1.68        | 1.52     |
| 2   | P     | 33  | ALA  | CA-CB | 5.47  | 1.62        | 1.53     |
| 2   | P     | 22  | PHE  | C-O   | 5.46  | 1.30        | 1.24     |
| 2   | H     | 17  | ASP  | CB-CG | -5.45 | 1.38        | 1.52     |
| 1   | K     | 6   | ILE  | CA-CB | 5.44  | 1.61        | 1.54     |
| 2   | J     | 28  | VAL  | CA-CB | -5.44 | 1.48        | 1.54     |
| 2   | L     | 31  | PHE  | N-CA  | -5.44 | 1.40        | 1.46     |
| 2   | S     | 26  | ALA  | C-O   | 5.41  | 1.30        | 1.24     |
| 1   | M     | 30  | VAL  | CA-CB | -5.40 | 1.48        | 1.54     |
| 1   | O     | 41  | PHE  | CA-C  | 5.39  | 1.58        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 18  | ALA  | C-O   | 5.38  | 1.30        | 1.24     |
| 1   | M     | 49  | VAL  | CA-C  | 5.34  | 1.59        | 1.52     |
| 1   | K     | 33  | ALA  | CA-CB | -5.32 | 1.45        | 1.53     |
| 1   | K     | 49  | VAL  | N-CA  | 5.31  | 1.52        | 1.46     |
| 1   | R     | 48  | GLY  | CA-C  | 5.22  | 1.59        | 1.51     |
| 1   | C     | 23  | VAL  | C-O   | 5.20  | 1.30        | 1.24     |
| 2   | P     | 16  | ILE  | CA-CB | 5.19  | 1.60        | 1.54     |
| 1   | I     | 36  | SER  | C-O   | -5.18 | 1.17        | 1.24     |
| 2   | B     | 34  | PHE  | C-O   | 5.18  | 1.30        | 1.24     |
| 2   | P     | 6   | GLU  | CA-CB | 5.18  | 1.61        | 1.53     |
| 1   | E     | 52  | ALA  | N-CA  | 5.18  | 1.52        | 1.46     |
| 1   | O     | 33  | ALA  | CA-C  | 5.16  | 1.59        | 1.52     |
| 1   | K     | 8   | THR  | CA-CB | 5.10  | 1.62        | 1.53     |
| 2   | F     | 37  | THR  | CA-CB | 5.08  | 1.61        | 1.54     |
| 1   | C     | 49  | VAL  | CA-C  | 5.07  | 1.59        | 1.52     |
| 1   | I     | 43  | ALA  | CA-CB | 5.02  | 1.61        | 1.53     |
| 1   | A     | 28  | ILE  | CA-CB | -5.01 | 1.48        | 1.54     |
| 1   | E     | 18  | ALA  | N-CA  | -5.01 | 1.40        | 1.46     |
| 1   | M     | 8   | THR  | C-O   | -5.00 | 1.17        | 1.24     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 49  | VAL  | N-CA-C  | 6.01  | 112.64      | 106.21   |
| 1   | M     | 14  | ILE  | CB-CA-C | -5.21 | 105.66      | 111.80   |
| 1   | C     | 14  | ILE  | CB-CA-C | -5.20 | 105.67      | 111.80   |

All (12) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | C     | 52  | ALA  | CA   |
| 1   | C     | 53  | ALA  | CA   |
| 1   | E     | 51  | LYS  | CA   |
| 1   | G     | 50  | LYS  | CA   |
| 1   | I     | 49  | VAL  | CA   |
| 1   | I     | 50  | LYS  | CA   |
| 1   | K     | 51  | LYS  | CA   |
| 1   | M     | 49  | VAL  | CA   |
| 1   | M     | 51  | LYS  | CA   |
| 1   | M     | 52  | ALA  | CA   |
| 1   | R     | 50  | LYS  | CA   |
| 1   | R     | 53  | ALA  | CA   |

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 50  | LYS  | Peptide |
| 1   | A     | 51  | LYS  | Peptide |
| 1   | C     | 52  | ALA  | Peptide |
| 1   | I     | 51  | LYS  | Peptide |
| 1   | K     | 50  | LYS  | Peptide |
| 1   | M     | 51  | LYS  | Peptide |
| 1   | O     | 50  | LYS  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 403   | 0        | 422      | 25      | 0            |
| 1   | C     | 403   | 0        | 422      | 27      | 0            |
| 1   | E     | 403   | 0        | 422      | 28      | 0            |
| 1   | G     | 403   | 0        | 422      | 19      | 0            |
| 1   | I     | 403   | 0        | 422      | 20      | 0            |
| 1   | K     | 403   | 0        | 422      | 26      | 0            |
| 1   | M     | 403   | 0        | 422      | 32      | 0            |
| 1   | O     | 403   | 0        | 422      | 17      | 0            |
| 1   | R     | 403   | 0        | 422      | 20      | 0            |
| 2   | B     | 323   | 0        | 321      | 25      | 0            |
| 2   | D     | 323   | 0        | 321      | 19      | 0            |
| 2   | F     | 323   | 0        | 321      | 23      | 0            |
| 2   | H     | 323   | 0        | 321      | 18      | 0            |
| 2   | J     | 323   | 0        | 321      | 22      | 0            |
| 2   | L     | 323   | 0        | 321      | 22      | 0            |
| 2   | N     | 323   | 0        | 321      | 28      | 0            |
| 2   | P     | 323   | 0        | 321      | 30      | 0            |
| 2   | S     | 323   | 0        | 321      | 11      | 0            |
| 3   | A     | 132   | 0        | 146      | 22      | 0            |
| 3   | B     | 66    | 0        | 74       | 7       | 0            |
| 3   | C     | 132   | 0        | 148      | 11      | 0            |
| 3   | D     | 66    | 0        | 74       | 5       | 0            |
| 3   | E     | 132   | 0        | 147      | 10      | 0            |
| 3   | F     | 66    | 0        | 74       | 9       | 0            |
| 3   | G     | 132   | 0        | 147      | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | H     | 66    | 0        | 73       | 8       | 0            |
| 3   | I     | 132   | 0        | 148      | 29      | 0            |
| 3   | J     | 66    | 0        | 73       | 15      | 0            |
| 3   | K     | 132   | 0        | 146      | 14      | 0            |
| 3   | L     | 66    | 0        | 74       | 21      | 0            |
| 3   | M     | 132   | 0        | 147      | 22      | 0            |
| 3   | N     | 66    | 0        | 74       | 14      | 0            |
| 3   | O     | 132   | 0        | 147      | 20      | 0            |
| 3   | P     | 66    | 0        | 73       | 11      | 0            |
| 3   | R     | 132   | 0        | 147      | 27      | 0            |
| 3   | S     | 66    | 0        | 74       | 10      | 0            |
| 4   | A     | 32    | 0        | 62       | 11      | 0            |
| 4   | B     | 16    | 0        | 31       | 2       | 0            |
| 4   | C     | 32    | 0        | 62       | 6       | 0            |
| 4   | D     | 16    | 0        | 31       | 3       | 0            |
| 4   | E     | 32    | 0        | 62       | 14      | 0            |
| 4   | F     | 16    | 0        | 31       | 7       | 0            |
| 4   | G     | 32    | 0        | 62       | 17      | 0            |
| 4   | H     | 16    | 0        | 31       | 3       | 0            |
| 4   | I     | 48    | 0        | 93       | 15      | 0            |
| 4   | J     | 16    | 0        | 31       | 1       | 0            |
| 4   | K     | 32    | 0        | 62       | 12      | 0            |
| 4   | L     | 16    | 0        | 31       | 5       | 0            |
| 4   | M     | 32    | 0        | 62       | 6       | 0            |
| 4   | N     | 16    | 0        | 31       | 2       | 0            |
| 4   | O     | 16    | 0        | 31       | 7       | 0            |
| 4   | P     | 16    | 0        | 31       | 3       | 0            |
| 4   | R     | 48    | 0        | 93       | 12      | 0            |
| 5   | D     | 52    | 0        | 66       | 5       | 0            |
| 5   | F     | 52    | 0        | 66       | 5       | 0            |
| 5   | H     | 52    | 0        | 66       | 5       | 0            |
| 5   | J     | 52    | 0        | 66       | 1       | 0            |
| 5   | L     | 52    | 0        | 66       | 4       | 0            |
| 5   | N     | 52    | 0        | 66       | 4       | 0            |
| 5   | P     | 52    | 0        | 66       | 4       | 0            |
| 5   | R     | 52    | 0        | 66       | 4       | 0            |
| 5   | S     | 52    | 0        | 66       | 5       | 0            |
| 6   | A     | 33    | 0        | 0        | 10      | 0            |
| 6   | B     | 26    | 0        | 0        | 6       | 0            |
| 6   | C     | 24    | 0        | 0        | 3       | 0            |
| 6   | D     | 27    | 0        | 0        | 7       | 0            |
| 6   | E     | 40    | 0        | 0        | 20      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | F     | 28    | 0        | 0        | 8       | 0            |
| 6   | G     | 41    | 0        | 0        | 22      | 0            |
| 6   | H     | 37    | 0        | 0        | 5       | 0            |
| 6   | I     | 38    | 0        | 0        | 11      | 0            |
| 6   | J     | 39    | 0        | 0        | 14      | 0            |
| 6   | K     | 47    | 0        | 0        | 28      | 0            |
| 6   | L     | 29    | 0        | 0        | 2       | 0            |
| 6   | M     | 36    | 0        | 0        | 10      | 0            |
| 6   | N     | 30    | 0        | 0        | 8       | 0            |
| 6   | O     | 33    | 0        | 0        | 11      | 0            |
| 6   | P     | 32    | 0        | 0        | 8       | 0            |
| 6   | R     | 39    | 0        | 0        | 23      | 0            |
| 6   | S     | 34    | 0        | 0        | 4       | 0            |
| All | All   | 9829  | 0        | 10104    | 622     | 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 32.

All (622) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:M:1:CXM:SD      | 1:M:1:CXM:CE     | 2.21                     | 1.28              |
| 1:G:48:GLY:HA2    | 6:G:1839:HOH:O   | 1.32                     | 1.24              |
| 4:I:1825:LDA:HM22 | 6:I:1845:HOH:O   | 1.06                     | 1.24              |
| 4:H:1804:LDA:H92  | 6:H:1825:HOH:O   | 1.38                     | 1.22              |
| 1:E:49:VAL:HG11   | 6:E:1850:HOH:O   | 1.45                     | 1.15              |
| 3:I:1705:BCL:H8   | 3:I:1705:BCL:H41 | 1.25                     | 1.15              |
| 6:A:1831:HOH:O    | 2:D:21:VAL:HG11  | 1.53                     | 1.08              |
| 3:R:1709:BCL:H2   | 6:R:1831:HOH:O   | 1.54                     | 1.07              |
| 3:G:1504:BCL:H143 | 6:G:1853:HOH:O   | 1.54                     | 1.05              |
| 3:O:1708:BCL:H2   | 6:O:1833:HOH:O   | 1.59                     | 1.02              |
| 2:P:33:ALA:O      | 2:P:37:THR:HB    | 1.58                     | 1.02              |
| 4:I:1812:LDA:HM23 | 6:I:1829:HOH:O   | 1.59                     | 1.01              |
| 3:O:1708:BCL:C2   | 6:O:1833:HOH:O   | 2.08                     | 1.01              |
| 2:D:6:GLU:HB3     | 6:D:1825:HOH:O   | 1.61                     | 1.01              |
| 3:J:1605:BCL:O2D  | 6:J:1813:HOH:O   | 1.79                     | 1.01              |
| 4:G:1824:LDA:CM1  | 6:G:1828:HOH:O   | 2.08                     | 1.00              |
| 4:E:1822:LDA:CM2  | 6:E:1859:HOH:O   | 2.09                     | 0.99              |
| 1:G:48:GLY:O      | 6:G:1832:HOH:O   | 1.79                     | 0.98              |
| 1:I:48:GLY:HA2    | 6:I:1836:HOH:O   | 1.63                     | 0.98              |
| 1:I:48:GLY:CA     | 6:I:1836:HOH:O   | 2.10                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1501:BCL:H191 | 3:R:1709:BCL:HED1 | 1.41                     | 0.97              |
| 3:A:1501:BCL:CAA  | 3:A:1501:BCL:O1D  | 2.14                     | 0.96              |
| 1:E:14:ILE:HG22   | 6:E:1835:HOH:O    | 1.65                     | 0.96              |
| 2:L:39:TRP:CE2    | 3:L:1606:BCL:CMC  | 2.49                     | 0.95              |
| 3:J:1605:BCL:CBD  | 6:J:1813:HOH:O    | 2.12                     | 0.95              |
| 2:P:23:LEU:HB2    | 3:P:1608:BCL:H2   | 1.46                     | 0.95              |
| 4:G:1824:LDA:HM11 | 6:G:1828:HOH:O    | 1.66                     | 0.94              |
| 3:M:1707:BCL:O2D  | 6:M:1859:HOH:O    | 1.86                     | 0.94              |
| 1:E:44:TYR:CZ     | 6:E:1862:HOH:O    | 2.19                     | 0.94              |
| 3:A:1501:BCL:O1D  | 3:A:1501:BCL:HAA2 | 1.68                     | 0.93              |
| 1:C:13:ALA:HB2    | 6:D:1826:HOH:O    | 1.67                     | 0.92              |
| 1:M:51:LYS:HG2    | 1:M:52:ALA:O      | 1.69                     | 0.92              |
| 2:F:33:ALA:O      | 2:F:37:THR:HB     | 1.68                     | 0.92              |
| 2:N:33:ALA:O      | 2:N:37:THR:HB     | 1.68                     | 0.92              |
| 4:O:1820:LDA:HM12 | 6:O:1823:HOH:O    | 1.70                     | 0.91              |
| 2:H:33:ALA:O      | 2:H:37:THR:HB     | 1.70                     | 0.91              |
| 4:R:1818:LDA:H92  | 6:R:1852:HOH:O    | 1.70                     | 0.90              |
| 1:C:14:ILE:HG21   | 4:C:1815:LDA:H21  | 1.53                     | 0.90              |
| 3:M:1707:BCL:CBD  | 6:M:1859:HOH:O    | 2.20                     | 0.89              |
| 1:M:51:LYS:HA     | 1:M:52:ALA:HB2    | 1.52                     | 0.89              |
| 1:C:36:SER:OG     | 4:E:1822:LDA:HM21 | 1.72                     | 0.88              |
| 2:D:33:ALA:O      | 2:D:37:THR:HB     | 1.74                     | 0.87              |
| 2:S:33:ALA:O      | 2:S:37:THR:HG22   | 1.74                     | 0.87              |
| 2:D:9:GLU:OE1     | 6:D:1809:HOH:O    | 1.91                     | 0.87              |
| 6:K:1864:HOH:O    | 4:L:1806:LDA:H82  | 1.75                     | 0.86              |
| 2:P:33:ALA:HB1    | 6:P:1837:HOH:O    | 1.76                     | 0.86              |
| 1:R:5:LYS:HD3     | 6:R:1835:HOH:O    | 1.75                     | 0.85              |
| 2:L:33:ALA:O      | 2:L:37:THR:HB     | 1.77                     | 0.85              |
| 2:J:33:ALA:O      | 2:J:37:THR:HB     | 1.76                     | 0.85              |
| 3:R:1709:BCL:H92  | 3:R:1709:BCL:H41  | 1.59                     | 0.84              |
| 1:I:48:GLY:N      | 6:I:1836:HOH:O    | 2.10                     | 0.84              |
| 2:J:41:HIS:NE2    | 1:K:49:VAL:HG12   | 1.92                     | 0.84              |
| 1:I:5:LYS:HG3     | 6:J:1823:HOH:O    | 1.78                     | 0.83              |
| 4:K:1810:LDA:HM22 | 1:M:14:ILE:HD11   | 1.58                     | 0.83              |
| 1:K:31:HIS:CE1    | 3:L:1606:BCL:HMD3 | 2.13                     | 0.83              |
| 4:O:1820:LDA:HM23 | 6:O:1823:HOH:O    | 1.76                     | 0.83              |
| 3:I:1705:BCL:H41  | 3:I:1705:BCL:C8   | 2.06                     | 0.82              |
| 6:K:1848:HOH:O    | 1:M:13:ALA:HB2    | 1.79                     | 0.82              |
| 3:A:1501:BCL:C19  | 3:R:1709:BCL:HED1 | 2.08                     | 0.82              |
| 4:O:1820:LDA:H122 | 6:O:1850:HOH:O    | 1.80                     | 0.81              |
| 2:P:37:THR:HG22   | 2:P:39:TRP:H      | 1.45                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1501:BCL:H62  | 3:R:1709:BCL:HED2 | 1.59                     | 0.81              |
| 3:J:1605:BCL:CBB  | 6:K:1864:HOH:O    | 2.28                     | 0.81              |
| 6:R:1835:HOH:O    | 2:S:5:ALA:HB1     | 1.81                     | 0.81              |
| 2:L:39:TRP:CE2    | 3:L:1606:BCL:HMC3 | 2.14                     | 0.80              |
| 3:R:1709:BCL:CAD  | 3:S:1609:BCL:H203 | 2.10                     | 0.80              |
| 4:I:1825:LDA:H92  | 6:K:1842:HOH:O    | 1.80                     | 0.80              |
| 4:A:1816:LDA:H31  | 1:C:14:ILE:HD13   | 1.64                     | 0.80              |
| 1:A:14:ILE:HG21   | 4:A:1816:LDA:H42  | 1.62                     | 0.80              |
| 2:B:4:THR:OG1     | 2:B:7:GLN:HG3     | 1.81                     | 0.80              |
| 6:A:1850:HOH:O    | 2:B:8:SER:HB2     | 1.82                     | 0.80              |
| 2:P:41:HIS:NE2    | 1:R:49:VAL:CG1    | 2.46                     | 0.79              |
| 3:M:1707:BCL:H41  | 3:M:1707:BCL:H8   | 1.65                     | 0.78              |
| 2:B:37:THR:HG23   | 2:B:39:TRP:H      | 1.47                     | 0.78              |
| 3:G:1704:BCL:CED  | 3:I:1505:BCL:H191 | 2.14                     | 0.78              |
| 3:R:1709:BCL:H102 | 6:S:419:HOH:O     | 1.85                     | 0.77              |
| 4:K:1810:LDA:H21  | 1:M:14:ILE:HD13   | 1.68                     | 0.76              |
| 3:R:1709:BCL:H41  | 3:R:1709:BCL:C9   | 2.16                     | 0.76              |
| 1:I:5:LYS:CG      | 6:J:1823:HOH:O    | 2.32                     | 0.75              |
| 4:O:1820:LDA:HM22 | 1:R:32:LEU:HD22   | 1.67                     | 0.75              |
| 2:S:37:THR:HG23   | 2:S:39:TRP:H      | 1.49                     | 0.75              |
| 2:P:33:ALA:CB     | 6:P:1837:HOH:O    | 2.31                     | 0.75              |
| 1:M:48:GLY:HA2    | 6:M:1829:HOH:O    | 1.86                     | 0.75              |
| 4:I:1812:LDA:H121 | 6:K:1856:HOH:O    | 1.85                     | 0.75              |
| 4:G:1824:LDA:CM2  | 6:G:1828:HOH:O    | 2.35                     | 0.75              |
| 2:S:23:LEU:HB2    | 3:S:1609:BCL:H2   | 1.67                     | 0.74              |
| 2:F:10:GLU:OE1    | 5:F:1403:RG1:O2'  | 2.03                     | 0.74              |
| 4:R:1818:LDA:C11  | 6:R:1856:HOH:O    | 2.35                     | 0.74              |
| 1:A:14:ILE:HD13   | 4:A:1816:LDA:H22  | 1.68                     | 0.74              |
| 4:A:1816:LDA:C3   | 1:C:14:ILE:HD13   | 2.18                     | 0.74              |
| 2:L:39:TRP:CD2    | 3:L:1606:BCL:CMC  | 2.71                     | 0.74              |
| 4:R:1818:LDA:H122 | 6:R:1856:HOH:O    | 1.88                     | 0.74              |
| 1:E:18:ALA:O      | 6:E:1860:HOH:O    | 2.05                     | 0.74              |
| 1:A:31:HIS:CE1    | 3:B:1601:BCL:HMD3 | 2.22                     | 0.73              |
| 2:H:32:LEU:HD12   | 4:H:1804:LDA:H122 | 1.70                     | 0.73              |
| 1:M:41:PHE:HB3    | 1:M:42:PRO:HD3    | 1.69                     | 0.73              |
| 3:I:1705:BCL:H8   | 3:I:1705:BCL:C4   | 2.15                     | 0.73              |
| 2:N:39:TRP:CE2    | 3:N:1607:BCL:CMC  | 2.72                     | 0.73              |
| 2:P:39:TRP:CE2    | 3:P:1608:BCL:HMC2 | 2.24                     | 0.73              |
| 4:G:1824:LDA:HM21 | 6:G:1843:HOH:O    | 1.89                     | 0.72              |
| 4:G:1824:LDA:H31  | 6:G:1844:HOH:O    | 1.86                     | 0.72              |
| 4:R:1818:LDA:C9   | 6:R:1852:HOH:O    | 2.30                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:1817:LDA:H11  | 6:A:1820:HOH:O    | 1.90                     | 0.72              |
| 2:D:37:THR:HG22   | 2:D:39:TRP:H      | 1.54                     | 0.71              |
| 3:P:1608:BCL:HBB2 | 3:P:1608:BCL:HMB3 | 1.70                     | 0.71              |
| 1:M:33:ALA:HA     | 4:M:1827:LDA:HM11 | 1.70                     | 0.71              |
| 3:P:1608:BCL:HBC1 | 6:P:1837:HOH:O    | 1.90                     | 0.71              |
| 4:G:1824:LDA:HM23 | 6:I:1859:HOH:O    | 1.89                     | 0.71              |
| 4:E:1822:LDA:HM22 | 6:E:1859:HOH:O    | 1.83                     | 0.71              |
| 2:H:23:LEU:HB2    | 3:H:1604:BCL:H2   | 1.72                     | 0.71              |
| 1:E:14:ILE:CG2    | 6:E:1835:HOH:O    | 2.30                     | 0.70              |
| 1:A:20:LEU:HD13   | 3:R:1709:BCL:HED3 | 1.73                     | 0.70              |
| 2:N:39:TRP:CD2    | 3:N:1607:BCL:HMC2 | 2.26                     | 0.70              |
| 3:O:1508:BCL:HHC  | 3:O:1508:BCL:OBB  | 1.89                     | 0.70              |
| 4:R:1818:LDA:C9   | 6:R:1856:HOH:O    | 2.39                     | 0.70              |
| 2:B:1:ALA:N       | 6:B:278:HOH:O     | 2.23                     | 0.70              |
| 2:H:39:TRP:CE3    | 3:H:1604:BCL:CBC  | 2.75                     | 0.70              |
| 1:M:49:VAL:HG12   | 6:M:1843:HOH:O    | 1.91                     | 0.70              |
| 4:N:1807:LDA:HM12 | 6:N:1810:HOH:O    | 1.92                     | 0.70              |
| 4:G:1824:LDA:C6   | 6:G:1865:HOH:O    | 2.38                     | 0.70              |
| 1:K:48:GLY:HA2    | 6:K:1829:HOH:O    | 1.90                     | 0.70              |
| 4:R:1818:LDA:C10  | 6:R:1856:HOH:O    | 2.40                     | 0.70              |
| 3:K:1506:BCL:HMC3 | 4:L:1806:LDA:H51  | 1.71                     | 0.70              |
| 4:K:1810:LDA:H101 | 6:K:1856:HOH:O    | 1.92                     | 0.70              |
| 2:P:41:HIS:NE2    | 1:R:49:VAL:HG13   | 2.06                     | 0.70              |
| 3:R:1509:BCL:O1D  | 3:R:1509:BCL:H2A  | 1.92                     | 0.69              |
| 3:M:1707:BCL:H41  | 3:M:1707:BCL:C7   | 2.22                     | 0.69              |
| 1:E:44:TYR:CE1    | 6:E:1862:HOH:O    | 2.44                     | 0.69              |
| 1:E:49:VAL:CG1    | 6:E:1850:HOH:O    | 2.16                     | 0.69              |
| 2:J:26:ALA:HB1    | 6:J:1825:HOH:O    | 1.92                     | 0.69              |
| 2:F:2:THR:HG22    | 6:F:1823:HOH:O    | 1.92                     | 0.69              |
| 3:K:1706:BCL:HBB2 | 3:K:1706:BCL:HHC  | 1.73                     | 0.69              |
| 2:P:41:HIS:NE2    | 1:R:49:VAL:HG12   | 2.07                     | 0.69              |
| 1:G:41:PHE:HB3    | 1:G:42:PRO:HD3    | 1.75                     | 0.68              |
| 2:N:39:TRP:CE2    | 3:N:1607:BCL:HMC2 | 2.27                     | 0.68              |
| 4:R:1818:LDA:H71  | 6:R:1852:HOH:O    | 1.93                     | 0.68              |
| 3:I:1705:BCL:HHB  | 2:J:19:THR:HG21   | 1.76                     | 0.68              |
| 1:R:48:GLY:HA2    | 6:R:1823:HOH:O    | 1.92                     | 0.68              |
| 6:A:1850:HOH:O    | 2:B:3:LEU:HB2     | 1.94                     | 0.68              |
| 1:K:30:VAL:CG2    | 5:L:1406:RG1:HM03 | 2.24                     | 0.68              |
| 1:R:37:HIS:ND1    | 6:R:1845:HOH:O    | 2.27                     | 0.68              |
| 3:J:1605:BCL:CGD  | 6:J:1813:HOH:O    | 2.27                     | 0.68              |
| 3:G:1704:BCL:C10  | 6:H:1808:HOH:O    | 2.40                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:N:17:ASP:CG     | 6:N:1829:HOH:O    | 2.35                     | 0.67              |
| 3:A:1501:BCL:O1D  | 3:A:1501:BCL:C2A  | 2.42                     | 0.67              |
| 3:O:1508:BCL:O1D  | 3:O:1508:BCL:HAA2 | 1.95                     | 0.67              |
| 6:E:1862:HOH:O    | 4:F:1803:LDA:C3   | 2.42                     | 0.67              |
| 2:F:41:HIS:CE1    | 1:G:49:VAL:H      | 2.12                     | 0.67              |
| 1:A:35:LEU:HD21   | 1:R:37:HIS:CD2    | 2.30                     | 0.67              |
| 3:R:1709:BCL:C10  | 6:S:419:HOH:O     | 2.41                     | 0.66              |
| 1:I:41:PHE:HB3    | 1:I:42:PRO:HD3    | 1.78                     | 0.66              |
| 4:I:1825:LDA:HM11 | 6:I:1859:HOH:O    | 1.95                     | 0.66              |
| 2:J:41:HIS:NE2    | 1:K:49:VAL:CG1    | 2.58                     | 0.66              |
| 3:F:1603:BCL:H62  | 3:F:1603:BCL:H112 | 1.76                     | 0.66              |
| 4:K:1810:LDA:H21  | 1:M:14:ILE:CD1    | 2.25                     | 0.66              |
| 3:G:1704:BCL:H101 | 6:H:1808:HOH:O    | 1.96                     | 0.65              |
| 1:A:14:ILE:HG21   | 4:A:1816:LDA:C4   | 2.26                     | 0.65              |
| 2:B:41:HIS:O      | 6:B:186:HOH:O     | 2.13                     | 0.65              |
| 5:F:1403:RG1:O1'  | 6:F:1827:HOH:O    | 2.13                     | 0.65              |
| 3:N:1607:BCL:HBB2 | 3:N:1607:BCL:HMB3 | 1.78                     | 0.65              |
| 1:I:51:LYS:HB2    | 1:I:52:ALA:HA     | 1.77                     | 0.65              |
| 3:F:1603:BCL:C10  | 3:F:1603:BCL:H142 | 2.26                     | 0.65              |
| 4:E:1823:LDA:H11  | 6:E:1854:HOH:O    | 1.97                     | 0.65              |
| 3:G:1704:BCL:CB D | 6:G:1854:HOH:O    | 2.44                     | 0.64              |
| 1:O:41:PHE:HB3    | 1:O:42:PRO:HD3    | 1.77                     | 0.64              |
| 1:C:31:HIS:CE1    | 3:D:1602:BCL:HMD3 | 2.32                     | 0.64              |
| 4:E:1823:LDA:HM21 | 6:E:1853:HOH:O    | 1.96                     | 0.64              |
| 4:I:1825:LDA:C9   | 6:K:1842:HOH:O    | 2.41                     | 0.64              |
| 1:R:5:LYS:CD      | 6:R:1835:HOH:O    | 2.37                     | 0.64              |
| 1:C:36:SER:OG     | 4:E:1822:LDA:CM2  | 2.43                     | 0.64              |
| 1:K:14:ILE:HG21   | 4:K:1810:LDA:H31  | 1.79                     | 0.64              |
| 1:K:30:VAL:HG22   | 5:L:1406:RG1:HM03 | 1.80                     | 0.64              |
| 2:B:41:HIS:NE2    | 1:C:49:VAL:HG12   | 2.13                     | 0.64              |
| 1:E:49:VAL:HG21   | 6:E:1849:HOH:O    | 1.96                     | 0.63              |
| 2:D:37:THR:CG2    | 2:D:39:TRP:H      | 2.11                     | 0.63              |
| 4:F:1803:LDA:C8   | 6:F:1809:HOH:O    | 2.44                     | 0.63              |
| 2:B:19:THR:CG2    | 3:B:1601:BCL:H42  | 2.27                     | 0.63              |
| 3:M:1707:BCL:H41  | 3:M:1707:BCL:C8   | 2.27                     | 0.63              |
| 3:M:1707:BCL:H141 | 2:N:30:HIS:ND1    | 2.12                     | 0.63              |
| 2:P:34:PHE:C      | 2:P:34:PHE:CD2    | 2.77                     | 0.63              |
| 4:G:1824:LDA:H52  | 6:G:1865:HOH:O    | 1.98                     | 0.63              |
| 2:N:23:LEU:HD22   | 3:N:1607:BCL:H61  | 1.79                     | 0.63              |
| 1:A:48:GLY:HA2    | 6:A:1843:HOH:O    | 1.98                     | 0.63              |
| 3:G:1704:BCL:HAA1 | 3:G:1704:BCL:O1D  | 1.98                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:39:TRP:CE2    | 3:H:1604:BCL:HMC2 | 2.34                     | 0.63              |
| 2:J:30:HIS:CE1    | 6:J:1825:HOH:O    | 2.50                     | 0.63              |
| 2:P:37:THR:CG2    | 2:P:39:TRP:H      | 2.12                     | 0.63              |
| 2:D:41:HIS:NE2    | 1:E:49:VAL:HG23   | 2.14                     | 0.62              |
| 4:O:1820:LDA:C12  | 6:O:1850:HOH:O    | 2.42                     | 0.62              |
| 2:D:38:PRO:O      | 1:E:47:GLY:HA3    | 1.99                     | 0.62              |
| 4:G:1824:LDA:C5   | 6:G:1865:HOH:O    | 2.46                     | 0.62              |
| 3:I:1705:BCL:H2   | 3:J:1605:BCL:H192 | 1.82                     | 0.62              |
| 2:B:4:THR:H       | 2:B:7:GLN:HE21    | 1.47                     | 0.62              |
| 3:A:1701:BCL:HHC  | 3:A:1701:BCL:HBB2 | 1.82                     | 0.62              |
| 4:G:1824:LDA:H61  | 6:G:1865:HOH:O    | 1.99                     | 0.62              |
| 1:R:16:ILE:HB     | 1:R:17:PRO:HD3    | 1.82                     | 0.62              |
| 3:R:1709:BCL:C2   | 6:R:1831:HOH:O    | 2.28                     | 0.62              |
| 4:E:1822:LDA:HM23 | 6:E:1859:HOH:O    | 1.82                     | 0.62              |
| 2:H:37:THR:HG22   | 2:H:39:TRP:H      | 1.65                     | 0.62              |
| 2:J:7:GLN:NE2     | 6:J:1812:HOH:O    | 2.31                     | 0.62              |
| 6:K:1861:HOH:O    | 1:M:12:PRO:C      | 2.43                     | 0.62              |
| 4:I:1812:LDA:C2   | 6:K:1860:HOH:O    | 2.47                     | 0.61              |
| 3:G:1704:BCL:HED2 | 3:I:1505:BCL:H191 | 1.81                     | 0.61              |
| 2:J:6:GLU:CD      | 6:J:1821:HOH:O    | 2.42                     | 0.61              |
| 3:R:1709:BCL:H41  | 3:R:1709:BCL:C8   | 2.31                     | 0.61              |
| 2:P:41:HIS:CD2    | 1:R:49:VAL:N      | 2.69                     | 0.61              |
| 2:F:37:THR:CG2    | 2:F:39:TRP:H      | 2.14                     | 0.60              |
| 3:G:1704:BCL:O1D  | 3:I:1505:BCL:C5   | 2.49                     | 0.60              |
| 3:G:1704:BCL:HHB  | 2:H:19:THR:HG21   | 1.83                     | 0.60              |
| 3:A:1501:BCL:HMB1 | 3:A:1501:BCL:CBB  | 2.32                     | 0.60              |
| 2:F:9:GLU:OE1     | 6:F:1804:HOH:O    | 2.15                     | 0.60              |
| 2:J:37:THR:HG23   | 2:J:39:TRP:H      | 1.67                     | 0.60              |
| 3:C:1702:BCL:HHC  | 3:C:1702:BCL:HBB2 | 1.84                     | 0.60              |
| 3:M:1707:BCL:O1D  | 3:O:1508:BCL:C5   | 2.50                     | 0.60              |
| 2:P:34:PHE:CG     | 6:P:1817:HOH:O    | 2.51                     | 0.60              |
| 3:F:1603:BCL:H112 | 3:F:1603:BCL:C6   | 2.31                     | 0.60              |
| 3:A:1501:BCL:O1D  | 3:A:1501:BCL:CBA  | 2.49                     | 0.60              |
| 4:G:1824:LDA:HM21 | 6:G:1828:HOH:O    | 1.99                     | 0.60              |
| 2:H:33:ALA:N      | 6:H:1825:HOH:O    | 2.35                     | 0.60              |
| 3:K:1506:BCL:HBB1 | 6:K:1851:HOH:O    | 2.02                     | 0.59              |
| 2:L:39:TRP:HA     | 6:M:1862:HOH:O    | 2.01                     | 0.59              |
| 3:O:1708:BCL:H91  | 3:P:1608:BCL:HHB  | 1.84                     | 0.59              |
| 1:A:41:PHE:HB3    | 1:A:42:PRO:HD3    | 1.84                     | 0.59              |
| 3:A:1701:BCL:C1D  | 6:A:1831:HOH:O    | 2.49                     | 0.59              |
| 2:J:37:THR:CG2    | 2:J:39:TRP:H      | 2.15                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:48:GLY:CA     | 6:R:1823:HOH:O    | 2.49                     | 0.59              |
| 3:M:1707:BCL:H143 | 2:N:27:LEU:HD23   | 1.83                     | 0.59              |
| 3:M:1707:BCL:CED  | 3:O:1508:BCL:H191 | 2.33                     | 0.59              |
| 2:D:33:ALA:HB2    | 6:D:1806:HOH:O    | 2.00                     | 0.59              |
| 1:M:5:LYS:HE3     | 6:M:1856:HOH:O    | 2.01                     | 0.59              |
| 6:E:1862:HOH:O    | 4:F:1803:LDA:H42  | 2.02                     | 0.59              |
| 1:A:14:ILE:CD1    | 4:A:1816:LDA:H22  | 2.33                     | 0.58              |
| 2:F:4:THR:HG1     | 2:F:7:GLN:CD      | 2.11                     | 0.58              |
| 1:G:14:ILE:HD13   | 4:G:1814:LDA:C4   | 2.33                     | 0.58              |
| 5:N:1407:RG1:HM82 | 3:O:1508:BCL:HAA1 | 1.84                     | 0.58              |
| 2:J:41:HIS:HB3    | 1:K:50:LYS:NZ     | 2.18                     | 0.58              |
| 2:B:41:HIS:NE2    | 1:C:49:VAL:CG1    | 2.66                     | 0.58              |
| 3:A:1701:BCL:CHD  | 6:A:1831:HOH:O    | 2.51                     | 0.58              |
| 2:P:34:PHE:CD1    | 6:P:1817:HOH:O    | 2.55                     | 0.58              |
| 3:G:1704:BCL:C7   | 6:G:1863:HOH:O    | 2.52                     | 0.58              |
| 3:M:1707:BCL:O1D  | 3:M:1707:BCL:HAA1 | 2.04                     | 0.58              |
| 4:R:1818:LDA:H92  | 6:R:1856:HOH:O    | 2.02                     | 0.58              |
| 6:E:1862:HOH:O    | 4:F:1803:LDA:C4   | 2.51                     | 0.57              |
| 3:P:1608:BCL:CAC  | 6:P:1837:HOH:O    | 2.51                     | 0.57              |
| 3:K:1706:BCL:H191 | 6:M:1849:HOH:O    | 2.04                     | 0.57              |
| 3:R:1509:BCL:HBB3 | 3:R:1509:BCL:HMB1 | 1.86                     | 0.57              |
| 3:M:1707:BCL:H71  | 6:N:1831:HOH:O    | 2.04                     | 0.57              |
| 5:P:1408:RG1:HM82 | 3:R:1509:BCL:HAA1 | 1.87                     | 0.57              |
| 2:S:33:ALA:O      | 2:S:37:THR:CG2    | 2.50                     | 0.57              |
| 4:M:1827:LDA:HM22 | 1:O:32:LEU:HD22   | 1.85                     | 0.57              |
| 5:P:1408:RG1:HM82 | 3:R:1509:BCL:CAA  | 2.35                     | 0.57              |
| 1:C:8:THR:HG22    | 2:D:3:LEU:O       | 2.05                     | 0.57              |
| 2:H:37:THR:CG2    | 2:H:39:TRP:H      | 2.18                     | 0.57              |
| 3:C:1702:BCL:H42  | 3:E:1503:BCL:CMA  | 2.35                     | 0.57              |
| 2:L:37:THR:CG2    | 2:L:39:TRP:H      | 2.18                     | 0.57              |
| 2:L:39:TRP:CZ2    | 3:L:1606:BCL:CMC  | 2.88                     | 0.57              |
| 4:R:1818:LDA:C12  | 6:R:1856:HOH:O    | 2.48                     | 0.56              |
| 1:C:5:LYS:NZ      | 2:D:9:GLU:OE2     | 2.34                     | 0.56              |
| 2:L:39:TRP:CD2    | 3:L:1606:BCL:HMC1 | 2.40                     | 0.56              |
| 2:J:41:HIS:CD2    | 1:K:49:VAL:N      | 2.74                     | 0.56              |
| 2:D:41:HIS:NE2    | 1:E:49:VAL:CG2    | 2.69                     | 0.56              |
| 1:C:9:VAL:CG2     | 1:E:12:PRO:HB2    | 2.36                     | 0.56              |
| 1:E:37:HIS:CD2    | 1:G:35:LEU:HD21   | 2.41                     | 0.55              |
| 4:K:1810:LDA:HM22 | 1:M:14:ILE:CD1    | 2.31                     | 0.55              |
| 1:R:5:LYS:CE      | 6:R:1835:HOH:O    | 2.54                     | 0.55              |
| 1:A:44:TYR:HB2    | 4:B:1801:LDA:HM22 | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:23:LEU:HD13   | 3:D:1602:BCL:H2   | 1.87                     | 0.55              |
| 3:I:1705:BCL:C4   | 3:I:1705:BCL:C9   | 2.84                     | 0.55              |
| 1:K:14:ILE:HG21   | 4:K:1810:LDA:C5   | 2.36                     | 0.55              |
| 2:B:33:ALA:O      | 2:B:37:THR:HB     | 2.07                     | 0.55              |
| 1:G:50:LYS:NZ     | 6:G:1840:HOH:O    | 2.29                     | 0.55              |
| 3:R:1709:BCL:H92  | 3:R:1709:BCL:C4   | 2.33                     | 0.55              |
| 3:A:1501:BCL:H191 | 3:R:1709:BCL:CED  | 2.26                     | 0.55              |
| 2:L:41:HIS:NE2    | 1:M:49:VAL:N      | 2.54                     | 0.55              |
| 3:C:1702:BCL:CAD  | 3:D:1602:BCL:H192 | 2.36                     | 0.55              |
| 2:F:37:THR:HG22   | 2:F:39:TRP:H      | 1.71                     | 0.55              |
| 4:I:1812:LDA:H21  | 6:K:1860:HOH:O    | 2.05                     | 0.55              |
| 2:P:39:TRP:HB2    | 6:R:1857:HOH:O    | 2.07                     | 0.55              |
| 2:D:41:HIS:CD2    | 1:E:49:VAL:N      | 2.75                     | 0.55              |
| 4:F:1803:LDA:C7   | 6:F:1809:HOH:O    | 2.54                     | 0.55              |
| 1:C:41:PHE:HB3    | 1:C:42:PRO:HD3    | 1.88                     | 0.54              |
| 1:A:5:LYS:HG2     | 5:D:1402:RG1:HM12 | 1.90                     | 0.54              |
| 1:K:41:PHE:HB3    | 1:K:42:PRO:HD3    | 1.88                     | 0.54              |
| 2:L:39:TRP:CE2    | 3:L:1606:BCL:HMC2 | 2.37                     | 0.54              |
| 1:M:14:ILE:HG13   | 4:M:1811:LDA:H12  | 1.90                     | 0.54              |
| 3:R:1709:BCL:H122 | 3:R:1709:BCL:H91  | 1.88                     | 0.54              |
| 2:H:2:THR:CG2     | 6:H:1822:HOH:O    | 2.55                     | 0.54              |
| 3:M:1707:BCL:HED3 | 3:O:1508:BCL:H62  | 1.90                     | 0.54              |
| 2:N:38:PRO:O      | 1:O:47:GLY:HA3    | 2.07                     | 0.54              |
| 3:C:1702:BCL:H42  | 3:E:1503:BCL:HMA2 | 1.90                     | 0.54              |
| 3:L:1606:BCL:HBA2 | 3:L:1606:BCL:HMA3 | 1.89                     | 0.54              |
| 5:H:1404:RG1:HM01 | 1:I:32:LEU:HD21   | 1.89                     | 0.54              |
| 2:B:18:GLY:HA2    | 3:R:1709:BCL:CMD  | 2.38                     | 0.53              |
| 1:G:48:GLY:CA     | 6:G:1839:HOH:O    | 2.15                     | 0.53              |
| 3:L:1606:BCL:HMC1 | 3:L:1606:BCL:HBC2 | 1.89                     | 0.53              |
| 3:N:1607:BCL:HMC2 | 3:N:1607:BCL:HBC3 | 1.90                     | 0.53              |
| 1:A:28:ILE:HG22   | 1:A:32:LEU:HD12   | 1.88                     | 0.53              |
| 3:G:1704:BCL:HHC  | 3:G:1704:BCL:HBB2 | 1.90                     | 0.53              |
| 3:M:1707:BCL:HHC  | 3:M:1707:BCL:HBB2 | 1.89                     | 0.53              |
| 1:A:39:THR:OG1    | 1:C:46:GLN:NE2    | 2.33                     | 0.53              |
| 1:C:16:ILE:HB     | 1:C:17:PRO:HD3    | 1.89                     | 0.53              |
| 3:E:1703:BCL:H11  | 3:F:1603:BCL:H192 | 1.90                     | 0.53              |
| 2:J:7:GLN:NE2     | 6:J:1818:HOH:O    | 2.41                     | 0.53              |
| 3:I:1705:BCL:H92  | 3:I:1705:BCL:H43  | 1.90                     | 0.53              |
| 1:E:41:PHE:HB3    | 1:E:42:PRO:HD3    | 1.91                     | 0.53              |
| 2:N:37:THR:CG2    | 2:N:39:TRP:H      | 2.22                     | 0.53              |
| 3:R:1709:BCL:H41  | 3:R:1709:BCL:H8   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:16:ILE:HB     | 1:A:17:PRO:HD3    | 1.91                     | 0.52              |
| 3:G:1704:BCL:O1D  | 3:I:1505:BCL:H62  | 2.09                     | 0.52              |
| 4:G:1824:LDA:H11  | 6:G:1843:HOH:O    | 2.09                     | 0.52              |
| 1:G:50:LYS:N      | 6:G:1832:HOH:O    | 2.29                     | 0.52              |
| 1:K:4:GLY:N       | 6:K:1840:HOH:O    | 2.41                     | 0.52              |
| 4:C:1815:LDA:HM21 | 1:E:14:ILE:HD13   | 1.91                     | 0.52              |
| 2:N:39:TRP:CD2    | 3:N:1607:BCL:CMC  | 2.90                     | 0.52              |
| 3:E:1503:BCL:OBB  | 3:E:1503:BCL:HHC  | 2.10                     | 0.52              |
| 3:M:1707:BCL:CGD  | 6:M:1859:HOH:O    | 2.35                     | 0.52              |
| 2:S:33:ALA:HB2    | 6:S:296:HOH:O     | 2.08                     | 0.52              |
| 3:I:1705:BCL:C2   | 3:J:1605:BCL:H192 | 2.39                     | 0.52              |
| 6:C:1838:HOH:O    | 3:D:1602:BCL:H121 | 2.10                     | 0.52              |
| 3:E:1703:BCL:H2   | 3:F:1603:BCL:H162 | 1.92                     | 0.52              |
| 3:A:1701:BCL:CMD  | 2:D:18:GLY:HA2    | 2.40                     | 0.52              |
| 1:C:9:VAL:HG21    | 1:E:12:PRO:HB2    | 1.92                     | 0.52              |
| 3:J:1605:BCL:C19  | 6:K:1854:HOH:O    | 2.57                     | 0.52              |
| 3:L:1606:BCL:CMA  | 6:L:1835:HOH:O    | 2.58                     | 0.52              |
| 1:K:9:VAL:HB      | 6:K:1861:HOH:O    | 2.09                     | 0.52              |
| 6:K:1864:HOH:O    | 4:L:1806:LDA:C8   | 2.47                     | 0.52              |
| 1:M:47:GLY:N      | 6:M:1862:HOH:O    | 2.43                     | 0.51              |
| 3:A:1501:BCL:O1D  | 3:A:1501:BCL:H2A  | 2.10                     | 0.51              |
| 1:G:14:ILE:HD13   | 4:G:1814:LDA:H42  | 1.91                     | 0.51              |
| 3:R:1509:BCL:HMD3 | 2:S:30:HIS:CE1    | 2.46                     | 0.51              |
| 1:E:1:CXM:HG2     | 3:E:1703:BCL:CHC  | 2.41                     | 0.51              |
| 1:M:31:HIS:CE1    | 3:N:1607:BCL:HMD1 | 2.45                     | 0.51              |
| 1:O:44:TYR:CE1    | 4:P:1808:LDA:H11  | 2.45                     | 0.51              |
| 2:L:39:TRP:CD2    | 3:L:1606:BCL:HMC2 | 2.44                     | 0.51              |
| 3:P:1608:BCL:HMB3 | 3:P:1608:BCL:CBB  | 2.39                     | 0.51              |
| 3:I:1705:BCL:C4   | 3:I:1705:BCL:H92  | 2.40                     | 0.51              |
| 1:M:6:ILE:N       | 5:P:1408:RG1:HM32 | 2.25                     | 0.51              |
| 1:O:1:CXM:HG2     | 3:O:1708:BCL:CHC  | 2.40                     | 0.51              |
| 4:A:1816:LDA:C3   | 1:C:14:ILE:CD1    | 2.88                     | 0.51              |
| 3:E:1703:BCL:HHC  | 3:E:1703:BCL:HBB2 | 1.93                     | 0.51              |
| 3:I:1505:BCL:HMC3 | 4:J:1805:LDA:H51  | 1.93                     | 0.51              |
| 1:K:1:CXM:C       | 6:K:1840:HOH:O    | 2.59                     | 0.51              |
| 4:O:1820:LDA:CM1  | 6:O:1823:HOH:O    | 2.45                     | 0.51              |
| 1:I:18:ALA:HA     | 4:I:1813:LDA:H91  | 1.93                     | 0.51              |
| 2:L:37:THR:HG22   | 2:L:39:TRP:H      | 1.75                     | 0.51              |
| 2:P:38:PRO:O      | 1:R:47:GLY:HA3    | 2.11                     | 0.51              |
| 2:F:41:HIS:CE1    | 1:G:49:VAL:N      | 2.79                     | 0.51              |
| 1:M:30:VAL:HG22   | 5:N:1407:RG1:HM03 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:49:VAL:HG22   | 1:R:49:VAL:O      | 2.10                     | 0.51              |
| 4:C:1815:LDA:HM11 | 1:E:14:ILE:CD1    | 2.42                     | 0.50              |
| 3:I:1705:BCL:C8   | 3:I:1705:BCL:C4   | 2.83                     | 0.50              |
| 2:J:41:HIS:NE2    | 1:K:49:VAL:N      | 2.59                     | 0.50              |
| 3:K:1706:BCL:CMD  | 2:N:18:GLY:HA2    | 2.40                     | 0.50              |
| 3:A:1501:BCL:O1D  | 3:A:1501:BCL:HBA1 | 2.11                     | 0.50              |
| 3:I:1705:BCL:H141 | 6:J:1825:HOH:O    | 2.11                     | 0.50              |
| 3:L:1606:BCL:HMA2 | 6:L:1835:HOH:O    | 2.11                     | 0.50              |
| 1:A:20:LEU:HD13   | 3:R:1709:BCL:CED  | 2.41                     | 0.50              |
| 2:F:41:HIS:HB3    | 1:G:50:LYS:HE2    | 1.92                     | 0.50              |
| 2:N:39:TRP:CE2    | 3:N:1607:BCL:HMC3 | 2.45                     | 0.50              |
| 1:K:30:VAL:HG23   | 5:L:1406:RG1:HM03 | 1.93                     | 0.50              |
| 1:G:19:LEU:O      | 1:G:23:VAL:HG23   | 2.11                     | 0.50              |
| 2:D:7:GLN:HB3     | 6:D:1829:HOH:O    | 2.10                     | 0.50              |
| 2:N:20:ARG:NH1    | 6:N:1812:HOH:O    | 2.45                     | 0.49              |
| 1:O:31:HIS:CE1    | 3:P:1608:BCL:HMD1 | 2.47                     | 0.49              |
| 3:O:1708:BCL:HED3 | 5:S:1409:RG1:HM42 | 1.92                     | 0.49              |
| 1:E:25:VAL:HG11   | 4:E:1823:LDA:C12  | 2.43                     | 0.49              |
| 4:I:1812:LDA:H111 | 6:K:1863:HOH:O    | 2.11                     | 0.49              |
| 1:C:14:ILE:HG21   | 4:C:1815:LDA:C2   | 2.36                     | 0.49              |
| 3:J:1605:BCL:HMC3 | 6:K:1851:HOH:O    | 2.12                     | 0.49              |
| 3:M:1707:BCL:H101 | 6:N:1831:HOH:O    | 2.13                     | 0.49              |
| 4:R:1818:LDA:C7   | 6:R:1852:HOH:O    | 2.57                     | 0.49              |
| 1:M:51:LYS:HA     | 1:M:52:ALA:CB     | 2.29                     | 0.49              |
| 2:N:17:ASP:CB     | 6:N:1829:HOH:O    | 2.60                     | 0.49              |
| 3:R:1509:BCL:HMB1 | 3:R:1509:BCL:CBB  | 2.42                     | 0.49              |
| 4:E:1823:LDA:CM2  | 6:E:1853:HOH:O    | 2.57                     | 0.49              |
| 2:H:37:THR:HG22   | 2:H:39:TRP:HB3    | 1.94                     | 0.49              |
| 1:K:51:LYS:HD3    | 1:K:52:ALA:O      | 2.12                     | 0.49              |
| 3:G:1704:BCL:H91  | 3:G:1704:BCL:H122 | 1.94                     | 0.49              |
| 2:B:34:PHE:CD1    | 2:B:40:LEU:HD12   | 2.48                     | 0.48              |
| 2:L:39:TRP:CZ2    | 3:L:1606:BCL:HMC3 | 2.46                     | 0.48              |
| 2:J:41:HIS:HB3    | 1:K:50:LYS:HZ1    | 1.77                     | 0.48              |
| 3:M:1707:BCL:HED1 | 3:O:1508:BCL:H191 | 1.94                     | 0.48              |
| 1:A:49:VAL:HG12   | 2:S:41:HIS:NE2    | 2.28                     | 0.48              |
| 3:M:1707:BCL:HBC3 | 3:N:1607:BCL:H143 | 1.95                     | 0.48              |
| 3:K:1706:BCL:HHC  | 3:K:1706:BCL:CBB  | 2.42                     | 0.48              |
| 2:B:6:GLU:CG      | 6:B:597:HOH:O     | 2.62                     | 0.48              |
| 3:F:1603:BCL:H142 | 3:F:1603:BCL:H101 | 1.95                     | 0.48              |
| 1:R:5:LYS:NZ      | 2:S:9:GLU:OE2     | 2.46                     | 0.48              |
| 3:O:1508:BCL:HAA2 | 3:O:1508:BCL:CGD  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:1708:BCL:H3C  | 6:O:1822:HOH:O    | 2.14                     | 0.48              |
| 1:C:14:ILE:HG13   | 4:C:1815:LDA:O1   | 2.13                     | 0.48              |
| 3:F:1603:BCL:HBB2 | 3:F:1603:BCL:HMB3 | 1.95                     | 0.47              |
| 1:I:5:LYS:HG2     | 6:J:1823:HOH:O    | 2.09                     | 0.47              |
| 6:C:1843:HOH:O    | 4:E:1822:LDA:C3   | 2.62                     | 0.47              |
| 3:G:1704:BCL:C6   | 6:G:1863:HOH:O    | 2.62                     | 0.47              |
| 3:I:1705:BCL:H2   | 3:J:1605:BCL:H161 | 1.95                     | 0.47              |
| 1:O:5:LYS:CE      | 2:P:5:ALA:HB1     | 2.44                     | 0.47              |
| 2:P:39:TRP:CD2    | 3:P:1608:BCL:HMC2 | 2.49                     | 0.47              |
| 3:R:1709:BCL:C3D  | 3:S:1609:BCL:H203 | 2.44                     | 0.47              |
| 3:S:1609:BCL:OBB  | 3:S:1609:BCL:HHC  | 2.14                     | 0.47              |
| 2:H:39:TRP:CE3    | 3:H:1604:BCL:HBC2 | 2.47                     | 0.47              |
| 3:G:1704:BCL:HED1 | 3:I:1505:BCL:H191 | 1.92                     | 0.47              |
| 1:O:4:GLY:HA2     | 2:P:12:HIS:CD2    | 2.49                     | 0.47              |
| 1:M:14:ILE:HG13   | 4:M:1811:LDA:C1   | 2.44                     | 0.47              |
| 3:M:1707:BCL:C4D  | 3:N:1607:BCL:H172 | 2.45                     | 0.47              |
| 4:M:1811:LDA:H41  | 1:O:14:ILE:HD12   | 1.95                     | 0.47              |
| 4:O:1820:LDA:CM2  | 6:O:1823:HOH:O    | 2.49                     | 0.47              |
| 4:A:1816:LDA:H32  | 1:C:14:ILE:CD1    | 2.44                     | 0.47              |
| 2:F:37:THR:HG22   | 2:F:39:TRP:HB3    | 1.96                     | 0.47              |
| 1:I:8:THR:HG22    | 2:J:3:LEU:O       | 2.15                     | 0.47              |
| 2:L:39:TRP:CZ2    | 3:L:1606:BCL:HMC2 | 2.50                     | 0.47              |
| 1:M:1:CXM:CN      | 2:N:16:ILE:HD11   | 2.44                     | 0.47              |
| 1:R:50:LYS:O      | 1:R:51:LYS:HB2    | 2.14                     | 0.47              |
| 6:C:1843:HOH:O    | 4:E:1822:LDA:C2   | 2.63                     | 0.47              |
| 2:F:4:THR:OG1     | 2:F:7:GLN:CD      | 2.58                     | 0.47              |
| 2:N:37:THR:HG22   | 2:N:39:TRP:HB3    | 1.96                     | 0.47              |
| 3:S:1609:BCL:HBB2 | 3:S:1609:BCL:HMB3 | 1.96                     | 0.47              |
| 6:E:1862:HOH:O    | 4:F:1803:LDA:H31  | 2.08                     | 0.47              |
| 3:B:1601:BCL:HHC  | 3:B:1601:BCL:OBB  | 2.14                     | 0.47              |
| 1:M:1:CXM:HG2     | 3:M:1707:BCL:CHC  | 2.45                     | 0.47              |
| 2:D:37:THR:HG22   | 2:D:39:TRP:HB3    | 1.97                     | 0.46              |
| 4:G:1824:LDA:HM12 | 6:G:1828:HOH:O    | 1.94                     | 0.46              |
| 1:O:5:LYS:HE2     | 2:P:5:ALA:HB1     | 1.96                     | 0.46              |
| 3:B:1601:BCL:H62  | 3:B:1601:BCL:H112 | 1.97                     | 0.46              |
| 1:R:14:ILE:HD11   | 4:R:1818:LDA:H11  | 1.97                     | 0.46              |
| 3:C:1502:BCL:CHD  | 6:D:1806:HOH:O    | 2.62                     | 0.46              |
| 4:E:1823:LDA:HM11 | 6:E:1853:HOH:O    | 2.14                     | 0.46              |
| 3:I:1705:BCL:H41  | 3:I:1705:BCL:C9   | 2.46                     | 0.46              |
| 1:K:14:ILE:HG21   | 4:K:1810:LDA:H52  | 1.95                     | 0.46              |
| 2:L:4:THR:OG1     | 2:L:7:GLN:HG3     | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:1606:BCL:H2A  | 3:L:1606:BCL:CGD  | 2.45                     | 0.46              |
| 3:S:1609:BCL:H43  | 6:S:515:HOH:O     | 2.14                     | 0.46              |
| 6:R:1831:HOH:O    | 3:S:1609:BCL:C19  | 2.62                     | 0.46              |
| 3:J:1605:BCL:HAA1 | 6:J:1825:HOH:O    | 2.14                     | 0.46              |
| 1:M:30:VAL:CG2    | 5:N:1407:RG1:HM03 | 2.46                     | 0.46              |
| 2:H:39:TRP:CD2    | 3:H:1604:BCL:HBC3 | 2.51                     | 0.46              |
| 1:M:1:CXM:SD      | 2:N:20:ARG:NH2    | 2.88                     | 0.46              |
| 3:J:1605:BCL:HBB3 | 6:K:1864:HOH:O    | 2.03                     | 0.46              |
| 3:C:1702:BCL:CMD  | 2:F:18:GLY:HA2    | 2.45                     | 0.46              |
| 2:J:37:THR:HG22   | 2:J:39:TRP:HB3    | 1.97                     | 0.46              |
| 3:A:1501:BCL:HMB1 | 3:A:1501:BCL:HBB3 | 1.98                     | 0.46              |
| 3:O:1708:BCL:HBC3 | 6:O:1822:HOH:O    | 2.16                     | 0.46              |
| 2:F:38:PRO:O      | 1:G:47:GLY:HA3    | 2.16                     | 0.45              |
| 2:H:11:LEU:CD1    | 5:H:1404:RG1:H41  | 2.47                     | 0.45              |
| 4:K:1826:LDA:C12  | 6:K:1863:HOH:O    | 2.64                     | 0.45              |
| 3:G:1504:BCL:HMB1 | 3:G:1504:BCL:HBB3 | 1.99                     | 0.45              |
| 3:K:1506:BCL:CMC  | 4:L:1806:LDA:H51  | 2.45                     | 0.45              |
| 4:I:1825:LDA:HM12 | 6:I:1840:HOH:O    | 2.16                     | 0.45              |
| 4:K:1826:LDA:H121 | 6:K:1847:HOH:O    | 2.17                     | 0.45              |
| 2:P:37:THR:HG22   | 2:P:39:TRP:N      | 2.23                     | 0.45              |
| 1:I:51:LYS:HB2    | 1:I:52:ALA:CA     | 2.45                     | 0.45              |
| 1:I:14:ILE:HD11   | 6:I:1862:HOH:O    | 2.15                     | 0.45              |
| 2:J:37:THR:CG2    | 2:J:39:TRP:HB3    | 2.47                     | 0.45              |
| 2:P:3:LEU:HD21    | 6:P:1824:HOH:O    | 2.16                     | 0.45              |
| 2:B:4:THR:HG23    | 2:B:7:GLN:NE2     | 2.32                     | 0.45              |
| 3:G:1704:BCL:CED  | 1:I:20:LEU:HD13   | 2.47                     | 0.45              |
| 5:H:1404:RG1:H7   | 5:H:1404:RG1:HM31 | 1.83                     | 0.45              |
| 2:N:17:ASP:HB3    | 6:N:1829:HOH:O    | 2.15                     | 0.45              |
| 1:O:4:GLY:HA2     | 2:P:12:HIS:CG     | 2.52                     | 0.45              |
| 2:B:19:THR:HG21   | 3:B:1601:BCL:H42  | 1.99                     | 0.45              |
| 2:B:37:THR:CG2    | 2:B:39:TRP:H      | 2.25                     | 0.45              |
| 2:F:2:THR:HG21    | 6:F:1825:HOH:O    | 2.17                     | 0.45              |
| 3:G:1704:BCL:C4D  | 3:H:1604:BCL:H172 | 2.47                     | 0.45              |
| 2:H:41:HIS:CD2    | 1:I:49:VAL:C      | 2.95                     | 0.45              |
| 3:G:1704:BCL:CMD  | 2:J:18:GLY:HA2    | 2.46                     | 0.45              |
| 5:H:1404:RG1:H11  | 5:H:1404:RG1:HM41 | 1.87                     | 0.45              |
| 3:I:1705:BCL:C9   | 3:I:1705:BCL:H43  | 2.47                     | 0.45              |
| 1:A:7:TRP:C       | 6:A:1850:HOH:O    | 2.60                     | 0.45              |
| 1:A:21:GLY:HA3    | 4:A:1817:LDA:H101 | 1.99                     | 0.45              |
| 1:A:49:VAL:CG1    | 2:S:41:HIS:NE2    | 2.80                     | 0.45              |
| 3:B:1601:BCL:H2   | 6:B:282:HOH:O     | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:29:ALA:HA     | 4:H:1804:LDA:H112 | 1.99                     | 0.45              |
| 3:A:1701:BCL:H92  | 3:B:1601:BCL:H92  | 1.99                     | 0.44              |
| 3:I:1705:BCL:HHC  | 3:I:1705:BCL:HBB2 | 1.99                     | 0.44              |
| 1:E:51:LYS:O      | 1:E:52:ALA:HB2    | 2.18                     | 0.44              |
| 3:I:1705:BCL:C14  | 6:J:1825:HOH:O    | 2.65                     | 0.44              |
| 2:L:36:ALA:HB1    | 4:L:1806:LDA:H32  | 1.99                     | 0.44              |
| 3:E:1703:BCL:HHB  | 2:F:19:THR:HG21   | 1.98                     | 0.44              |
| 2:P:19:THR:CG2    | 3:P:1608:BCL:H42  | 2.47                     | 0.44              |
| 3:K:1506:BCL:HMB1 | 3:K:1506:BCL:HBB3 | 1.99                     | 0.44              |
| 1:E:1:CXM:HE2     | 6:F:1820:HOH:O    | 2.17                     | 0.44              |
| 3:J:1605:BCL:HBB1 | 6:K:1864:HOH:O    | 2.06                     | 0.44              |
| 1:K:9:VAL:HG12    | 6:K:1853:HOH:O    | 2.17                     | 0.44              |
| 1:C:23:VAL:HG13   | 3:D:1602:BCL:HED1 | 1.98                     | 0.44              |
| 2:J:39:TRP:CD2    | 3:J:1605:BCL:HBC2 | 2.53                     | 0.44              |
| 5:L:1406:RG1:H11  | 5:L:1406:RG1:HM41 | 1.86                     | 0.44              |
| 4:M:1811:LDA:H21  | 1:O:14:ILE:CD1    | 2.47                     | 0.44              |
| 2:B:27:LEU:O      | 2:B:28:VAL:C      | 2.57                     | 0.44              |
| 2:B:38:PRO:O      | 1:C:47:GLY:HA3    | 2.18                     | 0.44              |
| 5:D:1402:RG1:HM31 | 5:D:1402:RG1:H7   | 1.82                     | 0.44              |
| 1:E:25:VAL:HG11   | 4:E:1823:LDA:H111 | 1.99                     | 0.44              |
| 1:M:39:THR:OG1    | 1:O:46:GLN:NE2    | 2.37                     | 0.44              |
| 1:A:43:ALA:HA     | 6:A:1825:HOH:O    | 2.17                     | 0.43              |
| 2:B:37:THR:CG2    | 2:B:39:TRP:HB3    | 2.48                     | 0.43              |
| 3:C:1502:BCL:HMB1 | 3:C:1502:BCL:HBB3 | 2.00                     | 0.43              |
| 1:R:41:PHE:HB3    | 1:R:42:PRO:CD     | 2.48                     | 0.43              |
| 2:D:6:GLU:CB      | 6:D:1825:HOH:O    | 2.41                     | 0.43              |
| 2:L:39:TRP:CE3    | 3:L:1606:BCL:HMC2 | 2.53                     | 0.43              |
| 3:O:1708:BCL:HHC  | 3:O:1708:BCL:HBB2 | 2.00                     | 0.43              |
| 3:I:1505:BCL:HMB1 | 3:I:1505:BCL:HBB3 | 2.00                     | 0.43              |
| 4:K:1826:LDA:H121 | 6:K:1863:HOH:O    | 2.17                     | 0.43              |
| 2:N:37:THR:HG23   | 2:N:39:TRP:H      | 1.83                     | 0.43              |
| 4:E:1822:LDA:O1   | 6:E:1859:HOH:O    | 2.20                     | 0.43              |
| 1:K:16:ILE:HB     | 1:K:17:PRO:HD3    | 1.99                     | 0.43              |
| 5:R:1401:RG1:H20  | 5:R:1401:RG1:HM61 | 1.85                     | 0.43              |
| 2:B:6:GLU:HG2     | 6:B:597:HOH:O     | 2.18                     | 0.43              |
| 5:J:1405:RG1:H7   | 5:J:1405:RG1:HM31 | 1.84                     | 0.43              |
| 3:L:1606:BCL:HBA2 | 3:L:1606:BCL:CMA  | 2.49                     | 0.43              |
| 3:H:1604:BCL:HBB2 | 3:H:1604:BCL:HMB3 | 2.00                     | 0.43              |
| 3:M:1507:BCL:HAA2 | 3:M:1507:BCL:HBD  | 2.00                     | 0.43              |
| 3:M:1707:BCL:H91  | 3:M:1707:BCL:H112 | 1.77                     | 0.43              |
| 2:N:33:ALA:CB     | 3:N:1607:BCL:HBC1 | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:8:THR:HG22    | 2:B:3:LEU:O       | 2.19                     | 0.43              |
| 3:A:1501:BCL:H3C  | 4:B:1801:LDA:H71  | 2.01                     | 0.43              |
| 1:E:14:ILE:HG13   | 4:G:1814:LDA:H12  | 2.00                     | 0.43              |
| 2:F:41:HIS:HB3    | 1:G:50:LYS:CG     | 2.49                     | 0.43              |
| 3:G:1704:BCL:CGD  | 6:G:1854:HOH:O    | 2.64                     | 0.43              |
| 3:I:1705:BCL:C4   | 3:K:1506:BCL:HMA2 | 2.47                     | 0.43              |
| 1:E:4:GLY:HA2     | 2:F:12:HIS:CD2    | 2.54                     | 0.43              |
| 2:F:41:HIS:HE1    | 1:G:49:VAL:H      | 1.60                     | 0.43              |
| 3:I:1705:BCL:O1A  | 3:K:1506:BCL:H2   | 2.19                     | 0.43              |
| 2:F:14:TYR:CE1    | 5:F:1403:RG1:HM11 | 2.53                     | 0.43              |
| 3:F:1603:BCL:C10  | 3:F:1603:BCL:C14  | 2.97                     | 0.43              |
| 5:H:1404:RG1:HM22 | 5:H:1404:RG1:H1'  | 1.73                     | 0.43              |
| 1:A:49:VAL:N      | 2:S:41:HIS:CD2    | 2.87                     | 0.42              |
| 1:A:50:LYS:HG3    | 6:A:1833:HOH:O    | 2.18                     | 0.42              |
| 1:E:1:CXM:HE3     | 1:E:1:CXM:HB2     | 1.92                     | 0.42              |
| 3:I:1705:BCL:C2   | 6:K:1854:HOH:O    | 2.67                     | 0.42              |
| 5:S:1409:RG1:H7   | 5:S:1409:RG1:HM31 | 1.77                     | 0.42              |
| 3:J:1605:BCL:HMB3 | 3:J:1605:BCL:HBB2 | 2.00                     | 0.42              |
| 2:N:29:ALA:HB1    | 4:N:1807:LDA:H112 | 2.01                     | 0.42              |
| 4:R:1818:LDA:C8   | 6:R:1852:HOH:O    | 2.64                     | 0.42              |
| 4:K:1826:LDA:HM22 | 4:K:1826:LDA:H22  | 1.87                     | 0.42              |
| 1:M:14:ILE:HG22   | 6:M:1852:HOH:O    | 2.19                     | 0.42              |
| 1:G:26:ILE:HG12   | 1:I:28:ILE:HD11   | 2.01                     | 0.42              |
| 2:J:41:HIS:CE1    | 1:K:49:VAL:HG12   | 2.53                     | 0.42              |
| 1:K:40:TRP:HH2    | 3:K:1506:BCL:CBC  | 2.32                     | 0.42              |
| 5:N:1407:RG1:H7   | 5:N:1407:RG1:HM31 | 1.85                     | 0.42              |
| 2:P:13:LYS:NZ     | 6:P:1835:HOH:O    | 2.52                     | 0.42              |
| 5:R:1401:RG1:HM31 | 5:R:1401:RG1:H7   | 1.80                     | 0.42              |
| 3:C:1702:BCL:OBD  | 5:F:1403:RG1:H11  | 2.19                     | 0.42              |
| 2:F:23:LEU:HB2    | 3:F:1603:BCL:H2   | 2.01                     | 0.42              |
| 3:A:1701:BCL:OBD  | 5:D:1402:RG1:H11  | 2.19                     | 0.42              |
| 6:I:1847:HOH:O    | 2:J:6:GLU:HA      | 2.20                     | 0.42              |
| 2:N:4:THR:H       | 2:N:7:GLN:HE21    | 1.67                     | 0.42              |
| 1:O:44:TYR:HB2    | 4:P:1808:LDA:HM11 | 2.02                     | 0.42              |
| 3:P:1608:BCL:CBB  | 3:P:1608:BCL:CMB  | 2.97                     | 0.42              |
| 3:A:1501:BCL:HED3 | 2:B:22:PHE:CE1    | 2.55                     | 0.42              |
| 2:L:39:TRP:CG     | 3:L:1606:BCL:HMC1 | 2.54                     | 0.42              |
| 2:N:37:THR:HG22   | 2:N:39:TRP:H      | 1.85                     | 0.42              |
| 2:P:17:ASP:O      | 2:P:21:VAL:HG23   | 2.20                     | 0.42              |
| 3:A:1501:BCL:HHC  | 3:A:1501:BCL:OBB  | 2.20                     | 0.42              |
| 5:P:1408:RG1:H7   | 5:P:1408:RG1:HM31 | 1.91                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:13:ALA:HB1    | 4:A:1817:LDA:HM11 | 2.02                     | 0.42              |
| 5:D:1402:RG1:H15  | 5:D:1402:RG1:HM51 | 1.92                     | 0.42              |
| 5:S:1409:RG1:C17  | 3:S:1609:BCL:H12  | 2.50                     | 0.42              |
| 1:C:44:TYR:CD1    | 4:D:1802:LDA:HM21 | 2.55                     | 0.41              |
| 2:F:37:THR:HG23   | 2:F:39:TRP:H      | 1.84                     | 0.41              |
| 1:I:14:ILE:HD13   | 4:I:1812:LDA:HM12 | 2.02                     | 0.41              |
| 2:N:9:GLU:O       | 2:N:13:LYS:HD2    | 2.19                     | 0.41              |
| 3:O:1508:BCL:H12  | 2:P:22:PHE:HE1    | 1.85                     | 0.41              |
| 5:S:1409:RG1:H15  | 5:S:1409:RG1:HM51 | 1.91                     | 0.41              |
| 5:F:1403:RG1:HM13 | 5:F:1403:RG1:H1'  | 1.79                     | 0.41              |
| 1:G:5:LYS:HE2     | 2:H:9:GLU:OE2     | 2.20                     | 0.41              |
| 3:M:1507:BCL:H61  | 3:M:1507:BCL:H102 | 1.93                     | 0.41              |
| 1:O:43:ALA:HB2    | 6:O:1830:HOH:O    | 2.20                     | 0.41              |
| 1:C:5:LYS:O       | 1:C:8:THR:OG1     | 2.32                     | 0.41              |
| 3:C:1702:BCL:H41  | 3:C:1702:BCL:C8   | 2.49                     | 0.41              |
| 3:I:1705:BCL:CMD  | 2:L:18:GLY:HA2    | 2.50                     | 0.41              |
| 4:I:1812:LDA:H22  | 6:K:1860:HOH:O    | 2.13                     | 0.41              |
| 4:I:1825:LDA:CM1  | 6:I:1859:HOH:O    | 2.60                     | 0.41              |
| 1:M:41:PHE:O      | 1:M:44:TYR:HB3    | 2.19                     | 0.41              |
| 1:O:49:VAL:O      | 1:O:49:VAL:HG13   | 2.21                     | 0.41              |
| 3:C:1702:BCL:H192 | 2:D:39:TRP:HZ2    | 1.85                     | 0.41              |
| 3:G:1504:BCL:HHC  | 3:G:1504:BCL:OBB  | 2.20                     | 0.41              |
| 1:I:18:ALA:HA     | 4:I:1813:LDA:C9   | 2.50                     | 0.41              |
| 1:M:16:ILE:HB     | 1:M:17:PRO:HD3    | 2.02                     | 0.41              |
| 5:R:1401:RG1:O5'  | 5:R:1401:RG1:CM1  | 2.68                     | 0.41              |
| 1:I:16:ILE:HB     | 1:I:17:PRO:HD3    | 2.02                     | 0.41              |
| 1:I:31:HIS:ND1    | 3:J:1605:BCL:HMD1 | 2.36                     | 0.41              |
| 3:K:1706:BCL:HBC3 | 3:K:1706:BCL:H2C  | 1.87                     | 0.41              |
| 3:O:1508:BCL:H3C  | 4:P:1808:LDA:H51  | 2.02                     | 0.41              |
| 1:O:32:LEU:HD23   | 1:O:32:LEU:HA     | 1.84                     | 0.41              |
| 1:C:44:TYR:CD1    | 4:D:1802:LDA:H11  | 2.55                     | 0.41              |
| 1:K:48:GLY:CA     | 6:K:1829:HOH:O    | 2.60                     | 0.41              |
| 1:C:16:ILE:O      | 1:C:20:LEU:HG     | 2.21                     | 0.41              |
| 4:C:1815:LDA:HM11 | 1:E:14:ILE:HD13   | 2.03                     | 0.41              |
| 1:E:1:CXM:HG2     | 3:E:1703:BCL:HHC  | 2.03                     | 0.41              |
| 3:E:1703:BCL:H161 | 3:E:1703:BCL:H202 | 1.74                     | 0.41              |
| 4:F:1803:LDA:H82  | 6:F:1809:HOH:O    | 2.17                     | 0.41              |
| 1:K:1:CXM:C       | 1:K:1:CXM:ON1     | 2.69                     | 0.41              |
| 1:K:50:LYS:O      | 1:K:51:LYS:CB     | 2.69                     | 0.41              |
| 2:L:38:PRO:O      | 1:M:47:GLY:HA3    | 2.21                     | 0.41              |
| 3:L:1606:BCL:HHB  | 3:L:1606:BCL:HMA1 | 1.93                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:M:31:HIS:ND1    | 3:N:1607:BCL:HMD1 | 2.36                     | 0.41              |
| 3:O:1708:BCL:HHC  | 3:O:1708:BCL:CBB  | 2.51                     | 0.41              |
| 2:P:6:GLU:HG2     | 2:P:10:GLU:OE2    | 2.21                     | 0.41              |
| 1:A:5:LYS:HE3     | 2:B:5:ALA:HB1     | 2.01                     | 0.41              |
| 2:L:37:THR:HG22   | 2:L:39:TRP:HB3    | 2.02                     | 0.41              |
| 2:N:4:THR:H       | 2:N:7:GLN:NE2     | 2.19                     | 0.41              |
| 6:B:517:HOH:O     | 1:R:5:LYS:HE2     | 2.21                     | 0.40              |
| 5:D:1402:RG1:H11  | 5:D:1402:RG1:HM41 | 1.98                     | 0.40              |
| 2:F:41:HIS:HB3    | 1:G:50:LYS:CE     | 2.51                     | 0.40              |
| 4:G:1824:LDA:HM22 | 4:G:1824:LDA:H22  | 1.78                     | 0.40              |
| 3:O:1508:BCL:CHD  | 3:O:1508:BCL:HBC2 | 2.50                     | 0.40              |
| 1:C:44:TYR:CE1    | 4:D:1802:LDA:H11  | 2.56                     | 0.40              |
| 3:G:1704:BCL:O1D  | 3:I:1505:BCL:C6   | 2.69                     | 0.40              |
| 2:N:5:ALA:HB3     | 6:N:1826:HOH:O    | 2.20                     | 0.40              |
| 3:R:1709:BCL:H92  | 3:S:1609:BCL:H51  | 2.03                     | 0.40              |
| 3:C:1502:BCL:HHC  | 3:C:1502:BCL:OBB  | 2.21                     | 0.40              |
| 2:H:39:TRP:NE1    | 3:H:1604:BCL:HMC2 | 2.35                     | 0.40              |
| 3:R:1709:BCL:C4D  | 3:S:1609:BCL:H172 | 2.52                     | 0.40              |
| 3:A:1501:BCL:HED3 | 2:B:22:PHE:CZ     | 2.56                     | 0.40              |
| 3:K:1506:BCL:HMB1 | 3:K:1506:BCL:CBB  | 2.51                     | 0.40              |
| 2:L:23:LEU:HB2    | 3:L:1606:BCL:H2   | 2.04                     | 0.40              |
| 2:N:39:TRP:CZ3    | 3:N:1607:BCL:HBC3 | 2.57                     | 0.40              |
| 2:P:41:HIS:HA     | 6:R:1823:HOH:O    | 2.22                     | 0.40              |
| 3:G:1704:BCL:O1D  | 3:I:1505:BCL:H52  | 2.22                     | 0.40              |
| 3:K:1506:BCL:HBC1 | 3:L:1606:BCL:CBC  | 2.51                     | 0.40              |
| 2:P:37:THR:HG23   | 2:P:38:PRO:HD2    | 2.02                     | 0.40              |
| 5:R:1401:RG1:H11  | 5:R:1401:RG1:HM41 | 1.87                     | 0.40              |
| 5:S:1409:RG1:H20  | 5:S:1409:RG1:HM61 | 1.79                     | 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   | A     | 51/53 (96%)   | 46 (90%)  | 5 (10%) | 0        | 100         | 100 |
| 1   | C     | 51/53 (96%)   | 47 (92%)  | 1 (2%)  | 3 (6%)   | 1           | 0   |
| 1   | E     | 51/53 (96%)   | 46 (90%)  | 2 (4%)  | 3 (6%)   | 1           | 0   |
| 1   | G     | 51/53 (96%)   | 51 (100%) | 0       | 0        | 100         | 100 |
| 1   | I     | 51/53 (96%)   | 48 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 1   | K     | 51/53 (96%)   | 47 (92%)  | 3 (6%)  | 1 (2%)   | 6           | 4   |
| 1   | M     | 51/53 (96%)   | 47 (92%)  | 1 (2%)  | 3 (6%)   | 1           | 0   |
| 1   | O     | 51/53 (96%)   | 47 (92%)  | 3 (6%)  | 1 (2%)   | 6           | 4   |
| 1   | R     | 51/53 (96%)   | 46 (90%)  | 2 (4%)  | 3 (6%)   | 1           | 0   |
| 2   | B     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | D     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | F     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | H     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | J     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | L     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | N     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| 2   | P     | 39/41 (95%)   | 38 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | S     | 39/41 (95%)   | 39 (100%) | 0       | 0        | 100         | 100 |
| All | All   | 810/846 (96%) | 775 (96%) | 21 (3%) | 14 (2%)  | 7           | 6   |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 50  | LYS  |
| 1   | E     | 51  | LYS  |
| 1   | E     | 52  | ALA  |
| 1   | K     | 50  | LYS  |
| 1   | M     | 50  | LYS  |
| 1   | M     | 51  | LYS  |
| 1   | M     | 52  | ALA  |
| 1   | R     | 51  | LYS  |
| 1   | C     | 51  | LYS  |
| 1   | R     | 50  | LYS  |
| 1   | R     | 52  | ALA  |
| 1   | C     | 52  | ALA  |
| 1   | E     | 50  | LYS  |
| 1   | O     | 50  | LYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A     | 40/40 (100%)   | 38 (95%)  | 2 (5%)   | 22          | 32 |
| 1   | C     | 40/40 (100%)   | 37 (92%)  | 3 (8%)   | 12          | 16 |
| 1   | E     | 40/40 (100%)   | 36 (90%)  | 4 (10%)  | 7           | 7  |
| 1   | G     | 40/40 (100%)   | 36 (90%)  | 4 (10%)  | 7           | 7  |
| 1   | I     | 40/40 (100%)   | 35 (88%)  | 5 (12%)  | 4           | 4  |
| 1   | K     | 40/40 (100%)   | 38 (95%)  | 2 (5%)   | 22          | 32 |
| 1   | M     | 40/40 (100%)   | 38 (95%)  | 2 (5%)   | 22          | 32 |
| 1   | O     | 40/40 (100%)   | 38 (95%)  | 2 (5%)   | 22          | 32 |
| 1   | R     | 40/40 (100%)   | 37 (92%)  | 3 (8%)   | 12          | 16 |
| 2   | B     | 33/33 (100%)   | 29 (88%)  | 4 (12%)  | 5           | 4  |
| 2   | D     | 33/33 (100%)   | 29 (88%)  | 4 (12%)  | 5           | 4  |
| 2   | F     | 33/33 (100%)   | 29 (88%)  | 4 (12%)  | 5           | 4  |
| 2   | H     | 33/33 (100%)   | 29 (88%)  | 4 (12%)  | 5           | 4  |
| 2   | J     | 33/33 (100%)   | 31 (94%)  | 2 (6%)   | 17          | 24 |
| 2   | L     | 33/33 (100%)   | 28 (85%)  | 5 (15%)  | 3           | 2  |
| 2   | N     | 33/33 (100%)   | 30 (91%)  | 3 (9%)   | 9           | 10 |
| 2   | P     | 33/33 (100%)   | 28 (85%)  | 5 (15%)  | 3           | 2  |
| 2   | S     | 33/33 (100%)   | 29 (88%)  | 4 (12%)  | 5           | 4  |
| All | All   | 657/657 (100%) | 595 (91%) | 62 (9%)  | 8           | 8  |

All (62) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | LYS  |
| 1   | A     | 51  | LYS  |
| 2   | B     | 2   | THR  |
| 2   | B     | 6   | GLU  |
| 2   | B     | 13  | LYS  |
| 2   | B     | 37  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 5   | LYS  |
| 1   | C     | 9   | VAL  |
| 1   | C     | 50  | LYS  |
| 2   | D     | 2   | THR  |
| 2   | D     | 10  | GLU  |
| 2   | D     | 35  | SER  |
| 2   | D     | 37  | THR  |
| 1   | E     | 5   | LYS  |
| 1   | E     | 9   | VAL  |
| 1   | E     | 14  | ILE  |
| 1   | E     | 49  | VAL  |
| 2   | F     | 2   | THR  |
| 2   | F     | 13  | LYS  |
| 2   | F     | 17  | ASP  |
| 2   | F     | 37  | THR  |
| 1   | G     | 14  | ILE  |
| 1   | G     | 36  | SER  |
| 1   | G     | 50  | LYS  |
| 1   | G     | 51  | LYS  |
| 2   | H     | 2   | THR  |
| 2   | H     | 13  | LYS  |
| 2   | H     | 17  | ASP  |
| 2   | H     | 37  | THR  |
| 1   | I     | 5   | LYS  |
| 1   | I     | 14  | ILE  |
| 1   | I     | 36  | SER  |
| 1   | I     | 50  | LYS  |
| 1   | I     | 51  | LYS  |
| 2   | J     | 2   | THR  |
| 2   | J     | 37  | THR  |
| 1   | K     | 14  | ILE  |
| 1   | K     | 50  | LYS  |
| 2   | L     | 2   | THR  |
| 2   | L     | 6   | GLU  |
| 2   | L     | 13  | LYS  |
| 2   | L     | 17  | ASP  |
| 2   | L     | 37  | THR  |
| 1   | M     | 5   | LYS  |
| 1   | M     | 9   | VAL  |
| 2   | N     | 2   | THR  |
| 2   | N     | 13  | LYS  |
| 2   | N     | 37  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 9   | VAL  |
| 1   | O     | 16  | ILE  |
| 2   | P     | 2   | THR  |
| 2   | P     | 13  | LYS  |
| 2   | P     | 17  | ASP  |
| 2   | P     | 34  | PHE  |
| 2   | P     | 37  | THR  |
| 1   | R     | 16  | ILE  |
| 1   | R     | 36  | SER  |
| 1   | R     | 50  | LYS  |
| 2   | S     | 2   | THR  |
| 2   | S     | 6   | GLU  |
| 2   | S     | 10  | GLU  |
| 2   | S     | 37  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | GLN  |
| 2   | B     | 7   | GLN  |
| 1   | C     | 3   | GLN  |
| 1   | C     | 37  | HIS  |
| 2   | D     | 7   | GLN  |
| 1   | E     | 37  | HIS  |
| 2   | H     | 7   | GLN  |
| 1   | I     | 37  | HIS  |
| 1   | K     | 37  | HIS  |
| 2   | L     | 7   | GLN  |
| 1   | M     | 3   | GLN  |
| 2   | N     | 7   | GLN  |
| 1   | O     | 3   | GLN  |
| 1   | R     | 37  | HIS  |
| 2   | S     | 7   | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | CXM  | E     | 1   | 3,1  | 9,10,11      | 1.38 | 2 (22%)  | 9,11,13     | 1.37 | 1 (11%)  |
| 1   | CXM  | I     | 1   | 3,1  | 9,10,11      | 1.36 | 1 (11%)  | 9,11,13     | 1.50 | 1 (11%)  |
| 1   | CXM  | K     | 1   | 3,1  | 9,10,11      | 1.49 | 2 (22%)  | 9,11,13     | 1.61 | 1 (11%)  |
| 1   | CXM  | A     | 1   | 3,1  | 9,10,11      | 1.50 | 2 (22%)  | 9,11,13     | 1.37 | 2 (22%)  |
| 1   | CXM  | R     | 1   | 3,1  | 9,10,11      | 1.63 | 1 (11%)  | 9,11,13     | 1.33 | 1 (11%)  |
| 1   | CXM  | O     | 1   | 3,1  | 9,10,11      | 1.49 | 1 (11%)  | 9,11,13     | 1.34 | 1 (11%)  |
| 1   | CXM  | C     | 1   | 3,1  | 9,10,11      | 2.27 | 2 (22%)  | 9,11,13     | 1.33 | 1 (11%)  |
| 1   | CXM  | M     | 1   | 3,1  | 9,10,11      | 2.88 | 2 (22%)  | 9,11,13     | 1.14 | 2 (22%)  |
| 1   | CXM  | G     | 1   | 3,1  | 9,10,11      | 1.77 | 2 (22%)  | 9,11,13     | 1.17 | 2 (22%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 1   | CXM  | E     | 1   | 3,1  | -       | 2/9/10/12 | -     |
| 1   | CXM  | I     | 1   | 3,1  | -       | 2/9/10/12 | -     |
| 1   | CXM  | K     | 1   | 3,1  | -       | 3/9/10/12 | -     |
| 1   | CXM  | A     | 1   | 3,1  | -       | 3/9/10/12 | -     |
| 1   | CXM  | R     | 1   | 3,1  | -       | 4/9/10/12 | -     |
| 1   | CXM  | O     | 1   | 3,1  | -       | 4/9/10/12 | -     |
| 1   | CXM  | C     | 1   | 3,1  | -       | 1/9/10/12 | -     |
| 1   | CXM  | M     | 1   | 3,1  | -       | 2/9/10/12 | -     |
| 1   | CXM  | G     | 1   | 3,1  | -       | 3/9/10/12 | -     |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 1   | CXM  | CE-SD  | 7.04  | 2.21        | 1.78     |
| 1   | C     | 1   | CXM  | ON1-CN | 5.27  | 1.31        | 1.21     |
| 1   | M     | 1   | CXM  | ON1-CN | 4.56  | 1.30        | 1.21     |
| 1   | R     | 1   | CXM  | ON1-CN | 3.99  | 1.29        | 1.21     |
| 1   | G     | 1   | CXM  | CE-SD  | 3.54  | 2.00        | 1.78     |
| 1   | G     | 1   | CXM  | ON1-CN | 3.45  | 1.28        | 1.21     |
| 1   | O     | 1   | CXM  | ON1-CN | 3.45  | 1.28        | 1.21     |
| 1   | C     | 1   | CXM  | CE-SD  | 3.01  | 1.97        | 1.78     |
| 1   | A     | 1   | CXM  | CA-N   | 2.55  | 1.50        | 1.46     |
| 1   | E     | 1   | CXM  | CE-SD  | 2.33  | 1.93        | 1.78     |
| 1   | K     | 1   | CXM  | ON1-CN | 2.27  | 1.25        | 1.21     |
| 1   | I     | 1   | CXM  | CN-N   | -2.20 | 1.31        | 1.35     |
| 1   | A     | 1   | CXM  | ON1-CN | 2.16  | 1.25        | 1.21     |
| 1   | E     | 1   | CXM  | ON1-CN | 2.10  | 1.25        | 1.21     |
| 1   | K     | 1   | CXM  | CA-N   | 2.02  | 1.49        | 1.46     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | K     | 1   | CXM  | ON1-CN-N | -3.92 | 118.42      | 124.86   |
| 1   | I     | 1   | CXM  | ON1-CN-N | -3.75 | 118.70      | 124.86   |
| 1   | R     | 1   | CXM  | ON1-CN-N | -3.65 | 118.86      | 124.86   |
| 1   | C     | 1   | CXM  | ON1-CN-N | -3.52 | 119.09      | 124.86   |
| 1   | O     | 1   | CXM  | ON1-CN-N | -3.47 | 119.16      | 124.86   |
| 1   | E     | 1   | CXM  | ON1-CN-N | -2.93 | 120.05      | 124.86   |
| 1   | A     | 1   | CXM  | ON1-CN-N | -2.82 | 120.23      | 124.86   |
| 1   | G     | 1   | CXM  | ON1-CN-N | -2.66 | 120.50      | 124.86   |
| 1   | G     | 1   | CXM  | O-C-CA   | -2.14 | 119.26      | 124.77   |
| 1   | M     | 1   | CXM  | ON1-CN-N | -2.14 | 121.35      | 124.86   |
| 1   | M     | 1   | CXM  | C-CA-N   | 2.10  | 113.56      | 109.50   |
| 1   | A     | 1   | CXM  | C-CA-N   | 2.05  | 113.45      | 109.50   |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | A     | 1   | CXM  | C-CA-CB-CG  |
| 1   | G     | 1   | CXM  | O-C-CA-CB   |
| 1   | K     | 1   | CXM  | O-C-CA-CB   |
| 1   | R     | 1   | CXM  | O-C-CA-CB   |
| 1   | O     | 1   | CXM  | CB-CG-SD-CE |
| 1   | O     | 1   | CXM  | ON1-CN-N-CA |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | G     | 1   | CXM  | C-CA-CB-CG  |
| 1   | R     | 1   | CXM  | ON1-CN-N-CA |
| 1   | A     | 1   | CXM  | C-CA-N-CN   |
| 1   | E     | 1   | CXM  | C-CA-N-CN   |
| 1   | K     | 1   | CXM  | C-CA-N-CN   |
| 1   | M     | 1   | CXM  | C-CA-N-CN   |
| 1   | G     | 1   | CXM  | CB-CA-N-CN  |
| 1   | I     | 1   | CXM  | CB-CA-N-CN  |
| 1   | M     | 1   | CXM  | CB-CA-N-CN  |
| 1   | O     | 1   | CXM  | CB-CA-N-CN  |
| 1   | I     | 1   | CXM  | C-CA-N-CN   |
| 1   | O     | 1   | CXM  | C-CA-N-CN   |
| 1   | A     | 1   | CXM  | CB-CA-N-CN  |
| 1   | C     | 1   | CXM  | CB-CA-N-CN  |
| 1   | E     | 1   | CXM  | CB-CA-N-CN  |
| 1   | K     | 1   | CXM  | CB-CA-N-CN  |
| 1   | R     | 1   | CXM  | CB-CA-N-CN  |
| 1   | R     | 1   | CXM  | C-CA-CB-CG  |

There are no ring outliers.

4 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | E     | 1   | CXM  | 4       | 0            |
| 1   | K     | 1   | CXM  | 2       | 0            |
| 1   | O     | 1   | CXM  | 1       | 0            |
| 1   | M     | 1   | CXM  | 4       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

63 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | LDA  | C     | 1815 | -    | 13,15,15     | 2.08 | 2 (15%)     | 14,17,17    | 0.34 | 0           |
| 3   | BCL  | K     | 1506 | 1    | 69,74,74     | 2.46 | 26 (37%)    | 79,115,115  | 2.36 | 24 (30%)    |
| 5   | RG1  | R     | 1401 | -    | 52,52,52     | 1.10 | 3 (5%)      | 66,67,67    | 1.81 | 16 (24%)    |
| 4   | LDA  | P     | 1808 | -    | 13,15,15     | 1.91 | 2 (15%)     | 14,17,17    | 0.57 | 0           |
| 4   | LDA  | D     | 1802 | -    | 13,15,15     | 2.30 | 2 (15%)     | 14,17,17    | 0.61 | 0           |
| 3   | BCL  | E     | 1503 | 1    | 69,74,74     | 1.90 | 16 (23%)    | 79,115,115  | 2.30 | 23 (29%)    |
| 4   | LDA  | L     | 1806 | -    | 13,15,15     | 2.03 | 2 (15%)     | 14,17,17    | 0.58 | 0           |
| 3   | BCL  | H     | 1604 | 2    | 69,74,74     | 2.07 | 22 (31%)    | 79,115,115  | 2.30 | 29 (36%)    |
| 3   | BCL  | R     | 1509 | 1    | 69,74,74     | 2.21 | 22 (31%)    | 79,115,115  | 2.41 | 26 (32%)    |
| 4   | LDA  | M     | 1811 | -    | 13,15,15     | 1.84 | 1 (7%)      | 14,17,17    | 0.49 | 0           |
| 3   | BCL  | C     | 1702 | 1    | 69,74,74     | 2.10 | 20 (28%)    | 79,115,115  | 2.11 | 20 (25%)    |
| 3   | BCL  | L     | 1606 | 2    | 69,74,74     | 2.26 | 26 (37%)    | 79,115,115  | 2.81 | 27 (34%)    |
| 5   | RG1  | D     | 1402 | -    | 52,52,52     | 1.20 | 6 (11%)     | 66,67,67    | 1.71 | 17 (25%)    |
| 5   | RG1  | N     | 1407 | -    | 52,52,52     | 1.18 | 3 (5%)      | 66,67,67    | 1.68 | 15 (22%)    |
| 3   | BCL  | K     | 1706 | 1    | 69,74,74     | 2.04 | 21 (30%)    | 79,115,115  | 2.27 | 22 (27%)    |
| 4   | LDA  | E     | 1822 | -    | 13,15,15     | 1.95 | 2 (15%)     | 14,17,17    | 0.51 | 0           |
| 3   | BCL  | A     | 1501 | 1    | 69,74,74     | 2.18 | 19 (27%)    | 79,115,115  | 2.31 | 26 (32%)    |
| 3   | BCL  | G     | 1704 | 1    | 69,74,74     | 2.06 | 20 (28%)    | 79,115,115  | 2.23 | 26 (32%)    |
| 4   | LDA  | C     | 1821 | -    | 13,15,15     | 1.87 | 1 (7%)      | 14,17,17    | 0.40 | 0           |
| 3   | BCL  | F     | 1603 | 2    | 69,74,74     | 1.84 | 18 (26%)    | 79,115,115  | 2.23 | 21 (26%)    |
| 4   | LDA  | R     | 1809 | -    | 13,15,15     | 1.89 | 1 (7%)      | 14,17,17    | 0.52 | 0           |
| 4   | LDA  | I     | 1812 | -    | 13,15,15     | 2.28 | 1 (7%)      | 14,17,17    | 0.37 | 0           |
| 3   | BCL  | D     | 1602 | 2    | 69,74,74     | 2.19 | 25 (36%)    | 79,115,115  | 2.37 | 23 (29%)    |
| 3   | BCL  | P     | 1608 | 2    | 69,74,74     | 2.23 | 22 (31%)    | 79,115,115  | 2.34 | 22 (27%)    |
| 4   | LDA  | K     | 1810 | -    | 13,15,15     | 2.06 | 1 (7%)      | 14,17,17    | 0.49 | 0           |
| 5   | RG1  | P     | 1408 | -    | 52,52,52     | 1.30 | 8 (15%)     | 66,67,67    | 1.67 | 15 (22%)    |
| 3   | BCL  | E     | 1703 | 1    | 69,74,74     | 1.95 | 17 (24%)    | 79,115,115  | 2.03 | 23 (29%)    |
| 4   | LDA  | E     | 1823 | -    | 13,15,15     | 1.74 | 1 (7%)      | 14,17,17    | 0.45 | 0           |
| 4   | LDA  | A     | 1817 | -    | 13,15,15     | 2.07 | 2 (15%)     | 14,17,17    | 0.43 | 0           |
| 4   | LDA  | K     | 1826 | -    | 13,15,15     | 1.94 | 2 (15%)     | 14,17,17    | 0.53 | 0           |
| 3   | BCL  | O     | 1508 | 1    | 69,74,74     | 1.85 | 18 (26%)    | 79,115,115  | 2.24 | 26 (32%)    |
| 3   | BCL  | S     | 1609 | 2    | 69,74,74     | 1.99 | 18 (26%)    | 79,115,115  | 2.37 | 27 (34%)    |
| 5   | RG1  | F     | 1403 | -    | 52,52,52     | 1.27 | 3 (5%)      | 66,67,67    | 1.66 | 18 (27%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | LDA  | O     | 1820 | -    | 13,15,15     | 2.01 | 1 (7%)   | 14,17,17    | 0.42 | 0        |
| 4   | LDA  | M     | 1827 | -    | 13,15,15     | 1.92 | 1 (7%)   | 14,17,17    | 0.42 | 0        |
| 4   | LDA  | I     | 1825 | -    | 13,15,15     | 1.95 | 1 (7%)   | 14,17,17    | 0.51 | 0        |
| 3   | BCL  | G     | 1504 | 1    | 69,74,74     | 2.04 | 20 (28%) | 79,115,115  | 2.15 | 24 (30%) |
| 3   | BCL  | M     | 1507 | 1    | 69,74,74     | 2.03 | 19 (27%) | 79,115,115  | 2.41 | 23 (29%) |
| 4   | LDA  | B     | 1801 | -    | 13,15,15     | 2.03 | 1 (7%)   | 14,17,17    | 0.43 | 0        |
| 4   | LDA  | F     | 1803 | -    | 13,15,15     | 2.13 | 1 (7%)   | 14,17,17    | 0.57 | 0        |
| 4   | LDA  | I     | 1813 | -    | 13,15,15     | 1.92 | 1 (7%)   | 14,17,17    | 0.40 | 0        |
| 4   | LDA  | J     | 1805 | -    | 13,15,15     | 1.80 | 1 (7%)   | 14,17,17    | 0.30 | 0        |
| 4   | LDA  | G     | 1824 | -    | 13,15,15     | 1.99 | 1 (7%)   | 14,17,17    | 0.34 | 0        |
| 4   | LDA  | H     | 1804 | -    | 13,15,15     | 2.45 | 2 (15%)  | 14,17,17    | 0.56 | 0        |
| 3   | BCL  | I     | 1705 | 1    | 69,74,74     | 2.13 | 27 (39%) | 79,115,115  | 2.17 | 21 (26%) |
| 3   | BCL  | B     | 1601 | 2    | 69,74,74     | 1.97 | 21 (30%) | 79,115,115  | 2.57 | 21 (26%) |
| 3   | BCL  | N     | 1607 | 2    | 69,74,74     | 2.11 | 20 (28%) | 79,115,115  | 2.37 | 23 (29%) |
| 3   | BCL  | O     | 1708 | 1    | 69,74,74     | 2.22 | 24 (34%) | 79,115,115  | 2.13 | 22 (27%) |
| 4   | LDA  | N     | 1807 | -    | 13,15,15     | 1.82 | 1 (7%)   | 14,17,17    | 0.37 | 0        |
| 4   | LDA  | R     | 1818 | -    | 13,15,15     | 1.91 | 1 (7%)   | 14,17,17    | 0.45 | 0        |
| 4   | LDA  | R     | 1819 | -    | 13,15,15     | 2.14 | 2 (15%)  | 14,17,17    | 0.42 | 0        |
| 5   | RG1  | H     | 1404 | -    | 52,52,52     | 1.31 | 7 (13%)  | 66,67,67    | 1.74 | 16 (24%) |
| 4   | LDA  | A     | 1816 | -    | 13,15,15     | 2.22 | 2 (15%)  | 14,17,17    | 0.35 | 0        |
| 3   | BCL  | M     | 1707 | 1    | 69,74,74     | 2.34 | 20 (28%) | 79,115,115  | 2.06 | 21 (26%) |
| 4   | LDA  | G     | 1814 | -    | 13,15,15     | 2.02 | 1 (7%)   | 14,17,17    | 0.44 | 0        |
| 3   | BCL  | A     | 1701 | 1    | 69,74,74     | 2.60 | 26 (37%) | 79,115,115  | 2.31 | 23 (29%) |
| 3   | BCL  | J     | 1605 | 2    | 69,74,74     | 2.24 | 25 (36%) | 79,115,115  | 2.47 | 25 (31%) |
| 3   | BCL  | I     | 1505 | 1    | 69,74,74     | 2.04 | 20 (28%) | 79,115,115  | 2.07 | 23 (29%) |
| 3   | BCL  | C     | 1502 | 1    | 69,74,74     | 2.10 | 20 (28%) | 79,115,115  | 2.30 | 27 (34%) |
| 5   | RG1  | S     | 1409 | -    | 52,52,52     | 1.34 | 7 (13%)  | 66,67,67    | 1.65 | 17 (25%) |
| 5   | RG1  | J     | 1405 | -    | 52,52,52     | 1.19 | 5 (9%)   | 66,67,67    | 1.69 | 17 (25%) |
| 3   | BCL  | R     | 1709 | 1    | 69,74,74     | 2.37 | 30 (43%) | 79,115,115  | 2.18 | 22 (27%) |
| 5   | RG1  | L     | 1406 | -    | 52,52,52     | 1.27 | 6 (11%)  | 66,67,67    | 1.62 | 16 (24%) |

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   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 4   | LDA  | C     | 1815 | -    | -         | 6/13/13/13    | -       |
| 3   | BCL  | K     | 1506 | 1    | 1/1/21/25 | 8/41/137/137  | -       |
| 5   | RG1  | R     | 1401 | -    | -         | 5/51/71/71    | 0/1/1/1 |
| 4   | LDA  | P     | 1808 | -    | -         | 8/13/13/13    | -       |
| 4   | LDA  | D     | 1802 | -    | -         | 8/13/13/13    | -       |
| 3   | BCL  | E     | 1503 | 1    | -         | 7/41/137/137  | -       |
| 4   | LDA  | L     | 1806 | -    | -         | 10/13/13/13   | -       |
| 3   | BCL  | H     | 1604 | 2    | 1/1/21/25 | 10/41/137/137 | -       |
| 3   | BCL  | R     | 1509 | 1    | 1/1/21/25 | 9/41/137/137  | -       |
| 4   | LDA  | M     | 1811 | -    | -         | 7/13/13/13    | -       |
| 3   | BCL  | C     | 1702 | 1    | 1/1/21/25 | 18/41/137/137 | -       |
| 3   | BCL  | L     | 1606 | 2    | 3/3/21/25 | 6/41/137/137  | -       |
| 5   | RG1  | D     | 1402 | -    | -         | 4/51/71/71    | 0/1/1/1 |
| 5   | RG1  | N     | 1407 | -    | -         | 4/51/71/71    | 0/1/1/1 |
| 3   | BCL  | K     | 1706 | 1    | 1/1/21/25 | 11/41/137/137 | -       |
| 4   | LDA  | E     | 1822 | -    | -         | 7/13/13/13    | -       |
| 3   | BCL  | A     | 1501 | 1    | 1/1/21/25 | 5/41/137/137  | -       |
| 3   | BCL  | G     | 1704 | 1    | 1/1/21/25 | 10/41/137/137 | -       |
| 4   | LDA  | C     | 1821 | -    | -         | 5/13/13/13    | -       |
| 3   | BCL  | F     | 1603 | 2    | -         | 10/41/137/137 | -       |
| 4   | LDA  | R     | 1809 | -    | -         | 10/13/13/13   | -       |
| 4   | LDA  | I     | 1812 | -    | -         | 7/13/13/13    | -       |
| 3   | BCL  | D     | 1602 | 2    | -         | 8/41/137/137  | -       |
| 3   | BCL  | P     | 1608 | 2    | 2/2/21/25 | 13/41/137/137 | -       |
| 4   | LDA  | K     | 1810 | -    | -         | 7/13/13/13    | -       |
| 5   | RG1  | P     | 1408 | -    | -         | 7/51/71/71    | 0/1/1/1 |
| 3   | BCL  | E     | 1703 | 1    | -         | 16/41/137/137 | -       |
| 4   | LDA  | E     | 1823 | -    | -         | 5/13/13/13    | -       |
| 4   | LDA  | A     | 1817 | -    | -         | 8/13/13/13    | -       |
| 4   | LDA  | K     | 1826 | -    | -         | 6/13/13/13    | -       |
| 3   | BCL  | O     | 1508 | 1    | 2/2/21/25 | 9/41/137/137  | -       |
| 3   | BCL  | S     | 1609 | 2    | 1/1/21/25 | 13/41/137/137 | -       |
| 5   | RG1  | F     | 1403 | -    | -         | 4/51/71/71    | 0/1/1/1 |
| 4   | LDA  | O     | 1820 | -    | -         | 5/13/13/13    | -       |
| 4   | LDA  | M     | 1827 | -    | -         | 4/13/13/13    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 4   | LDA  | I     | 1825 | -    | -         | 8/13/13/13    | -       |
| 3   | BCL  | G     | 1504 | 1    | -         | 7/41/137/137  | -       |
| 3   | BCL  | M     | 1507 | 1    | -         | 3/41/137/137  | -       |
| 4   | LDA  | B     | 1801 | -    | -         | 8/13/13/13    | -       |
| 4   | LDA  | F     | 1803 | -    | -         | 9/13/13/13    | -       |
| 4   | LDA  | I     | 1813 | -    | -         | 4/13/13/13    | -       |
| 4   | LDA  | J     | 1805 | -    | -         | 9/13/13/13    | -       |
| 4   | LDA  | G     | 1824 | -    | -         | 4/13/13/13    | -       |
| 4   | LDA  | H     | 1804 | -    | -         | 6/13/13/13    | -       |
| 3   | BCL  | N     | 1607 | 2    | 1/1/21/25 | 17/41/137/137 | -       |
| 3   | BCL  | O     | 1708 | 1    | 1/1/21/25 | 10/41/137/137 | -       |
| 3   | BCL  | B     | 1601 | 2    | 1/1/21/25 | 8/41/137/137  | -       |
| 3   | BCL  | I     | 1705 | 1    | -         | 6/41/137/137  | -       |
| 4   | LDA  | N     | 1807 | -    | -         | 6/13/13/13    | -       |
| 4   | LDA  | R     | 1818 | -    | -         | 5/13/13/13    | -       |
| 4   | LDA  | R     | 1819 | -    | -         | 8/13/13/13    | -       |
| 5   | RG1  | H     | 1404 | -    | -         | 9/51/71/71    | 0/1/1/1 |
| 4   | LDA  | A     | 1816 | -    | -         | 6/13/13/13    | -       |
| 3   | BCL  | M     | 1707 | 1    | 1/1/21/25 | 15/41/137/137 | -       |
| 4   | LDA  | G     | 1814 | -    | -         | 8/13/13/13    | -       |
| 3   | BCL  | A     | 1701 | 1    | 1/1/21/25 | 15/41/137/137 | -       |
| 3   | BCL  | J     | 1605 | 2    | 1/1/21/25 | 8/41/137/137  | -       |
| 3   | BCL  | I     | 1505 | 1    | -         | 5/41/137/137  | -       |
| 3   | BCL  | C     | 1502 | 1    | 1/1/21/25 | 6/41/137/137  | -       |
| 5   | RG1  | S     | 1409 | -    | -         | 3/51/71/71    | 0/1/1/1 |
| 5   | RG1  | J     | 1405 | -    | -         | 5/51/71/71    | 0/1/1/1 |
| 3   | BCL  | R     | 1709 | 1    | 1/1/21/25 | 17/41/137/137 | -       |
| 5   | RG1  | L     | 1406 | -    | -         | 5/51/71/71    | 0/1/1/1 |

All (667) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | C     | 1702 | BCL  | C2-C3   | 8.61  | 1.52        | 1.33     |
| 3   | K     | 1506 | BCL  | CAC-C3C | -8.21 | 1.38        | 1.54     |
| 3   | A     | 1701 | BCL  | C2-C3   | 7.68  | 1.50        | 1.33     |
| 3   | S     | 1609 | BCL  | C2-C3   | 7.66  | 1.50        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | J     | 1605 | BCL  | C2-C3   | 7.50  | 1.50        | 1.33     |
| 4   | I     | 1812 | LDA  | O1-N1   | -7.43 | 1.23        | 1.42     |
| 3   | O     | 1708 | BCL  | C2-C3   | 7.43  | 1.50        | 1.33     |
| 3   | G     | 1704 | BCL  | C2-C3   | 7.33  | 1.49        | 1.33     |
| 3   | M     | 1707 | BCL  | CBD-CGD | -7.27 | 1.30        | 1.52     |
| 3   | A     | 1701 | BCL  | C3C-C4C | -7.23 | 1.42        | 1.51     |
| 3   | E     | 1503 | BCL  | C2-C3   | 7.10  | 1.49        | 1.33     |
| 3   | R     | 1709 | BCL  | C2-C3   | 6.94  | 1.49        | 1.33     |
| 3   | N     | 1607 | BCL  | C2-C3   | 6.93  | 1.49        | 1.33     |
| 3   | A     | 1501 | BCL  | C2-C3   | 6.88  | 1.48        | 1.33     |
| 4   | F     | 1803 | LDA  | O1-N1   | -6.81 | 1.25        | 1.42     |
| 3   | M     | 1707 | BCL  | C2-C3   | 6.80  | 1.48        | 1.33     |
| 4   | K     | 1810 | LDA  | O1-N1   | -6.76 | 1.25        | 1.42     |
| 4   | O     | 1820 | LDA  | O1-N1   | -6.76 | 1.25        | 1.42     |
| 4   | D     | 1802 | LDA  | O1-N1   | -6.75 | 1.25        | 1.42     |
| 3   | M     | 1507 | BCL  | C2-C3   | 6.72  | 1.48        | 1.33     |
| 3   | K     | 1506 | BCL  | C2-C3   | 6.70  | 1.48        | 1.33     |
| 4   | G     | 1824 | LDA  | O1-N1   | -6.67 | 1.25        | 1.42     |
| 3   | B     | 1601 | BCL  | C2-C3   | 6.66  | 1.48        | 1.33     |
| 3   | D     | 1602 | BCL  | C2-C3   | 6.65  | 1.48        | 1.33     |
| 4   | I     | 1813 | LDA  | O1-N1   | -6.58 | 1.26        | 1.42     |
| 4   | I     | 1825 | LDA  | O1-N1   | -6.57 | 1.26        | 1.42     |
| 3   | M     | 1707 | BCL  | C3B-C4B | 6.50  | 1.54        | 1.41     |
| 4   | A     | 1817 | LDA  | O1-N1   | -6.48 | 1.26        | 1.42     |
| 4   | L     | 1806 | LDA  | O1-N1   | -6.47 | 1.26        | 1.42     |
| 4   | C     | 1815 | LDA  | O1-N1   | -6.47 | 1.26        | 1.42     |
| 3   | P     | 1608 | BCL  | C2-C3   | 6.45  | 1.47        | 1.33     |
| 3   | R     | 1709 | BCL  | C3B-C4B | 6.45  | 1.53        | 1.41     |
| 3   | F     | 1603 | BCL  | C2-C3   | 6.42  | 1.47        | 1.33     |
| 3   | H     | 1604 | BCL  | C2-C3   | 6.41  | 1.47        | 1.33     |
| 4   | M     | 1827 | LDA  | O1-N1   | -6.37 | 1.26        | 1.42     |
| 3   | E     | 1703 | BCL  | C2-C3   | 6.32  | 1.47        | 1.33     |
| 4   | G     | 1814 | LDA  | O1-N1   | -6.28 | 1.26        | 1.42     |
| 3   | C     | 1502 | BCL  | C2-C3   | 6.26  | 1.47        | 1.33     |
| 4   | B     | 1801 | LDA  | O1-N1   | -6.24 | 1.26        | 1.42     |
| 4   | H     | 1804 | LDA  | C1-N1   | -6.19 | 1.45        | 1.51     |
| 4   | H     | 1804 | LDA  | O1-N1   | -6.18 | 1.27        | 1.42     |
| 3   | G     | 1504 | BCL  | C2-C3   | 6.17  | 1.47        | 1.33     |
| 4   | A     | 1816 | LDA  | O1-N1   | -6.16 | 1.27        | 1.42     |
| 4   | R     | 1819 | LDA  | O1-N1   | -6.15 | 1.27        | 1.42     |
| 4   | R     | 1818 | LDA  | O1-N1   | -6.15 | 1.27        | 1.42     |
| 4   | K     | 1826 | LDA  | O1-N1   | -6.15 | 1.27        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | K     | 1706 | BCL  | C2-C3   | 6.13  | 1.47        | 1.33     |
| 3   | R     | 1509 | BCL  | C2-C3   | 6.07  | 1.47        | 1.33     |
| 4   | C     | 1821 | LDA  | O1-N1   | -6.07 | 1.27        | 1.42     |
| 4   | E     | 1822 | LDA  | O1-N1   | -6.07 | 1.27        | 1.42     |
| 4   | P     | 1808 | LDA  | O1-N1   | -6.07 | 1.27        | 1.42     |
| 3   | C     | 1502 | BCL  | C3B-C4B | 6.00  | 1.53        | 1.41     |
| 4   | R     | 1809 | LDA  | O1-N1   | -5.99 | 1.27        | 1.42     |
| 4   | E     | 1823 | LDA  | O1-N1   | -5.97 | 1.27        | 1.42     |
| 3   | E     | 1503 | BCL  | MG-NB   | -5.92 | 1.94        | 2.05     |
| 4   | M     | 1811 | LDA  | O1-N1   | -5.91 | 1.27        | 1.42     |
| 3   | E     | 1703 | BCL  | O1D-CGD | 5.82  | 1.35        | 1.21     |
| 3   | K     | 1506 | BCL  | C3B-C4B | 5.75  | 1.52        | 1.41     |
| 3   | O     | 1508 | BCL  | C2-C3   | 5.67  | 1.46        | 1.33     |
| 3   | I     | 1705 | BCL  | C3B-C4B | 5.66  | 1.52        | 1.41     |
| 3   | L     | 1606 | BCL  | C2C-C3C | -5.65 | 1.39        | 1.54     |
| 4   | N     | 1807 | LDA  | O1-N1   | -5.56 | 1.28        | 1.42     |
| 3   | P     | 1608 | BCL  | C3B-C4B | 5.53  | 1.52        | 1.41     |
| 3   | N     | 1607 | BCL  | CMC-C2C | -5.52 | 1.41        | 1.53     |
| 3   | L     | 1606 | BCL  | C2-C3   | 5.51  | 1.45        | 1.33     |
| 4   | J     | 1805 | LDA  | O1-N1   | -5.50 | 1.28        | 1.42     |
| 3   | P     | 1608 | BCL  | O1D-CGD | 5.43  | 1.34        | 1.21     |
| 3   | O     | 1708 | BCL  | C3B-C4B | 5.37  | 1.51        | 1.41     |
| 3   | R     | 1509 | BCL  | C3A-C2A | -5.37 | 1.40        | 1.54     |
| 3   | M     | 1507 | BCL  | MG-NB   | -5.35 | 1.95        | 2.05     |
| 3   | I     | 1705 | BCL  | C2-C3   | 5.28  | 1.45        | 1.33     |
| 3   | A     | 1701 | BCL  | C3B-C4B | 5.28  | 1.51        | 1.41     |
| 3   | J     | 1605 | BCL  | C1D-C2D | 5.18  | 1.55        | 1.45     |
| 3   | K     | 1506 | BCL  | CAA-C2A | 5.17  | 1.63        | 1.54     |
| 3   | H     | 1604 | BCL  | C3C-C4C | -5.15 | 1.45        | 1.51     |
| 3   | I     | 1505 | BCL  | C3B-C4B | 5.15  | 1.51        | 1.41     |
| 3   | D     | 1602 | BCL  | C3B-C4B | 5.11  | 1.51        | 1.41     |
| 3   | J     | 1605 | BCL  | CBD-CGD | -5.10 | 1.37        | 1.52     |
| 3   | R     | 1709 | BCL  | CHB-C1B | 5.02  | 1.50        | 1.39     |
| 3   | C     | 1502 | BCL  | C1D-ND  | 5.01  | 1.44        | 1.37     |
| 3   | I     | 1505 | BCL  | CHC-C4B | 5.00  | 1.50        | 1.39     |
| 3   | C     | 1702 | BCL  | O1D-CGD | 4.96  | 1.33        | 1.21     |
| 3   | R     | 1509 | BCL  | OBD-CAD | 4.94  | 1.31        | 1.22     |
| 3   | S     | 1609 | BCL  | MG-NB   | -4.88 | 1.96        | 2.05     |
| 3   | K     | 1706 | BCL  | C1D-C2D | 4.85  | 1.54        | 1.45     |
| 3   | G     | 1504 | BCL  | O1D-CGD | 4.84  | 1.33        | 1.21     |
| 3   | A     | 1501 | BCL  | C3B-C4B | 4.82  | 1.50        | 1.41     |
| 5   | N     | 1407 | RG1  | O1'-C1  | -4.81 | 1.40        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | K     | 1506 | BCL  | O1D-CGD | 4.81  | 1.33        | 1.21     |
| 3   | A     | 1701 | BCL  | CHD-C1D | 4.80  | 1.47        | 1.38     |
| 3   | M     | 1507 | BCL  | C3B-C4B | 4.80  | 1.50        | 1.41     |
| 5   | F     | 1403 | RG1  | C19-C18 | 4.78  | 1.56        | 1.46     |
| 3   | A     | 1701 | BCL  | CAC-C3C | -4.78 | 1.44        | 1.54     |
| 3   | D     | 1602 | BCL  | CHB-C1B | 4.78  | 1.50        | 1.39     |
| 3   | G     | 1704 | BCL  | CBD-CGD | -4.77 | 1.38        | 1.52     |
| 3   | M     | 1707 | BCL  | C1D-C2D | 4.76  | 1.54        | 1.45     |
| 3   | M     | 1707 | BCL  | CHB-C1B | 4.72  | 1.50        | 1.39     |
| 3   | I     | 1505 | BCL  | CHB-C1B | 4.71  | 1.50        | 1.39     |
| 3   | A     | 1501 | BCL  | MG-NB   | -4.69 | 1.96        | 2.05     |
| 3   | I     | 1705 | BCL  | C1D-C2D | 4.68  | 1.54        | 1.45     |
| 3   | C     | 1502 | BCL  | CHB-C4A | 4.68  | 1.49        | 1.37     |
| 3   | A     | 1501 | BCL  | OBD-CAD | 4.66  | 1.30        | 1.22     |
| 3   | M     | 1507 | BCL  | C3D-C2D | 4.66  | 1.51        | 1.39     |
| 3   | L     | 1606 | BCL  | CHC-C4B | 4.65  | 1.49        | 1.39     |
| 3   | G     | 1504 | BCL  | C1D-C2D | 4.64  | 1.54        | 1.45     |
| 3   | R     | 1709 | BCL  | C1D-ND  | 4.63  | 1.43        | 1.37     |
| 3   | A     | 1701 | BCL  | C1D-C2D | 4.61  | 1.54        | 1.45     |
| 3   | C     | 1702 | BCL  | C3B-C4B | 4.60  | 1.50        | 1.41     |
| 3   | N     | 1607 | BCL  | C2C-C3C | -4.58 | 1.42        | 1.54     |
| 4   | D     | 1802 | LDA  | C1-N1   | -4.57 | 1.46        | 1.51     |
| 3   | H     | 1604 | BCL  | CHB-C1B | 4.54  | 1.49        | 1.39     |
| 3   | A     | 1701 | BCL  | CHB-C1B | 4.54  | 1.49        | 1.39     |
| 3   | P     | 1608 | BCL  | OBD-CAD | 4.52  | 1.30        | 1.22     |
| 3   | B     | 1601 | BCL  | MG-NB   | -4.52 | 1.96        | 2.05     |
| 3   | N     | 1607 | BCL  | C3B-C4B | 4.51  | 1.50        | 1.41     |
| 3   | H     | 1604 | BCL  | CHC-C4B | 4.51  | 1.49        | 1.39     |
| 3   | P     | 1608 | BCL  | CHB-C4A | 4.50  | 1.49        | 1.37     |
| 3   | O     | 1708 | BCL  | CHD-C1D | 4.50  | 1.47        | 1.38     |
| 3   | F     | 1603 | BCL  | C3D-C2D | 4.48  | 1.51        | 1.39     |
| 3   | O     | 1708 | BCL  | O1D-CGD | 4.47  | 1.32        | 1.21     |
| 3   | G     | 1504 | BCL  | MG-NA   | 4.47  | 2.16        | 2.06     |
| 3   | D     | 1602 | BCL  | MG-NA   | 4.42  | 2.16        | 2.06     |
| 3   | O     | 1508 | BCL  | OBD-CAD | 4.42  | 1.30        | 1.22     |
| 3   | J     | 1605 | BCL  | C3B-C4B | 4.40  | 1.49        | 1.41     |
| 3   | K     | 1706 | BCL  | OBB-CAB | 4.39  | 1.33        | 1.23     |
| 3   | L     | 1606 | BCL  | MG-NC   | 4.39  | 2.16        | 2.06     |
| 4   | A     | 1816 | LDA  | C1-N1   | -4.37 | 1.47        | 1.51     |
| 3   | M     | 1707 | BCL  | MG-NA   | 4.37  | 2.16        | 2.06     |
| 3   | I     | 1505 | BCL  | C2-C3   | 4.37  | 1.43        | 1.33     |
| 3   | K     | 1506 | BCL  | O2D-CGD | 4.37  | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | O     | 1708 | BCL  | CHB-C4A | 4.36  | 1.48        | 1.37     |
| 3   | A     | 1701 | BCL  | MG-NA   | 4.34  | 2.16        | 2.06     |
| 4   | R     | 1819 | LDA  | C1-N1   | -4.33 | 1.47        | 1.51     |
| 3   | F     | 1603 | BCL  | C3B-C4B | 4.31  | 1.49        | 1.41     |
| 3   | C     | 1702 | BCL  | CHB-C4A | 4.31  | 1.48        | 1.37     |
| 3   | L     | 1606 | BCL  | MG-NB   | -4.29 | 1.97        | 2.05     |
| 3   | C     | 1502 | BCL  | CHB-C1B | 4.29  | 1.49        | 1.39     |
| 3   | L     | 1606 | BCL  | CHC-C1C | 4.27  | 1.48        | 1.37     |
| 3   | A     | 1701 | BCL  | OBD-CAD | 4.26  | 1.29        | 1.22     |
| 3   | C     | 1702 | BCL  | C3D-C2D | 4.26  | 1.50        | 1.39     |
| 3   | G     | 1704 | BCL  | CHB-C1B | 4.24  | 1.48        | 1.39     |
| 3   | J     | 1605 | BCL  | MG-NA   | 4.24  | 2.16        | 2.06     |
| 3   | S     | 1609 | BCL  | CHB-C1B | 4.23  | 1.48        | 1.39     |
| 3   | K     | 1706 | BCL  | O1D-CGD | 4.23  | 1.31        | 1.21     |
| 3   | P     | 1608 | BCL  | CHB-C1B | 4.22  | 1.48        | 1.39     |
| 3   | E     | 1703 | BCL  | C1D-C2D | 4.19  | 1.53        | 1.45     |
| 3   | M     | 1707 | BCL  | CHB-C4A | 4.18  | 1.48        | 1.37     |
| 3   | M     | 1707 | BCL  | OBD-CAD | 4.17  | 1.29        | 1.22     |
| 3   | P     | 1608 | BCL  | CHC-C4B | 4.17  | 1.48        | 1.39     |
| 3   | G     | 1504 | BCL  | CHB-C1B | 4.17  | 1.48        | 1.39     |
| 3   | J     | 1605 | BCL  | CHB-C1B | 4.16  | 1.48        | 1.39     |
| 3   | R     | 1509 | BCL  | CHC-C1C | 4.15  | 1.48        | 1.37     |
| 3   | K     | 1706 | BCL  | CHB-C1B | 4.15  | 1.48        | 1.39     |
| 3   | E     | 1703 | BCL  | C3D-C2D | 4.13  | 1.50        | 1.39     |
| 3   | A     | 1501 | BCL  | MG-NA   | 4.12  | 2.16        | 2.06     |
| 3   | I     | 1705 | BCL  | CHD-C1D | 4.12  | 1.46        | 1.38     |
| 3   | L     | 1606 | BCL  | CMC-C2C | -4.12 | 1.44        | 1.53     |
| 3   | H     | 1604 | BCL  | O1D-CGD | 4.12  | 1.31        | 1.21     |
| 3   | N     | 1607 | BCL  | CHB-C1B | 4.11  | 1.48        | 1.39     |
| 3   | B     | 1601 | BCL  | C1D-C2D | 4.11  | 1.53        | 1.45     |
| 3   | O     | 1508 | BCL  | C14-C13 | -4.10 | 1.40        | 1.52     |
| 3   | C     | 1702 | BCL  | C1D-C2D | 4.08  | 1.53        | 1.45     |
| 3   | E     | 1503 | BCL  | C3D-C2D | 4.07  | 1.50        | 1.39     |
| 3   | K     | 1506 | BCL  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 3   | R     | 1509 | BCL  | O1D-CGD | 4.07  | 1.31        | 1.21     |
| 3   | L     | 1606 | BCL  | O1D-CGD | 4.06  | 1.31        | 1.21     |
| 3   | O     | 1508 | BCL  | CBD-CGD | -4.05 | 1.40        | 1.52     |
| 3   | G     | 1704 | BCL  | CHB-C4A | 4.04  | 1.47        | 1.37     |
| 3   | A     | 1501 | BCL  | CHB-C1B | 4.03  | 1.48        | 1.39     |
| 3   | E     | 1703 | BCL  | C3B-C4B | 4.02  | 1.49        | 1.41     |
| 3   | R     | 1509 | BCL  | CHC-C4B | 4.02  | 1.48        | 1.39     |
| 3   | I     | 1505 | BCL  | C1B-C2B | 4.02  | 1.52        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | I     | 1505 | BCL  | C1D-C2D | 3.98  | 1.53        | 1.45     |
| 3   | A     | 1701 | BCL  | O1D-CGD | 3.97  | 1.31        | 1.21     |
| 3   | G     | 1704 | BCL  | C1B-C2B | 3.96  | 1.52        | 1.43     |
| 3   | A     | 1501 | BCL  | O1A-CGA | 3.94  | 1.34        | 1.22     |
| 3   | O     | 1708 | BCL  | C3D-C2D | 3.94  | 1.49        | 1.39     |
| 3   | A     | 1701 | BCL  | O1A-CGA | 3.92  | 1.34        | 1.22     |
| 3   | K     | 1706 | BCL  | C3B-C4B | 3.92  | 1.48        | 1.41     |
| 3   | D     | 1602 | BCL  | C3D-C2D | 3.90  | 1.49        | 1.39     |
| 3   | N     | 1607 | BCL  | MG-NA   | 3.88  | 2.15        | 2.06     |
| 3   | J     | 1605 | BCL  | CHB-C4A | 3.88  | 1.47        | 1.37     |
| 3   | L     | 1606 | BCL  | CHB-C1B | 3.87  | 1.48        | 1.39     |
| 3   | O     | 1508 | BCL  | C1D-C2D | 3.87  | 1.53        | 1.45     |
| 3   | G     | 1504 | BCL  | CHB-C4A | 3.87  | 1.47        | 1.37     |
| 3   | S     | 1609 | BCL  | C3D-C2D | 3.86  | 1.49        | 1.39     |
| 3   | E     | 1503 | BCL  | C3B-C4B | 3.85  | 1.48        | 1.41     |
| 3   | R     | 1709 | BCL  | C3D-C2D | 3.85  | 1.49        | 1.39     |
| 3   | O     | 1508 | BCL  | OBB-CAB | 3.85  | 1.32        | 1.23     |
| 3   | H     | 1604 | BCL  | C3B-C4B | 3.84  | 1.48        | 1.41     |
| 3   | R     | 1509 | BCL  | C3B-C4B | 3.84  | 1.48        | 1.41     |
| 3   | E     | 1703 | BCL  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 3   | P     | 1608 | BCL  | C2C-C3C | -3.81 | 1.44        | 1.54     |
| 3   | N     | 1607 | BCL  | C3D-C2D | 3.81  | 1.49        | 1.39     |
| 3   | B     | 1601 | BCL  | CHC-C4B | 3.78  | 1.47        | 1.39     |
| 3   | K     | 1506 | BCL  | C1B-C2B | 3.77  | 1.52        | 1.43     |
| 3   | K     | 1706 | BCL  | C3D-C2D | 3.76  | 1.49        | 1.39     |
| 3   | M     | 1507 | BCL  | O1D-CGD | 3.76  | 1.30        | 1.21     |
| 3   | O     | 1708 | BCL  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 3   | C     | 1502 | BCL  | CHC-C4B | 3.74  | 1.47        | 1.39     |
| 3   | R     | 1709 | BCL  | C1D-C2D | 3.74  | 1.52        | 1.45     |
| 3   | A     | 1501 | BCL  | CHB-C4A | 3.72  | 1.47        | 1.37     |
| 3   | A     | 1701 | BCL  | C3D-C2D | 3.71  | 1.49        | 1.39     |
| 3   | R     | 1709 | BCL  | MG-NA   | 3.70  | 2.15        | 2.06     |
| 3   | O     | 1508 | BCL  | O1A-CGA | 3.69  | 1.33        | 1.22     |
| 3   | I     | 1705 | BCL  | O1A-CGA | 3.69  | 1.33        | 1.22     |
| 3   | D     | 1602 | BCL  | C2A-C1A | -3.69 | 1.43        | 1.52     |
| 3   | A     | 1501 | BCL  | O1D-CGD | 3.67  | 1.30        | 1.21     |
| 3   | I     | 1505 | BCL  | O2D-CGD | 3.67  | 1.42        | 1.33     |
| 3   | D     | 1602 | BCL  | CHB-C4A | 3.67  | 1.46        | 1.37     |
| 3   | R     | 1509 | BCL  | C1D-C2D | 3.66  | 1.52        | 1.45     |
| 3   | I     | 1505 | BCL  | MG-NC   | 3.65  | 2.14        | 2.06     |
| 3   | G     | 1704 | BCL  | C3B-C4B | 3.64  | 1.48        | 1.41     |
| 5   | S     | 1409 | RG1  | O1'-C1  | -3.62 | 1.42        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | I     | 1705 | BCL  | O2D-CGD | 3.61  | 1.42        | 1.33     |
| 3   | A     | 1701 | BCL  | O2D-CGD | 3.58  | 1.42        | 1.33     |
| 3   | A     | 1701 | BCL  | OBB-CAB | 3.57  | 1.31        | 1.23     |
| 5   | S     | 1409 | RG1  | C2-C1   | 3.56  | 1.58        | 1.53     |
| 3   | R     | 1509 | BCL  | OBB-CAB | 3.56  | 1.31        | 1.23     |
| 3   | L     | 1606 | BCL  | C3B-C4B | 3.55  | 1.48        | 1.41     |
| 3   | D     | 1602 | BCL  | MG-NB   | -3.55 | 1.98        | 2.05     |
| 3   | B     | 1601 | BCL  | CHB-C1B | 3.55  | 1.47        | 1.39     |
| 3   | H     | 1604 | BCL  | OBB-CAB | 3.55  | 1.31        | 1.23     |
| 3   | I     | 1705 | BCL  | C3D-C2D | 3.54  | 1.48        | 1.39     |
| 3   | O     | 1708 | BCL  | C1D-C2D | 3.54  | 1.52        | 1.45     |
| 3   | F     | 1603 | BCL  | CHB-C4A | 3.53  | 1.46        | 1.37     |
| 3   | O     | 1708 | BCL  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 3   | G     | 1504 | BCL  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 3   | G     | 1704 | BCL  | MG-NC   | 3.52  | 2.14        | 2.06     |
| 3   | K     | 1506 | BCL  | CHB-C4A | 3.51  | 1.46        | 1.37     |
| 3   | D     | 1602 | BCL  | O1A-CGA | 3.50  | 1.33        | 1.22     |
| 3   | R     | 1509 | BCL  | C3D-C2D | 3.50  | 1.48        | 1.39     |
| 3   | I     | 1505 | BCL  | CHC-C1C | 3.48  | 1.46        | 1.37     |
| 3   | M     | 1507 | BCL  | O2D-CGD | 3.47  | 1.41        | 1.33     |
| 5   | H     | 1404 | RG1  | C2-C1   | 3.47  | 1.58        | 1.53     |
| 3   | K     | 1506 | BCL  | C2C-C3C | -3.46 | 1.45        | 1.54     |
| 3   | S     | 1609 | BCL  | C3B-C4B | 3.46  | 1.48        | 1.41     |
| 3   | J     | 1605 | BCL  | MG-NB   | -3.46 | 1.98        | 2.05     |
| 5   | J     | 1405 | RG1  | O1'-C1  | -3.45 | 1.42        | 1.46     |
| 3   | N     | 1607 | BCL  | C1B-C2B | 3.45  | 1.51        | 1.43     |
| 3   | I     | 1705 | BCL  | CAA-C2A | 3.44  | 1.60        | 1.54     |
| 3   | D     | 1602 | BCL  | O2A-CGA | 3.44  | 1.43        | 1.33     |
| 3   | R     | 1509 | BCL  | O1A-CGA | 3.44  | 1.32        | 1.22     |
| 3   | A     | 1701 | BCL  | CHB-C4A | 3.44  | 1.46        | 1.37     |
| 3   | R     | 1509 | BCL  | MG-NB   | -3.44 | 1.99        | 2.05     |
| 3   | P     | 1608 | BCL  | MG-NC   | 3.43  | 2.14        | 2.06     |
| 3   | E     | 1703 | BCL  | MG-NC   | 3.41  | 2.14        | 2.06     |
| 3   | H     | 1604 | BCL  | O1A-CGA | 3.41  | 1.32        | 1.22     |
| 3   | B     | 1601 | BCL  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 3   | G     | 1704 | BCL  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 3   | L     | 1606 | BCL  | C3A-C4A | -3.40 | 1.40        | 1.51     |
| 3   | C     | 1502 | BCL  | C1B-C2B | 3.40  | 1.51        | 1.43     |
| 3   | B     | 1601 | BCL  | O1D-CGD | 3.40  | 1.29        | 1.21     |
| 3   | P     | 1608 | BCL  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 3   | I     | 1505 | BCL  | O1A-CGA | 3.39  | 1.32        | 1.22     |
| 3   | K     | 1706 | BCL  | CHC-C1C | 3.39  | 1.46        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | R     | 1509 | BCL  | CHB-C4A | 3.36  | 1.46        | 1.37     |
| 3   | H     | 1604 | BCL  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 3   | G     | 1504 | BCL  | C4B-NB  | 3.35  | 1.42        | 1.37     |
| 4   | A     | 1817 | LDA  | C1-N1   | -3.34 | 1.48        | 1.51     |
| 3   | R     | 1709 | BCL  | CHB-C4A | 3.34  | 1.46        | 1.37     |
| 3   | I     | 1705 | BCL  | C4D-CHA | 3.34  | 1.49        | 1.38     |
| 3   | A     | 1701 | BCL  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 3   | R     | 1709 | BCL  | CHC-C4B | 3.33  | 1.46        | 1.39     |
| 3   | R     | 1709 | BCL  | CHD-C1D | 3.33  | 1.44        | 1.38     |
| 3   | P     | 1608 | BCL  | CMC-C2C | -3.32 | 1.46        | 1.53     |
| 3   | A     | 1501 | BCL  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 3   | H     | 1604 | BCL  | CHB-C4A | 3.31  | 1.46        | 1.37     |
| 3   | I     | 1705 | BCL  | C1B-C2B | 3.30  | 1.50        | 1.43     |
| 3   | G     | 1704 | BCL  | C3C-C4C | -3.30 | 1.47        | 1.51     |
| 3   | M     | 1707 | BCL  | C3C-C4C | -3.29 | 1.47        | 1.51     |
| 3   | A     | 1501 | BCL  | C3C-C4C | 3.29  | 1.55        | 1.51     |
| 3   | J     | 1605 | BCL  | C4D-CHA | 3.28  | 1.49        | 1.38     |
| 3   | A     | 1501 | BCL  | CBD-CGD | -3.28 | 1.42        | 1.52     |
| 3   | M     | 1707 | BCL  | C1B-C2B | 3.27  | 1.50        | 1.43     |
| 3   | L     | 1606 | BCL  | C3A-C2A | -3.27 | 1.45        | 1.54     |
| 3   | L     | 1606 | BCL  | CMA-C3A | -3.27 | 1.46        | 1.53     |
| 3   | J     | 1605 | BCL  | O1A-CGA | 3.26  | 1.32        | 1.22     |
| 3   | P     | 1608 | BCL  | MG-NA   | 3.24  | 2.14        | 2.06     |
| 3   | K     | 1506 | BCL  | C3B-CAB | 3.23  | 1.56        | 1.46     |
| 3   | A     | 1701 | BCL  | CHD-C4C | 3.23  | 1.48        | 1.39     |
| 3   | R     | 1709 | BCL  | CHC-C1C | 3.23  | 1.45        | 1.37     |
| 3   | K     | 1506 | BCL  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 3   | G     | 1704 | BCL  | MG-NA   | 3.22  | 2.13        | 2.06     |
| 3   | R     | 1709 | BCL  | MG-NC   | 3.22  | 2.13        | 2.06     |
| 3   | F     | 1603 | BCL  | C5-C3   | 3.22  | 1.57        | 1.51     |
| 3   | O     | 1708 | BCL  | MG-NA   | 3.20  | 2.13        | 2.06     |
| 3   | M     | 1507 | BCL  | CHC-C1C | 3.19  | 1.45        | 1.37     |
| 3   | R     | 1509 | BCL  | C3C-C4C | -3.19 | 1.47        | 1.51     |
| 3   | S     | 1609 | BCL  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 3   | O     | 1708 | BCL  | C4D-CHA | 3.18  | 1.49        | 1.38     |
| 3   | O     | 1708 | BCL  | CHC-C1C | 3.17  | 1.45        | 1.37     |
| 3   | S     | 1609 | BCL  | O1D-CGD | 3.17  | 1.29        | 1.21     |
| 4   | K     | 1826 | LDA  | C1-N1   | -3.16 | 1.48        | 1.51     |
| 3   | F     | 1603 | BCL  | CHD-C1D | 3.16  | 1.44        | 1.38     |
| 3   | A     | 1501 | BCL  | CHC-C1C | 3.16  | 1.45        | 1.37     |
| 3   | C     | 1502 | BCL  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 3   | B     | 1601 | BCL  | C3D-C2D | 3.14  | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | E     | 1822 | LDA  | C1-N1   | -3.14 | 1.48        | 1.51     |
| 3   | C     | 1702 | BCL  | CHB-C1B | 3.13  | 1.46        | 1.39     |
| 3   | C     | 1502 | BCL  | CHC-C1C | 3.13  | 1.45        | 1.37     |
| 3   | O     | 1508 | BCL  | CHB-C4A | 3.13  | 1.45        | 1.37     |
| 3   | C     | 1502 | BCL  | MG-NB   | -3.13 | 1.99        | 2.05     |
| 3   | D     | 1602 | BCL  | C4D-CHA | 3.12  | 1.49        | 1.38     |
| 3   | I     | 1705 | BCL  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 3   | N     | 1607 | BCL  | C4D-CHA | 3.11  | 1.49        | 1.38     |
| 3   | G     | 1504 | BCL  | CHC-C1C | 3.11  | 1.45        | 1.37     |
| 3   | M     | 1707 | BCL  | MG-NC   | 3.11  | 2.13        | 2.06     |
| 3   | K     | 1506 | BCL  | O2A-CGA | 3.10  | 1.42        | 1.33     |
| 3   | I     | 1705 | BCL  | C3B-CAB | 3.10  | 1.56        | 1.46     |
| 5   | L     | 1406 | RG1  | C16-C17 | 3.09  | 1.52        | 1.43     |
| 3   | K     | 1706 | BCL  | O1A-CGA | 3.09  | 1.31        | 1.22     |
| 3   | A     | 1701 | BCL  | C2C-C3C | -3.09 | 1.46        | 1.54     |
| 3   | M     | 1507 | BCL  | OBB-CAB | 3.08  | 1.30        | 1.23     |
| 3   | A     | 1501 | BCL  | O2D-CGD | 3.07  | 1.40        | 1.33     |
| 3   | E     | 1503 | BCL  | O1A-CGA | 3.07  | 1.31        | 1.22     |
| 3   | R     | 1709 | BCL  | O1D-CGD | 3.07  | 1.29        | 1.21     |
| 3   | N     | 1607 | BCL  | CBD-CGD | -3.06 | 1.43        | 1.52     |
| 3   | R     | 1709 | BCL  | C5-C3   | 3.06  | 1.57        | 1.51     |
| 3   | L     | 1606 | BCL  | C4D-CHA | 3.05  | 1.48        | 1.38     |
| 3   | K     | 1506 | BCL  | C4D-CHA | 3.05  | 1.48        | 1.38     |
| 3   | B     | 1601 | BCL  | C3B-C4B | 3.04  | 1.47        | 1.41     |
| 3   | I     | 1705 | BCL  | CHB-C1B | 3.03  | 1.46        | 1.39     |
| 3   | S     | 1609 | BCL  | CHB-C4A | 3.03  | 1.45        | 1.37     |
| 5   | H     | 1404 | RG1  | C23-C22 | 3.03  | 1.52        | 1.46     |
| 3   | M     | 1707 | BCL  | CBD-CAD | -3.03 | 1.43        | 1.56     |
| 3   | E     | 1503 | BCL  | OBD-CAD | 3.02  | 1.27        | 1.22     |
| 3   | J     | 1605 | BCL  | CHC-C4B | 3.02  | 1.46        | 1.39     |
| 3   | R     | 1509 | BCL  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 3   | G     | 1704 | BCL  | CBD-CAD | -3.01 | 1.43        | 1.56     |
| 3   | D     | 1602 | BCL  | MG-NC   | 3.01  | 2.13        | 2.06     |
| 3   | D     | 1602 | BCL  | C1B-C2B | 3.00  | 1.50        | 1.43     |
| 3   | S     | 1609 | BCL  | O2A-CGA | 3.00  | 1.42        | 1.33     |
| 3   | I     | 1505 | BCL  | OBB-CAB | 3.00  | 1.30        | 1.23     |
| 3   | O     | 1508 | BCL  | MG-NB   | -2.99 | 1.99        | 2.05     |
| 3   | A     | 1501 | BCL  | C4D-CHA | 2.99  | 1.48        | 1.38     |
| 3   | F     | 1603 | BCL  | OBD-CAD | 2.98  | 1.27        | 1.22     |
| 3   | A     | 1701 | BCL  | C4D-CHA | 2.98  | 1.48        | 1.38     |
| 3   | J     | 1605 | BCL  | O2A-CGA | 2.98  | 1.42        | 1.33     |
| 3   | N     | 1607 | BCL  | OBD-CAD | 2.98  | 1.27        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | S     | 1409 | RG1  | C24-C25 | 2.97  | 1.52        | 1.43     |
| 3   | O     | 1708 | BCL  | OBB-CAB | 2.97  | 1.30        | 1.23     |
| 3   | L     | 1606 | BCL  | OBD-CAD | 2.97  | 1.27        | 1.22     |
| 3   | C     | 1502 | BCL  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 3   | E     | 1503 | BCL  | MG-NC   | 2.97  | 2.13        | 2.06     |
| 3   | E     | 1503 | BCL  | CHB-C4A | 2.97  | 1.45        | 1.37     |
| 3   | G     | 1704 | BCL  | C1D-C2D | 2.95  | 1.51        | 1.45     |
| 3   | E     | 1503 | BCL  | O1D-CGD | 2.95  | 1.28        | 1.21     |
| 5   | F     | 1403 | RG1  | C24-C25 | 2.95  | 1.52        | 1.43     |
| 3   | F     | 1603 | BCL  | O2D-CGD | 2.95  | 1.40        | 1.33     |
| 3   | S     | 1609 | BCL  | MG-NC   | 2.95  | 2.13        | 2.06     |
| 3   | O     | 1708 | BCL  | CHC-C4B | 2.94  | 1.46        | 1.39     |
| 3   | R     | 1709 | BCL  | O1A-CGA | 2.94  | 1.31        | 1.22     |
| 5   | P     | 1408 | RG1  | C23-C22 | 2.94  | 1.52        | 1.46     |
| 5   | L     | 1406 | RG1  | C16-C15 | 2.93  | 1.44        | 1.36     |
| 3   | L     | 1606 | BCL  | CHD-C1D | 2.93  | 1.44        | 1.38     |
| 3   | M     | 1707 | BCL  | CHD-C1D | 2.92  | 1.44        | 1.38     |
| 3   | C     | 1702 | BCL  | O1A-CGA | 2.92  | 1.31        | 1.22     |
| 3   | K     | 1706 | BCL  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 3   | K     | 1706 | BCL  | C1B-C2B | 2.92  | 1.50        | 1.43     |
| 3   | N     | 1607 | BCL  | C1D-ND  | 2.91  | 1.41        | 1.37     |
| 3   | G     | 1504 | BCL  | C3D-C2D | 2.91  | 1.46        | 1.39     |
| 5   | F     | 1403 | RG1  | C11-C10 | 2.91  | 1.52        | 1.43     |
| 3   | R     | 1709 | BCL  | OBB-CAB | 2.91  | 1.29        | 1.23     |
| 3   | B     | 1601 | BCL  | O2D-CGD | 2.91  | 1.40        | 1.33     |
| 3   | A     | 1701 | BCL  | O2A-CGA | 2.89  | 1.41        | 1.33     |
| 3   | K     | 1706 | BCL  | CHD-C1D | 2.89  | 1.44        | 1.38     |
| 3   | D     | 1602 | BCL  | O1D-CGD | 2.89  | 1.28        | 1.21     |
| 3   | N     | 1607 | BCL  | O1A-CGA | 2.88  | 1.31        | 1.22     |
| 5   | H     | 1404 | RG1  | C27-C26 | 2.88  | 1.52        | 1.46     |
| 3   | B     | 1601 | BCL  | CHD-C1D | 2.88  | 1.44        | 1.38     |
| 3   | J     | 1605 | BCL  | CBA-CGA | -2.88 | 1.42        | 1.50     |
| 3   | D     | 1602 | BCL  | OBD-CAD | 2.88  | 1.27        | 1.22     |
| 3   | G     | 1704 | BCL  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 3   | K     | 1706 | BCL  | MG-NA   | 2.87  | 2.13        | 2.06     |
| 3   | I     | 1505 | BCL  | CHB-C4A | 2.87  | 1.44        | 1.37     |
| 3   | J     | 1605 | BCL  | MG-NC   | 2.87  | 2.13        | 2.06     |
| 3   | C     | 1502 | BCL  | C3D-C2D | 2.87  | 1.46        | 1.39     |
| 3   | M     | 1507 | BCL  | CHB-C1B | 2.87  | 1.45        | 1.39     |
| 3   | O     | 1708 | BCL  | MG-NC   | 2.86  | 2.13        | 2.06     |
| 3   | G     | 1504 | BCL  | CBD-CGD | -2.86 | 1.43        | 1.52     |
| 3   | M     | 1507 | BCL  | CHB-C4A | 2.86  | 1.44        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | R     | 1509 | BCL  | CHB-C1B | 2.85  | 1.45        | 1.39     |
| 3   | P     | 1608 | BCL  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 3   | A     | 1501 | BCL  | CHC-C4B | 2.85  | 1.45        | 1.39     |
| 3   | R     | 1709 | BCL  | CHD-C4C | 2.84  | 1.47        | 1.39     |
| 3   | L     | 1606 | BCL  | O1A-CGA | 2.84  | 1.31        | 1.22     |
| 3   | P     | 1608 | BCL  | OBB-CAB | 2.84  | 1.29        | 1.23     |
| 3   | M     | 1507 | BCL  | MG-NC   | 2.83  | 2.13        | 2.06     |
| 3   | K     | 1706 | BCL  | OBD-CAD | 2.83  | 1.27        | 1.22     |
| 3   | R     | 1709 | BCL  | C2A-C1A | -2.83 | 1.45        | 1.52     |
| 3   | J     | 1605 | BCL  | O1D-CGD | 2.82  | 1.28        | 1.21     |
| 5   | L     | 1406 | RG1  | C11-C10 | 2.82  | 1.51        | 1.43     |
| 3   | E     | 1703 | BCL  | C3B-CAB | 2.82  | 1.55        | 1.46     |
| 3   | M     | 1507 | BCL  | C1D-C2D | 2.82  | 1.50        | 1.45     |
| 3   | N     | 1607 | BCL  | CHD-C1D | 2.82  | 1.43        | 1.38     |
| 3   | M     | 1707 | BCL  | O1A-CGA | 2.82  | 1.30        | 1.22     |
| 3   | P     | 1608 | BCL  | O2D-CGD | 2.82  | 1.40        | 1.33     |
| 3   | R     | 1709 | BCL  | C1B-C2B | 2.82  | 1.49        | 1.43     |
| 3   | C     | 1502 | BCL  | MG-NA   | 2.82  | 2.13        | 2.06     |
| 3   | N     | 1607 | BCL  | CHB-C4A | 2.82  | 1.44        | 1.37     |
| 5   | D     | 1402 | RG1  | C2-C1   | 2.81  | 1.57        | 1.53     |
| 3   | S     | 1609 | BCL  | MG-NA   | 2.79  | 2.12        | 2.06     |
| 3   | D     | 1602 | BCL  | CBD-CGD | -2.79 | 1.44        | 1.52     |
| 3   | B     | 1601 | BCL  | C4B-NB  | -2.79 | 1.34        | 1.37     |
| 3   | P     | 1608 | BCL  | C1B-C2B | 2.79  | 1.49        | 1.43     |
| 3   | J     | 1605 | BCL  | C3D-C2D | 2.79  | 1.46        | 1.39     |
| 3   | R     | 1709 | BCL  | C4D-CHA | 2.79  | 1.47        | 1.38     |
| 5   | D     | 1402 | RG1  | C11-C10 | 2.78  | 1.51        | 1.43     |
| 3   | L     | 1606 | BCL  | O2A-CGA | 2.78  | 1.41        | 1.33     |
| 3   | F     | 1603 | BCL  | C1D-C2D | 2.78  | 1.50        | 1.45     |
| 3   | O     | 1508 | BCL  | MG-NA   | 2.78  | 2.12        | 2.06     |
| 3   | R     | 1509 | BCL  | C1B-C2B | 2.78  | 1.49        | 1.43     |
| 5   | R     | 1401 | RG1  | CM1-C1  | 2.77  | 1.58        | 1.52     |
| 3   | S     | 1609 | BCL  | C4D-CHA | 2.77  | 1.47        | 1.38     |
| 3   | R     | 1709 | BCL  | CBD-CGD | -2.77 | 1.44        | 1.52     |
| 3   | K     | 1506 | BCL  | C1D-ND  | 2.77  | 1.41        | 1.37     |
| 3   | I     | 1705 | BCL  | MG-NA   | 2.75  | 2.12        | 2.06     |
| 3   | D     | 1602 | BCL  | O2D-CGD | 2.73  | 1.39        | 1.33     |
| 3   | A     | 1701 | BCL  | CBD-CGD | -2.73 | 1.44        | 1.52     |
| 5   | D     | 1402 | RG1  | C7-C6   | 2.73  | 1.51        | 1.43     |
| 3   | M     | 1507 | BCL  | C2A-C1A | -2.73 | 1.46        | 1.52     |
| 3   | L     | 1606 | BCL  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 3   | I     | 1505 | BCL  | O1D-CGD | 2.72  | 1.28        | 1.21     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | R     | 1509 | BCL  | C3B-CAB | 2.72  | 1.55        | 1.46     |
| 3   | C     | 1702 | BCL  | CHC-C1C | 2.72  | 1.44        | 1.37     |
| 3   | E     | 1703 | BCL  | CHB-C4A | 2.72  | 1.44        | 1.37     |
| 3   | K     | 1506 | BCL  | O1A-CGA | 2.70  | 1.30        | 1.22     |
| 3   | E     | 1503 | BCL  | O2A-CGA | 2.70  | 1.41        | 1.33     |
| 3   | G     | 1504 | BCL  | C3B-C4B | 2.69  | 1.46        | 1.41     |
| 3   | C     | 1502 | BCL  | O1A-CGA | 2.69  | 1.30        | 1.22     |
| 3   | B     | 1601 | BCL  | O2A-CGA | 2.69  | 1.41        | 1.33     |
| 5   | P     | 1408 | RG1  | C24-C25 | 2.69  | 1.51        | 1.43     |
| 3   | G     | 1704 | BCL  | O1A-CGA | 2.69  | 1.30        | 1.22     |
| 3   | O     | 1508 | BCL  | C3B-C2B | 2.69  | 1.51        | 1.42     |
| 3   | H     | 1604 | BCL  | O2D-CGD | 2.69  | 1.39        | 1.33     |
| 3   | M     | 1507 | BCL  | C3B-C2B | 2.68  | 1.51        | 1.42     |
| 3   | C     | 1702 | BCL  | CHC-C4B | 2.68  | 1.45        | 1.39     |
| 3   | O     | 1708 | BCL  | CHD-C4C | 2.67  | 1.46        | 1.39     |
| 5   | L     | 1406 | RG1  | C19-C18 | 2.67  | 1.51        | 1.46     |
| 3   | O     | 1508 | BCL  | O1D-CGD | 2.66  | 1.28        | 1.21     |
| 3   | D     | 1602 | BCL  | CHC-C1C | 2.66  | 1.44        | 1.37     |
| 3   | G     | 1504 | BCL  | C3B-C2B | 2.66  | 1.51        | 1.42     |
| 3   | I     | 1705 | BCL  | CBD-CGD | -2.66 | 1.44        | 1.52     |
| 3   | R     | 1709 | BCL  | C1B-NB  | 2.65  | 1.41        | 1.37     |
| 3   | C     | 1502 | BCL  | C2A-C1A | -2.65 | 1.46        | 1.52     |
| 3   | I     | 1705 | BCL  | OBB-CAB | 2.65  | 1.29        | 1.23     |
| 3   | I     | 1505 | BCL  | C2A-C1A | -2.65 | 1.46        | 1.52     |
| 3   | E     | 1703 | BCL  | OBB-CAB | 2.65  | 1.29        | 1.23     |
| 3   | P     | 1608 | BCL  | CHD-C1D | 2.65  | 1.43        | 1.38     |
| 3   | N     | 1607 | BCL  | MG-ND   | -2.64 | 2.00        | 2.05     |
| 3   | P     | 1608 | BCL  | O1A-CGA | 2.64  | 1.30        | 1.22     |
| 5   | R     | 1401 | RG1  | C8-C9   | 2.64  | 1.51        | 1.46     |
| 3   | R     | 1509 | BCL  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 3   | L     | 1606 | BCL  | CHB-C4A | 2.64  | 1.44        | 1.37     |
| 3   | F     | 1603 | BCL  | CMC-C2C | -2.64 | 1.47        | 1.53     |
| 3   | K     | 1706 | BCL  | C9-C8   | 2.64  | 1.61        | 1.52     |
| 3   | K     | 1506 | BCL  | MG-NB   | -2.64 | 2.00        | 2.05     |
| 3   | I     | 1505 | BCL  | CBD-CGD | -2.63 | 1.44        | 1.52     |
| 3   | K     | 1706 | BCL  | CHB-C4A | 2.63  | 1.44        | 1.37     |
| 3   | C     | 1502 | BCL  | O1D-CGD | 2.63  | 1.27        | 1.21     |
| 3   | H     | 1604 | BCL  | C2A-C1A | -2.62 | 1.46        | 1.52     |
| 3   | A     | 1501 | BCL  | CBD-CAD | -2.62 | 1.44        | 1.56     |
| 3   | K     | 1506 | BCL  | C3B-C2B | 2.62  | 1.51        | 1.42     |
| 3   | L     | 1606 | BCL  | C3B-C2B | 2.62  | 1.51        | 1.42     |
| 3   | H     | 1604 | BCL  | C2C-C1C | -2.61 | 1.43        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 1601 | BCL  | MG-NA   | 2.61  | 2.12        | 2.06     |
| 5   | N     | 1407 | RG1  | C27-C26 | 2.61  | 1.51        | 1.46     |
| 3   | K     | 1706 | BCL  | C1D-ND  | 2.61  | 1.41        | 1.37     |
| 3   | G     | 1504 | BCL  | MG-NB   | -2.60 | 2.00        | 2.05     |
| 3   | E     | 1703 | BCL  | MG-ND   | -2.59 | 2.00        | 2.05     |
| 3   | D     | 1602 | BCL  | CHD-C1D | 2.59  | 1.43        | 1.38     |
| 3   | R     | 1509 | BCL  | CHD-C1D | 2.58  | 1.43        | 1.38     |
| 3   | R     | 1709 | BCL  | C3C-C4C | -2.58 | 1.48        | 1.51     |
| 3   | A     | 1701 | BCL  | C5-C3   | 2.58  | 1.56        | 1.51     |
| 3   | H     | 1604 | BCL  | CHC-C1C | 2.57  | 1.44        | 1.37     |
| 3   | K     | 1506 | BCL  | CBD-CGD | -2.57 | 1.44        | 1.52     |
| 3   | S     | 1609 | BCL  | CHD-C1D | 2.57  | 1.43        | 1.38     |
| 3   | S     | 1609 | BCL  | CBB-CAB | -2.57 | 1.45        | 1.50     |
| 3   | J     | 1605 | BCL  | C3A-C2A | -2.56 | 1.47        | 1.54     |
| 3   | A     | 1501 | BCL  | O2A-CGA | 2.56  | 1.40        | 1.33     |
| 3   | G     | 1504 | BCL  | MG-ND   | -2.56 | 2.00        | 2.05     |
| 3   | M     | 1507 | BCL  | C2C-C3C | -2.56 | 1.47        | 1.54     |
| 3   | I     | 1705 | BCL  | C3D-CAD | 2.56  | 1.53        | 1.45     |
| 3   | I     | 1505 | BCL  | CHD-C1D | 2.56  | 1.43        | 1.38     |
| 5   | J     | 1405 | RG1  | C8-C9   | 2.55  | 1.51        | 1.46     |
| 3   | D     | 1602 | BCL  | OBB-CAB | 2.55  | 1.29        | 1.23     |
| 3   | O     | 1508 | BCL  | CHB-C1B | 2.55  | 1.45        | 1.39     |
| 3   | F     | 1603 | BCL  | O1A-CGA | 2.54  | 1.30        | 1.22     |
| 3   | E     | 1503 | BCL  | C3B-C2B | 2.54  | 1.51        | 1.42     |
| 5   | N     | 1407 | RG1  | C15-C14 | 2.54  | 1.51        | 1.43     |
| 3   | A     | 1701 | BCL  | MG-NC   | 2.54  | 2.12        | 2.06     |
| 3   | M     | 1707 | BCL  | C4D-CHA | 2.53  | 1.47        | 1.38     |
| 3   | I     | 1705 | BCL  | O1D-CGD | 2.52  | 1.27        | 1.21     |
| 3   | S     | 1609 | BCL  | O2D-CGD | 2.52  | 1.39        | 1.33     |
| 3   | P     | 1608 | BCL  | CBA-CGA | -2.52 | 1.43        | 1.50     |
| 3   | G     | 1704 | BCL  | C4B-NB  | 2.51  | 1.41        | 1.37     |
| 3   | L     | 1606 | BCL  | OBB-CAB | 2.51  | 1.28        | 1.23     |
| 3   | D     | 1602 | BCL  | C3C-C4C | -2.51 | 1.48        | 1.51     |
| 5   | H     | 1404 | RG1  | CM5-C13 | -2.51 | 1.45        | 1.50     |
| 3   | J     | 1605 | BCL  | CAA-C2A | -2.51 | 1.49        | 1.54     |
| 3   | J     | 1605 | BCL  | O2D-CED | -2.50 | 1.39        | 1.45     |
| 3   | M     | 1707 | BCL  | CHC-C4B | 2.50  | 1.45        | 1.39     |
| 5   | P     | 1408 | RG1  | CM7-C22 | -2.49 | 1.45        | 1.50     |
| 3   | M     | 1707 | BCL  | CHC-C1C | 2.49  | 1.43        | 1.37     |
| 3   | B     | 1601 | BCL  | CHC-C1C | 2.49  | 1.43        | 1.37     |
| 3   | K     | 1506 | BCL  | MG-NC   | 2.49  | 2.12        | 2.06     |
| 3   | P     | 1608 | BCL  | CHC-C1C | 2.48  | 1.43        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | K     | 1506 | BCL  | CHB-C1B | 2.48  | 1.45        | 1.39     |
| 3   | E     | 1703 | BCL  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 3   | A     | 1701 | BCL  | C1B-NB  | 2.48  | 1.41        | 1.37     |
| 3   | C     | 1702 | BCL  | C4D-CHA | 2.48  | 1.46        | 1.38     |
| 3   | A     | 1701 | BCL  | CHC-C1C | 2.48  | 1.43        | 1.37     |
| 3   | I     | 1705 | BCL  | CHB-C4A | 2.47  | 1.43        | 1.37     |
| 3   | H     | 1604 | BCL  | C1D-C2D | 2.47  | 1.50        | 1.45     |
| 3   | M     | 1707 | BCL  | C5-C3   | 2.47  | 1.56        | 1.51     |
| 3   | N     | 1607 | BCL  | C3C-C4C | -2.46 | 1.48        | 1.51     |
| 3   | I     | 1705 | BCL  | MG-NC   | 2.46  | 2.12        | 2.06     |
| 5   | D     | 1402 | RG1  | C28-C27 | -2.46 | 1.28        | 1.34     |
| 3   | K     | 1506 | BCL  | CBD-CAD | -2.46 | 1.45        | 1.56     |
| 3   | F     | 1603 | BCL  | O2D-CED | -2.45 | 1.39        | 1.45     |
| 3   | G     | 1704 | BCL  | CBD-CHA | -2.45 | 1.38        | 1.51     |
| 3   | B     | 1601 | BCL  | O1A-CGA | 2.44  | 1.29        | 1.22     |
| 3   | O     | 1508 | BCL  | C4D-CHA | 2.44  | 1.46        | 1.38     |
| 3   | D     | 1602 | BCL  | C3B-C2B | 2.44  | 1.50        | 1.42     |
| 3   | H     | 1604 | BCL  | O2A-CGA | 2.44  | 1.40        | 1.33     |
| 3   | K     | 1506 | BCL  | CHC-C1C | 2.43  | 1.43        | 1.37     |
| 3   | O     | 1708 | BCL  | C3B-CAB | 2.43  | 1.54        | 1.46     |
| 5   | R     | 1401 | RG1  | C11-C10 | 2.43  | 1.50        | 1.43     |
| 3   | N     | 1607 | BCL  | C1D-C2D | 2.42  | 1.50        | 1.45     |
| 3   | M     | 1507 | BCL  | C1D-ND  | 2.42  | 1.41        | 1.37     |
| 3   | I     | 1505 | BCL  | C4B-NB  | 2.42  | 1.41        | 1.37     |
| 3   | G     | 1704 | BCL  | OBB-CAB | 2.42  | 1.28        | 1.23     |
| 3   | O     | 1708 | BCL  | O1A-CGA | 2.41  | 1.29        | 1.22     |
| 3   | R     | 1709 | BCL  | C3B-C2B | 2.41  | 1.50        | 1.42     |
| 5   | P     | 1408 | RG1  | C28-C29 | 2.40  | 1.50        | 1.43     |
| 5   | D     | 1402 | RG1  | C8-C9   | 2.40  | 1.51        | 1.46     |
| 3   | C     | 1702 | BCL  | C3B-C2B | 2.40  | 1.50        | 1.42     |
| 3   | D     | 1602 | BCL  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 3   | K     | 1706 | BCL  | C4D-CHA | 2.38  | 1.46        | 1.38     |
| 3   | O     | 1708 | BCL  | C4B-NB  | 2.38  | 1.41        | 1.37     |
| 3   | S     | 1609 | BCL  | C2A-C1A | -2.38 | 1.46        | 1.52     |
| 4   | C     | 1815 | LDA  | C1-N1   | -2.37 | 1.49        | 1.51     |
| 3   | D     | 1602 | BCL  | C1D-ND  | 2.36  | 1.41        | 1.37     |
| 5   | S     | 1409 | RG1  | C12-C13 | 2.36  | 1.51        | 1.46     |
| 5   | P     | 1408 | RG1  | CM5-C13 | -2.36 | 1.46        | 1.50     |
| 3   | E     | 1503 | BCL  | CBB-CAB | -2.35 | 1.45        | 1.50     |
| 3   | C     | 1502 | BCL  | CAC-C3C | -2.35 | 1.49        | 1.54     |
| 3   | O     | 1708 | BCL  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 5   | D     | 1402 | RG1  | O5'-C1' | 2.35  | 1.47        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | P     | 1408 | RG1  | C19-C18 | 2.35  | 1.51        | 1.46     |
| 3   | E     | 1703 | BCL  | C3B-C2B | 2.35  | 1.50        | 1.42     |
| 3   | F     | 1603 | BCL  | C3C-C4C | -2.34 | 1.48        | 1.51     |
| 3   | C     | 1502 | BCL  | C1D-C2D | 2.34  | 1.50        | 1.45     |
| 3   | E     | 1503 | BCL  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 3   | B     | 1601 | BCL  | MG-NC   | 2.34  | 2.11        | 2.06     |
| 3   | B     | 1601 | BCL  | C3A-C2A | -2.33 | 1.48        | 1.54     |
| 3   | M     | 1507 | BCL  | C3B-CAB | 2.33  | 1.54        | 1.46     |
| 3   | O     | 1708 | BCL  | CMD-C2D | -2.32 | 1.46        | 1.50     |
| 3   | G     | 1504 | BCL  | CHD-C1D | 2.32  | 1.42        | 1.38     |
| 3   | K     | 1706 | BCL  | O2D-CGD | 2.32  | 1.38        | 1.33     |
| 3   | R     | 1709 | BCL  | O2A-CGA | 2.32  | 1.40        | 1.33     |
| 3   | F     | 1603 | BCL  | O1D-CGD | 2.31  | 1.27        | 1.21     |
| 3   | G     | 1504 | BCL  | C3B-CAB | 2.31  | 1.54        | 1.46     |
| 3   | H     | 1604 | BCL  | MG-NA   | 2.31  | 2.11        | 2.06     |
| 3   | F     | 1603 | BCL  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 3   | K     | 1506 | BCL  | C1D-C2D | 2.30  | 1.49        | 1.45     |
| 3   | H     | 1604 | BCL  | C4D-CHA | 2.30  | 1.46        | 1.38     |
| 3   | I     | 1505 | BCL  | CBD-CAD | -2.30 | 1.46        | 1.56     |
| 3   | B     | 1601 | BCL  | C4D-CHA | 2.30  | 1.46        | 1.38     |
| 3   | H     | 1604 | BCL  | OBD-CAD | 2.29  | 1.26        | 1.22     |
| 3   | K     | 1506 | BCL  | MG-NA   | 2.29  | 2.11        | 2.06     |
| 3   | O     | 1508 | BCL  | C3D-C2D | 2.29  | 1.45        | 1.39     |
| 3   | I     | 1705 | BCL  | C4B-NB  | 2.28  | 1.40        | 1.37     |
| 3   | C     | 1702 | BCL  | MG-NC   | 2.28  | 2.11        | 2.06     |
| 3   | K     | 1506 | BCL  | OBB-CAB | 2.27  | 1.28        | 1.23     |
| 4   | P     | 1808 | LDA  | C1-N1   | -2.27 | 1.49        | 1.51     |
| 3   | I     | 1705 | BCL  | CHD-C4C | 2.27  | 1.45        | 1.39     |
| 3   | G     | 1504 | BCL  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 3   | C     | 1502 | BCL  | O2D-CGD | 2.27  | 1.38        | 1.33     |
| 3   | A     | 1501 | BCL  | C1D-C2D | 2.27  | 1.49        | 1.45     |
| 5   | S     | 1409 | RG1  | O5'-C1' | 2.26  | 1.47        | 1.41     |
| 3   | C     | 1502 | BCL  | C3B-CAB | 2.26  | 1.53        | 1.46     |
| 3   | E     | 1703 | BCL  | O1A-CGA | 2.25  | 1.29        | 1.22     |
| 3   | S     | 1609 | BCL  | C4B-NB  | -2.24 | 1.34        | 1.37     |
| 3   | N     | 1607 | BCL  | CHC-C1C | 2.24  | 1.43        | 1.37     |
| 3   | K     | 1706 | BCL  | C4B-NB  | 2.24  | 1.40        | 1.37     |
| 4   | L     | 1806 | LDA  | C1-N1   | 2.24  | 1.53        | 1.51     |
| 3   | I     | 1705 | BCL  | CHC-C4B | 2.24  | 1.44        | 1.39     |
| 3   | R     | 1709 | BCL  | C3B-CAB | 2.24  | 1.53        | 1.46     |
| 3   | C     | 1702 | BCL  | O2A-CGA | 2.23  | 1.39        | 1.33     |
| 3   | I     | 1505 | BCL  | C4D-CHA | 2.23  | 1.46        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | G     | 1704 | BCL  | C3B-CAB | 2.21  | 1.53        | 1.46     |
| 3   | I     | 1705 | BCL  | CHC-C1C | 2.21  | 1.43        | 1.37     |
| 5   | S     | 1409 | RG1  | CM6-C18 | -2.20 | 1.46        | 1.50     |
| 3   | C     | 1702 | BCL  | OBD-CAD | 2.20  | 1.26        | 1.22     |
| 3   | G     | 1504 | BCL  | C4D-CHA | 2.20  | 1.46        | 1.38     |
| 3   | O     | 1708 | BCL  | CBD-CGD | -2.20 | 1.45        | 1.52     |
| 3   | J     | 1605 | BCL  | C1B-C2B | 2.20  | 1.48        | 1.43     |
| 3   | L     | 1606 | BCL  | O2D-CED | -2.19 | 1.40        | 1.45     |
| 3   | F     | 1603 | BCL  | C1B-C2B | 2.19  | 1.48        | 1.43     |
| 3   | C     | 1702 | BCL  | C3C-C4C | -2.19 | 1.48        | 1.51     |
| 3   | M     | 1707 | BCL  | C1B-NB  | 2.19  | 1.40        | 1.37     |
| 3   | C     | 1702 | BCL  | CHD-C4C | 2.19  | 1.45        | 1.39     |
| 3   | C     | 1702 | BCL  | C2A-C1A | -2.17 | 1.47        | 1.52     |
| 3   | H     | 1604 | BCL  | C1B-C2B | 2.17  | 1.48        | 1.43     |
| 3   | I     | 1505 | BCL  | C3B-CAB | 2.17  | 1.53        | 1.46     |
| 3   | R     | 1709 | BCL  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 3   | I     | 1705 | BCL  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 3   | O     | 1708 | BCL  | OBD-CAD | 2.16  | 1.26        | 1.22     |
| 3   | R     | 1509 | BCL  | CBB-CAB | -2.16 | 1.46        | 1.50     |
| 3   | A     | 1701 | BCL  | C1B-C2B | 2.16  | 1.48        | 1.43     |
| 3   | R     | 1709 | BCL  | OBD-CAD | 2.16  | 1.26        | 1.22     |
| 3   | O     | 1508 | BCL  | CBD-CAD | -2.16 | 1.46        | 1.56     |
| 3   | G     | 1704 | BCL  | CMC-C2C | 2.16  | 1.57        | 1.53     |
| 3   | J     | 1605 | BCL  | CBD-CAD | -2.15 | 1.46        | 1.56     |
| 3   | R     | 1509 | BCL  | CAA-CBA | -2.15 | 1.46        | 1.52     |
| 5   | J     | 1405 | RG1  | C12-C13 | 2.14  | 1.50        | 1.46     |
| 5   | J     | 1405 | RG1  | C11-C10 | 2.14  | 1.49        | 1.43     |
| 5   | J     | 1405 | RG1  | C15-C14 | 2.14  | 1.49        | 1.43     |
| 3   | D     | 1602 | BCL  | CHC-C4B | 2.13  | 1.44        | 1.39     |
| 3   | F     | 1603 | BCL  | CHC-C1C | 2.13  | 1.43        | 1.37     |
| 3   | B     | 1601 | BCL  | CHB-C4A | 2.13  | 1.43        | 1.37     |
| 3   | R     | 1709 | BCL  | C1-C2   | 2.13  | 1.55        | 1.49     |
| 3   | J     | 1605 | BCL  | C3B-C2B | 2.11  | 1.49        | 1.42     |
| 5   | L     | 1406 | RG1  | O2'-C2' | 2.11  | 1.48        | 1.43     |
| 3   | E     | 1703 | BCL  | CHB-C1B | 2.11  | 1.44        | 1.39     |
| 3   | I     | 1705 | BCL  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 3   | C     | 1702 | BCL  | C5-C3   | 2.11  | 1.55        | 1.51     |
| 5   | P     | 1408 | RG1  | O5'-C1' | 2.11  | 1.47        | 1.41     |
| 5   | L     | 1406 | RG1  | C20-C21 | 2.11  | 1.49        | 1.43     |
| 5   | H     | 1404 | RG1  | C11-C10 | 2.11  | 1.49        | 1.43     |
| 3   | J     | 1605 | BCL  | C1A-CHA | 2.10  | 1.51        | 1.43     |
| 3   | H     | 1604 | BCL  | C5-C3   | 2.10  | 1.55        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | F     | 1603 | BCL  | C3B-C2B | 2.10  | 1.49        | 1.42     |
| 5   | P     | 1408 | RG1  | C11-C10 | 2.09  | 1.49        | 1.43     |
| 3   | O     | 1508 | BCL  | C3B-C4B | 2.09  | 1.45        | 1.41     |
| 3   | R     | 1709 | BCL  | C4B-NB  | 2.08  | 1.40        | 1.37     |
| 3   | I     | 1705 | BCL  | MG-ND   | 2.08  | 2.09        | 2.05     |
| 3   | J     | 1605 | BCL  | C4B-NB  | -2.08 | 1.35        | 1.37     |
| 3   | P     | 1608 | BCL  | C3C-C4C | -2.08 | 1.49        | 1.51     |
| 3   | L     | 1606 | BCL  | CAC-C3C | -2.07 | 1.50        | 1.54     |
| 3   | B     | 1601 | BCL  | C3B-C2B | 2.07  | 1.49        | 1.42     |
| 3   | L     | 1606 | BCL  | C1D-C2D | 2.07  | 1.49        | 1.45     |
| 3   | G     | 1704 | BCL  | C1A-CHA | 2.07  | 1.51        | 1.43     |
| 3   | K     | 1706 | BCL  | CHD-C4C | 2.07  | 1.45        | 1.39     |
| 3   | E     | 1703 | BCL  | CHD-C1D | 2.07  | 1.42        | 1.38     |
| 3   | O     | 1508 | BCL  | C1B-C2B | 2.06  | 1.48        | 1.43     |
| 3   | L     | 1606 | BCL  | MG-NA   | 2.06  | 2.11        | 2.06     |
| 3   | N     | 1607 | BCL  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 3   | H     | 1604 | BCL  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 3   | M     | 1707 | BCL  | O1D-CGD | 2.06  | 1.26        | 1.21     |
| 3   | E     | 1503 | BCL  | C1D-ND  | 2.06  | 1.40        | 1.37     |
| 3   | O     | 1708 | BCL  | C3B-C2B | 2.05  | 1.49        | 1.42     |
| 3   | S     | 1609 | BCL  | C3B-CAB | 2.05  | 1.53        | 1.46     |
| 3   | C     | 1702 | BCL  | MG-NA   | 2.04  | 2.11        | 2.06     |
| 3   | E     | 1703 | BCL  | C4D-CHA | 2.04  | 1.45        | 1.38     |
| 3   | M     | 1507 | BCL  | CHC-C4B | 2.04  | 1.44        | 1.39     |
| 3   | M     | 1507 | BCL  | MG-NA   | 2.03  | 2.11        | 2.06     |
| 5   | H     | 1404 | RG1  | C7-C6   | 2.03  | 1.49        | 1.43     |
| 3   | E     | 1503 | BCL  | O2D-CGD | 2.02  | 1.38        | 1.33     |
| 3   | G     | 1504 | BCL  | C1B-C2B | 2.02  | 1.47        | 1.43     |
| 3   | J     | 1605 | BCL  | CHC-C1C | 2.01  | 1.42        | 1.37     |
| 3   | E     | 1503 | BCL  | C2A-C1A | -2.01 | 1.47        | 1.52     |
| 5   | H     | 1404 | RG1  | C4-C5   | 2.01  | 1.55        | 1.51     |
| 3   | P     | 1608 | BCL  | C1D-C2D | 2.01  | 1.49        | 1.45     |
| 5   | S     | 1409 | RG1  | C19-C18 | 2.00  | 1.50        | 1.46     |

All (787) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 3   | L     | 1606 | BCL  | C4A-NA-C1A | -14.45 | 100.09      | 106.68   |
| 3   | B     | 1601 | BCL  | C4A-NA-C1A | -13.44 | 100.55      | 106.68   |
| 3   | R     | 1509 | BCL  | C4A-NA-C1A | -12.21 | 101.11      | 106.68   |
| 3   | M     | 1507 | BCL  | C4A-NA-C1A | -11.78 | 101.30      | 106.68   |
| 3   | D     | 1602 | BCL  | C4A-NA-C1A | -11.64 | 101.37      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 3   | J     | 1605 | BCL  | C4A-NA-C1A | -10.51 | 101.89      | 106.68   |
| 3   | E     | 1503 | BCL  | C4A-NA-C1A | -10.47 | 101.90      | 106.68   |
| 3   | N     | 1607 | BCL  | C4A-NA-C1A | -10.09 | 102.08      | 106.68   |
| 3   | F     | 1603 | BCL  | C4A-NA-C1A | -9.82  | 102.20      | 106.68   |
| 3   | C     | 1502 | BCL  | C4A-NA-C1A | -9.45  | 102.37      | 106.68   |
| 3   | J     | 1605 | BCL  | C1C-NC-C4C | -9.28  | 102.44      | 106.68   |
| 3   | A     | 1701 | BCL  | C4A-NA-C1A | -9.22  | 102.47      | 106.68   |
| 3   | K     | 1506 | BCL  | C4A-NA-C1A | -9.17  | 102.50      | 106.68   |
| 3   | P     | 1608 | BCL  | C1C-NC-C4C | -9.07  | 102.54      | 106.68   |
| 3   | A     | 1501 | BCL  | C4A-NA-C1A | -8.93  | 102.61      | 106.68   |
| 3   | L     | 1606 | BCL  | C1C-NC-C4C | -8.86  | 102.64      | 106.68   |
| 3   | S     | 1609 | BCL  | C4A-NA-C1A | -8.85  | 102.64      | 106.68   |
| 3   | K     | 1706 | BCL  | C4A-NA-C1A | -8.74  | 102.69      | 106.68   |
| 3   | I     | 1505 | BCL  | C4A-NA-C1A | -8.72  | 102.70      | 106.68   |
| 3   | S     | 1609 | BCL  | C1C-NC-C4C | -8.48  | 102.81      | 106.68   |
| 3   | O     | 1508 | BCL  | C4A-NA-C1A | -8.36  | 102.86      | 106.68   |
| 3   | C     | 1702 | BCL  | C4A-NA-C1A | -8.34  | 102.87      | 106.68   |
| 3   | G     | 1704 | BCL  | C1-C2-C3   | -8.19  | 112.78      | 126.20   |
| 3   | G     | 1504 | BCL  | C4A-NA-C1A | -8.15  | 102.96      | 106.68   |
| 3   | P     | 1608 | BCL  | C4A-NA-C1A | -8.11  | 102.98      | 106.68   |
| 3   | O     | 1708 | BCL  | C4A-NA-C1A | -7.99  | 103.04      | 106.68   |
| 3   | K     | 1706 | BCL  | C1-C2-C3   | -7.87  | 113.31      | 126.20   |
| 3   | R     | 1709 | BCL  | C4A-NA-C1A | -7.84  | 103.10      | 106.68   |
| 3   | M     | 1707 | BCL  | C1-C2-C3   | -7.70  | 113.58      | 126.20   |
| 3   | H     | 1604 | BCL  | C4A-NA-C1A | -7.63  | 103.20      | 106.68   |
| 3   | K     | 1506 | BCL  | C1-C2-C3   | -7.63  | 113.69      | 126.20   |
| 3   | I     | 1705 | BCL  | C1-C2-C3   | -7.60  | 113.75      | 126.20   |
| 3   | I     | 1705 | BCL  | C4A-NA-C1A | -7.58  | 103.22      | 106.68   |
| 3   | A     | 1701 | BCL  | C1-C2-C3   | -7.32  | 114.20      | 126.20   |
| 3   | O     | 1708 | BCL  | C1-C2-C3   | -7.14  | 114.49      | 126.20   |
| 3   | B     | 1601 | BCL  | C1C-NC-C4C | -7.08  | 103.45      | 106.68   |
| 3   | N     | 1607 | BCL  | C1C-NC-C4C | -6.93  | 103.52      | 106.68   |
| 3   | E     | 1703 | BCL  | C1-C2-C3   | -6.86  | 114.96      | 126.20   |
| 3   | I     | 1505 | BCL  | C1-C2-C3   | -6.86  | 114.97      | 126.20   |
| 3   | R     | 1709 | BCL  | C1-C2-C3   | -6.78  | 115.09      | 126.20   |
| 3   | M     | 1507 | BCL  | C1C-NC-C4C | -6.71  | 103.62      | 106.68   |
| 3   | C     | 1702 | BCL  | C1-C2-C3   | -6.64  | 115.32      | 126.20   |
| 3   | A     | 1501 | BCL  | C1-C2-C3   | -6.62  | 115.36      | 126.20   |
| 3   | H     | 1604 | BCL  | C1C-NC-C4C | -6.55  | 103.69      | 106.68   |
| 3   | D     | 1602 | BCL  | C1-C2-C3   | -6.50  | 115.54      | 126.20   |
| 3   | G     | 1704 | BCL  | C4A-NA-C1A | -6.43  | 103.75      | 106.68   |
| 3   | E     | 1703 | BCL  | C4A-NA-C1A | -6.39  | 103.76      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | N     | 1607 | BCL  | C1-C2-C3    | -6.26 | 115.93      | 126.20   |
| 3   | R     | 1509 | BCL  | C1-C2-C3    | -6.15 | 116.12      | 126.20   |
| 3   | E     | 1503 | BCL  | C1-C2-C3    | -5.99 | 116.38      | 126.20   |
| 3   | G     | 1504 | BCL  | C1-C2-C3    | -5.98 | 116.40      | 126.20   |
| 3   | A     | 1501 | BCL  | C1C-NC-C4C  | -5.95 | 103.97      | 106.68   |
| 5   | H     | 1404 | RG1  | C16-C17-C18 | -5.81 | 119.14      | 127.28   |
| 3   | L     | 1606 | BCL  | C1-C2-C3    | -5.77 | 116.75      | 126.20   |
| 5   | J     | 1405 | RG1  | C16-C17-C18 | -5.72 | 119.25      | 127.28   |
| 3   | K     | 1706 | BCL  | C1C-NC-C4C  | -5.69 | 104.08      | 106.68   |
| 3   | P     | 1608 | BCL  | C1-C2-C3    | -5.69 | 116.87      | 126.20   |
| 5   | R     | 1401 | RG1  | C16-C17-C18 | -5.64 | 119.38      | 127.28   |
| 3   | C     | 1502 | BCL  | C1-C2-C3    | -5.62 | 117.00      | 126.20   |
| 3   | E     | 1503 | BCL  | C1C-NC-C4C  | -5.58 | 104.13      | 106.68   |
| 3   | K     | 1506 | BCL  | C1C-NC-C4C  | -5.53 | 104.15      | 106.68   |
| 5   | D     | 1402 | RG1  | C16-C17-C18 | -5.53 | 119.52      | 127.28   |
| 3   | B     | 1601 | BCL  | C1-C2-C3    | -5.40 | 117.36      | 126.20   |
| 3   | M     | 1707 | BCL  | C4A-NA-C1A  | -5.38 | 104.22      | 106.68   |
| 3   | K     | 1506 | BCL  | C2C-C3C-C4C | 5.38  | 109.40      | 101.34   |
| 3   | F     | 1603 | BCL  | C1-C2-C3    | -5.32 | 117.47      | 126.20   |
| 3   | H     | 1604 | BCL  | C1-C2-C3    | -5.31 | 117.49      | 126.20   |
| 3   | A     | 1701 | BCL  | C1C-NC-C4C  | -5.24 | 104.29      | 106.68   |
| 3   | J     | 1605 | BCL  | C1-C2-C3    | -5.23 | 117.63      | 126.20   |
| 3   | F     | 1603 | BCL  | CHB-C1B-NB  | 5.22  | 131.87      | 124.05   |
| 3   | N     | 1607 | BCL  | CHB-C1B-NB  | 5.21  | 131.87      | 124.05   |
| 3   | M     | 1507 | BCL  | C1-C2-C3    | -5.17 | 117.73      | 126.20   |
| 3   | B     | 1601 | BCL  | CHB-C1B-NB  | 5.16  | 131.79      | 124.05   |
| 3   | A     | 1701 | BCL  | CHB-C1B-NB  | 5.09  | 131.68      | 124.05   |
| 5   | N     | 1407 | RG1  | C16-C17-C18 | -5.09 | 120.14      | 127.28   |
| 3   | R     | 1509 | BCL  | O2D-CGD-CBD | 5.08  | 120.12      | 111.23   |
| 3   | S     | 1609 | BCL  | CHB-C1B-NB  | 5.07  | 131.66      | 124.05   |
| 3   | M     | 1507 | BCL  | CHB-C1B-NB  | 5.07  | 131.66      | 124.05   |
| 3   | R     | 1709 | BCL  | O2D-CGD-CBD | 5.06  | 120.08      | 111.23   |
| 3   | A     | 1501 | BCL  | CHB-C1B-NB  | 5.02  | 131.58      | 124.05   |
| 3   | O     | 1508 | BCL  | C1-C2-C3    | -5.02 | 117.97      | 126.20   |
| 3   | D     | 1602 | BCL  | CHB-C1B-NB  | 5.02  | 131.57      | 124.05   |
| 3   | J     | 1605 | BCL  | CHB-C1B-NB  | 4.98  | 131.52      | 124.05   |
| 3   | L     | 1606 | BCL  | CHB-C1B-NB  | 4.97  | 131.50      | 124.05   |
| 3   | G     | 1704 | BCL  | C3D-C2D-C1D | -4.95 | 99.07       | 105.83   |
| 3   | G     | 1704 | BCL  | C1C-NC-C4C  | -4.93 | 104.43      | 106.68   |
| 3   | O     | 1508 | BCL  | C1C-NC-C4C  | -4.92 | 104.44      | 106.68   |
| 3   | D     | 1602 | BCL  | C1C-NC-C4C  | -4.89 | 104.45      | 106.68   |
| 3   | R     | 1709 | BCL  | CHB-C1B-NB  | 4.83  | 131.30      | 124.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | I     | 1705 | BCL  | OBB-CAB-C3B | -4.83 | 111.90      | 120.43   |
| 3   | G     | 1504 | BCL  | CHB-C1B-NB  | 4.83  | 131.29      | 124.05   |
| 3   | O     | 1508 | BCL  | OBB-CAB-C3B | -4.82 | 111.91      | 120.43   |
| 3   | I     | 1705 | BCL  | CHB-C1B-NB  | 4.82  | 131.28      | 124.05   |
| 5   | P     | 1408 | RG1  | C16-C17-C18 | -4.80 | 120.54      | 127.28   |
| 3   | E     | 1703 | BCL  | C1C-NC-C4C  | -4.79 | 104.49      | 106.68   |
| 3   | E     | 1703 | BCL  | CHB-C1B-NB  | 4.77  | 131.21      | 124.05   |
| 5   | S     | 1409 | RG1  | C16-C17-C18 | -4.71 | 120.67      | 127.28   |
| 3   | O     | 1708 | BCL  | CHB-C1B-NB  | 4.69  | 131.09      | 124.05   |
| 5   | R     | 1401 | RG1  | C7-C6-C5    | -4.69 | 121.10      | 127.69   |
| 3   | O     | 1508 | BCL  | C3D-C2D-C1D | -4.67 | 99.45       | 105.83   |
| 3   | O     | 1508 | BCL  | CHB-C1B-NB  | 4.67  | 131.06      | 124.05   |
| 3   | C     | 1502 | BCL  | C6-C5-C3    | -4.67 | 102.09      | 113.47   |
| 3   | L     | 1606 | BCL  | O2D-CGD-O1D | -4.66 | 114.78      | 123.85   |
| 3   | H     | 1604 | BCL  | CHB-C1B-NB  | 4.65  | 131.03      | 124.05   |
| 3   | K     | 1706 | BCL  | CHB-C1B-NB  | 4.64  | 131.02      | 124.05   |
| 3   | C     | 1502 | BCL  | C1C-NC-C4C  | -4.64 | 104.56      | 106.68   |
| 3   | C     | 1502 | BCL  | OBB-CAB-C3B | -4.63 | 112.24      | 120.43   |
| 3   | L     | 1606 | BCL  | OBB-CAB-C3B | -4.62 | 112.26      | 120.43   |
| 5   | D     | 1402 | RG1  | C7-C6-C5    | -4.60 | 121.23      | 127.69   |
| 3   | I     | 1705 | BCL  | C1C-NC-C4C  | -4.59 | 104.59      | 106.68   |
| 3   | E     | 1503 | BCL  | C3D-C2D-C1D | -4.57 | 99.59       | 105.83   |
| 3   | A     | 1701 | BCL  | OBB-CAB-C3B | -4.57 | 112.35      | 120.43   |
| 3   | F     | 1603 | BCL  | C3D-C2D-C1D | -4.57 | 99.60       | 105.83   |
| 3   | C     | 1702 | BCL  | CHB-C1B-NB  | 4.56  | 130.89      | 124.05   |
| 3   | P     | 1608 | BCL  | CHB-C1B-NB  | 4.55  | 130.88      | 124.05   |
| 5   | R     | 1401 | RG1  | C28-C29-C30 | -4.54 | 120.54      | 127.48   |
| 3   | J     | 1605 | BCL  | OBB-CAB-C3B | -4.53 | 112.42      | 120.43   |
| 3   | A     | 1501 | BCL  | O2D-CGD-CBD | 4.52  | 119.14      | 111.23   |
| 3   | G     | 1704 | BCL  | CHB-C1B-NB  | 4.52  | 130.82      | 124.05   |
| 3   | O     | 1708 | BCL  | OBB-CAB-C3B | -4.51 | 112.47      | 120.43   |
| 3   | C     | 1502 | BCL  | C3D-C2D-C1D | -4.50 | 99.68       | 105.83   |
| 3   | E     | 1503 | BCL  | CHB-C1B-NB  | 4.49  | 130.78      | 124.05   |
| 5   | F     | 1403 | RG1  | C11-C10-C9  | -4.48 | 120.99      | 127.28   |
| 3   | M     | 1507 | BCL  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 3   | S     | 1609 | BCL  | C3D-C2D-C1D | -4.48 | 99.72       | 105.83   |
| 3   | O     | 1708 | BCL  | O2A-CGA-O1A | -4.47 | 112.44      | 123.63   |
| 3   | C     | 1702 | BCL  | OBB-CAB-C3B | -4.43 | 112.60      | 120.43   |
| 3   | M     | 1707 | BCL  | C3D-C2D-C1D | -4.42 | 99.80       | 105.83   |
| 3   | G     | 1504 | BCL  | C1C-NC-C4C  | -4.42 | 104.66      | 106.68   |
| 3   | L     | 1606 | BCL  | C3D-C2D-C1D | -4.40 | 99.83       | 105.83   |
| 3   | M     | 1707 | BCL  | C1C-NC-C4C  | -4.34 | 104.70      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms        | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------------|-------|-------------|----------|
| 3   | C     | 1502 | BCL  | CHB-C1B-NB   | 4.33  | 130.55      | 124.05   |
| 3   | M     | 1707 | BCL  | CHB-C1B-NB   | 4.33  | 130.54      | 124.05   |
| 3   | S     | 1609 | BCL  | C1-C2-C3     | -4.32 | 119.12      | 126.20   |
| 3   | H     | 1604 | BCL  | C3D-C2D-C1D  | -4.32 | 99.93       | 105.83   |
| 3   | B     | 1601 | BCL  | C3D-C2D-C1D  | -4.32 | 99.94       | 105.83   |
| 3   | N     | 1607 | BCL  | O2D-CGD-CBD  | 4.31  | 118.76      | 111.23   |
| 3   | B     | 1601 | BCL  | OB B-CAB-C3B | -4.31 | 112.82      | 120.43   |
| 3   | R     | 1509 | BCL  | C3A-C2A-C1A  | -4.29 | 94.91       | 101.34   |
| 5   | N     | 1407 | RG1  | C7-C6-C5     | -4.28 | 121.67      | 127.69   |
| 3   | S     | 1609 | BCL  | O2D-CGD-CBD  | 4.28  | 118.70      | 111.23   |
| 3   | K     | 1506 | BCL  | C3D-C2D-C1D  | -4.27 | 100.01      | 105.83   |
| 3   | N     | 1607 | BCL  | C3D-C2D-C1D  | -4.23 | 100.05      | 105.83   |
| 5   | S     | 1409 | RG1  | C7-C6-C5     | -4.22 | 121.75      | 127.69   |
| 3   | A     | 1501 | BCL  | OB B-CAB-C3B | -4.21 | 113.00      | 120.43   |
| 3   | M     | 1707 | BCL  | OB B-CAB-C3B | -4.20 | 113.00      | 120.43   |
| 3   | R     | 1709 | BCL  | C3D-C2D-C1D  | -4.20 | 100.09      | 105.83   |
| 3   | N     | 1607 | BCL  | OB B-CAB-C3B | -4.17 | 113.05      | 120.43   |
| 3   | G     | 1504 | BCL  | O2A-CGA-O1A  | -4.17 | 113.20      | 123.63   |
| 3   | B     | 1601 | BCL  | O2D-CGD-CBD  | 4.17  | 118.52      | 111.23   |
| 5   | F     | 1403 | RG1  | C16-C17-C18  | -4.13 | 121.49      | 127.28   |
| 3   | C     | 1702 | BCL  | C3D-C2D-C1D  | -4.09 | 100.25      | 105.83   |
| 3   | L     | 1606 | BCL  | O2D-CGD-CBD  | 4.09  | 118.37      | 111.23   |
| 3   | O     | 1508 | BCL  | O2D-CGD-CBD  | 4.07  | 118.35      | 111.23   |
| 3   | D     | 1602 | BCL  | OB B-CAB-C3B | -4.05 | 113.27      | 120.43   |
| 3   | S     | 1609 | BCL  | OB B-CAB-C3B | -4.04 | 113.29      | 120.43   |
| 3   | M     | 1707 | BCL  | O2A-CGA-O1A  | -4.04 | 113.53      | 123.63   |
| 3   | K     | 1706 | BCL  | O2A-CGA-O1A  | -4.03 | 113.55      | 123.63   |
| 3   | K     | 1706 | BCL  | O2D-CGD-CBD  | 4.02  | 118.26      | 111.23   |
| 3   | G     | 1504 | BCL  | C3D-C2D-C1D  | -4.02 | 100.34      | 105.83   |
| 5   | L     | 1406 | RG1  | C7-C6-C5     | -4.02 | 122.04      | 127.69   |
| 3   | R     | 1509 | BCL  | CHB-C1B-NB   | 4.02  | 130.07      | 124.05   |
| 3   | I     | 1505 | BCL  | CHB-C1B-NB   | 4.01  | 130.07      | 124.05   |
| 3   | H     | 1604 | BCL  | O2D-CGD-CBD  | 4.01  | 118.25      | 111.23   |
| 3   | J     | 1605 | BCL  | C3D-C2D-C1D  | -4.00 | 100.38      | 105.83   |
| 3   | R     | 1509 | BCL  | C3D-C2D-C1D  | -3.98 | 100.40      | 105.83   |
| 5   | L     | 1406 | RG1  | C11-C10-C9   | -3.97 | 121.70      | 127.28   |
| 3   | D     | 1602 | BCL  | C3D-C2D-C1D  | -3.97 | 100.41      | 105.83   |
| 5   | R     | 1401 | RG1  | C16-C15-C14  | -3.95 | 115.45      | 123.52   |
| 5   | P     | 1408 | RG1  | C7-C6-C5     | -3.94 | 122.14      | 127.69   |
| 3   | C     | 1502 | BCL  | O2D-CGD-CBD  | 3.94  | 118.12      | 111.23   |
| 3   | I     | 1705 | BCL  | O2A-CGA-O1A  | -3.93 | 113.79      | 123.63   |
| 3   | I     | 1505 | BCL  | C3D-C2D-C1D  | -3.93 | 100.47      | 105.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | P     | 1608 | BCL  | C3D-C2D-C1D | -3.93 | 100.47      | 105.83   |
| 3   | I     | 1505 | BCL  | OBB-CAB-C3B | -3.92 | 113.50      | 120.43   |
| 3   | N     | 1607 | BCL  | O2A-CGA-O1A | -3.92 | 113.82      | 123.63   |
| 3   | G     | 1704 | BCL  | OBB-CAB-C3B | -3.92 | 113.51      | 120.43   |
| 3   | J     | 1605 | BCL  | CBA-CAA-C2A | -3.90 | 102.19      | 113.79   |
| 3   | K     | 1706 | BCL  | OBB-CAB-C3B | -3.89 | 113.55      | 120.43   |
| 5   | N     | 1407 | RG1  | C1-O1'-C1'  | -3.89 | 111.82      | 119.78   |
| 3   | G     | 1704 | BCL  | O2A-CGA-O1A | -3.89 | 113.90      | 123.63   |
| 3   | E     | 1703 | BCL  | O2A-CGA-O1A | -3.89 | 113.91      | 123.63   |
| 3   | C     | 1502 | BCL  | O2A-CGA-O1A | -3.89 | 113.91      | 123.63   |
| 3   | P     | 1608 | BCL  | CMC-C2C-C1C | 3.87  | 122.17      | 111.77   |
| 3   | K     | 1506 | BCL  | CHB-C1B-NB  | 3.85  | 129.82      | 124.05   |
| 3   | M     | 1507 | BCL  | O2A-CGA-O1A | -3.83 | 114.05      | 123.63   |
| 3   | R     | 1509 | BCL  | O2A-CGA-O1A | -3.82 | 114.08      | 123.63   |
| 3   | M     | 1507 | BCL  | OBB-CAB-C3B | -3.81 | 113.69      | 120.43   |
| 3   | F     | 1603 | BCL  | O2D-CGD-CBD | 3.80  | 117.87      | 111.23   |
| 3   | R     | 1709 | BCL  | OBB-CAB-C3B | -3.79 | 113.72      | 120.43   |
| 3   | R     | 1709 | BCL  | O2A-CGA-O1A | -3.78 | 114.16      | 123.63   |
| 3   | J     | 1605 | BCL  | O2D-CGD-CBD | 3.78  | 117.84      | 111.23   |
| 3   | F     | 1603 | BCL  | C1C-NC-C4C  | -3.77 | 104.96      | 106.68   |
| 3   | A     | 1701 | BCL  | O2A-CGA-O1A | -3.77 | 114.19      | 123.63   |
| 3   | O     | 1508 | BCL  | O2A-CGA-O1A | -3.77 | 114.19      | 123.63   |
| 3   | I     | 1705 | BCL  | O2D-CGD-CBD | 3.77  | 117.82      | 111.23   |
| 5   | S     | 1409 | RG1  | CM7-C22-C23 | 3.77  | 123.84      | 118.09   |
| 3   | K     | 1706 | BCL  | C3D-C2D-C1D | -3.76 | 100.70      | 105.83   |
| 3   | E     | 1503 | BCL  | O2D-CGD-CBD | 3.75  | 117.79      | 111.23   |
| 5   | P     | 1408 | RG1  | C24-C25-C26 | -3.75 | 122.02      | 127.28   |
| 5   | H     | 1404 | RG1  | C7-C6-C5    | -3.74 | 122.43      | 127.69   |
| 3   | A     | 1701 | BCL  | C3D-C2D-C1D | -3.73 | 100.74      | 105.83   |
| 3   | E     | 1503 | BCL  | O2A-CGA-O1A | -3.72 | 114.32      | 123.63   |
| 5   | L     | 1406 | RG1  | C16-C15-C14 | -3.72 | 115.90      | 123.52   |
| 3   | A     | 1501 | BCL  | C3D-C2D-C1D | -3.71 | 100.77      | 105.83   |
| 3   | P     | 1608 | BCL  | OBB-CAB-C3B | -3.71 | 113.88      | 120.43   |
| 3   | E     | 1703 | BCL  | C3D-C2D-C1D | -3.71 | 100.77      | 105.83   |
| 3   | F     | 1603 | BCL  | C6-C5-C3    | -3.70 | 104.46      | 113.47   |
| 3   | G     | 1704 | BCL  | C6-C5-C3    | -3.69 | 104.48      | 113.47   |
| 3   | F     | 1603 | BCL  | OBB-CAB-C3B | -3.68 | 113.92      | 120.43   |
| 3   | B     | 1601 | BCL  | O2A-CGA-O1A | -3.68 | 114.44      | 123.63   |
| 5   | P     | 1408 | RG1  | C16-C15-C14 | -3.66 | 116.03      | 123.52   |
| 3   | H     | 1604 | BCL  | CMC-C2C-C1C | 3.65  | 121.59      | 111.77   |
| 3   | G     | 1704 | BCL  | C4D-C3D-CAD | -3.62 | 104.17      | 108.11   |
| 3   | M     | 1507 | BCL  | O2D-CGD-CBD | 3.62  | 117.56      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | H     | 1604 | BCL  | C3C-C2C-C1C | 3.61  | 107.70      | 101.87   |
| 3   | H     | 1604 | BCL  | OBB-CAB-C3B | -3.61 | 114.06      | 120.43   |
| 3   | F     | 1603 | BCL  | O2A-CGA-O1A | -3.60 | 114.61      | 123.63   |
| 3   | E     | 1503 | BCL  | OBB-CAB-C3B | -3.60 | 114.06      | 120.43   |
| 5   | L     | 1406 | RG1  | C1-O1'-C1'  | -3.60 | 112.41      | 119.78   |
| 3   | O     | 1508 | BCL  | O2D-CGD-O1D | -3.60 | 116.84      | 123.85   |
| 3   | I     | 1705 | BCL  | C4-C3-C5    | 3.60  | 121.47      | 115.23   |
| 3   | G     | 1504 | BCL  | C6-C5-C3    | -3.60 | 104.71      | 113.47   |
| 3   | I     | 1505 | BCL  | O2A-CGA-O1A | -3.59 | 114.64      | 123.63   |
| 3   | G     | 1704 | BCL  | O2D-CGD-CBD | 3.59  | 117.51      | 111.23   |
| 3   | A     | 1501 | BCL  | CHB-C1B-C2B | -3.58 | 117.02      | 127.43   |
| 3   | C     | 1702 | BCL  | O2A-CGA-O1A | -3.58 | 114.67      | 123.63   |
| 3   | A     | 1701 | BCL  | CHB-C1B-C2B | -3.57 | 117.08      | 127.43   |
| 5   | H     | 1404 | RG1  | CM3-C5-C4   | 3.56  | 121.40      | 115.23   |
| 3   | L     | 1606 | BCL  | C2A-C3A-C4A | 3.55  | 107.60      | 101.87   |
| 3   | H     | 1604 | BCL  | CBA-CAA-C2A | -3.55 | 103.24      | 113.79   |
| 5   | J     | 1405 | RG1  | C1-O1'-C1'  | -3.54 | 112.53      | 119.78   |
| 3   | F     | 1603 | BCL  | CHB-C1B-C2B | -3.52 | 117.20      | 127.43   |
| 3   | P     | 1608 | BCL  | CBA-CAA-C2A | -3.52 | 103.31      | 113.79   |
| 3   | L     | 1606 | BCL  | C3C-C2C-C1C | 3.52  | 107.55      | 101.87   |
| 3   | S     | 1609 | BCL  | C14-C13-C12 | 3.51  | 123.79      | 111.27   |
| 3   | E     | 1703 | BCL  | CHB-C1B-C2B | -3.50 | 117.26      | 127.43   |
| 3   | C     | 1502 | BCL  | O2D-CGD-O1D | -3.50 | 117.03      | 123.85   |
| 5   | P     | 1408 | RG1  | C11-C10-C9  | -3.50 | 122.38      | 127.28   |
| 5   | J     | 1405 | RG1  | C20-C21-C22 | -3.49 | 122.38      | 127.28   |
| 3   | K     | 1506 | BCL  | C6-C5-C3    | -3.49 | 104.98      | 113.47   |
| 3   | R     | 1709 | BCL  | CMD-C2D-C1D | 3.48  | 130.86      | 124.73   |
| 3   | L     | 1606 | BCL  | CHB-C1B-C2B | -3.48 | 117.32      | 127.43   |
| 3   | D     | 1602 | BCL  | O2D-CGD-CBD | 3.47  | 117.30      | 111.23   |
| 3   | I     | 1705 | BCL  | C3D-C2D-C1D | -3.46 | 101.10      | 105.83   |
| 3   | K     | 1506 | BCL  | CBC-CAC-C3C | -3.46 | 106.07      | 113.41   |
| 3   | G     | 1704 | BCL  | CHA-C1A-NA  | -3.45 | 118.58      | 126.39   |
| 3   | S     | 1609 | BCL  | O2D-CGD-O1D | -3.44 | 117.15      | 123.85   |
| 3   | L     | 1606 | BCL  | O2A-CGA-O1A | -3.44 | 115.03      | 123.63   |
| 3   | M     | 1507 | BCL  | CHB-C1B-C2B | -3.44 | 117.45      | 127.43   |
| 3   | S     | 1609 | BCL  | CBA-CAA-C2A | -3.43 | 103.59      | 113.79   |
| 3   | O     | 1708 | BCL  | C3D-C2D-C1D | -3.43 | 101.16      | 105.83   |
| 3   | R     | 1709 | BCL  | O2A-CGA-CBA | 3.42  | 122.27      | 111.83   |
| 3   | R     | 1709 | BCL  | CHB-C1B-C2B | -3.42 | 117.50      | 127.43   |
| 3   | S     | 1609 | BCL  | CHC-C4B-NB  | 3.41  | 129.16      | 124.05   |
| 3   | A     | 1501 | BCL  | O2D-CGD-O1D | -3.40 | 117.22      | 123.85   |
| 3   | B     | 1601 | BCL  | CHB-C1B-C2B | -3.40 | 117.55      | 127.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | N     | 1407 | RG1  | C11-C10-C9  | -3.39 | 122.53      | 127.28   |
| 3   | I     | 1705 | BCL  | CHB-C1B-C2B | -3.38 | 117.62      | 127.43   |
| 3   | O     | 1708 | BCL  | O2A-CGA-CBA | 3.37  | 122.12      | 111.83   |
| 3   | O     | 1708 | BCL  | CHB-C1B-C2B | -3.37 | 117.63      | 127.43   |
| 3   | D     | 1602 | BCL  | CHB-C1B-C2B | -3.37 | 117.63      | 127.43   |
| 5   | N     | 1407 | RG1  | C16-C15-C14 | -3.37 | 116.63      | 123.52   |
| 3   | I     | 1505 | BCL  | CMD-C2D-C1D | 3.35  | 130.63      | 124.73   |
| 3   | H     | 1604 | BCL  | CMC-C2C-C3C | 3.35  | 126.95      | 113.98   |
| 3   | C     | 1702 | BCL  | CHB-C1B-C2B | -3.33 | 117.75      | 127.43   |
| 3   | J     | 1605 | BCL  | CHB-C1B-C2B | -3.33 | 117.75      | 127.43   |
| 3   | D     | 1602 | BCL  | O2A-CGA-O1A | -3.33 | 115.30      | 123.63   |
| 3   | E     | 1703 | BCL  | C4-C3-C5    | 3.32  | 121.00      | 115.23   |
| 5   | D     | 1402 | RG1  | C28-C29-C30 | -3.32 | 122.41      | 127.48   |
| 3   | M     | 1707 | BCL  | CHB-C1B-C2B | -3.31 | 117.82      | 127.43   |
| 3   | A     | 1701 | BCL  | C2C-C3C-C4C | 3.30  | 106.29      | 101.34   |
| 5   | S     | 1409 | RG1  | C16-C15-C14 | -3.30 | 116.76      | 123.52   |
| 5   | R     | 1401 | RG1  | C11-C10-C9  | -3.30 | 122.65      | 127.28   |
| 3   | S     | 1609 | BCL  | CHB-C1B-C2B | -3.29 | 117.89      | 127.43   |
| 3   | K     | 1506 | BCL  | C1D-CHD-C4C | -3.29 | 118.70      | 126.62   |
| 3   | K     | 1706 | BCL  | O2D-CGD-O1D | -3.27 | 117.48      | 123.85   |
| 3   | M     | 1707 | BCL  | CMD-C2D-C1D | 3.27  | 130.48      | 124.73   |
| 3   | G     | 1504 | BCL  | OBb-CAB-C3B | -3.25 | 114.68      | 120.43   |
| 3   | A     | 1501 | BCL  | O2A-CGA-O1A | -3.24 | 115.52      | 123.63   |
| 3   | K     | 1506 | BCL  | CBA-CAA-C2A | -3.23 | 104.17      | 113.79   |
| 3   | E     | 1703 | BCL  | OBb-CAB-C3B | -3.23 | 114.72      | 120.43   |
| 3   | N     | 1607 | BCL  | CHB-C1B-C2B | -3.22 | 118.08      | 127.43   |
| 3   | K     | 1506 | BCL  | O2A-CGA-O1A | -3.22 | 115.57      | 123.63   |
| 3   | E     | 1503 | BCL  | C6-C5-C3    | -3.22 | 105.64      | 113.47   |
| 5   | J     | 1405 | RG1  | C25-C24-C23 | -3.21 | 113.91      | 123.20   |
| 3   | A     | 1501 | BCL  | CBA-CAA-C2A | -3.20 | 104.26      | 113.79   |
| 3   | K     | 1706 | BCL  | CHB-C1B-C2B | -3.20 | 118.14      | 127.43   |
| 3   | H     | 1604 | BCL  | C6-C5-C3    | -3.20 | 105.67      | 113.47   |
| 3   | D     | 1602 | BCL  | C6-C5-C3    | -3.20 | 105.68      | 113.47   |
| 3   | A     | 1701 | BCL  | C1D-CHD-C4C | -3.19 | 118.93      | 126.62   |
| 3   | R     | 1509 | BCL  | O2D-CGD-O1D | -3.19 | 117.64      | 123.85   |
| 3   | S     | 1609 | BCL  | OBd-CAD-C3D | -3.18 | 120.99      | 128.42   |
| 3   | H     | 1604 | BCL  | CHB-C1B-C2B | -3.16 | 118.25      | 127.43   |
| 3   | J     | 1605 | BCL  | C6-C5-C3    | -3.15 | 105.80      | 113.47   |
| 3   | E     | 1503 | BCL  | CHB-C1B-C2B | -3.15 | 118.29      | 127.43   |
| 3   | J     | 1605 | BCL  | C4D-C3D-CAD | -3.15 | 104.69      | 108.11   |
| 3   | R     | 1509 | BCL  | OBb-CAB-C3B | -3.15 | 114.87      | 120.43   |
| 3   | B     | 1601 | BCL  | O2D-CGD-O1D | -3.13 | 117.75      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | R     | 1401 | RG1  | C20-C21-C22 | -3.12 | 122.90      | 127.28   |
| 5   | H     | 1404 | RG1  | C16-C15-C14 | -3.12 | 117.13      | 123.52   |
| 5   | S     | 1409 | RG1  | C20-C21-C22 | -3.11 | 122.91      | 127.28   |
| 3   | O     | 1508 | BCL  | CMD-C2D-C1D | 3.11  | 130.20      | 124.73   |
| 5   | D     | 1402 | RG1  | C15-C14-C13 | -3.10 | 122.92      | 127.28   |
| 3   | B     | 1601 | BCL  | C6-C5-C3    | -3.10 | 105.92      | 113.47   |
| 3   | M     | 1707 | BCL  | O2A-CGA-CBA | 3.10  | 121.27      | 111.83   |
| 3   | P     | 1608 | BCL  | O2D-CGD-CBD | 3.09  | 116.64      | 111.23   |
| 5   | J     | 1405 | RG1  | C7-C6-C5    | -3.08 | 123.35      | 127.69   |
| 3   | K     | 1506 | BCL  | CAC-C3C-C4C | 3.08  | 119.43      | 112.58   |
| 3   | R     | 1709 | BCL  | C1C-NC-C4C  | -3.08 | 105.27      | 106.68   |
| 3   | G     | 1504 | BCL  | CHB-C1B-C2B | -3.08 | 118.48      | 127.43   |
| 3   | E     | 1503 | BCL  | CBA-CAA-C2A | -3.08 | 104.63      | 113.79   |
| 5   | F     | 1403 | RG1  | C12-C13-C14 | -3.08 | 114.17      | 119.01   |
| 3   | O     | 1708 | BCL  | C6-C5-C3    | -3.07 | 105.98      | 113.47   |
| 3   | O     | 1508 | BCL  | CHB-C1B-C2B | -3.07 | 118.50      | 127.43   |
| 3   | N     | 1607 | BCL  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 5   | F     | 1403 | RG1  | CM3-C5-C4   | 3.07  | 120.56      | 115.23   |
| 3   | O     | 1508 | BCL  | C6-C5-C3    | -3.06 | 106.00      | 113.47   |
| 3   | F     | 1603 | BCL  | C1-O2A-CGA  | 3.06  | 124.05      | 116.65   |
| 3   | C     | 1702 | BCL  | C1-O2A-CGA  | 3.05  | 124.04      | 116.65   |
| 3   | E     | 1503 | BCL  | CHC-C4B-NB  | 3.05  | 128.63      | 124.05   |
| 3   | R     | 1509 | BCL  | C6-C5-C3    | -3.05 | 106.04      | 113.47   |
| 3   | R     | 1509 | BCL  | CHB-C1B-C2B | -3.05 | 118.58      | 127.43   |
| 3   | I     | 1705 | BCL  | C6-C5-C3    | -3.04 | 106.05      | 113.47   |
| 3   | P     | 1608 | BCL  | CHB-C1B-C2B | -3.04 | 118.60      | 127.43   |
| 3   | O     | 1508 | BCL  | CHC-C4B-NB  | 3.04  | 128.61      | 124.05   |
| 3   | E     | 1703 | BCL  | CMD-C2D-C1D | 3.03  | 130.07      | 124.73   |
| 3   | M     | 1507 | BCL  | C1-O2A-CGA  | 3.03  | 123.98      | 116.65   |
| 3   | C     | 1502 | BCL  | CMD-C2D-C1D | 3.02  | 130.05      | 124.73   |
| 3   | H     | 1604 | BCL  | C3C-C4C-CHD | -3.02 | 117.03      | 123.39   |
| 3   | S     | 1609 | BCL  | O2A-CGA-O1A | -3.02 | 116.08      | 123.63   |
| 3   | P     | 1608 | BCL  | O2A-CGA-O1A | -3.01 | 116.09      | 123.63   |
| 3   | H     | 1604 | BCL  | O2A-CGA-O1A | -3.01 | 116.10      | 123.63   |
| 5   | F     | 1403 | RG1  | C24-C25-C26 | -3.01 | 123.06      | 127.28   |
| 5   | D     | 1402 | RG1  | C16-C15-C14 | -3.01 | 117.37      | 123.52   |
| 3   | I     | 1505 | BCL  | CBA-CAA-C2A | -3.00 | 104.86      | 113.79   |
| 5   | R     | 1401 | RG1  | C1-O1'-C1'  | -3.00 | 113.64      | 119.78   |
| 3   | I     | 1705 | BCL  | O2A-CGA-CBA | 3.00  | 120.97      | 111.83   |
| 5   | L     | 1406 | RG1  | C16-C17-C18 | -2.99 | 123.08      | 127.28   |
| 5   | F     | 1403 | RG1  | CM5-C13-C12 | 2.99  | 122.66      | 118.09   |
| 3   | E     | 1703 | BCL  | OBD-CAD-C3D | -2.99 | 121.43      | 128.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | H     | 1604 | BCL  | C2D-C1D-ND  | 2.98  | 113.08      | 110.13   |
| 3   | C     | 1702 | BCL  | O2D-CGD-CBD | 2.98  | 116.44      | 111.23   |
| 3   | M     | 1707 | BCL  | CHA-C1A-NA  | -2.98 | 119.64      | 126.39   |
| 5   | S     | 1409 | RG1  | CM3-C5-C4   | 2.97  | 120.39      | 115.23   |
| 3   | A     | 1701 | BCL  | CMD-C2D-C1D | 2.97  | 129.96      | 124.73   |
| 3   | M     | 1707 | BCL  | C4-C3-C5    | 2.97  | 120.38      | 115.23   |
| 3   | K     | 1706 | BCL  | CHC-C4B-NB  | 2.97  | 128.50      | 124.05   |
| 3   | G     | 1504 | BCL  | O2D-CGD-CBD | 2.97  | 116.41      | 111.23   |
| 3   | F     | 1603 | BCL  | O2D-CGD-O1D | -2.97 | 118.08      | 123.85   |
| 3   | G     | 1704 | BCL  | O2A-CGA-CBA | 2.96  | 120.87      | 111.83   |
| 3   | A     | 1701 | BCL  | O2D-CGD-CBD | 2.96  | 116.41      | 111.23   |
| 3   | B     | 1601 | BCL  | CHC-C4B-NB  | 2.96  | 128.49      | 124.05   |
| 5   | J     | 1405 | RG1  | C16-C15-C14 | -2.95 | 117.48      | 123.52   |
| 3   | R     | 1709 | BCL  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 3   | S     | 1609 | BCL  | C6-C5-C3    | -2.94 | 106.30      | 113.47   |
| 3   | A     | 1501 | BCL  | CGD-CBD-CAD | 2.94  | 120.38      | 110.85   |
| 3   | O     | 1508 | BCL  | O2A-C1-C2   | -2.94 | 96.79       | 108.11   |
| 3   | N     | 1607 | BCL  | C6-C5-C3    | -2.93 | 106.33      | 113.47   |
| 3   | N     | 1607 | BCL  | CBA-CAA-C2A | -2.93 | 105.08      | 113.79   |
| 3   | E     | 1503 | BCL  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 3   | M     | 1507 | BCL  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 3   | B     | 1601 | BCL  | O2A-CGA-CBA | 2.92  | 120.75      | 111.83   |
| 3   | D     | 1602 | BCL  | CBA-CAA-C2A | -2.91 | 105.14      | 113.79   |
| 3   | B     | 1601 | BCL  | CBA-CAA-C2A | -2.91 | 105.15      | 113.79   |
| 5   | H     | 1404 | RG1  | C25-C24-C23 | -2.90 | 114.79      | 123.20   |
| 3   | A     | 1701 | BCL  | CHC-C4B-NB  | 2.89  | 128.39      | 124.05   |
| 5   | R     | 1401 | RG1  | CM7-C22-C23 | 2.89  | 122.50      | 118.09   |
| 5   | L     | 1406 | RG1  | C20-C21-C22 | -2.89 | 123.23      | 127.28   |
| 3   | C     | 1502 | BCL  | CHB-C1B-C2B | -2.88 | 119.06      | 127.43   |
| 3   | K     | 1506 | BCL  | CHB-C1B-C2B | -2.87 | 119.10      | 127.43   |
| 5   | H     | 1404 | RG1  | CM7-C22-C23 | 2.86  | 122.46      | 118.09   |
| 5   | S     | 1409 | RG1  | CM5-C13-C12 | 2.86  | 122.46      | 118.09   |
| 5   | R     | 1401 | RG1  | C25-C24-C23 | -2.86 | 114.91      | 123.20   |
| 3   | L     | 1606 | BCL  | OBD-CAD-C3D | -2.86 | 121.74      | 128.42   |
| 3   | I     | 1505 | BCL  | CHB-C1B-C2B | -2.85 | 119.14      | 127.43   |
| 3   | J     | 1605 | BCL  | CHC-C4B-NB  | 2.85  | 128.33      | 124.05   |
| 3   | A     | 1501 | BCL  | CHA-C1A-NA  | -2.85 | 119.93      | 126.39   |
| 3   | A     | 1701 | BCL  | OBB-CAB-CBB | 2.85  | 126.15      | 119.77   |
| 3   | G     | 1504 | BCL  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |
| 3   | J     | 1605 | BCL  | C3D-C4D-ND  | 2.84  | 114.60      | 109.99   |
| 3   | A     | 1501 | BCL  | CHC-C4B-NB  | 2.83  | 128.30      | 124.05   |
| 3   | G     | 1504 | BCL  | O2A-C1-C2   | -2.83 | 97.21       | 108.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | F     | 1403 | RG1  | C16-C15-C14 | -2.83 | 117.73      | 123.52   |
| 3   | N     | 1607 | BCL  | C1D-CHD-C4C | -2.83 | 119.80      | 126.62   |
| 3   | R     | 1509 | BCL  | CMA-C3A-C4A | 2.83  | 119.37      | 111.77   |
| 3   | R     | 1709 | BCL  | OBD-CAD-C3D | -2.83 | 121.81      | 128.42   |
| 5   | P     | 1408 | RG1  | CM3-C5-C4   | 2.82  | 120.12      | 115.23   |
| 5   | N     | 1407 | RG1  | C29-C28-C27 | -2.82 | 115.04      | 123.20   |
| 3   | M     | 1507 | BCL  | C6-C5-C3    | -2.82 | 106.61      | 113.47   |
| 3   | A     | 1701 | BCL  | C4-C3-C5    | 2.81  | 120.10      | 115.23   |
| 3   | R     | 1509 | BCL  | C1C-NC-C4C  | -2.81 | 105.40      | 106.68   |
| 3   | O     | 1708 | BCL  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 3   | K     | 1706 | BCL  | OBB-CAB-CBB | 2.80  | 126.05      | 119.77   |
| 3   | F     | 1603 | BCL  | C4-C3-C5    | 2.80  | 120.09      | 115.23   |
| 3   | S     | 1609 | BCL  | C1-O2A-CGA  | 2.80  | 123.43      | 116.65   |
| 5   | L     | 1406 | RG1  | C12-C13-C14 | -2.80 | 114.61      | 119.01   |
| 3   | G     | 1704 | BCL  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 3   | G     | 1704 | BCL  | CHB-C1B-C2B | -2.79 | 119.33      | 127.43   |
| 5   | P     | 1408 | RG1  | CM7-C22-C23 | 2.78  | 122.34      | 118.09   |
| 5   | D     | 1402 | RG1  | CM0-C30-CM9 | 2.78  | 120.98      | 114.59   |
| 3   | A     | 1701 | BCL  | O2A-CGA-CBA | 2.77  | 120.27      | 111.83   |
| 3   | K     | 1706 | BCL  | C6-C5-C3    | -2.76 | 106.73      | 113.47   |
| 5   | D     | 1402 | RG1  | CM4-C9-C8   | 2.76  | 122.31      | 118.09   |
| 5   | H     | 1404 | RG1  | C1-O1'-C1'  | -2.76 | 114.13      | 119.78   |
| 3   | M     | 1707 | BCL  | C4D-C3D-CAD | -2.76 | 105.11      | 108.11   |
| 3   | P     | 1608 | BCL  | CHC-C4B-NB  | 2.76  | 128.19      | 124.05   |
| 3   | R     | 1509 | BCL  | CMD-C2D-C1D | 2.76  | 129.58      | 124.73   |
| 3   | K     | 1506 | BCL  | C4-C3-C5    | 2.76  | 120.01      | 115.23   |
| 3   | K     | 1506 | BCL  | OBB-CAB-C3B | -2.75 | 115.57      | 120.43   |
| 3   | A     | 1501 | BCL  | CHA-C4D-ND  | 2.75  | 138.22      | 132.55   |
| 5   | H     | 1404 | RG1  | C11-C10-C9  | -2.74 | 123.43      | 127.28   |
| 3   | R     | 1509 | BCL  | CHC-C4B-NB  | 2.73  | 128.14      | 124.05   |
| 3   | D     | 1602 | BCL  | CHC-C4B-NB  | 2.73  | 128.14      | 124.05   |
| 3   | L     | 1606 | BCL  | OBB-CAB-CBB | 2.72  | 125.87      | 119.77   |
| 3   | G     | 1704 | BCL  | CBC-CAC-C3C | -2.72 | 107.64      | 113.41   |
| 3   | N     | 1607 | BCL  | O2A-CGA-CBA | 2.71  | 120.11      | 111.83   |
| 3   | R     | 1709 | BCL  | C4-C3-C5    | 2.71  | 119.93      | 115.23   |
| 3   | G     | 1504 | BCL  | CMD-C2D-C1D | 2.71  | 129.50      | 124.73   |
| 3   | N     | 1607 | BCL  | OBD-CAD-C3D | -2.71 | 122.09      | 128.42   |
| 5   | J     | 1405 | RG1  | C2-C3-C4    | -2.70 | 105.82      | 112.33   |
| 3   | I     | 1705 | BCL  | CHC-C4B-NB  | 2.70  | 128.10      | 124.05   |
| 3   | M     | 1707 | BCL  | C6-C5-C3    | -2.70 | 106.89      | 113.47   |
| 3   | K     | 1706 | BCL  | C4-C3-C5    | 2.70  | 119.92      | 115.23   |
| 3   | O     | 1708 | BCL  | C1C-NC-C4C  | -2.70 | 105.45      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | J     | 1405 | RG1  | C28-C27-C26 | -2.70 | 118.97      | 126.36   |
| 5   | H     | 1404 | RG1  | C28-C27-C26 | -2.70 | 118.97      | 126.36   |
| 3   | L     | 1606 | BCL  | C3A-C2A-C1A | -2.69 | 97.30       | 101.34   |
| 3   | M     | 1707 | BCL  | O2D-CGD-CBD | 2.69  | 115.94      | 111.23   |
| 5   | D     | 1402 | RG1  | C20-C21-C22 | -2.69 | 123.50      | 127.28   |
| 3   | C     | 1502 | BCL  | OBD-CAD-C3D | -2.68 | 122.15      | 128.42   |
| 3   | A     | 1501 | BCL  | C4-C3-C5    | 2.68  | 119.88      | 115.23   |
| 3   | C     | 1702 | BCL  | C1C-NC-C4C  | -2.68 | 105.46      | 106.68   |
| 3   | O     | 1708 | BCL  | CMD-C2D-C1D | 2.68  | 129.44      | 124.73   |
| 5   | H     | 1404 | RG1  | CM2-C1-C2   | -2.67 | 106.37      | 111.12   |
| 3   | C     | 1502 | BCL  | C4-C3-C5    | 2.67  | 119.87      | 115.23   |
| 5   | F     | 1403 | RG1  | C1-O1'-C1'  | -2.67 | 114.32      | 119.78   |
| 5   | L     | 1406 | RG1  | CM3-C5-C4   | 2.66  | 119.85      | 115.23   |
| 3   | D     | 1602 | BCL  | C4-C3-C5    | 2.66  | 119.85      | 115.23   |
| 5   | N     | 1407 | RG1  | CM3-C5-C4   | 2.66  | 119.85      | 115.23   |
| 3   | F     | 1603 | BCL  | CBA-CAA-C2A | -2.66 | 105.89      | 113.79   |
| 3   | A     | 1701 | BCL  | CBC-CAC-C3C | -2.65 | 107.78      | 113.41   |
| 3   | N     | 1607 | BCL  | CHC-C4B-NB  | 2.65  | 128.03      | 124.05   |
| 3   | C     | 1702 | BCL  | O2A-CGA-CBA | 2.65  | 119.92      | 111.83   |
| 3   | R     | 1709 | BCL  | CGD-CBD-CAD | -2.65 | 102.27      | 110.85   |
| 3   | A     | 1701 | BCL  | CAC-C3C-C4C | 2.65  | 118.46      | 112.58   |
| 3   | R     | 1509 | BCL  | C2A-C3A-C4A | 2.64  | 106.14      | 101.87   |
| 3   | M     | 1707 | BCL  | CHC-C4B-NB  | 2.64  | 128.01      | 124.05   |
| 5   | H     | 1404 | RG1  | C20-C21-C22 | -2.64 | 123.58      | 127.28   |
| 5   | S     | 1409 | RG1  | C28-C27-C26 | -2.64 | 119.13      | 126.36   |
| 3   | K     | 1706 | BCL  | CMD-C2D-C1D | 2.63  | 129.37      | 124.73   |
| 3   | C     | 1702 | BCL  | O2D-CGD-O1D | -2.63 | 118.72      | 123.85   |
| 3   | N     | 1607 | BCL  | OBB-CAB-CBB | 2.62  | 125.63      | 119.77   |
| 3   | H     | 1604 | BCL  | CAC-C3C-C4C | -2.62 | 106.78      | 112.58   |
| 3   | B     | 1601 | BCL  | OBB-CAB-CBB | 2.61  | 125.62      | 119.77   |
| 3   | J     | 1605 | BCL  | O2A-CGA-CBA | 2.61  | 119.80      | 111.83   |
| 5   | N     | 1407 | RG1  | C24-C25-C26 | -2.61 | 123.62      | 127.28   |
| 5   | H     | 1404 | RG1  | C28-C29-C30 | -2.61 | 123.50      | 127.48   |
| 3   | D     | 1602 | BCL  | C2D-C1D-ND  | 2.60  | 112.70      | 110.13   |
| 3   | C     | 1502 | BCL  | CHC-C4B-NB  | 2.60  | 127.95      | 124.05   |
| 3   | O     | 1708 | BCL  | C1D-CHD-C4C | -2.60 | 120.35      | 126.62   |
| 3   | L     | 1606 | BCL  | CHC-C4B-NB  | 2.60  | 127.95      | 124.05   |
| 3   | G     | 1704 | BCL  | CMD-C2D-C1D | 2.60  | 129.30      | 124.73   |
| 3   | R     | 1709 | BCL  | C1D-CHD-C4C | -2.60 | 120.36      | 126.62   |
| 3   | R     | 1509 | BCL  | O2A-C1-C2   | -2.59 | 98.13       | 108.11   |
| 3   | J     | 1605 | BCL  | O2A-CGA-O1A | -2.59 | 117.14      | 123.63   |
| 3   | E     | 1703 | BCL  | C6-C5-C3    | -2.59 | 107.16      | 113.47   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 1703 | BCL  | O2A-CGA-CBA | 2.59  | 119.73      | 111.83   |
| 5   | S     | 1409 | RG1  | C24-C25-C26 | -2.59 | 123.65      | 127.28   |
| 3   | E     | 1503 | BCL  | O2A-CGA-CBA | 2.59  | 119.73      | 111.83   |
| 5   | J     | 1405 | RG1  | CM3-C5-C4   | 2.59  | 119.72      | 115.23   |
| 3   | C     | 1502 | BCL  | C14-C13-C12 | 2.59  | 120.49      | 111.27   |
| 3   | K     | 1706 | BCL  | O2A-CGA-CBA | 2.58  | 119.70      | 111.83   |
| 5   | P     | 1408 | RG1  | C1'-O5'-C5' | 2.58  | 118.75      | 113.72   |
| 3   | P     | 1608 | BCL  | OBB-CAB-CBB | 2.58  | 125.54      | 119.77   |
| 5   | D     | 1402 | RG1  | C10-C11-C12 | -2.57 | 115.74      | 123.20   |
| 3   | K     | 1506 | BCL  | O2D-CGD-CBD | 2.57  | 115.73      | 111.23   |
| 3   | C     | 1502 | BCL  | CBA-CAA-C2A | -2.56 | 106.16      | 113.79   |
| 3   | R     | 1509 | BCL  | C4-C3-C5    | 2.56  | 119.68      | 115.23   |
| 5   | J     | 1405 | RG1  | C11-C10-C9  | -2.56 | 123.69      | 127.28   |
| 3   | G     | 1504 | BCL  | CHA-C1A-NA  | -2.56 | 120.60      | 126.39   |
| 3   | J     | 1605 | BCL  | C2D-C1D-ND  | 2.55  | 112.65      | 110.13   |
| 3   | R     | 1709 | BCL  | OBB-CAB-CBB | 2.55  | 125.48      | 119.77   |
| 3   | H     | 1604 | BCL  | OBD-CAD-C3D | -2.55 | 122.46      | 128.42   |
| 3   | E     | 1703 | BCL  | O2A-C1-C2   | -2.54 | 98.33       | 108.11   |
| 3   | I     | 1505 | BCL  | C1C-NC-C4C  | -2.54 | 105.52      | 106.68   |
| 3   | G     | 1504 | BCL  | O2A-CGA-CBA | 2.54  | 119.58      | 111.83   |
| 3   | H     | 1604 | BCL  | OBB-CAB-CBB | 2.53  | 125.45      | 119.77   |
| 3   | I     | 1705 | BCL  | C3D-C4D-ND  | 2.53  | 114.10      | 109.99   |
| 3   | O     | 1708 | BCL  | OBD-CAD-C3D | -2.53 | 122.50      | 128.42   |
| 5   | L     | 1406 | RG1  | C28-C29-C30 | -2.53 | 123.62      | 127.48   |
| 3   | D     | 1602 | BCL  | C1-O2A-CGA  | 2.52  | 122.76      | 116.65   |
| 5   | L     | 1406 | RG1  | O5'-C1'-C2' | 2.52  | 115.56      | 110.37   |
| 3   | O     | 1508 | BCL  | CHA-C4D-ND  | 2.52  | 137.75      | 132.55   |
| 3   | I     | 1505 | BCL  | C4-C3-C5    | 2.52  | 119.60      | 115.23   |
| 3   | R     | 1709 | BCL  | CHC-C4B-NB  | 2.52  | 127.82      | 124.05   |
| 3   | O     | 1708 | BCL  | CHC-C4B-NB  | 2.51  | 127.82      | 124.05   |
| 3   | G     | 1504 | BCL  | CHC-C4B-NB  | 2.51  | 127.81      | 124.05   |
| 3   | K     | 1706 | BCL  | C3D-C4D-ND  | 2.51  | 114.06      | 109.99   |
| 3   | M     | 1507 | BCL  | O2A-C1-C2   | -2.51 | 98.46       | 108.11   |
| 5   | D     | 1402 | RG1  | C28-C27-C26 | -2.50 | 119.50      | 126.36   |
| 3   | C     | 1702 | BCL  | CHC-C4B-NB  | 2.50  | 127.80      | 124.05   |
| 5   | N     | 1407 | RG1  | C20-C21-C22 | -2.50 | 123.77      | 127.28   |
| 3   | K     | 1706 | BCL  | C1D-CHD-C4C | -2.50 | 120.60      | 126.62   |
| 3   | S     | 1609 | BCL  | O2A-CGA-CBA | 2.49  | 119.44      | 111.83   |
| 5   | D     | 1402 | RG1  | CM5-C13-C12 | 2.49  | 121.90      | 118.09   |
| 3   | I     | 1505 | BCL  | O2A-C1-C2   | -2.49 | 98.51       | 108.11   |
| 3   | O     | 1508 | BCL  | C2D-C1D-ND  | 2.48  | 112.58      | 110.13   |
| 3   | C     | 1502 | BCL  | C2D-C1D-ND  | 2.48  | 112.58      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | L     | 1606 | BCL  | C1D-CHD-C4C | -2.48 | 120.63      | 126.62   |
| 3   | E     | 1503 | BCL  | OBD-CAD-C3D | -2.48 | 122.61      | 128.42   |
| 3   | B     | 1601 | BCL  | C1-O2A-CGA  | 2.48  | 122.65      | 116.65   |
| 3   | B     | 1601 | BCL  | OBD-CAD-C3D | -2.48 | 122.63      | 128.42   |
| 5   | S     | 1409 | RG1  | C25-C24-C23 | -2.47 | 116.03      | 123.20   |
| 3   | M     | 1707 | BCL  | C3D-C4D-ND  | 2.47  | 114.01      | 109.99   |
| 5   | D     | 1402 | RG1  | C24-C25-C26 | -2.47 | 123.81      | 127.28   |
| 3   | S     | 1609 | BCL  | C2D-C1D-ND  | 2.46  | 112.56      | 110.13   |
| 3   | M     | 1507 | BCL  | CBA-CAA-C2A | -2.46 | 106.47      | 113.79   |
| 3   | A     | 1501 | BCL  | C6-C5-C3    | -2.46 | 107.48      | 113.47   |
| 3   | D     | 1602 | BCL  | CHA-C4D-ND  | 2.46  | 137.62      | 132.55   |
| 3   | F     | 1603 | BCL  | OBB-CAB-CBB | 2.46  | 125.27      | 119.77   |
| 5   | F     | 1403 | RG1  | C29-C28-C27 | -2.46 | 116.08      | 123.20   |
| 3   | F     | 1603 | BCL  | C1D-ND-C4D  | 2.46  | 108.03      | 106.31   |
| 3   | O     | 1708 | BCL  | O2D-CGD-CBD | 2.45  | 115.52      | 111.23   |
| 3   | L     | 1606 | BCL  | O2A-CGA-CBA | 2.45  | 119.32      | 111.83   |
| 3   | G     | 1504 | BCL  | C1-O2A-CGA  | 2.45  | 122.59      | 116.65   |
| 3   | P     | 1608 | BCL  | C2D-C1D-ND  | 2.45  | 112.55      | 110.13   |
| 3   | K     | 1506 | BCL  | C3D-C4D-ND  | 2.44  | 113.95      | 109.99   |
| 3   | S     | 1609 | BCL  | CHD-C1D-C2D | -2.44 | 120.42      | 125.49   |
| 3   | O     | 1508 | BCL  | C4-C3-C5    | 2.43  | 119.45      | 115.23   |
| 3   | E     | 1703 | BCL  | CHC-C4B-NB  | 2.43  | 127.69      | 124.05   |
| 3   | D     | 1602 | BCL  | OBD-CAD-C3D | -2.43 | 122.74      | 128.42   |
| 3   | D     | 1602 | BCL  | C1D-CHD-C4C | -2.43 | 120.77      | 126.62   |
| 5   | D     | 1402 | RG1  | C29-C28-C27 | -2.43 | 116.17      | 123.20   |
| 3   | O     | 1508 | BCL  | C14-C13-C12 | 2.42  | 119.92      | 111.27   |
| 3   | N     | 1607 | BCL  | C2D-C1D-ND  | 2.42  | 112.52      | 110.13   |
| 3   | I     | 1505 | BCL  | C6-C5-C3    | -2.42 | 107.57      | 113.47   |
| 3   | G     | 1504 | BCL  | C4-C3-C5    | 2.42  | 119.43      | 115.23   |
| 3   | I     | 1505 | BCL  | C1D-CHD-C4C | -2.41 | 120.81      | 126.62   |
| 5   | J     | 1405 | RG1  | C24-C25-C26 | -2.41 | 123.90      | 127.28   |
| 5   | F     | 1403 | RG1  | CM0-C30-CM9 | 2.41  | 120.13      | 114.59   |
| 3   | E     | 1503 | BCL  | CHD-C1D-C2D | -2.41 | 120.48      | 125.49   |
| 3   | A     | 1501 | BCL  | OBB-CAB-CBB | 2.41  | 125.16      | 119.77   |
| 3   | M     | 1507 | BCL  | CHC-C4B-NB  | 2.41  | 127.66      | 124.05   |
| 5   | D     | 1402 | RG1  | C25-C24-C23 | -2.40 | 116.23      | 123.20   |
| 5   | L     | 1406 | RG1  | C29-C28-C27 | -2.40 | 116.25      | 123.20   |
| 3   | L     | 1606 | BCL  | C6-C5-C3    | -2.40 | 107.63      | 113.47   |
| 3   | C     | 1702 | BCL  | CBC-CAC-C3C | -2.39 | 108.33      | 113.41   |
| 5   | P     | 1408 | RG1  | C10-C11-C12 | -2.39 | 116.26      | 123.20   |
| 3   | G     | 1504 | BCL  | CBC-CAC-C3C | -2.39 | 108.34      | 113.41   |
| 3   | C     | 1502 | BCL  | O2A-CGA-CBA | 2.39  | 119.12      | 111.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | R     | 1509 | BCL  | C1D-CHD-C4C | -2.39 | 120.85      | 126.62   |
| 3   | L     | 1606 | BCL  | CBA-CAA-C2A | -2.39 | 106.69      | 113.79   |
| 5   | S     | 1409 | RG1  | C29-C28-C27 | -2.38 | 116.30      | 123.20   |
| 5   | N     | 1407 | RG1  | C15-C14-C13 | -2.38 | 123.94      | 127.28   |
| 5   | F     | 1403 | RG1  | C28-C27-C26 | -2.38 | 119.84      | 126.36   |
| 3   | O     | 1708 | BCL  | CBA-CAA-C2A | -2.38 | 106.71      | 113.79   |
| 3   | F     | 1603 | BCL  | CHC-C4B-NB  | 2.38  | 127.62      | 124.05   |
| 3   | E     | 1503 | BCL  | C2D-C1D-ND  | 2.38  | 112.48      | 110.13   |
| 5   | F     | 1403 | RG1  | C25-C24-C23 | -2.38 | 116.32      | 123.20   |
| 5   | L     | 1406 | RG1  | CM5-C13-C12 | 2.37  | 121.71      | 118.09   |
| 3   | H     | 1604 | BCL  | O2D-CGD-O1D | -2.37 | 119.24      | 123.85   |
| 3   | F     | 1603 | BCL  | O2A-CGA-CBA | 2.37  | 119.06      | 111.83   |
| 5   | F     | 1403 | RG1  | C6-C7-C8    | -2.37 | 116.34      | 123.20   |
| 3   | J     | 1605 | BCL  | CHA-C1A-NA  | -2.37 | 121.03      | 126.39   |
| 3   | G     | 1504 | BCL  | CBA-CAA-C2A | -2.37 | 106.75      | 113.79   |
| 3   | O     | 1508 | BCL  | CHA-C1A-NA  | -2.36 | 121.05      | 126.39   |
| 5   | S     | 1409 | RG1  | CM0-C30-CM9 | 2.36  | 120.02      | 114.59   |
| 5   | R     | 1401 | RG1  | C23-C22-C21 | -2.36 | 115.30      | 119.01   |
| 3   | G     | 1704 | BCL  | CHC-C4B-NB  | 2.36  | 127.59      | 124.05   |
| 3   | O     | 1508 | BCL  | OBB-CAB-CBB | 2.36  | 125.05      | 119.77   |
| 3   | D     | 1602 | BCL  | CHD-C1D-C2D | -2.35 | 120.60      | 125.49   |
| 3   | R     | 1709 | BCL  | CHA-C4D-ND  | 2.35  | 137.39      | 132.55   |
| 3   | I     | 1505 | BCL  | C3D-C4D-ND  | 2.35  | 113.80      | 109.99   |
| 5   | N     | 1407 | RG1  | C12-C13-C14 | -2.35 | 115.32      | 119.01   |
| 3   | J     | 1605 | BCL  | OBB-CAB-CBB | 2.34  | 125.02      | 119.77   |
| 3   | E     | 1703 | BCL  | CHA-C1A-NA  | -2.34 | 121.09      | 126.39   |
| 3   | O     | 1708 | BCL  | CHA-C4D-ND  | 2.34  | 137.37      | 132.55   |
| 3   | L     | 1606 | BCL  | C2D-C1D-ND  | 2.34  | 112.44      | 110.13   |
| 5   | P     | 1408 | RG1  | C1-O1'-C1'  | -2.33 | 115.00      | 119.78   |
| 3   | D     | 1602 | BCL  | O2D-CGD-O1D | -2.33 | 119.31      | 123.85   |
| 3   | O     | 1508 | BCL  | CHC-C4B-C3B | -2.33 | 122.46      | 131.72   |
| 3   | L     | 1606 | BCL  | C3D-C4D-ND  | 2.33  | 113.77      | 109.99   |
| 3   | H     | 1604 | BCL  | C2C-C3C-C4C | -2.33 | 97.85       | 101.34   |
| 3   | G     | 1504 | BCL  | CHA-C4D-ND  | 2.33  | 137.35      | 132.55   |
| 5   | J     | 1405 | RG1  | CM6-C18-C17 | -2.33 | 119.05      | 122.82   |
| 3   | A     | 1701 | BCL  | C6-C5-C3    | -2.32 | 107.81      | 113.47   |
| 3   | B     | 1601 | BCL  | C3D-C4D-ND  | 2.32  | 113.76      | 109.99   |
| 3   | S     | 1609 | BCL  | C5-C3-C2    | -2.32 | 115.95      | 121.17   |
| 5   | R     | 1401 | RG1  | CM5-C13-C12 | 2.32  | 121.63      | 118.09   |
| 5   | S     | 1409 | RG1  | C23-C22-C21 | -2.32 | 115.36      | 119.01   |
| 3   | M     | 1507 | BCL  | CHA-C1A-NA  | -2.31 | 121.16      | 126.39   |
| 3   | D     | 1602 | BCL  | OBB-CAB-CBB | 2.31  | 124.95      | 119.77   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | O     | 1708 | BCL  | C4-C3-C5    | 2.31  | 119.24      | 115.23   |
| 3   | P     | 1608 | BCL  | O2A-CGA-CBA | 2.31  | 118.88      | 111.83   |
| 3   | C     | 1702 | BCL  | OBb-CAB-CBB | 2.31  | 124.94      | 119.77   |
| 3   | R     | 1509 | BCL  | OBD-CAD-C3D | -2.31 | 123.02      | 128.42   |
| 3   | B     | 1601 | BCL  | C2D-C1D-ND  | 2.31  | 112.41      | 110.13   |
| 3   | L     | 1606 | BCL  | CHD-C1D-C2D | -2.30 | 120.69      | 125.49   |
| 3   | M     | 1507 | BCL  | C2D-C1D-ND  | 2.30  | 112.41      | 110.13   |
| 3   | H     | 1604 | BCL  | CHD-C1D-C2D | -2.30 | 120.70      | 125.49   |
| 3   | R     | 1509 | BCL  | CMA-C3A-C2A | 2.30  | 122.86      | 113.98   |
| 5   | R     | 1401 | RG1  | C28-C27-C26 | -2.30 | 120.07      | 126.36   |
| 3   | A     | 1501 | BCL  | C2D-C1D-ND  | 2.29  | 112.40      | 110.13   |
| 3   | A     | 1701 | BCL  | CHA-C1A-NA  | -2.29 | 121.20      | 126.39   |
| 3   | P     | 1608 | BCL  | CHA-C1A-NA  | -2.29 | 121.20      | 126.39   |
| 3   | M     | 1507 | BCL  | C1D-CHD-C4C | -2.29 | 121.10      | 126.62   |
| 5   | D     | 1402 | RG1  | C1'-C2'-C3' | 2.29  | 114.83      | 110.01   |
| 3   | K     | 1706 | BCL  | CBA-CAA-C2A | -2.29 | 106.98      | 113.79   |
| 3   | A     | 1501 | BCL  | C1D-CHD-C4C | -2.29 | 121.10      | 126.62   |
| 3   | K     | 1506 | BCL  | CHA-C1A-NA  | -2.29 | 121.21      | 126.39   |
| 3   | L     | 1606 | BCL  | C1-O2A-CGA  | 2.28  | 122.18      | 116.65   |
| 3   | O     | 1508 | BCL  | C5-C3-C2    | -2.28 | 116.04      | 121.17   |
| 3   | S     | 1609 | BCL  | CHC-C4B-C3B | -2.28 | 122.65      | 131.72   |
| 3   | N     | 1607 | BCL  | CHA-C1A-NA  | -2.28 | 121.22      | 126.39   |
| 5   | J     | 1405 | RG1  | C6-C7-C8    | -2.28 | 116.59      | 123.20   |
| 3   | G     | 1704 | BCL  | CBA-CAA-C2A | -2.28 | 107.00      | 113.79   |
| 3   | N     | 1607 | BCL  | CHA-C4D-ND  | 2.28  | 137.25      | 132.55   |
| 3   | R     | 1709 | BCL  | CBC-CAC-C3C | -2.28 | 108.58      | 113.41   |
| 3   | M     | 1507 | BCL  | O2A-CGA-CBA | 2.28  | 118.78      | 111.83   |
| 3   | C     | 1702 | BCL  | C3D-C4D-ND  | 2.27  | 113.68      | 109.99   |
| 3   | G     | 1704 | BCL  | C1D-CHD-C4C | -2.27 | 121.14      | 126.62   |
| 5   | S     | 1409 | RG1  | C20-C19-C18 | -2.27 | 120.14      | 126.36   |
| 3   | K     | 1506 | BCL  | O2A-C1-C2   | -2.27 | 99.38       | 108.11   |
| 3   | G     | 1704 | BCL  | C4-C3-C5    | 2.27  | 119.16      | 115.23   |
| 3   | M     | 1707 | BCL  | CHA-C4D-ND  | 2.27  | 137.23      | 132.55   |
| 5   | N     | 1407 | RG1  | C25-C24-C23 | -2.26 | 116.64      | 123.20   |
| 3   | H     | 1604 | BCL  | CHA-C1A-NA  | -2.26 | 121.28      | 126.39   |
| 5   | N     | 1407 | RG1  | CM4-C9-C8   | 2.26  | 121.54      | 118.09   |
| 3   | H     | 1604 | BCL  | O2A-CGA-CBA | 2.26  | 118.72      | 111.83   |
| 3   | P     | 1608 | BCL  | OBD-CAD-C3D | -2.26 | 123.14      | 128.42   |
| 3   | J     | 1605 | BCL  | CGD-CBD-CAD | 2.25  | 118.14      | 110.85   |
| 3   | G     | 1704 | BCL  | OBb-CAB-CBB | 2.25  | 124.82      | 119.77   |
| 3   | I     | 1505 | BCL  | OBD-CAD-C3D | -2.25 | 123.17      | 128.42   |
| 3   | E     | 1703 | BCL  | O2D-CGD-CBD | 2.25  | 115.16      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 1503 | BCL  | CHA-C1A-NA  | -2.24 | 121.31      | 126.39   |
| 5   | F     | 1403 | RG1  | C28-C29-C30 | -2.24 | 124.05      | 127.48   |
| 3   | C     | 1702 | BCL  | C4-C3-C5    | 2.24  | 119.12      | 115.23   |
| 3   | A     | 1701 | BCL  | C3D-C4D-ND  | 2.24  | 113.63      | 109.99   |
| 3   | E     | 1703 | BCL  | CHC-C4B-C3B | -2.24 | 122.82      | 131.72   |
| 3   | S     | 1609 | BCL  | CHA-C4D-ND  | 2.24  | 137.17      | 132.55   |
| 3   | H     | 1604 | BCL  | CMD-C2D-C1D | 2.24  | 128.67      | 124.73   |
| 3   | E     | 1503 | BCL  | CMD-C2D-C1D | 2.24  | 128.67      | 124.73   |
| 5   | J     | 1405 | RG1  | C29-C28-C27 | -2.24 | 116.71      | 123.20   |
| 3   | C     | 1502 | BCL  | C5-C3-C2    | -2.24 | 116.14      | 121.17   |
| 3   | I     | 1705 | BCL  | O2D-CGD-O1D | -2.24 | 119.49      | 123.85   |
| 3   | R     | 1709 | BCL  | CHA-C1A-NA  | -2.24 | 121.33      | 126.39   |
| 3   | E     | 1503 | BCL  | C4-C3-C5    | 2.23  | 119.10      | 115.23   |
| 3   | P     | 1608 | BCL  | C6-C5-C3    | -2.23 | 108.03      | 113.47   |
| 3   | P     | 1608 | BCL  | C4-C3-C5    | 2.23  | 119.10      | 115.23   |
| 5   | S     | 1409 | RG1  | C7-C8-C9    | -2.23 | 120.25      | 126.36   |
| 3   | G     | 1504 | BCL  | C1D-CHD-C4C | -2.23 | 121.24      | 126.62   |
| 3   | P     | 1608 | BCL  | C3C-C2C-C1C | 2.23  | 105.47      | 101.87   |
| 3   | I     | 1505 | BCL  | O2D-CGD-CBD | 2.23  | 115.13      | 111.23   |
| 3   | G     | 1704 | BCL  | C3D-C4D-ND  | 2.22  | 113.60      | 109.99   |
| 3   | C     | 1502 | BCL  | CHA-C1A-NA  | -2.22 | 121.37      | 126.39   |
| 3   | G     | 1504 | BCL  | C14-C13-C15 | -2.22 | 103.36      | 111.27   |
| 3   | J     | 1605 | BCL  | O2D-CGD-O1D | -2.22 | 119.53      | 123.85   |
| 3   | D     | 1602 | BCL  | O2A-CGA-CBA | 2.22  | 118.60      | 111.83   |
| 3   | M     | 1507 | BCL  | C2A-C1A-CHA | -2.22 | 120.02      | 123.87   |
| 3   | B     | 1601 | BCL  | C4-C3-C5    | 2.22  | 119.08      | 115.23   |
| 3   | K     | 1506 | BCL  | C1-O2A-CGA  | 2.21  | 122.01      | 116.65   |
| 3   | I     | 1705 | BCL  | C1D-CHD-C4C | -2.21 | 121.28      | 126.62   |
| 3   | R     | 1509 | BCL  | C3D-C4D-ND  | 2.21  | 113.58      | 109.99   |
| 5   | N     | 1407 | RG1  | CM5-C13-C12 | 2.21  | 121.46      | 118.09   |
| 5   | R     | 1401 | RG1  | C15-C14-C13 | -2.21 | 124.18      | 127.28   |
| 3   | I     | 1505 | BCL  | C11-C10-C8  | -2.21 | 108.63      | 115.97   |
| 3   | O     | 1508 | BCL  | O2A-CGA-CBA | 2.21  | 118.56      | 111.83   |
| 3   | C     | 1502 | BCL  | CHD-C1D-C2D | -2.21 | 120.90      | 125.49   |
| 3   | R     | 1709 | BCL  | C6-C5-C3    | -2.20 | 108.11      | 113.47   |
| 3   | C     | 1502 | BCL  | C2A-C1A-CHA | -2.19 | 120.06      | 123.87   |
| 3   | C     | 1502 | BCL  | C1D-CHD-C4C | -2.19 | 121.33      | 126.62   |
| 3   | R     | 1509 | BCL  | O2A-CGA-CBA | 2.19  | 118.52      | 111.83   |
| 3   | H     | 1604 | BCL  | C1D-CHD-C4C | -2.19 | 121.33      | 126.62   |
| 3   | P     | 1608 | BCL  | C3B-C4B-NB  | -2.19 | 106.87      | 109.76   |
| 5   | H     | 1404 | RG1  | CM4-C9-C8   | 2.19  | 121.43      | 118.09   |
| 5   | P     | 1408 | RG1  | C2-C3-C4    | -2.18 | 107.07      | 112.33   |

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| Mol | Chain | Res  | Type | Atoms        | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------------|-------|-------------|----------|
| 3   | H     | 1604 | BCL  | C4-C3-C5     | 2.18  | 119.02      | 115.23   |
| 5   | S     | 1409 | RG1  | C10-C11-C12  | -2.18 | 116.88      | 123.20   |
| 3   | I     | 1505 | BCL  | CHC-C4B-NB   | 2.18  | 127.32      | 124.05   |
| 5   | D     | 1402 | RG1  | CM7-C22-C23  | 2.18  | 121.41      | 118.09   |
| 3   | C     | 1702 | BCL  | C6-C5-C3     | -2.18 | 108.17      | 113.47   |
| 3   | F     | 1603 | BCL  | C2D-C1D-ND   | 2.18  | 112.28      | 110.13   |
| 3   | I     | 1705 | BCL  | CMD-C2D-C1D  | 2.17  | 128.55      | 124.73   |
| 3   | E     | 1703 | BCL  | O2D-CGD-O1D  | -2.17 | 119.62      | 123.85   |
| 3   | L     | 1606 | BCL  | C4D-C3D-CAD  | -2.17 | 105.75      | 108.11   |
| 3   | P     | 1608 | BCL  | CAB-C3B-C2B  | -2.17 | 123.24      | 127.74   |
| 3   | E     | 1703 | BCL  | C3D-C4D-ND   | 2.17  | 113.51      | 109.99   |
| 5   | N     | 1407 | RG1  | CM6-C18-C17  | -2.17 | 119.31      | 122.82   |
| 3   | I     | 1705 | BCL  | OB B-CAB-CBB | 2.16  | 124.62      | 119.77   |
| 3   | O     | 1508 | BCL  | C1-O2A-CGA   | 2.16  | 121.89      | 116.65   |
| 3   | G     | 1704 | BCL  | CHC-C4B-C3B  | -2.16 | 123.14      | 131.72   |
| 3   | C     | 1502 | BCL  | C3D-C4D-ND   | 2.16  | 113.50      | 109.99   |
| 5   | S     | 1409 | RG1  | C11-C10-C9   | -2.16 | 124.25      | 127.28   |
| 3   | O     | 1508 | BCL  | CGD-CBD-CAD  | 2.16  | 117.83      | 110.85   |
| 3   | R     | 1509 | BCL  | CHA-C1A-NA   | -2.16 | 121.51      | 126.39   |
| 3   | M     | 1507 | BCL  | C3D-C4D-ND   | 2.16  | 113.49      | 109.99   |
| 3   | S     | 1609 | BCL  | C4-C3-C5     | 2.16  | 118.97      | 115.23   |
| 3   | F     | 1603 | BCL  | CMD-C2D-C1D  | 2.15  | 128.52      | 124.73   |
| 3   | K     | 1506 | BCL  | O2D-CGD-O1D  | -2.15 | 119.66      | 123.85   |
| 5   | P     | 1408 | RG1  | C29-C28-C27  | -2.15 | 116.97      | 123.20   |
| 5   | P     | 1408 | RG1  | C21-C20-C19  | -2.15 | 116.97      | 123.20   |
| 5   | J     | 1405 | RG1  | CM0-C30-CM9  | 2.15  | 119.53      | 114.59   |
| 3   | M     | 1707 | BCL  | CAB-C3B-C2B  | -2.15 | 123.28      | 127.74   |
| 3   | G     | 1704 | BCL  | C2D-C1D-ND   | 2.15  | 112.25      | 110.13   |
| 3   | O     | 1508 | BCL  | OBD-CAD-C3D  | -2.15 | 123.40      | 128.42   |
| 3   | K     | 1706 | BCL  | CHC-C4B-C3B  | -2.14 | 123.21      | 131.72   |
| 3   | L     | 1606 | BCL  | C4-C3-C5     | 2.14  | 118.94      | 115.23   |
| 3   | I     | 1505 | BCL  | C1-O2A-CGA   | 2.14  | 121.82      | 116.65   |
| 3   | E     | 1703 | BCL  | C1D-CHD-C4C  | -2.13 | 121.48      | 126.62   |
| 3   | M     | 1707 | BCL  | OB B-CAB-CBB | 2.13  | 124.54      | 119.77   |
| 5   | J     | 1405 | RG1  | C10-C11-C12  | -2.13 | 117.03      | 123.20   |
| 3   | A     | 1501 | BCL  | C1-O2A-CGA   | 2.13  | 121.80      | 116.65   |
| 3   | K     | 1506 | BCL  | CMD-C2D-C1D  | 2.13  | 128.48      | 124.73   |
| 3   | A     | 1501 | BCL  | CHD-C1D-C2D  | -2.13 | 121.06      | 125.49   |
| 3   | C     | 1702 | BCL  | OBD-CAD-C3D  | -2.13 | 123.45      | 128.42   |
| 5   | R     | 1401 | RG1  | C10-C11-C12  | -2.13 | 117.04      | 123.20   |
| 3   | R     | 1509 | BCL  | CHC-C4B-C3B  | -2.12 | 123.29      | 131.72   |
| 3   | G     | 1504 | BCL  | C3D-C4D-ND   | 2.12  | 113.43      | 109.99   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | J     | 1605 | BCL  | CHC-C4B-C3B | -2.12 | 123.31      | 131.72   |
| 3   | O     | 1708 | BCL  | OBB-CAB-CBB | 2.11  | 124.50      | 119.77   |
| 3   | S     | 1609 | BCL  | OBB-CAB-CBB | 2.11  | 124.50      | 119.77   |
| 3   | C     | 1502 | BCL  | OBB-CAB-CBB | 2.11  | 124.48      | 119.77   |
| 3   | S     | 1609 | BCL  | C1D-CHD-C4C | -2.10 | 121.55      | 126.62   |
| 3   | E     | 1503 | BCL  | CHC-C4B-C3B | -2.10 | 123.38      | 131.72   |
| 5   | F     | 1403 | RG1  | C7-C6-C5    | -2.09 | 124.75      | 127.69   |
| 3   | L     | 1606 | BCL  | CMD-C2D-C3D | 2.09  | 132.49      | 127.69   |
| 3   | O     | 1708 | BCL  | C3D-C4D-ND  | 2.09  | 113.38      | 109.99   |
| 3   | C     | 1502 | BCL  | CHA-C4D-ND  | 2.09  | 136.86      | 132.55   |
| 5   | L     | 1406 | RG1  | C10-C11-C12 | -2.08 | 117.17      | 123.20   |
| 3   | G     | 1704 | BCL  | CGD-CBD-CAD | 2.08  | 117.58      | 110.85   |
| 5   | D     | 1402 | RG1  | CM3-C5-C4   | 2.08  | 118.83      | 115.23   |
| 3   | E     | 1703 | BCL  | CHA-C4D-ND  | 2.08  | 136.84      | 132.55   |
| 5   | H     | 1404 | RG1  | C6-C7-C8    | -2.08 | 117.18      | 123.20   |
| 5   | H     | 1404 | RG1  | C15-C14-C13 | -2.08 | 124.37      | 127.28   |
| 3   | I     | 1705 | BCL  | CHC-C4B-C3B | -2.08 | 123.47      | 131.72   |
| 3   | A     | 1501 | BCL  | CMD-C2D-C1D | 2.07  | 128.38      | 124.73   |
| 3   | F     | 1603 | BCL  | CHA-C1A-NA  | -2.07 | 121.70      | 126.39   |
| 3   | D     | 1602 | BCL  | CHA-C1A-NA  | -2.07 | 121.71      | 126.39   |
| 3   | I     | 1505 | BCL  | OBB-CAB-CBB | 2.06  | 124.39      | 119.77   |
| 3   | H     | 1604 | BCL  | C1-O2A-CGA  | 2.06  | 121.64      | 116.65   |
| 5   | R     | 1401 | RG1  | C20-C19-C18 | -2.06 | 120.71      | 126.36   |
| 3   | O     | 1708 | BCL  | CHA-C1A-NA  | -2.06 | 121.73      | 126.39   |
| 3   | E     | 1703 | BCL  | CBA-CAA-C2A | -2.06 | 107.67      | 113.79   |
| 3   | M     | 1507 | BCL  | CHD-C1D-C2D | -2.06 | 121.21      | 125.49   |
| 5   | H     | 1404 | RG1  | CM5-C13-C12 | 2.06  | 121.23      | 118.09   |
| 3   | A     | 1501 | BCL  | O2A-C1-C2   | -2.06 | 100.20      | 108.11   |
| 5   | F     | 1403 | RG1  | O5'-C5'-C6' | 2.05  | 111.53      | 106.44   |
| 3   | K     | 1506 | BCL  | C3C-C2C-C1C | -2.05 | 98.55       | 101.87   |
| 5   | L     | 1406 | RG1  | C1'-O5'-C5' | 2.05  | 117.73      | 113.72   |
| 3   | E     | 1503 | BCL  | C1D-CHD-C4C | -2.05 | 121.67      | 126.62   |
| 5   | F     | 1403 | RG1  | C20-C21-C22 | -2.05 | 124.40      | 127.28   |
| 3   | C     | 1702 | BCL  | CMD-C2D-C1D | 2.05  | 128.34      | 124.73   |
| 5   | F     | 1403 | RG1  | CM8-C26-C25 | -2.05 | 119.50      | 122.82   |
| 3   | M     | 1707 | BCL  | CHC-C4B-C3B | -2.05 | 123.58      | 131.72   |
| 3   | N     | 1607 | BCL  | CHC-C4B-C3B | -2.05 | 123.59      | 131.72   |
| 3   | R     | 1509 | BCL  | C1-O2A-CGA  | 2.05  | 121.61      | 116.65   |
| 3   | S     | 1609 | BCL  | CHA-C1A-NA  | -2.05 | 121.76      | 126.39   |
| 3   | I     | 1505 | BCL  | O2A-CGA-CBA | 2.04  | 118.06      | 111.83   |
| 3   | J     | 1605 | BCL  | C3C-C4C-CHD | -2.04 | 119.09      | 123.39   |
| 3   | A     | 1701 | BCL  | CHA-C4D-ND  | 2.04  | 136.76      | 132.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | L     | 1406 | RG1  | C25-C24-C23 | -2.04 | 117.29      | 123.20   |
| 3   | J     | 1605 | BCL  | C16-C15-C13 | -2.04 | 109.19      | 115.97   |
| 5   | P     | 1408 | RG1  | CM5-C13-C12 | 2.04  | 121.20      | 118.09   |
| 3   | G     | 1704 | BCL  | CHA-C4D-ND  | 2.04  | 136.75      | 132.55   |
| 5   | L     | 1406 | RG1  | CM0-C30-CM9 | 2.04  | 119.28      | 114.59   |
| 3   | N     | 1607 | BCL  | C4-C3-C5    | 2.04  | 118.76      | 115.23   |
| 3   | M     | 1507 | BCL  | CMD-C2D-C1D | 2.03  | 128.30      | 124.73   |
| 3   | K     | 1706 | BCL  | OBD-CAD-C3D | -2.03 | 123.68      | 128.42   |
| 3   | J     | 1605 | BCL  | C1-O2A-CGA  | 2.03  | 121.56      | 116.65   |
| 5   | R     | 1401 | RG1  | CM8-C26-C27 | 2.02  | 121.18      | 118.09   |
| 3   | B     | 1601 | BCL  | C1D-CHD-C4C | -2.02 | 121.74      | 126.62   |
| 3   | A     | 1701 | BCL  | CAB-C3B-C2B | -2.02 | 123.54      | 127.74   |
| 3   | E     | 1503 | BCL  | C5-C3-C2    | -2.02 | 116.63      | 121.17   |
| 3   | I     | 1705 | BCL  | C4D-C3D-CAD | -2.02 | 105.91      | 108.11   |
| 3   | K     | 1506 | BCL  | O2A-CGA-CBA | 2.01  | 117.97      | 111.83   |
| 3   | J     | 1605 | BCL  | C4-C3-C5    | 2.01  | 118.72      | 115.23   |
| 3   | N     | 1607 | BCL  | CMD-C2D-C1D | 2.01  | 128.27      | 124.73   |
| 3   | I     | 1505 | BCL  | CHA-C4D-ND  | 2.01  | 136.70      | 132.55   |
| 3   | H     | 1604 | BCL  | CHA-C4D-ND  | 2.01  | 136.70      | 132.55   |
| 5   | P     | 1408 | RG1  | CM8-C26-C25 | -2.01 | 119.56      | 122.82   |
| 3   | A     | 1501 | BCL  | C3D-C4D-ND  | 2.01  | 113.25      | 109.99   |
| 3   | A     | 1501 | BCL  | O2A-CGA-CBA | 2.01  | 117.96      | 111.83   |
| 3   | I     | 1705 | BCL  | CHA-C1A-NA  | -2.01 | 121.84      | 126.39   |
| 3   | S     | 1609 | BCL  | C3C-C4C-CHD | -2.01 | 119.16      | 123.39   |
| 5   | J     | 1405 | RG1  | C28-C29-C30 | -2.01 | 124.42      | 127.48   |
| 3   | K     | 1706 | BCL  | CHA-C1A-NA  | -2.00 | 121.85      | 126.39   |

All (23) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 3   | A     | 1501 | BCL  | CBD  |
| 3   | A     | 1701 | BCL  | C3C  |
| 3   | B     | 1601 | BCL  | C8   |
| 3   | C     | 1502 | BCL  | C13  |
| 3   | C     | 1702 | BCL  | C13  |
| 3   | G     | 1704 | BCL  | CBD  |
| 3   | H     | 1604 | BCL  | C2C  |
| 3   | J     | 1605 | BCL  | CBD  |
| 3   | K     | 1506 | BCL  | C3C  |
| 3   | K     | 1706 | BCL  | C8   |
| 3   | L     | 1606 | BCL  | C8   |
| 3   | L     | 1606 | BCL  | C3A  |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 3   | L     | 1606 | BCL  | C2C  |
| 3   | M     | 1707 | BCL  | CBD  |
| 3   | N     | 1607 | BCL  | C2C  |
| 3   | O     | 1508 | BCL  | C13  |
| 3   | O     | 1508 | BCL  | CBD  |
| 3   | O     | 1708 | BCL  | C8   |
| 3   | P     | 1608 | BCL  | C8   |
| 3   | P     | 1608 | BCL  | C2C  |
| 3   | R     | 1509 | BCL  | C3A  |
| 3   | R     | 1709 | BCL  | C13  |
| 3   | S     | 1609 | BCL  | C13  |

All (500) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 1701 | BCL  | C4C-C3C-CAC-CBC |
| 3   | C     | 1702 | BCL  | C1-C2-C3-C5     |
| 3   | E     | 1503 | BCL  | C2C-C3C-CAC-CBC |
| 3   | F     | 1603 | BCL  | C11-C10-C8-C7   |
| 3   | H     | 1604 | BCL  | C2C-C3C-CAC-CBC |
| 3   | H     | 1604 | BCL  | C4C-C3C-CAC-CBC |
| 3   | I     | 1705 | BCL  | C11-C10-C8-C9   |
| 3   | K     | 1506 | BCL  | C4C-C3C-CAC-CBC |
| 3   | P     | 1608 | BCL  | C2C-C3C-CAC-CBC |
| 3   | P     | 1608 | BCL  | C4C-C3C-CAC-CBC |
| 3   | R     | 1709 | BCL  | C2B-C3B-CAB-OBB |
| 3   | R     | 1709 | BCL  | C2B-C3B-CAB-CBB |
| 3   | R     | 1709 | BCL  | C4B-C3B-CAB-CBB |
| 4   | A     | 1817 | LDA  | C2-C1-N1-CM1    |
| 4   | A     | 1817 | LDA  | N1-C1-C2-C3     |
| 4   | B     | 1801 | LDA  | N1-C1-C2-C3     |
| 4   | C     | 1815 | LDA  | N1-C1-C2-C3     |
| 4   | D     | 1802 | LDA  | C2-C1-N1-CM1    |
| 4   | D     | 1802 | LDA  | N1-C1-C2-C3     |
| 4   | E     | 1822 | LDA  | N1-C1-C2-C3     |
| 4   | F     | 1803 | LDA  | C2-C1-N1-O1     |
| 4   | F     | 1803 | LDA  | C2-C1-N1-CM1    |
| 4   | F     | 1803 | LDA  | C2-C1-N1-CM2    |
| 4   | G     | 1814 | LDA  | C2-C1-N1-CM1    |
| 4   | G     | 1814 | LDA  | C2-C1-N1-CM2    |
| 4   | I     | 1812 | LDA  | N1-C1-C2-C3     |
| 4   | I     | 1825 | LDA  | C2-C1-N1-CM1    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | J     | 1805 | LDA  | C2-C1-N1-O1     |
| 4   | J     | 1805 | LDA  | N1-C1-C2-C3     |
| 4   | K     | 1810 | LDA  | N1-C1-C2-C3     |
| 4   | L     | 1806 | LDA  | C2-C1-N1-O1     |
| 4   | L     | 1806 | LDA  | C2-C1-N1-CM2    |
| 4   | L     | 1806 | LDA  | N1-C1-C2-C3     |
| 4   | M     | 1827 | LDA  | N1-C1-C2-C3     |
| 4   | O     | 1820 | LDA  | N1-C1-C2-C3     |
| 4   | P     | 1808 | LDA  | N1-C1-C2-C3     |
| 4   | R     | 1809 | LDA  | C2-C1-N1-O1     |
| 4   | R     | 1809 | LDA  | C2-C1-N1-CM1    |
| 4   | R     | 1809 | LDA  | C2-C1-N1-CM2    |
| 5   | F     | 1403 | RG1  | C25-C26-C27-C28 |
| 5   | F     | 1403 | RG1  | CM8-C26-C27-C28 |
| 5   | H     | 1404 | RG1  | O1'-C1-C2-C3    |
| 5   | H     | 1404 | RG1  | CM1-C1-C2-C3    |
| 5   | H     | 1404 | RG1  | CM2-C1-C2-C3    |
| 5   | P     | 1408 | RG1  | O1'-C1-C2-C3    |
| 5   | P     | 1408 | RG1  | CM2-C1-C2-C3    |
| 5   | P     | 1408 | RG1  | CM8-C26-C27-C28 |
| 3   | R     | 1709 | BCL  | O1D-CGD-O2D-CED |
| 3   | R     | 1709 | BCL  | CBD-CGD-O2D-CED |
| 3   | J     | 1605 | BCL  | C3-C5-C6-C7     |
| 3   | R     | 1709 | BCL  | C3-C5-C6-C7     |
| 3   | A     | 1501 | BCL  | CBD-CGD-O2D-CED |
| 3   | M     | 1707 | BCL  | CBD-CGD-O2D-CED |
| 3   | O     | 1708 | BCL  | CBD-CGD-O2D-CED |
| 3   | M     | 1707 | BCL  | C4-C3-C5-C6     |
| 3   | M     | 1707 | BCL  | C2-C3-C5-C6     |
| 3   | A     | 1701 | BCL  | C3-C5-C6-C7     |
| 3   | O     | 1708 | BCL  | C3-C5-C6-C7     |
| 3   | S     | 1609 | BCL  | C3-C5-C6-C7     |
| 5   | H     | 1404 | RG1  | C2-C3-C4-C5     |
| 3   | F     | 1603 | BCL  | C5-C6-C7-C8     |
| 5   | P     | 1408 | RG1  | O5'-C5'-C6'-O6' |
| 3   | H     | 1604 | BCL  | CBD-CGD-O2D-CED |
| 3   | M     | 1707 | BCL  | O1D-CGD-O2D-CED |
| 3   | G     | 1704 | BCL  | CBD-CGD-O2D-CED |
| 5   | P     | 1408 | RG1  | C4'-C5'-C6'-O6' |
| 3   | S     | 1609 | BCL  | CBD-CGD-O2D-CED |
| 5   | L     | 1406 | RG1  | O5'-C5'-C6'-O6' |
| 3   | D     | 1602 | BCL  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | L     | 1406 | RG1  | C4'-C5'-C6'-O6' |
| 3   | E     | 1703 | BCL  | C6-C7-C8-C9     |
| 3   | F     | 1603 | BCL  | C11-C12-C13-C14 |
| 3   | R     | 1709 | BCL  | C11-C10-C8-C9   |
| 3   | S     | 1609 | BCL  | C11-C12-C13-C14 |
| 3   | O     | 1708 | BCL  | O1D-CGD-O2D-CED |
| 5   | D     | 1402 | RG1  | CM8-C26-C27-C28 |
| 5   | H     | 1404 | RG1  | CM8-C26-C27-C28 |
| 5   | J     | 1405 | RG1  | CM8-C26-C27-C28 |
| 5   | R     | 1401 | RG1  | CM8-C26-C27-C28 |
| 5   | S     | 1409 | RG1  | CM8-C26-C27-C28 |
| 5   | H     | 1404 | RG1  | C25-C26-C27-C28 |
| 5   | R     | 1401 | RG1  | C25-C26-C27-C28 |
| 5   | J     | 1405 | RG1  | O5'-C5'-C6'-O6' |
| 3   | S     | 1609 | BCL  | C10-C11-C12-C13 |
| 3   | M     | 1707 | BCL  | C10-C11-C12-C13 |
| 3   | P     | 1608 | BCL  | C3-C5-C6-C7     |
| 5   | J     | 1405 | RG1  | C4'-C5'-C6'-O6' |
| 3   | B     | 1601 | BCL  | C6-C7-C8-C10    |
| 3   | C     | 1702 | BCL  | C11-C12-C13-C15 |
| 3   | P     | 1608 | BCL  | C6-C7-C8-C10    |
| 3   | A     | 1501 | BCL  | C15-C16-C17-C18 |
| 3   | O     | 1508 | BCL  | CBD-CGD-O2D-CED |
| 3   | A     | 1701 | BCL  | C10-C11-C12-C13 |
| 3   | C     | 1702 | BCL  | C15-C16-C17-C18 |
| 3   | F     | 1603 | BCL  | C8-C10-C11-C12  |
| 3   | C     | 1702 | BCL  | C5-C6-C7-C8     |
| 3   | K     | 1506 | BCL  | C8-C10-C11-C12  |
| 3   | M     | 1507 | BCL  | C15-C16-C17-C18 |
| 3   | E     | 1503 | BCL  | C8-C10-C11-C12  |
| 3   | M     | 1707 | BCL  | C8-C10-C11-C12  |
| 3   | A     | 1501 | BCL  | O1D-CGD-O2D-CED |
| 3   | N     | 1607 | BCL  | C8-C10-C11-C12  |
| 3   | H     | 1604 | BCL  | O1D-CGD-O2D-CED |
| 3   | C     | 1502 | BCL  | C10-C11-C12-C13 |
| 3   | D     | 1602 | BCL  | C13-C15-C16-C17 |
| 3   | G     | 1504 | BCL  | C8-C10-C11-C12  |
| 3   | M     | 1507 | BCL  | C8-C10-C11-C12  |
| 3   | P     | 1608 | BCL  | C5-C6-C7-C8     |
| 3   | D     | 1602 | BCL  | C10-C11-C12-C13 |
| 3   | O     | 1708 | BCL  | C10-C11-C12-C13 |
| 3   | E     | 1703 | BCL  | C4B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | E     | 1703 | BCL  | C4B-C3B-CAB-CBB |
| 3   | R     | 1709 | BCL  | C4B-C3B-CAB-OBB |
| 5   | D     | 1402 | RG1  | C25-C26-C27-C28 |
| 5   | J     | 1405 | RG1  | C25-C26-C27-C28 |
| 5   | P     | 1408 | RG1  | C25-C26-C27-C28 |
| 5   | S     | 1409 | RG1  | C25-C26-C27-C28 |
| 4   | R     | 1819 | LDA  | C3-C4-C5-C6     |
| 3   | N     | 1607 | BCL  | C16-C17-C18-C20 |
| 3   | G     | 1704 | BCL  | O1D-CGD-O2D-CED |
| 3   | C     | 1702 | BCL  | C3-C5-C6-C7     |
| 3   | I     | 1705 | BCL  | C3-C5-C6-C7     |
| 3   | M     | 1707 | BCL  | C5-C6-C7-C8     |
| 5   | D     | 1402 | RG1  | O5'-C5'-C6'-O6' |
| 3   | N     | 1607 | BCL  | C2-C1-O2A-CGA   |
| 3   | J     | 1605 | BCL  | C16-C17-C18-C20 |
| 4   | I     | 1813 | LDA  | C7-C8-C9-C10    |
| 4   | K     | 1826 | LDA  | C6-C7-C8-C9     |
| 4   | P     | 1808 | LDA  | C2-C3-C4-C5     |
| 4   | I     | 1813 | LDA  | C6-C7-C8-C9     |
| 4   | R     | 1809 | LDA  | C6-C7-C8-C9     |
| 4   | D     | 1802 | LDA  | C7-C8-C9-C10    |
| 4   | F     | 1803 | LDA  | C6-C7-C8-C9     |
| 4   | L     | 1806 | LDA  | C3-C4-C5-C6     |
| 4   | O     | 1820 | LDA  | C6-C7-C8-C9     |
| 3   | C     | 1502 | BCL  | C12-C13-C15-C16 |
| 4   | A     | 1816 | LDA  | C6-C7-C8-C9     |
| 4   | D     | 1802 | LDA  | C11-C10-C9-C8   |
| 4   | F     | 1803 | LDA  | C4-C5-C6-C7     |
| 4   | P     | 1808 | LDA  | C11-C10-C9-C8   |
| 3   | G     | 1704 | BCL  | C5-C6-C7-C8     |
| 4   | M     | 1827 | LDA  | C4-C5-C6-C7     |
| 3   | R     | 1509 | BCL  | C3A-C2A-CAA-CBA |
| 4   | A     | 1816 | LDA  | C7-C8-C9-C10    |
| 4   | J     | 1805 | LDA  | C3-C4-C5-C6     |
| 4   | E     | 1822 | LDA  | C5-C6-C7-C8     |
| 3   | A     | 1701 | BCL  | C8-C10-C11-C12  |
| 3   | G     | 1704 | BCL  | C8-C10-C11-C12  |
| 3   | M     | 1707 | BCL  | C16-C17-C18-C19 |
| 4   | L     | 1806 | LDA  | C5-C6-C7-C8     |
| 4   | R     | 1819 | LDA  | C5-C6-C7-C8     |
| 3   | S     | 1609 | BCL  | O1D-CGD-O2D-CED |
| 3   | E     | 1703 | BCL  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | E     | 1503 | BCL  | C15-C16-C17-C18 |
| 4   | G     | 1824 | LDA  | C3-C4-C5-C6     |
| 4   | K     | 1826 | LDA  | C5-C6-C7-C8     |
| 3   | O     | 1508 | BCL  | O1D-CGD-O2D-CED |
| 4   | K     | 1826 | LDA  | C2-C3-C4-C5     |
| 4   | C     | 1821 | LDA  | C7-C8-C9-C10    |
| 4   | H     | 1804 | LDA  | C3-C4-C5-C6     |
| 4   | N     | 1807 | LDA  | C11-C10-C9-C8   |
| 4   | C     | 1815 | LDA  | C5-C6-C7-C8     |
| 4   | M     | 1827 | LDA  | C7-C8-C9-C10    |
| 4   | I     | 1825 | LDA  | C11-C10-C9-C8   |
| 4   | G     | 1824 | LDA  | C6-C7-C8-C9     |
| 4   | B     | 1801 | LDA  | C2-C3-C4-C5     |
| 4   | G     | 1814 | LDA  | C5-C6-C7-C8     |
| 4   | J     | 1805 | LDA  | C2-C3-C4-C5     |
| 4   | O     | 1820 | LDA  | C11-C10-C9-C8   |
| 4   | R     | 1818 | LDA  | C7-C8-C9-C10    |
| 3   | C     | 1702 | BCL  | C11-C10-C8-C9   |
| 4   | A     | 1817 | LDA  | C1-C2-C3-C4     |
| 4   | K     | 1810 | LDA  | C1-C2-C3-C4     |
| 4   | A     | 1817 | LDA  | C11-C10-C9-C8   |
| 4   | C     | 1815 | LDA  | C6-C7-C8-C9     |
| 4   | C     | 1815 | LDA  | C2-C3-C4-C5     |
| 4   | I     | 1812 | LDA  | C2-C3-C4-C5     |
| 4   | O     | 1820 | LDA  | C7-C8-C9-C10    |
| 3   | M     | 1707 | BCL  | C15-C16-C17-C18 |
| 4   | E     | 1823 | LDA  | C5-C6-C7-C8     |
| 4   | C     | 1821 | LDA  | C3-C4-C5-C6     |
| 4   | I     | 1812 | LDA  | C7-C8-C9-C10    |
| 4   | N     | 1807 | LDA  | C5-C6-C7-C8     |
| 3   | M     | 1707 | BCL  | C16-C17-C18-C20 |
| 3   | R     | 1509 | BCL  | C8-C10-C11-C12  |
| 3   | C     | 1702 | BCL  | CBD-CGD-O2D-CED |
| 5   | L     | 1406 | RG1  | CM8-C26-C27-C28 |
| 4   | N     | 1807 | LDA  | C2-C3-C4-C5     |
| 3   | B     | 1601 | BCL  | C3-C5-C6-C7     |
| 4   | H     | 1804 | LDA  | C2-C3-C4-C5     |
| 4   | H     | 1804 | LDA  | C4-C5-C6-C7     |
| 4   | I     | 1825 | LDA  | C7-C8-C9-C10    |
| 3   | M     | 1707 | BCL  | CBA-CGA-O2A-C1  |
| 4   | L     | 1806 | LDA  | C1-C2-C3-C4     |
| 4   | G     | 1824 | LDA  | C7-C8-C9-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | I     | 1825 | LDA  | C3-C4-C5-C6     |
| 3   | E     | 1703 | BCL  | C15-C16-C17-C18 |
| 4   | A     | 1816 | LDA  | C1-C2-C3-C4     |
| 4   | A     | 1817 | LDA  | C3-C4-C5-C6     |
| 3   | E     | 1703 | BCL  | C5-C6-C7-C8     |
| 3   | K     | 1506 | BCL  | C15-C16-C17-C18 |
| 4   | E     | 1823 | LDA  | C7-C8-C9-C10    |
| 3   | R     | 1509 | BCL  | CBA-CGA-O2A-C1  |
| 4   | L     | 1806 | LDA  | C11-C10-C9-C8   |
| 4   | A     | 1817 | LDA  | C4-C5-C6-C7     |
| 4   | C     | 1821 | LDA  | C4-C5-C6-C7     |
| 3   | N     | 1607 | BCL  | CBD-CGD-O2D-CED |
| 4   | B     | 1801 | LDA  | C11-C10-C9-C8   |
| 4   | E     | 1822 | LDA  | C11-C10-C9-C8   |
| 3   | S     | 1609 | BCL  | C8-C10-C11-C12  |
| 4   | K     | 1810 | LDA  | C3-C4-C5-C6     |
| 4   | C     | 1821 | LDA  | C11-C10-C9-C8   |
| 4   | M     | 1811 | LDA  | C11-C10-C9-C8   |
| 4   | E     | 1822 | LDA  | C1-C2-C3-C4     |
| 3   | M     | 1707 | BCL  | O1A-CGA-O2A-C1  |
| 3   | R     | 1509 | BCL  | C1A-C2A-CAA-CBA |
| 3   | E     | 1703 | BCL  | C13-C15-C16-C17 |
| 4   | M     | 1811 | LDA  | C3-C4-C5-C6     |
| 3   | O     | 1708 | BCL  | C8-C10-C11-C12  |
| 3   | A     | 1701 | BCL  | C11-C10-C8-C7   |
| 3   | E     | 1703 | BCL  | C6-C7-C8-C10    |
| 3   | N     | 1607 | BCL  | C12-C13-C15-C16 |
| 3   | O     | 1508 | BCL  | C11-C12-C13-C15 |
| 3   | R     | 1709 | BCL  | C11-C12-C13-C15 |
| 3   | R     | 1709 | BCL  | C12-C13-C15-C16 |
| 3   | A     | 1701 | BCL  | C16-C17-C18-C20 |
| 3   | A     | 1701 | BCL  | C2C-C3C-CAC-CBC |
| 3   | K     | 1506 | BCL  | C2C-C3C-CAC-CBC |
| 4   | K     | 1810 | LDA  | C6-C7-C8-C9     |
| 4   | M     | 1811 | LDA  | C2-C3-C4-C5     |
| 3   | I     | 1505 | BCL  | C8-C10-C11-C12  |
| 3   | K     | 1706 | BCL  | C8-C10-C11-C12  |
| 3   | A     | 1701 | BCL  | C11-C10-C8-C9   |
| 3   | O     | 1508 | BCL  | C11-C12-C13-C14 |
| 3   | R     | 1509 | BCL  | C11-C12-C13-C14 |
| 3   | R     | 1509 | BCL  | C14-C13-C15-C16 |
| 3   | R     | 1709 | BCL  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 4   | O     | 1820 | LDA  | C3-C4-C5-C6     |
| 4   | C     | 1815 | LDA  | C11-C10-C9-C8   |
| 4   | L     | 1806 | LDA  | C4-C5-C6-C7     |
| 4   | A     | 1817 | LDA  | C7-C8-C9-C10    |
| 4   | D     | 1802 | LDA  | C5-C6-C7-C8     |
| 3   | L     | 1606 | BCL  | C3-C5-C6-C7     |
| 4   | L     | 1806 | LDA  | C2-C3-C4-C5     |
| 5   | N     | 1407 | RG1  | CM8-C26-C27-C28 |
| 3   | A     | 1701 | BCL  | C16-C17-C18-C19 |
| 4   | R     | 1809 | LDA  | C4-C5-C6-C7     |
| 5   | L     | 1406 | RG1  | C25-C26-C27-C28 |
| 3   | K     | 1706 | BCL  | C10-C11-C12-C13 |
| 3   | K     | 1706 | BCL  | C5-C6-C7-C8     |
| 3   | E     | 1703 | BCL  | CBA-CGA-O2A-C1  |
| 3   | C     | 1702 | BCL  | C2B-C3B-CAB-CBB |
| 3   | E     | 1703 | BCL  | C2B-C3B-CAB-OB  |
| 3   | E     | 1703 | BCL  | C2B-C3B-CAB-CBB |
| 4   | A     | 1816 | LDA  | C3-C4-C5-C6     |
| 4   | E     | 1822 | LDA  | C4-C5-C6-C7     |
| 4   | N     | 1807 | LDA  | C7-C8-C9-C10    |
| 3   | E     | 1703 | BCL  | O1A-CGA-O2A-C1  |
| 4   | C     | 1815 | LDA  | C4-C5-C6-C7     |
| 3   | N     | 1607 | BCL  | C10-C11-C12-C13 |
| 3   | H     | 1604 | BCL  | C16-C17-C18-C20 |
| 4   | F     | 1803 | LDA  | C2-C3-C4-C5     |
| 4   | H     | 1804 | LDA  | C5-C6-C7-C8     |
| 4   | M     | 1811 | LDA  | C7-C8-C9-C10    |
| 4   | R     | 1819 | LDA  | C9-C10-C11-C12  |
| 4   | E     | 1823 | LDA  | C2-C3-C4-C5     |
| 4   | F     | 1803 | LDA  | C3-C4-C5-C6     |
| 3   | D     | 1602 | BCL  | C8-C10-C11-C12  |
| 4   | I     | 1813 | LDA  | C5-C6-C7-C8     |
| 3   | C     | 1702 | BCL  | CBA-CGA-O2A-C1  |
| 4   | R     | 1818 | LDA  | C11-C10-C9-C8   |
| 4   | E     | 1822 | LDA  | C3-C4-C5-C6     |
| 4   | G     | 1814 | LDA  | C6-C7-C8-C9     |
| 4   | K     | 1810 | LDA  | C9-C10-C11-C12  |
| 4   | F     | 1803 | LDA  | C5-C6-C7-C8     |
| 3   | A     | 1501 | BCL  | C8-C10-C11-C12  |
| 4   | P     | 1808 | LDA  | C9-C10-C11-C12  |
| 4   | R     | 1818 | LDA  | C5-C6-C7-C8     |
| 3   | B     | 1601 | BCL  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | D     | 1602 | BCL  | C11-C12-C13-C14 |
| 3   | O     | 1708 | BCL  | C11-C10-C8-C9   |
| 3   | P     | 1608 | BCL  | C11-C12-C13-C14 |
| 4   | H     | 1804 | LDA  | C6-C7-C8-C9     |
| 4   | R     | 1818 | LDA  | C9-C10-C11-C12  |
| 4   | G     | 1814 | LDA  | C3-C4-C5-C6     |
| 4   | M     | 1811 | LDA  | C4-C5-C6-C7     |
| 4   | M     | 1827 | LDA  | C3-C4-C5-C6     |
| 5   | P     | 1408 | RG1  | CM1-C1-C2-C3    |
| 4   | J     | 1805 | LDA  | C9-C10-C11-C12  |
| 3   | I     | 1505 | BCL  | C12-C13-C15-C16 |
| 3   | I     | 1705 | BCL  | C11-C10-C8-C7   |
| 3   | R     | 1509 | BCL  | C11-C12-C13-C15 |
| 3   | R     | 1509 | BCL  | C12-C13-C15-C16 |
| 3   | R     | 1709 | BCL  | C13-C15-C16-C17 |
| 5   | N     | 1407 | RG1  | C27-C28-C29-C30 |
| 3   | R     | 1509 | BCL  | O1A-CGA-O2A-C1  |
| 3   | G     | 1504 | BCL  | C15-C16-C17-C18 |
| 3   | C     | 1702 | BCL  | C1-C2-C3-C4     |
| 4   | R     | 1818 | LDA  | C6-C7-C8-C9     |
| 5   | H     | 1404 | RG1  | C4'-C5'-C6'-O6' |
| 4   | I     | 1812 | LDA  | C6-C7-C8-C9     |
| 4   | J     | 1805 | LDA  | C5-C6-C7-C8     |
| 3   | N     | 1607 | BCL  | C1-C2-C3-C5     |
| 4   | G     | 1814 | LDA  | C4-C5-C6-C7     |
| 4   | I     | 1813 | LDA  | C3-C4-C5-C6     |
| 3   | G     | 1704 | BCL  | C4B-C3B-CAB-CBB |
| 3   | C     | 1502 | BCL  | C14-C13-C15-C16 |
| 3   | N     | 1607 | BCL  | C14-C13-C15-C16 |
| 4   | C     | 1821 | LDA  | C9-C10-C11-C12  |
| 3   | H     | 1604 | BCL  | C16-C17-C18-C19 |
| 4   | R     | 1819 | LDA  | C1-C2-C3-C4     |
| 3   | M     | 1507 | BCL  | C4C-C3C-CAC-CBC |
| 3   | J     | 1605 | BCL  | C16-C17-C18-C19 |
| 3   | N     | 1607 | BCL  | C16-C17-C18-C19 |
| 4   | I     | 1825 | LDA  | C6-C7-C8-C9     |
| 3   | C     | 1702 | BCL  | O1D-CGD-O2D-CED |
| 3   | E     | 1703 | BCL  | C16-C17-C18-C20 |
| 3   | K     | 1506 | BCL  | C16-C17-C18-C19 |
| 3   | C     | 1702 | BCL  | C6-C7-C8-C10    |
| 3   | F     | 1603 | BCL  | C11-C12-C13-C15 |
| 3   | K     | 1706 | BCL  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | R     | 1709 | BCL  | C11-C10-C8-C7   |
| 3   | H     | 1604 | BCL  | C3-C5-C6-C7     |
| 3   | O     | 1508 | BCL  | C8-C10-C11-C12  |
| 5   | N     | 1407 | RG1  | C25-C26-C27-C28 |
| 3   | O     | 1508 | BCL  | O1A-CGA-O2A-C1  |
| 3   | C     | 1702 | BCL  | O1A-CGA-O2A-C1  |
| 4   | I     | 1825 | LDA  | C1-C2-C3-C4     |
| 3   | C     | 1702 | BCL  | C2B-C3B-CAB-OBB |
| 3   | G     | 1704 | BCL  | C2B-C3B-CAB-OBB |
| 3   | G     | 1704 | BCL  | C2B-C3B-CAB-CBB |
| 3   | K     | 1706 | BCL  | C2B-C3B-CAB-OBB |
| 3   | K     | 1706 | BCL  | C2B-C3B-CAB-CBB |
| 3   | P     | 1608 | BCL  | O2A-C1-C2-C3    |
| 4   | I     | 1812 | LDA  | C4-C5-C6-C7     |
| 4   | R     | 1809 | LDA  | C3-C4-C5-C6     |
| 4   | B     | 1801 | LDA  | C7-C8-C9-C10    |
| 3   | R     | 1709 | BCL  | C16-C17-C18-C20 |
| 4   | R     | 1809 | LDA  | C5-C6-C7-C8     |
| 3   | C     | 1702 | BCL  | C6-C7-C8-C9     |
| 3   | E     | 1703 | BCL  | C11-C12-C13-C14 |
| 4   | B     | 1801 | LDA  | C6-C7-C8-C9     |
| 3   | O     | 1508 | BCL  | C10-C11-C12-C13 |
| 3   | B     | 1601 | BCL  | C2-C1-O2A-CGA   |
| 4   | A     | 1817 | LDA  | C2-C1-N1-CM2    |
| 4   | D     | 1802 | LDA  | C2-C1-N1-CM2    |
| 4   | J     | 1805 | LDA  | C2-C1-N1-CM2    |
| 4   | L     | 1806 | LDA  | C2-C1-N1-CM1    |
| 4   | P     | 1808 | LDA  | C1-C2-C3-C4     |
| 4   | P     | 1808 | LDA  | C6-C7-C8-C9     |
| 4   | R     | 1819 | LDA  | C6-C7-C8-C9     |
| 3   | M     | 1707 | BCL  | C1A-C2A-CAA-CBA |
| 3   | E     | 1703 | BCL  | CBD-CGD-O2D-CED |
| 3   | O     | 1708 | BCL  | C6-C7-C8-C10    |
| 4   | A     | 1816 | LDA  | C11-C10-C9-C8   |
| 4   | P     | 1808 | LDA  | C7-C8-C9-C10    |
| 4   | R     | 1809 | LDA  | C11-C10-C9-C8   |
| 5   | F     | 1403 | RG1  | C2-C1-O1'-C1'   |
| 5   | R     | 1401 | RG1  | C2-C1-O1'-C1'   |
| 5   | S     | 1409 | RG1  | C2-C1-O1'-C1'   |
| 3   | C     | 1702 | BCL  | C4B-C3B-CAB-CBB |
| 3   | G     | 1704 | BCL  | C4B-C3B-CAB-OBB |
| 3   | P     | 1608 | BCL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | I     | 1505 | BCL  | C14-C13-C15-C16 |
| 3   | K     | 1506 | BCL  | C11-C12-C13-C14 |
| 4   | J     | 1805 | LDA  | C1-C2-C3-C4     |
| 3   | G     | 1504 | BCL  | O1D-CGD-O2D-CED |
| 3   | O     | 1508 | BCL  | CBA-CGA-O2A-C1  |
| 3   | R     | 1709 | BCL  | C16-C17-C18-C19 |
| 3   | N     | 1607 | BCL  | O1A-CGA-O2A-C1  |
| 5   | H     | 1404 | RG1  | O5'-C5'-C6'-O6' |
| 4   | G     | 1824 | LDA  | C5-C6-C7-C8     |
| 3   | C     | 1502 | BCL  | C15-C16-C17-C18 |
| 4   | B     | 1801 | LDA  | C4-C5-C6-C7     |
| 4   | J     | 1805 | LDA  | C7-C8-C9-C10    |
| 4   | A     | 1816 | LDA  | C9-C10-C11-C12  |
| 4   | R     | 1819 | LDA  | C2-C3-C4-C5     |
| 4   | K     | 1826 | LDA  | C4-C5-C6-C7     |
| 3   | C     | 1502 | BCL  | O1D-CGD-O2D-CED |
| 3   | O     | 1708 | BCL  | C5-C6-C7-C8     |
| 4   | E     | 1822 | LDA  | C7-C8-C9-C10    |
| 4   | D     | 1802 | LDA  | C6-C7-C8-C9     |
| 3   | P     | 1608 | BCL  | O1A-CGA-O2A-C1  |
| 4   | R     | 1819 | LDA  | N1-C1-C2-C3     |
| 4   | G     | 1814 | LDA  | C11-C10-C9-C8   |
| 4   | K     | 1826 | LDA  | C11-C10-C9-C8   |
| 4   | F     | 1803 | LDA  | C7-C8-C9-C10    |
| 4   | B     | 1801 | LDA  | C1-C2-C3-C4     |
| 3   | N     | 1607 | BCL  | CBA-CGA-O2A-C1  |
| 4   | G     | 1814 | LDA  | C7-C8-C9-C10    |
| 3   | E     | 1503 | BCL  | C11-C12-C13-C14 |
| 3   | G     | 1504 | BCL  | C11-C12-C13-C14 |
| 3   | L     | 1606 | BCL  | C11-C10-C8-C9   |
| 3   | P     | 1608 | BCL  | CBA-CGA-O2A-C1  |
| 3   | L     | 1606 | BCL  | C13-C15-C16-C17 |
| 3   | J     | 1605 | BCL  | C5-C6-C7-C8     |
| 3   | L     | 1606 | BCL  | C10-C11-C12-C13 |
| 3   | G     | 1704 | BCL  | C11-C12-C13-C15 |
| 4   | B     | 1801 | LDA  | C3-C4-C5-C6     |
| 4   | R     | 1819 | LDA  | C4-C5-C6-C7     |
| 3   | A     | 1701 | BCL  | C15-C16-C17-C18 |
| 3   | C     | 1502 | BCL  | C8-C10-C11-C12  |
| 4   | I     | 1812 | LDA  | C11-C10-C9-C8   |
| 4   | M     | 1811 | LDA  | C6-C7-C8-C9     |
| 3   | N     | 1607 | BCL  | C4-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | F     | 1603 | BCL  | C11-C10-C8-C9   |
| 3   | N     | 1607 | BCL  | C6-C7-C8-C9     |
| 3   | N     | 1607 | BCL  | C11-C12-C13-C14 |
| 3   | P     | 1608 | BCL  | C11-C10-C8-C9   |
| 3   | S     | 1609 | BCL  | C11-C10-C8-C9   |
| 3   | A     | 1701 | BCL  | C2B-C3B-CAB-OBB |
| 3   | N     | 1607 | BCL  | C1-C2-C3-C4     |
| 3   | F     | 1603 | BCL  | C4-C3-C5-C6     |
| 3   | L     | 1606 | BCL  | C4-C3-C5-C6     |
| 3   | D     | 1602 | BCL  | C6-C7-C8-C10    |
| 3   | E     | 1503 | BCL  | C11-C12-C13-C15 |
| 3   | I     | 1505 | BCL  | C11-C12-C13-C15 |
| 3   | J     | 1605 | BCL  | C12-C13-C15-C16 |
| 3   | K     | 1506 | BCL  | C11-C12-C13-C15 |
| 3   | N     | 1607 | BCL  | C6-C7-C8-C10    |
| 3   | S     | 1609 | BCL  | C11-C10-C8-C7   |
| 4   | P     | 1808 | LDA  | C5-C6-C7-C8     |
| 4   | E     | 1823 | LDA  | C3-C4-C5-C6     |
| 4   | D     | 1802 | LDA  | C4-C5-C6-C7     |
| 4   | K     | 1810 | LDA  | C4-C5-C6-C7     |
| 5   | R     | 1401 | RG1  | CM1-C1-O1'-C1'  |
| 5   | R     | 1401 | RG1  | CM2-C1-O1'-C1'  |
| 4   | M     | 1811 | LDA  | C5-C6-C7-C8     |
| 3   | R     | 1709 | BCL  | C5-C6-C7-C8     |
| 3   | C     | 1702 | BCL  | C4B-C3B-CAB-OBB |
| 3   | K     | 1706 | BCL  | C4B-C3B-CAB-OBB |
| 3   | K     | 1706 | BCL  | C4B-C3B-CAB-CBB |
| 3   | G     | 1504 | BCL  | C3-C5-C6-C7     |
| 3   | D     | 1602 | BCL  | C6-C7-C8-C9     |
| 3   | I     | 1505 | BCL  | C11-C12-C13-C14 |
| 4   | H     | 1804 | LDA  | C9-C10-C11-C12  |
| 3   | I     | 1705 | BCL  | C13-C15-C16-C17 |
| 3   | N     | 1607 | BCL  | C2-C3-C5-C6     |
| 3   | K     | 1706 | BCL  | O1A-CGA-O2A-C1  |
| 3   | G     | 1704 | BCL  | C4-C3-C5-C6     |
| 3   | R     | 1709 | BCL  | C8-C10-C11-C12  |
| 3   | B     | 1601 | BCL  | O1A-CGA-O2A-C1  |
| 3   | G     | 1504 | BCL  | C12-C13-C15-C16 |
| 4   | R     | 1809 | LDA  | C7-C8-C9-C10    |
| 3   | E     | 1503 | BCL  | C14-C13-C15-C16 |
| 3   | F     | 1603 | BCL  | C14-C13-C15-C16 |
| 3   | G     | 1504 | BCL  | C14-C13-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | J     | 1605 | BCL  | C11-C10-C8-C9   |
| 3   | P     | 1608 | BCL  | C6-C7-C8-C9     |
| 4   | K     | 1810 | LDA  | C11-C10-C9-C8   |
| 3   | I     | 1705 | BCL  | C2-C1-O2A-CGA   |
| 4   | K     | 1826 | LDA  | C3-C4-C5-C6     |
| 3   | A     | 1701 | BCL  | C2B-C3B-CAB-CBB |
| 3   | M     | 1707 | BCL  | C2B-C3B-CAB-CBB |
| 5   | L     | 1406 | RG1  | C27-C28-C29-C30 |
| 4   | R     | 1809 | LDA  | C2-C3-C4-C5     |
| 4   | I     | 1825 | LDA  | C5-C6-C7-C8     |
| 3   | I     | 1705 | BCL  | O1A-CGA-O2A-C1  |
| 5   | D     | 1402 | RG1  | C4'-C5'-C6'-O6' |
| 3   | A     | 1701 | BCL  | C4B-C3B-CAB-CBB |
| 3   | H     | 1604 | BCL  | C11-C12-C13-C14 |
| 3   | O     | 1508 | BCL  | C11-C10-C8-C9   |
| 3   | E     | 1503 | BCL  | C12-C13-C15-C16 |
| 3   | F     | 1603 | BCL  | C12-C13-C15-C16 |
| 3   | H     | 1604 | BCL  | C6-C7-C8-C10    |
| 3   | J     | 1605 | BCL  | C11-C10-C8-C7   |
| 3   | L     | 1606 | BCL  | C11-C10-C8-C7   |
| 3   | O     | 1708 | BCL  | C11-C10-C8-C7   |
| 3   | S     | 1609 | BCL  | C6-C7-C8-C10    |
| 4   | I     | 1812 | LDA  | C2-C1-N1-CM1    |
| 4   | I     | 1825 | LDA  | C2-C1-N1-CM2    |
| 4   | N     | 1807 | LDA  | C6-C7-C8-C9     |
| 3   | B     | 1601 | BCL  | O1D-CGD-O2D-CED |
| 4   | E     | 1823 | LDA  | C9-C10-C11-C12  |
| 5   | H     | 1404 | RG1  | C17-C18-C19-C20 |
| 5   | J     | 1405 | RG1  | C21-C22-C23-C24 |
| 3   | O     | 1708 | BCL  | C15-C16-C17-C18 |
| 3   | D     | 1602 | BCL  | C16-C17-C18-C19 |
| 5   | F     | 1403 | RG1  | CM2-C1-C2-C3    |
| 5   | N     | 1407 | RG1  | CM2-C1-C2-C3    |
| 3   | E     | 1703 | BCL  | C12-C13-C15-C16 |
| 3   | P     | 1608 | BCL  | C11-C12-C13-C15 |
| 3   | M     | 1707 | BCL  | C2B-C3B-CAB-OBB |
| 3   | S     | 1609 | BCL  | O2A-C1-C2-C3    |
| 4   | N     | 1807 | LDA  | C3-C4-C5-C6     |
| 3   | C     | 1702 | BCL  | C2C-C3C-CAC-CBC |
| 3   | B     | 1601 | BCL  | C5-C6-C7-C8     |
| 3   | K     | 1506 | BCL  | C3A-C2A-CAA-CBA |
| 3   | A     | 1701 | BCL  | C4B-C3B-CAB-OBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | J     | 1605 | BCL  | C14-C13-C15-C16 |
| 3   | S     | 1609 | BCL  | C6-C7-C8-C9     |
| 3   | K     | 1706 | BCL  | CBA-CGA-O2A-C1  |
| 3   | A     | 1701 | BCL  | C2-C3-C5-C6     |
| 3   | S     | 1609 | BCL  | C5-C6-C7-C8     |
| 3   | K     | 1706 | BCL  | C4-C3-C5-C6     |
| 3   | F     | 1603 | BCL  | C15-C16-C17-C18 |
| 3   | A     | 1501 | BCL  | C1-C2-C3-C4     |
| 3   | B     | 1601 | BCL  | C1-C2-C3-C4     |
| 3   | H     | 1604 | BCL  | C1-C2-C3-C4     |
| 3   | S     | 1609 | BCL  | C1-C2-C3-C4     |

There are no ring outliers.

60 monomers are involved in 394 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | C     | 1815 | LDA  | 6       | 0            |
| 3   | K     | 1506 | BCL  | 9       | 0            |
| 5   | R     | 1401 | RG1  | 4       | 0            |
| 4   | P     | 1808 | LDA  | 3       | 0            |
| 4   | D     | 1802 | LDA  | 3       | 0            |
| 3   | E     | 1503 | BCL  | 3       | 0            |
| 4   | L     | 1806 | LDA  | 5       | 0            |
| 3   | H     | 1604 | BCL  | 8       | 0            |
| 3   | R     | 1509 | BCL  | 6       | 0            |
| 4   | M     | 1811 | LDA  | 4       | 0            |
| 3   | C     | 1702 | BCL  | 8       | 0            |
| 3   | L     | 1606 | BCL  | 21      | 0            |
| 5   | D     | 1402 | RG1  | 5       | 0            |
| 5   | N     | 1407 | RG1  | 4       | 0            |
| 3   | K     | 1706 | BCL  | 5       | 0            |
| 4   | E     | 1822 | LDA  | 8       | 0            |
| 3   | A     | 1501 | BCL  | 16      | 0            |
| 3   | G     | 1704 | BCL  | 20      | 0            |
| 3   | F     | 1603 | BCL  | 9       | 0            |
| 4   | I     | 1812 | LDA  | 7       | 0            |
| 3   | D     | 1602 | BCL  | 5       | 0            |
| 3   | P     | 1608 | BCL  | 11      | 0            |
| 4   | K     | 1810 | LDA  | 8       | 0            |
| 5   | P     | 1408 | RG1  | 4       | 0            |
| 3   | E     | 1703 | BCL  | 7       | 0            |
| 4   | E     | 1823 | LDA  | 6       | 0            |

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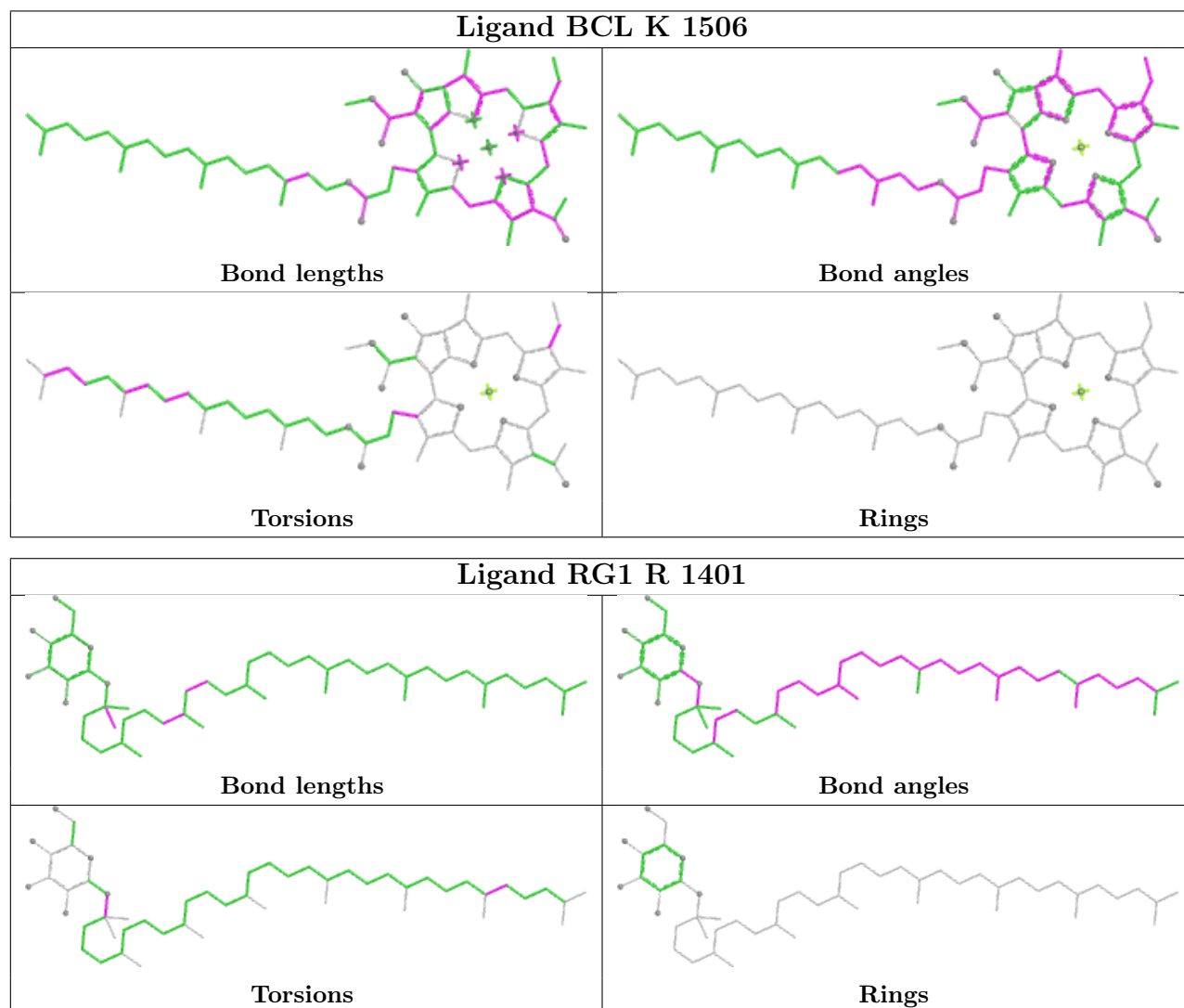


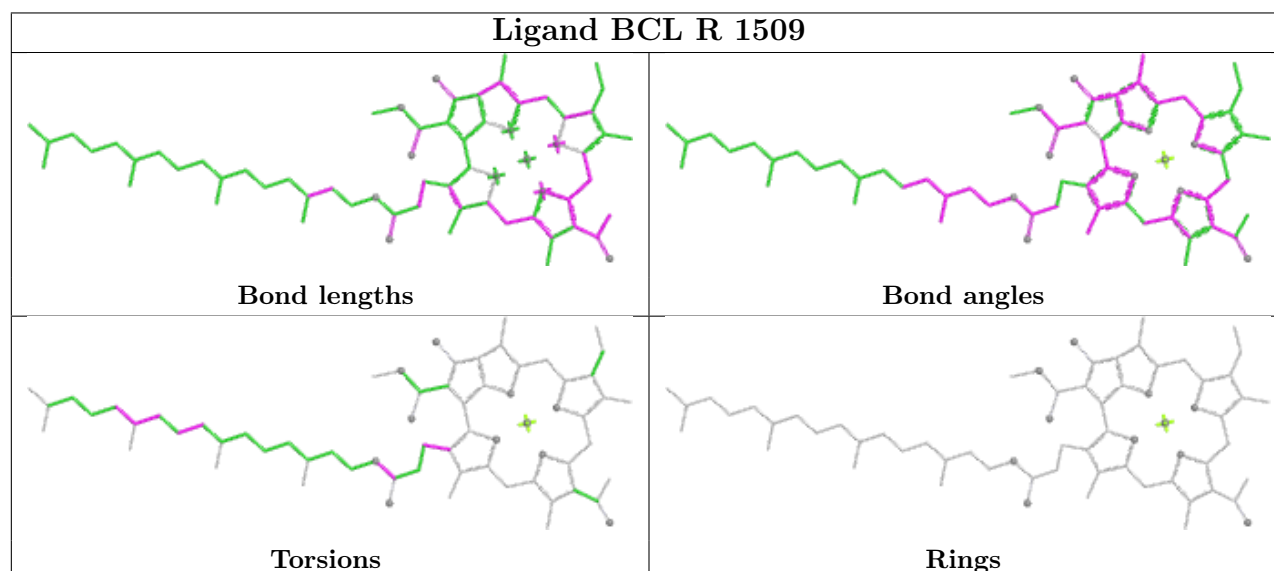
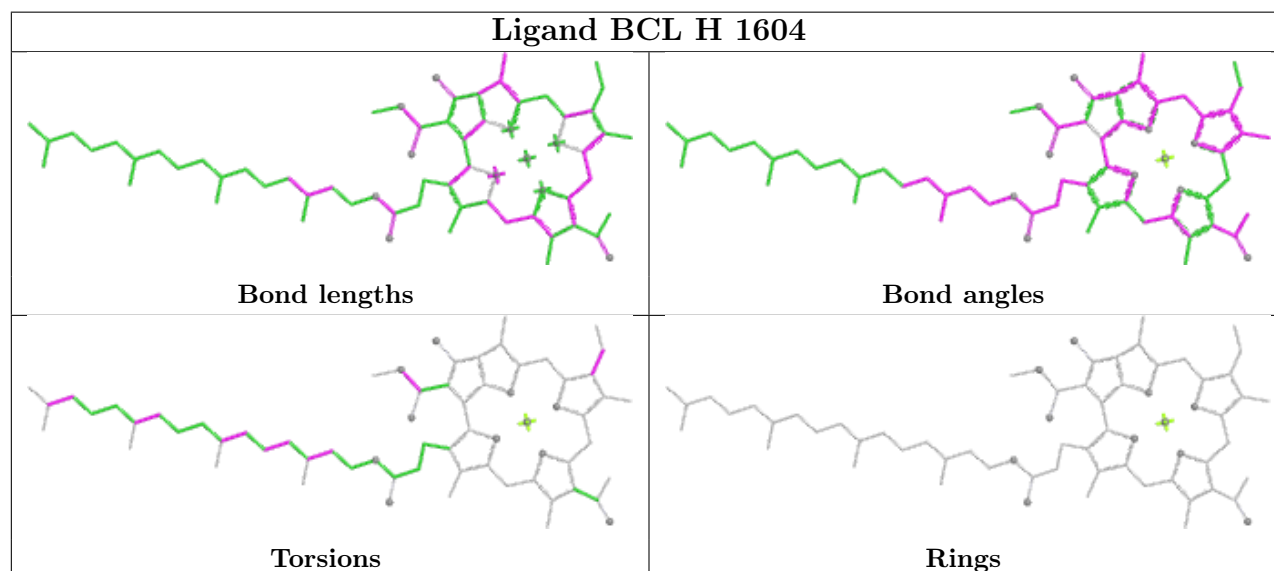
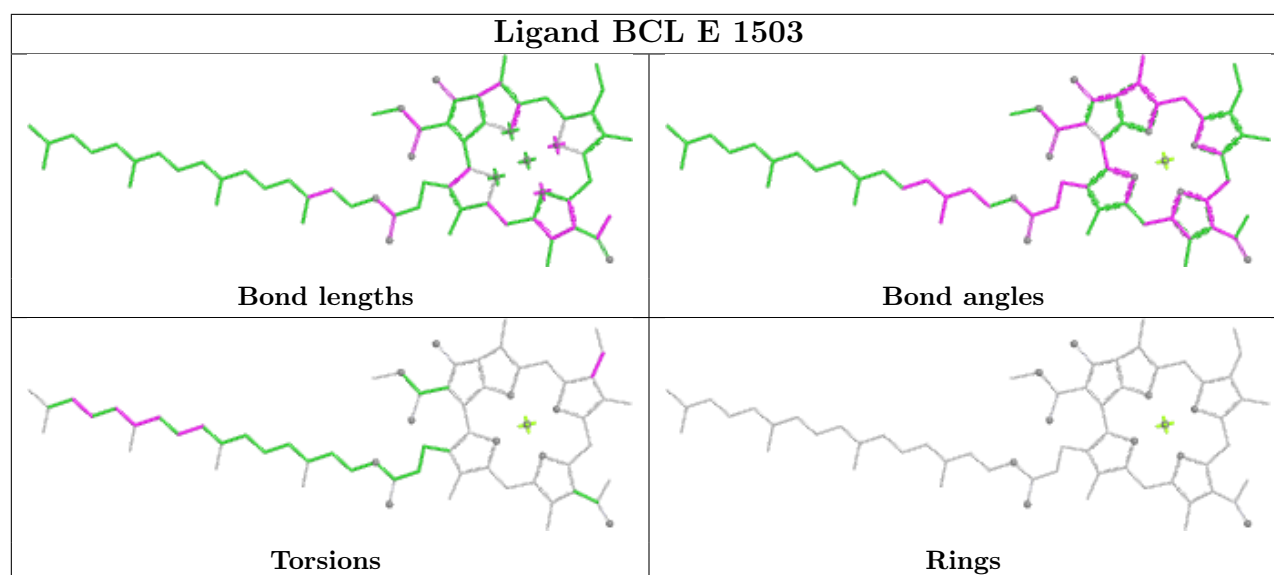
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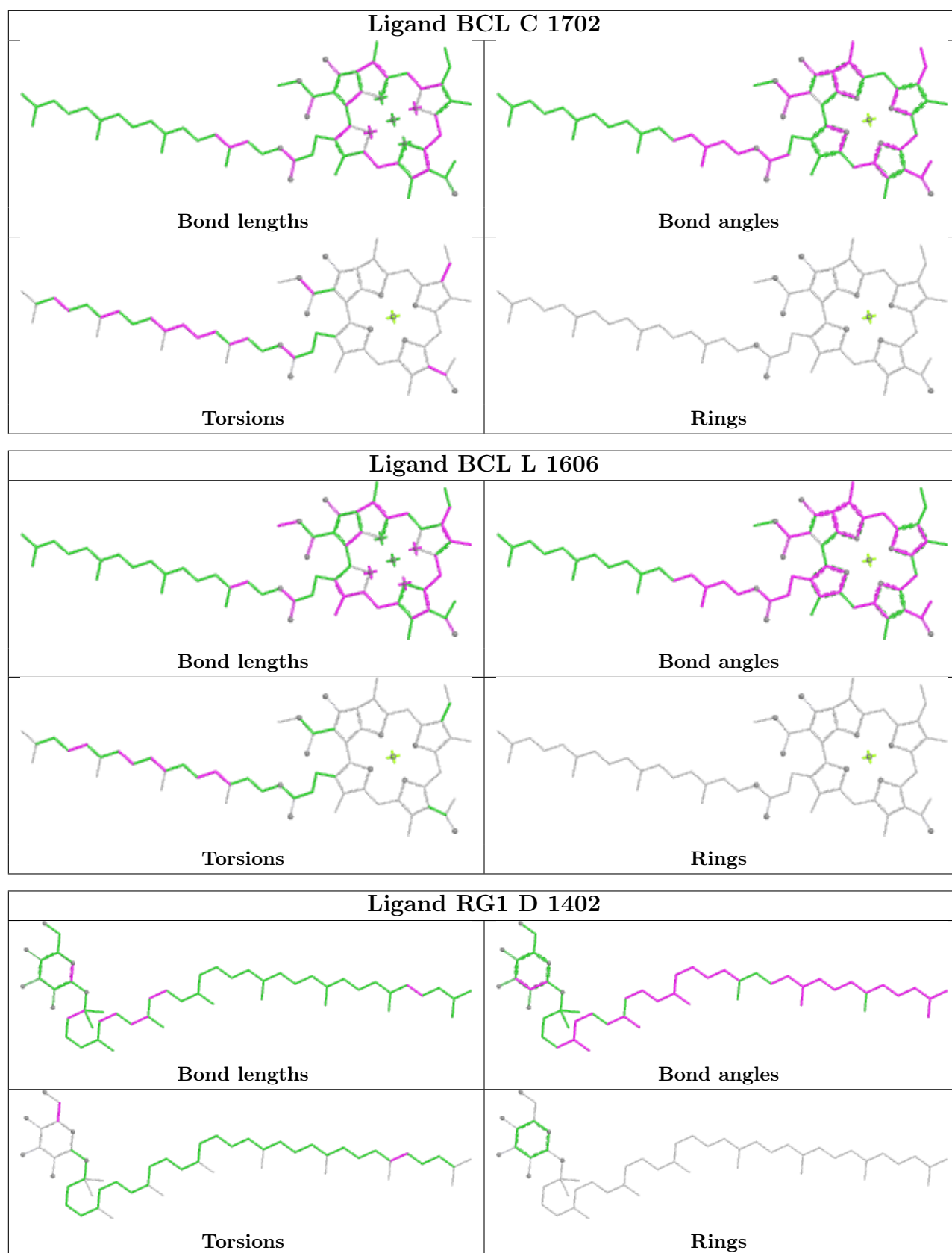
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1817 | LDA  | 3       | 0            |
| 4   | K     | 1826 | LDA  | 4       | 0            |
| 3   | O     | 1508 | BCL  | 11      | 0            |
| 3   | S     | 1609 | BCL  | 10      | 0            |
| 5   | F     | 1403 | RG1  | 5       | 0            |
| 4   | O     | 1820 | LDA  | 7       | 0            |
| 4   | M     | 1827 | LDA  | 2       | 0            |
| 4   | I     | 1825 | LDA  | 6       | 0            |
| 3   | G     | 1504 | BCL  | 3       | 0            |
| 3   | M     | 1507 | BCL  | 2       | 0            |
| 4   | B     | 1801 | LDA  | 2       | 0            |
| 4   | F     | 1803 | LDA  | 7       | 0            |
| 4   | I     | 1813 | LDA  | 2       | 0            |
| 4   | J     | 1805 | LDA  | 1       | 0            |
| 4   | G     | 1824 | LDA  | 14      | 0            |
| 4   | H     | 1804 | LDA  | 3       | 0            |
| 3   | I     | 1705 | BCL  | 20      | 0            |
| 3   | B     | 1601 | BCL  | 7       | 0            |
| 3   | N     | 1607 | BCL  | 14      | 0            |
| 3   | O     | 1708 | BCL  | 9       | 0            |
| 4   | N     | 1807 | LDA  | 2       | 0            |
| 4   | R     | 1818 | LDA  | 12      | 0            |
| 5   | H     | 1404 | RG1  | 5       | 0            |
| 4   | A     | 1816 | LDA  | 8       | 0            |
| 3   | M     | 1707 | BCL  | 20      | 0            |
| 4   | G     | 1814 | LDA  | 3       | 0            |
| 3   | A     | 1701 | BCL  | 6       | 0            |
| 3   | J     | 1605 | BCL  | 15      | 0            |
| 3   | I     | 1505 | BCL  | 9       | 0            |
| 3   | C     | 1502 | BCL  | 3       | 0            |
| 5   | S     | 1409 | RG1  | 5       | 0            |
| 5   | J     | 1405 | RG1  | 1       | 0            |
| 3   | R     | 1709 | BCL  | 21      | 0            |
| 5   | L     | 1406 | RG1  | 4       | 0            |

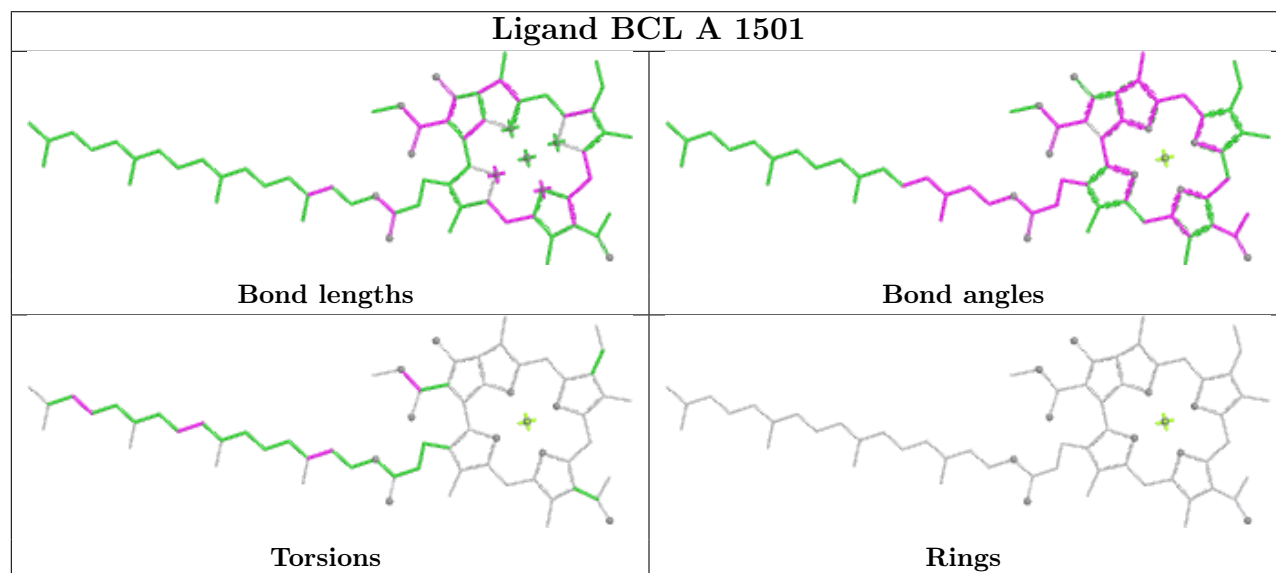
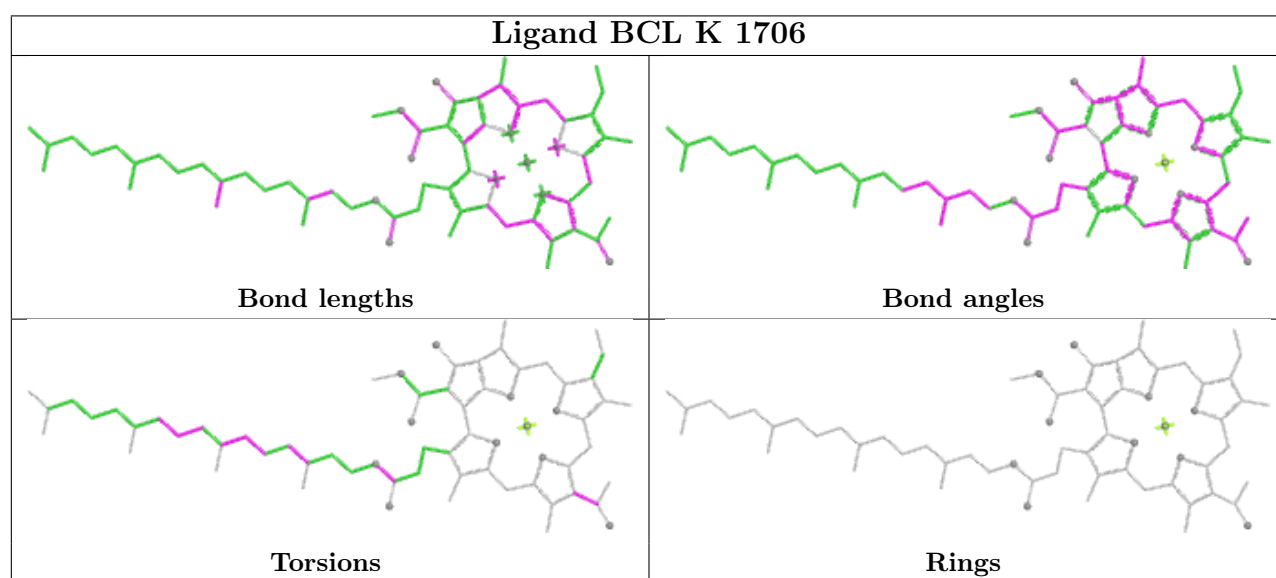
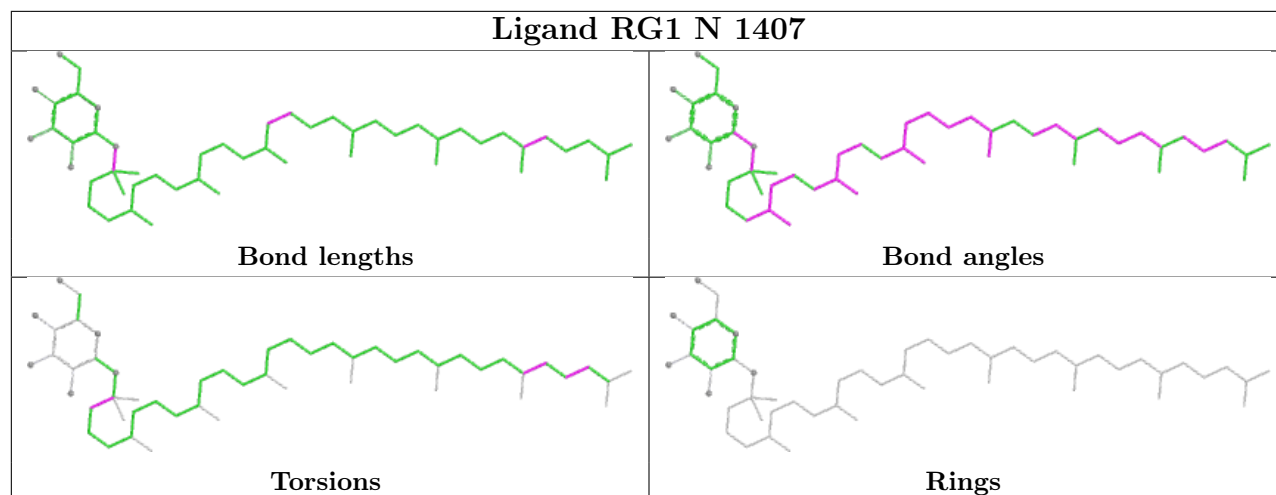
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

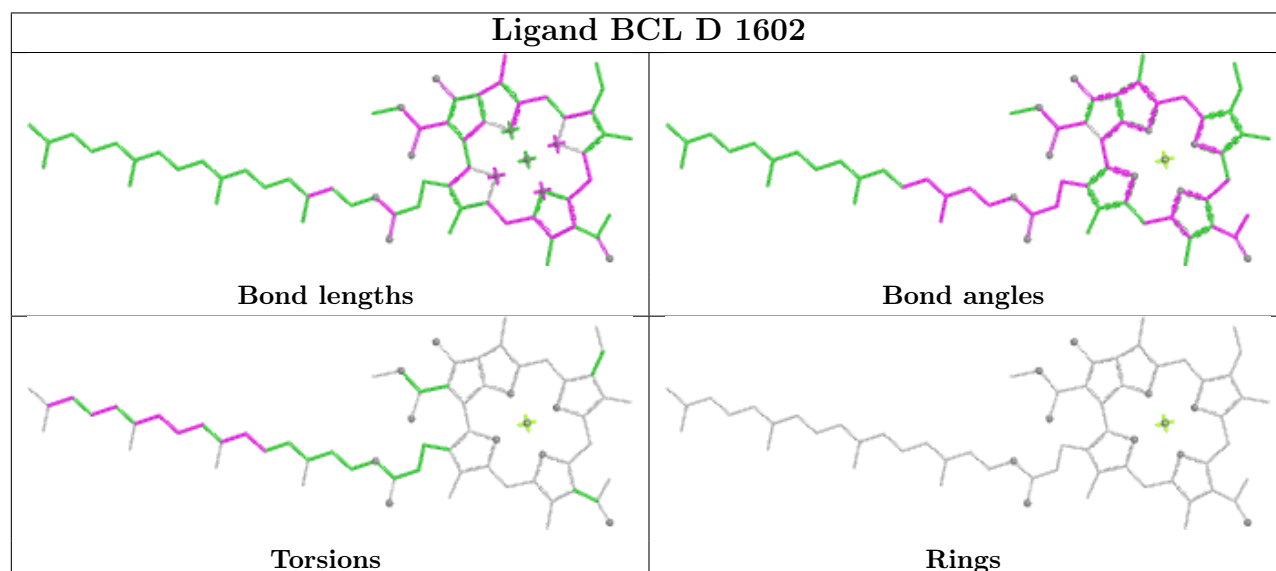
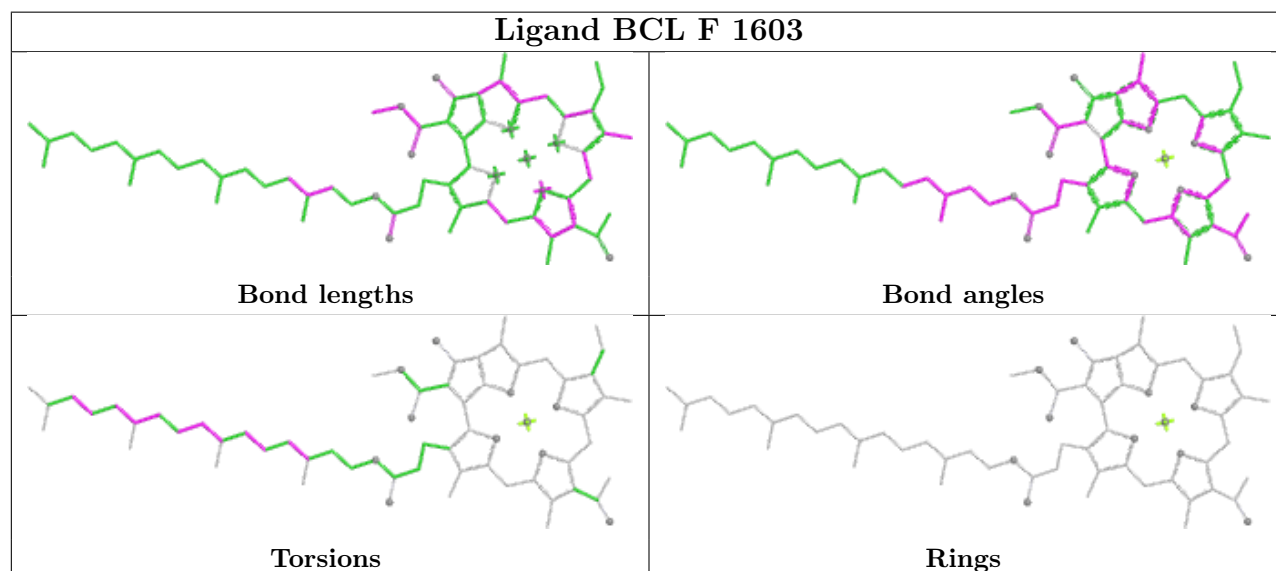
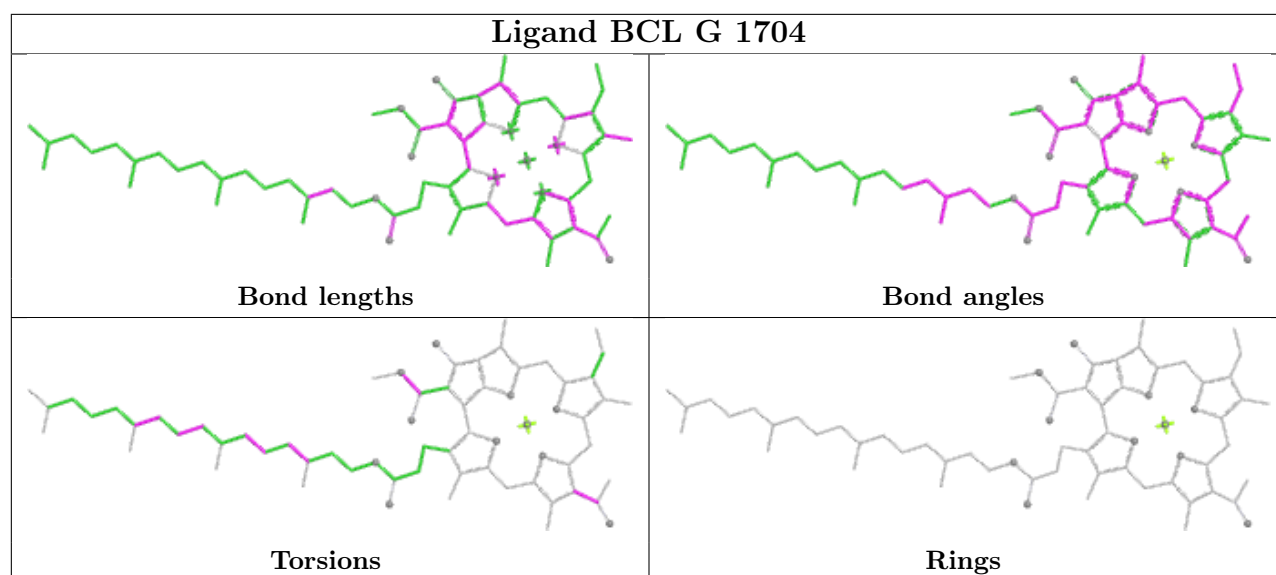
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

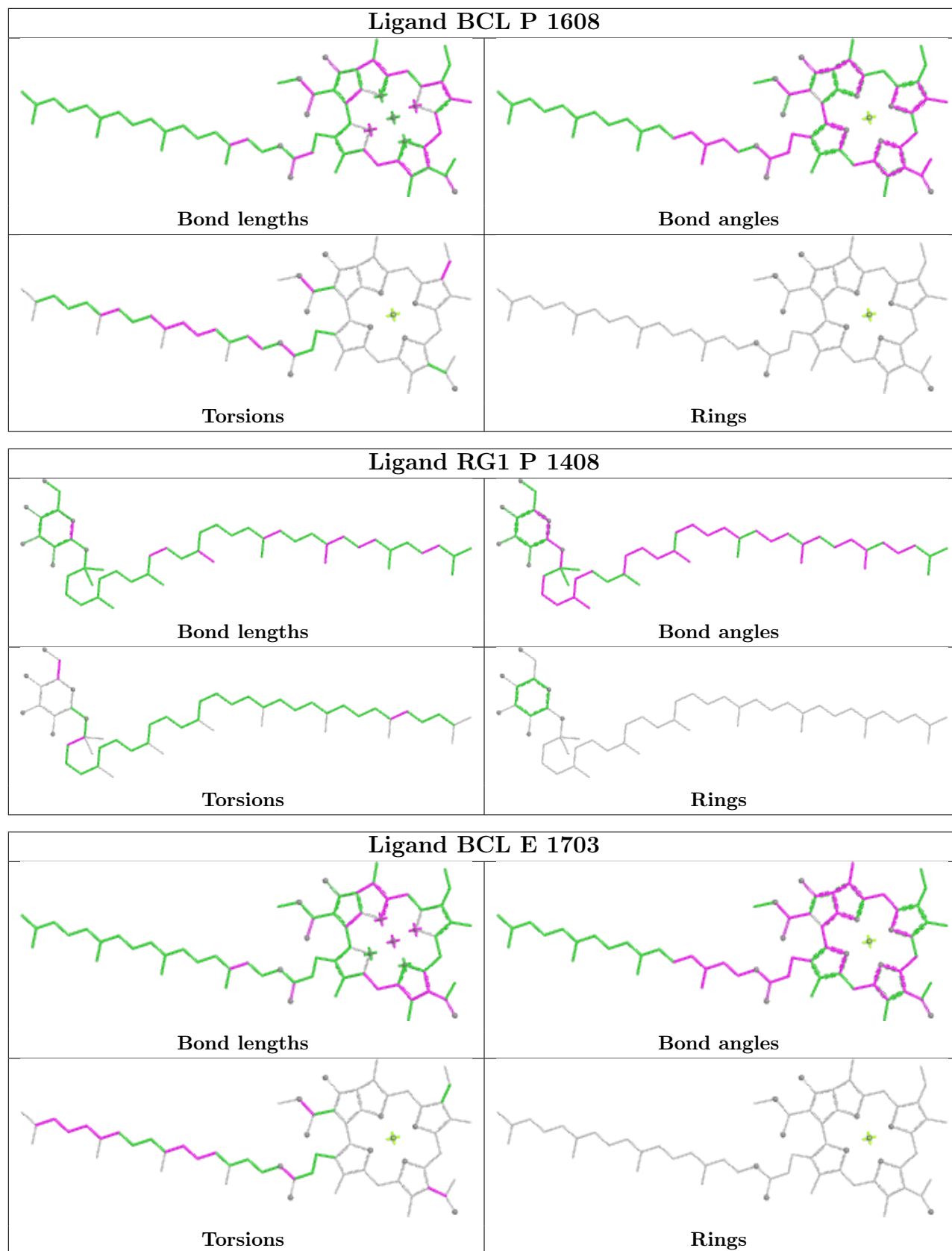


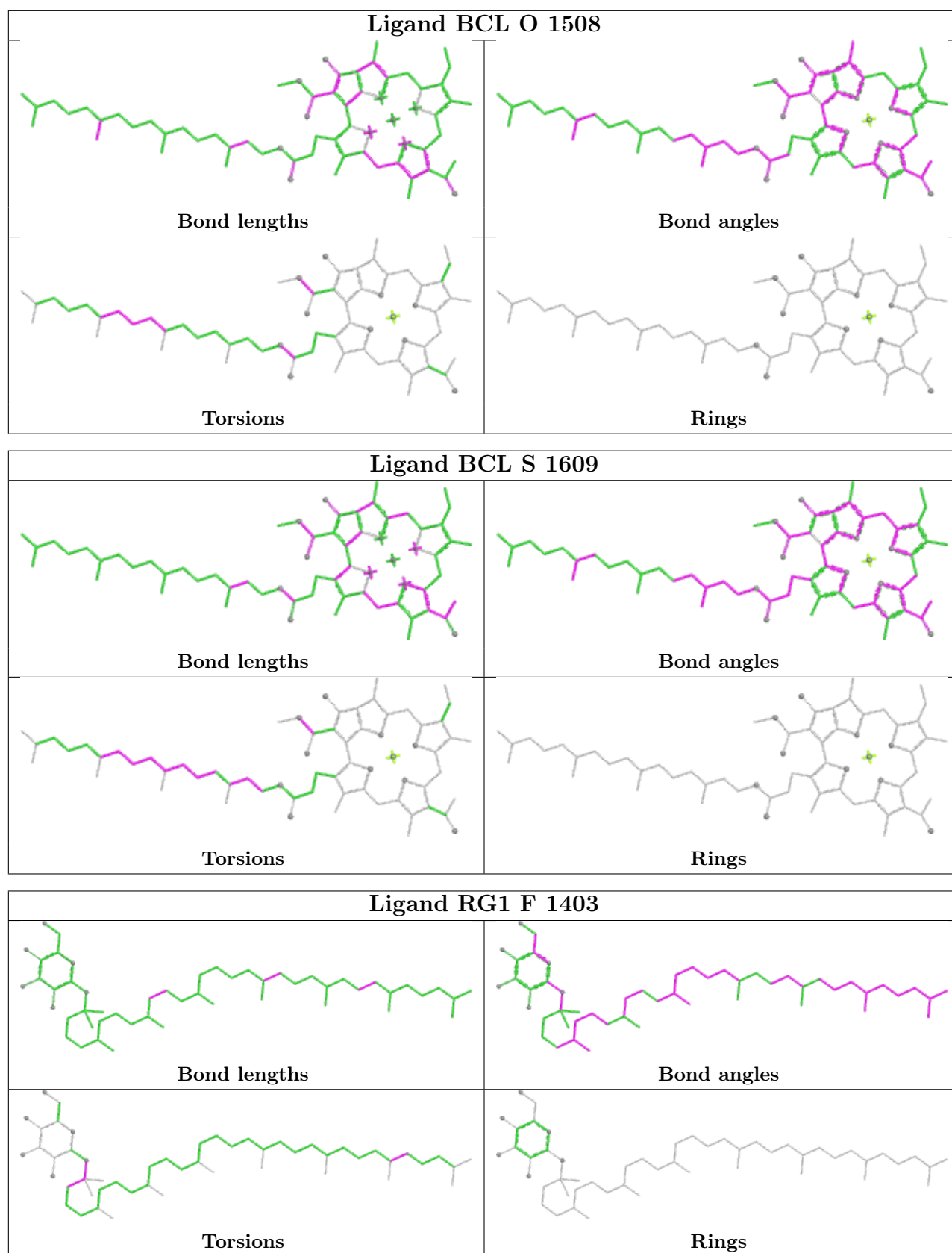




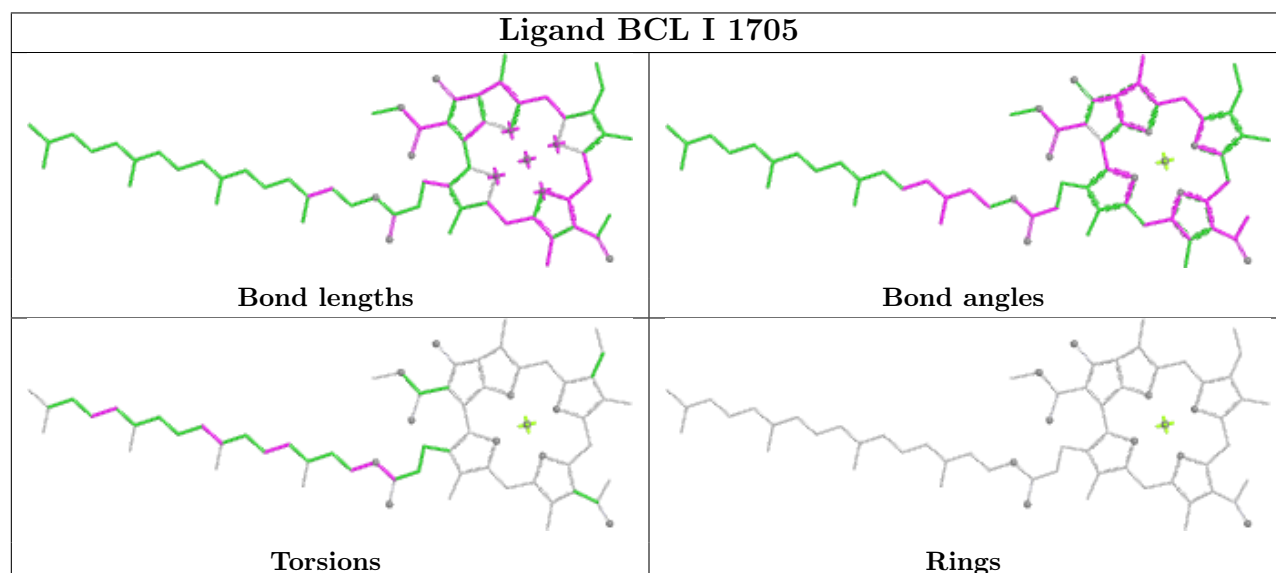
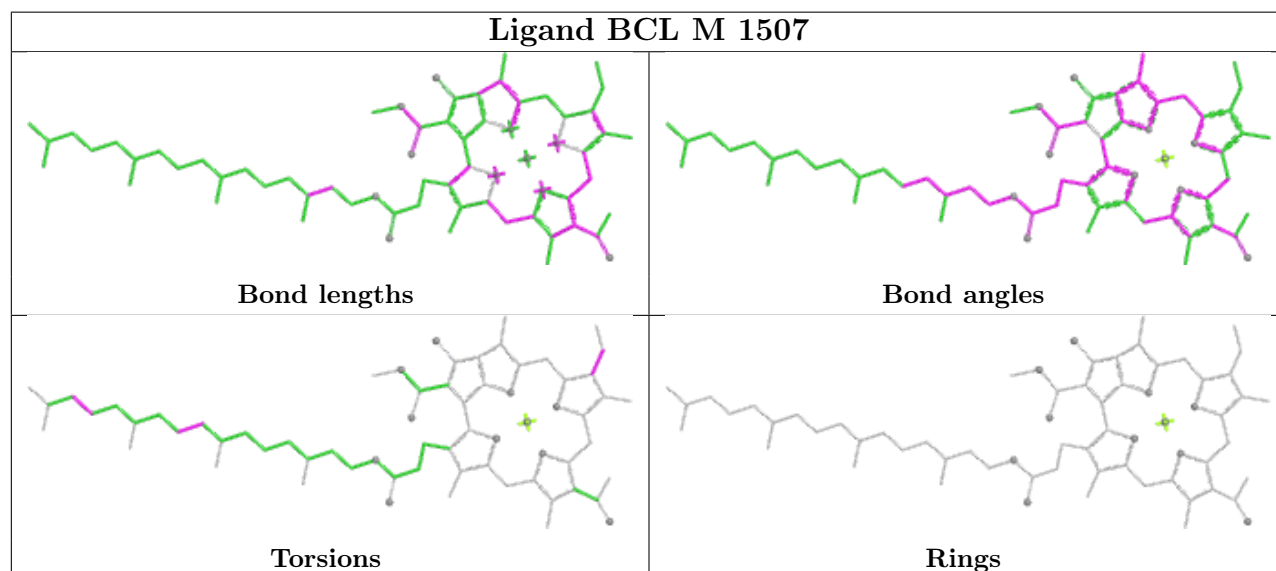
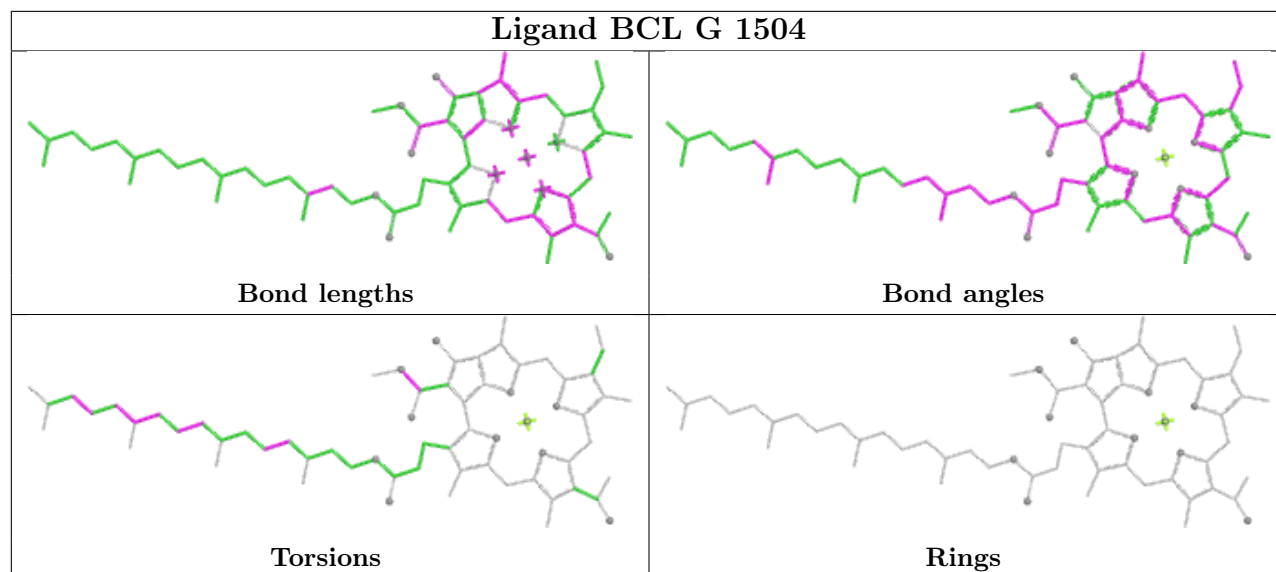


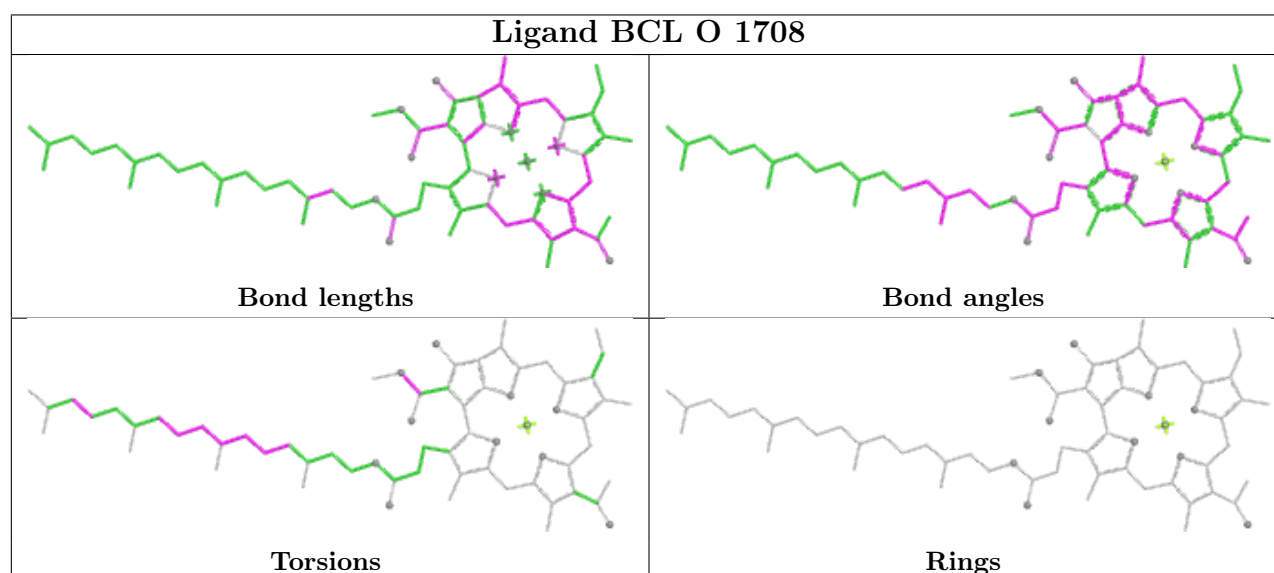
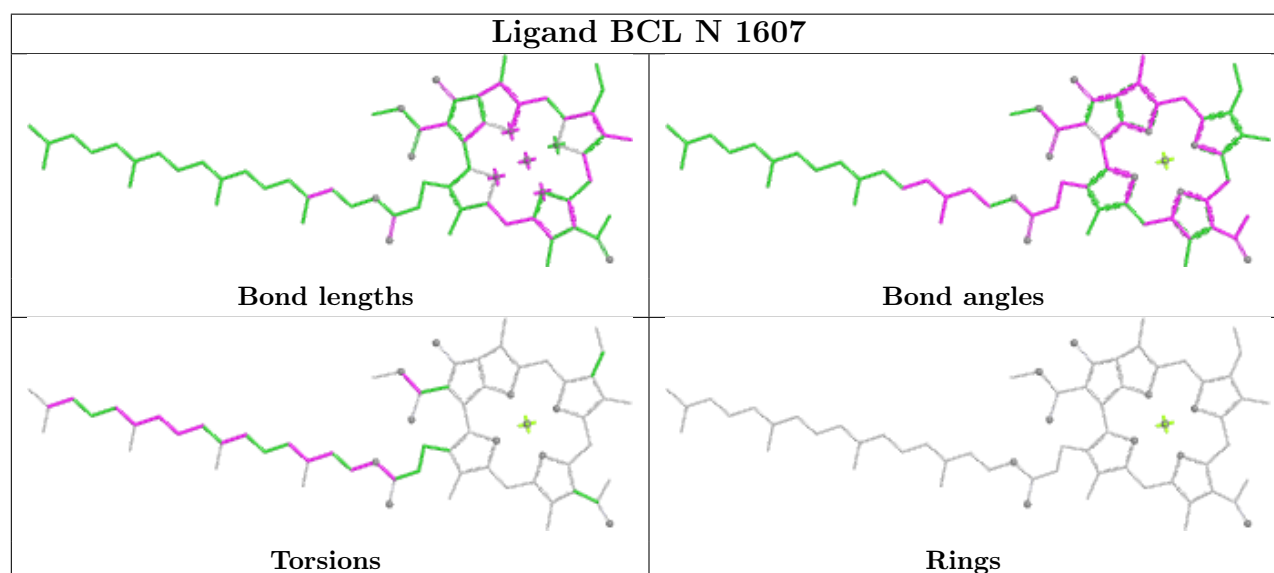
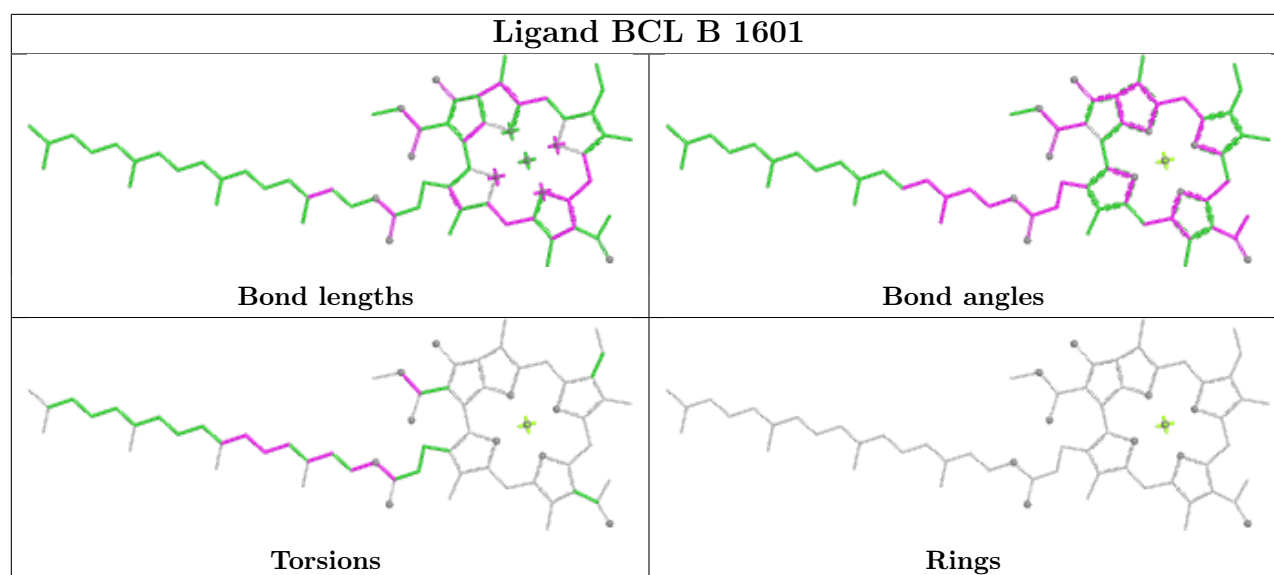


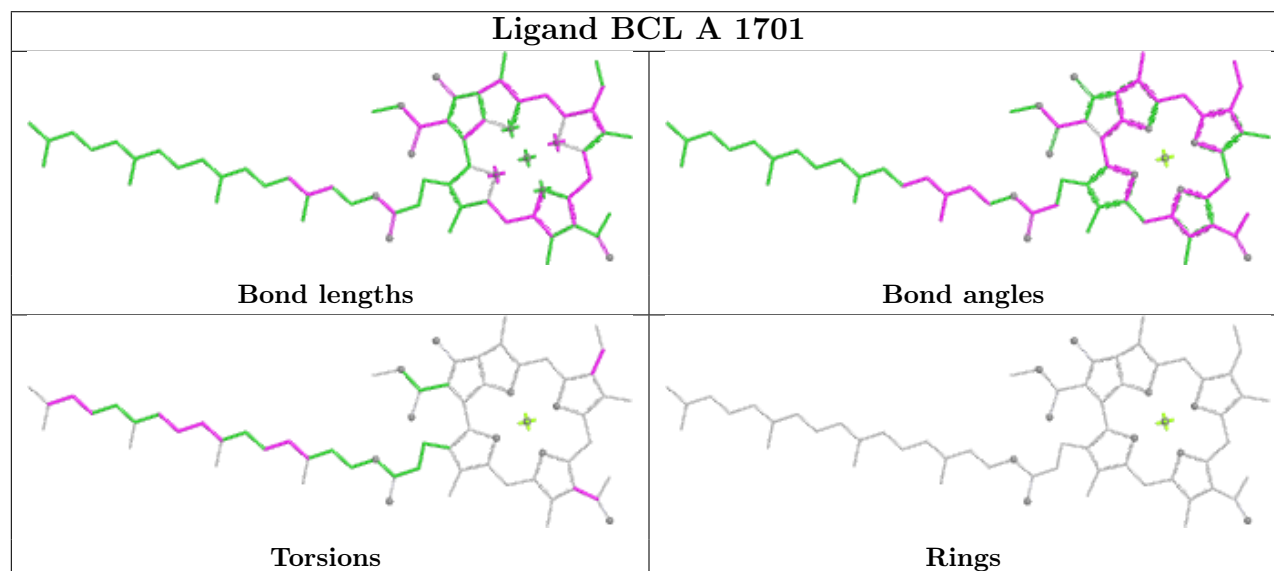
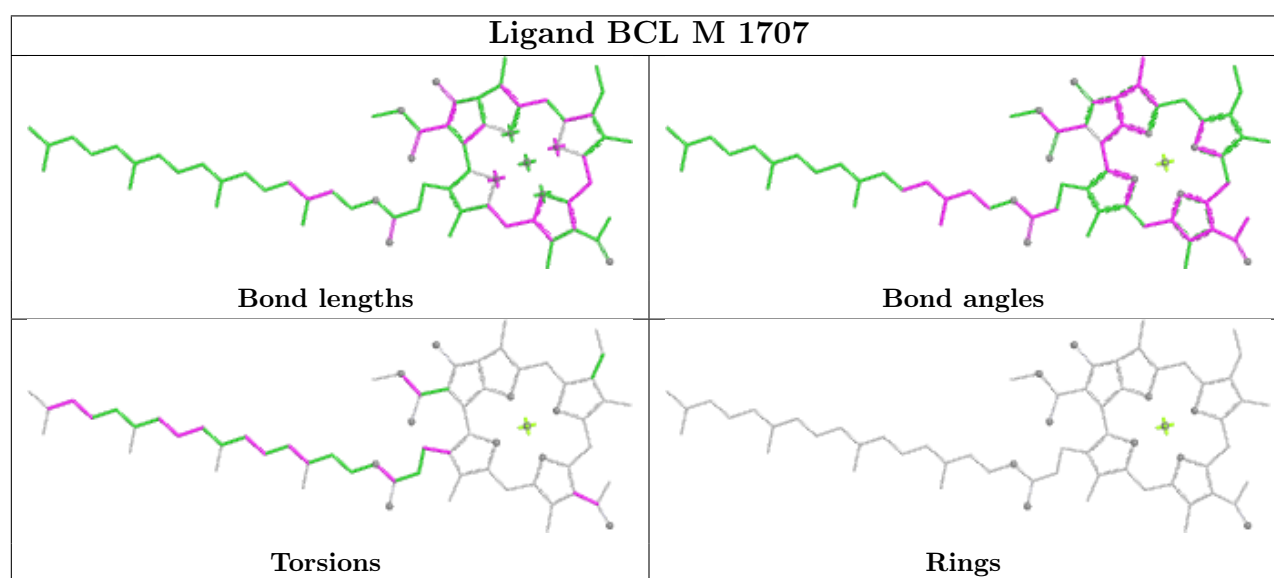
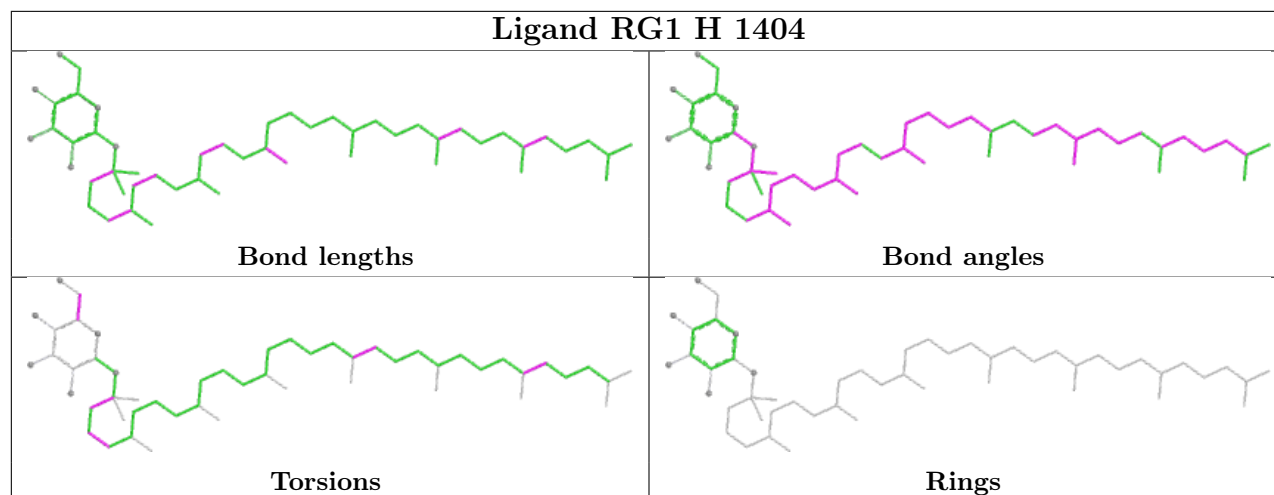


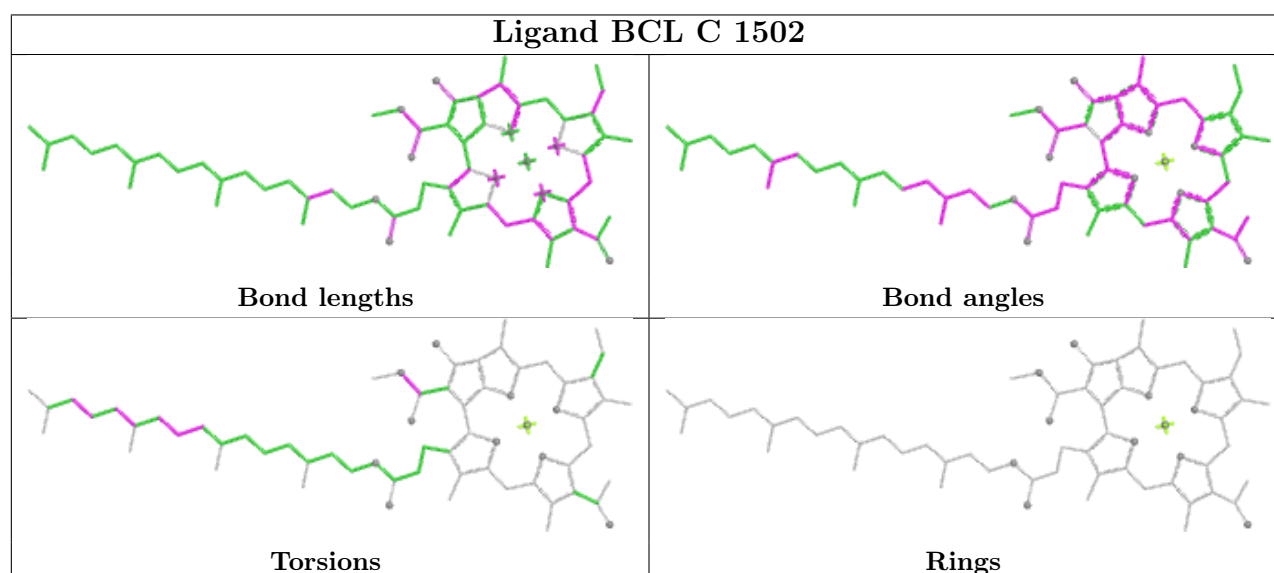
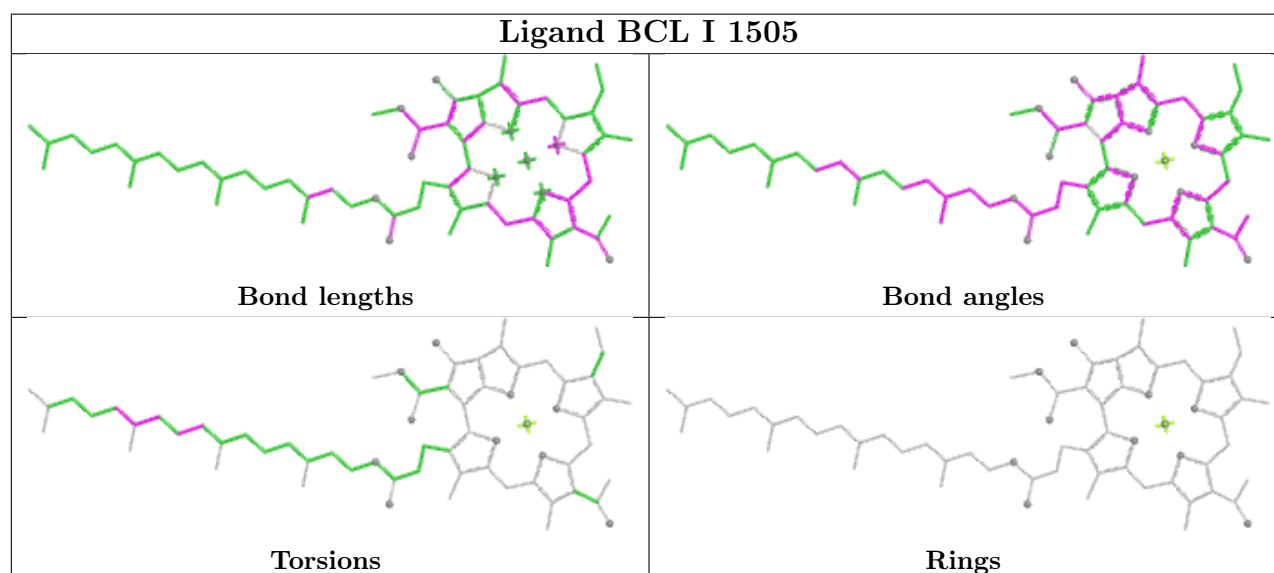
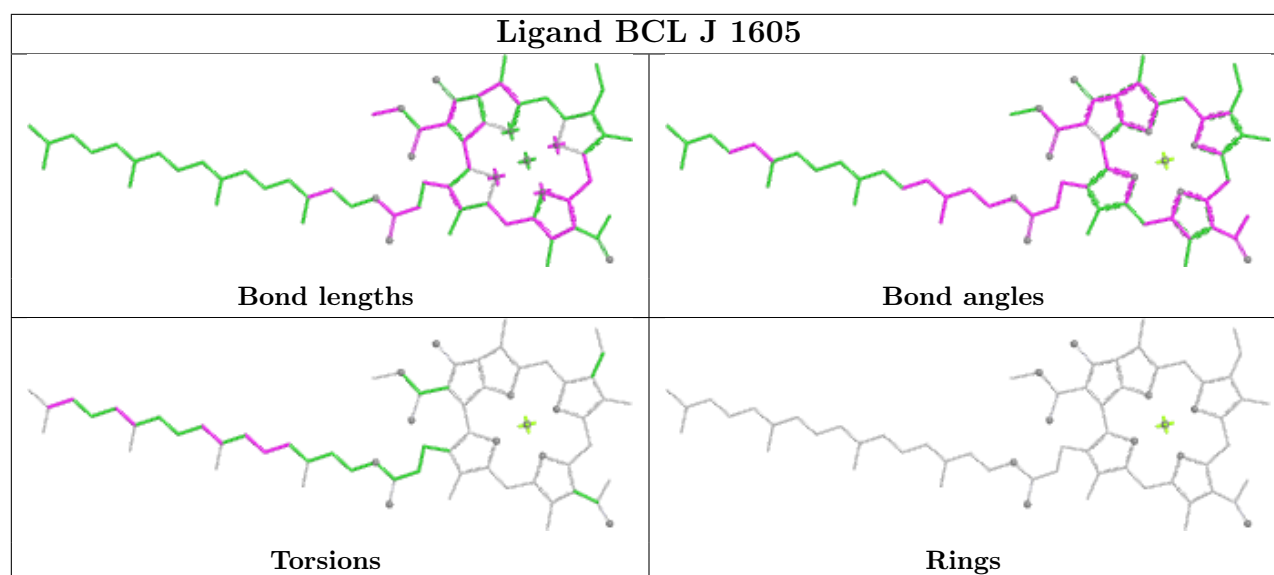


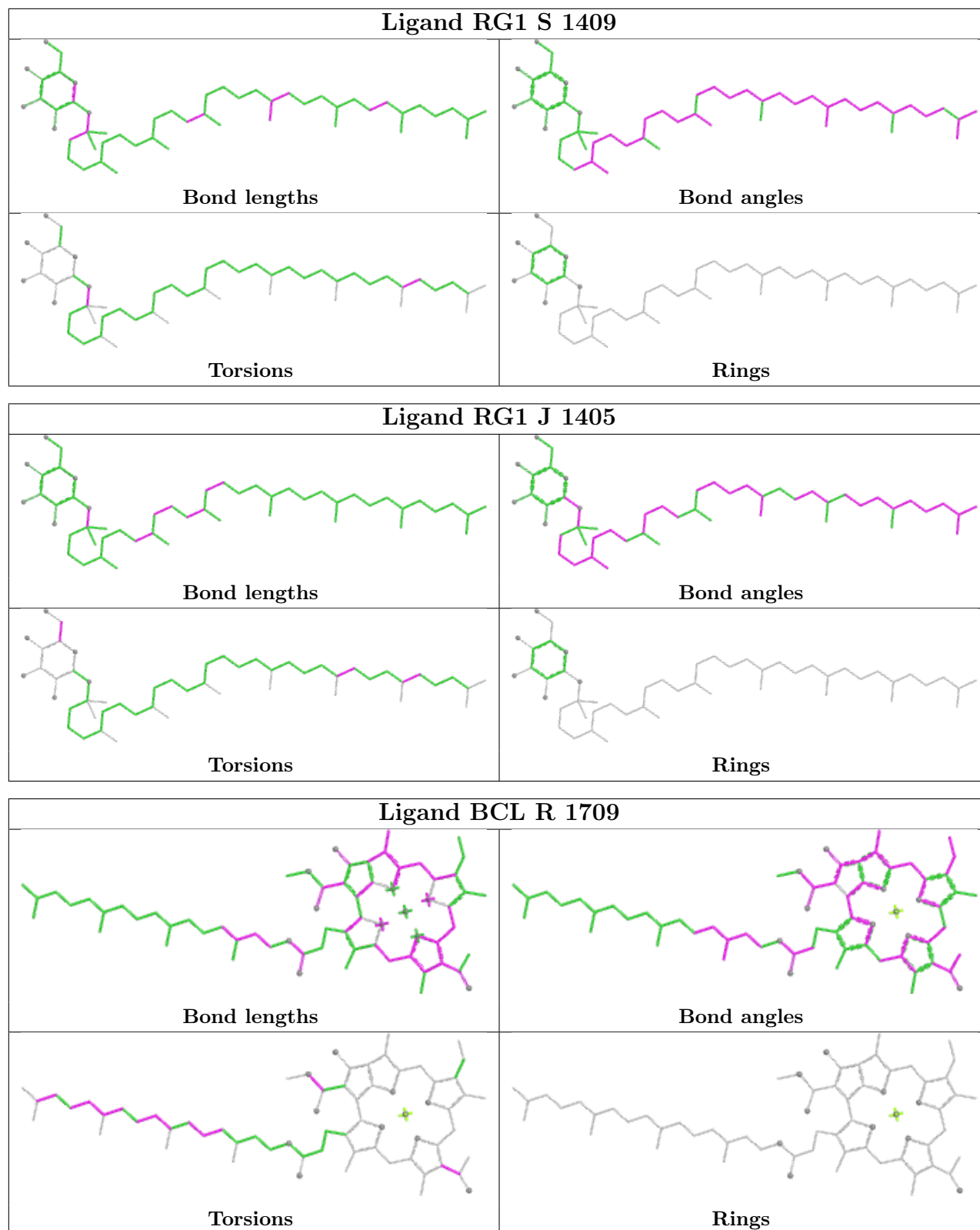


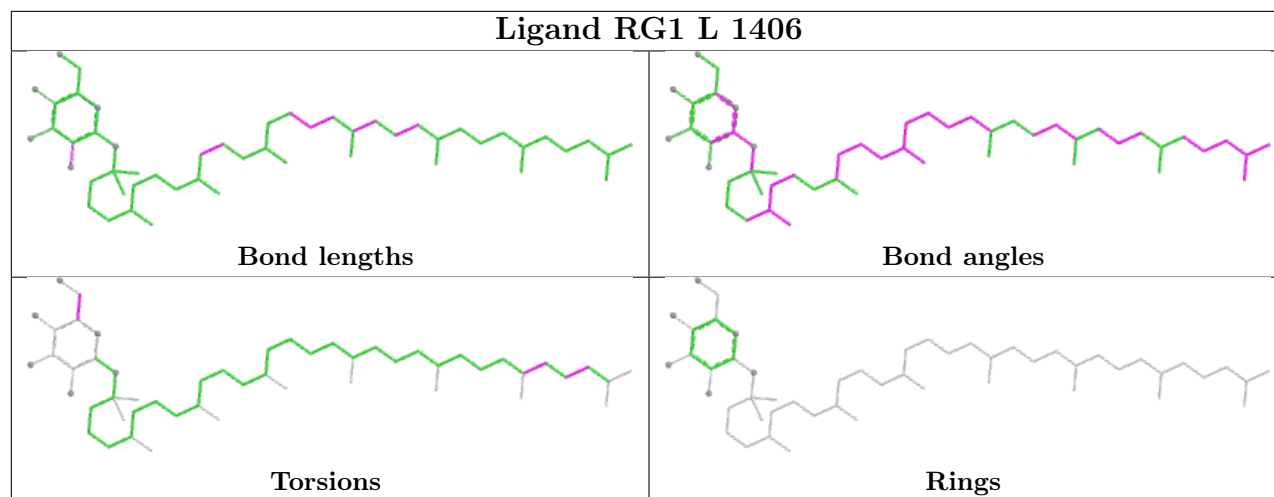












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 52/53 (98%)   | -0.35  | 2 (3%) 44 44  | 35, 41, 88, 98        | 0     |
| 1   | C     | 52/53 (98%)   | -0.20  | 3 (5%) 29 26  | 34, 41, 88, 102       | 0     |
| 1   | E     | 52/53 (98%)   | -0.17  | 3 (5%) 29 26  | 35, 40, 88, 101       | 0     |
| 1   | G     | 52/53 (98%)   | -0.14  | 4 (7%) 19 17  | 33, 40, 87, 99        | 0     |
| 1   | I     | 52/53 (98%)   | -0.20  | 3 (5%) 29 26  | 34, 39, 88, 100       | 0     |
| 1   | K     | 52/53 (98%)   | -0.24  | 2 (3%) 44 44  | 33, 40, 88, 100       | 0     |
| 1   | M     | 52/53 (98%)   | -0.09  | 5 (9%) 13 11  | 35, 40, 88, 101       | 0     |
| 1   | O     | 52/53 (98%)   | -0.20  | 3 (5%) 29 26  | 34, 41, 87, 100       | 0     |
| 1   | R     | 52/53 (98%)   | -0.27  | 3 (5%) 29 26  | 35, 41, 87, 97        | 0     |
| 2   | B     | 41/41 (100%)  | -0.16  | 0 100 100     | 42, 46, 54, 67        | 0     |
| 2   | D     | 41/41 (100%)  | -0.32  | 0 100 100     | 41, 46, 55, 64        | 0     |
| 2   | F     | 41/41 (100%)  | -0.35  | 0 100 100     | 38, 45, 52, 65        | 0     |
| 2   | H     | 41/41 (100%)  | -0.40  | 0 100 100     | 37, 45, 52, 64        | 0     |
| 2   | J     | 41/41 (100%)  | -0.35  | 0 100 100     | 40, 45, 53, 65        | 0     |
| 2   | L     | 41/41 (100%)  | -0.26  | 0 100 100     | 39, 43, 52, 65        | 0     |
| 2   | N     | 41/41 (100%)  | -0.30  | 0 100 100     | 41, 45, 52, 69        | 0     |
| 2   | P     | 41/41 (100%)  | -0.26  | 0 100 100     | 40, 46, 53, 68        | 0     |
| 2   | S     | 41/41 (100%)  | -0.28  | 0 100 100     | 41, 46, 54, 67        | 0     |
| All | All   | 837/846 (98%) | -0.25  | 28 (3%) 49 50 | 33, 43, 79, 102       | 0     |

All (28) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 49  | VAL  | 6.5  |
| 1   | G     | 49  | VAL  | 5.8  |
| 1   | E     | 52  | ALA  | 5.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 49  | VAL  | 4.8  |
| 1   | C     | 49  | VAL  | 4.6  |
| 1   | O     | 49  | VAL  | 4.4  |
| 1   | R     | 49  | VAL  | 4.4  |
| 1   | I     | 49  | VAL  | 4.4  |
| 1   | A     | 49  | VAL  | 4.2  |
| 1   | G     | 52  | ALA  | 4.1  |
| 1   | E     | 49  | VAL  | 4.1  |
| 1   | C     | 53  | ALA  | 4.1  |
| 1   | M     | 52  | ALA  | 3.8  |
| 1   | E     | 53  | ALA  | 3.4  |
| 1   | C     | 52  | ALA  | 3.4  |
| 1   | G     | 48  | GLY  | 3.3  |
| 1   | I     | 50  | LYS  | 3.3  |
| 1   | O     | 48  | GLY  | 3.3  |
| 1   | A     | 53  | ALA  | 3.1  |
| 1   | I     | 52  | ALA  | 3.0  |
| 1   | O     | 50  | LYS  | 2.8  |
| 1   | M     | 48  | GLY  | 2.7  |
| 1   | M     | 50  | LYS  | 2.4  |
| 1   | R     | 52  | ALA  | 2.4  |
| 1   | K     | 48  | GLY  | 2.4  |
| 1   | M     | 51  | LYS  | 2.4  |
| 1   | G     | 53  | ALA  | 2.2  |
| 1   | R     | 48  | GLY  | 2.1  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1   | CXM  | C     | 1   | 11/12 | 0.89 | 0.10 | 45,47,55,58                | 0     |
| 1   | CXM  | A     | 1   | 11/12 | 0.92 | 0.08 | 45,48,60,62                | 0     |
| 1   | CXM  | G     | 1   | 11/12 | 0.92 | 0.07 | 45,46,52,58                | 0     |
| 1   | CXM  | R     | 1   | 11/12 | 0.92 | 0.07 | 45,48,54,59                | 0     |
| 1   | CXM  | M     | 1   | 11/12 | 0.93 | 0.07 | 40,45,51,52                | 0     |
| 1   | CXM  | K     | 1   | 11/12 | 0.93 | 0.07 | 40,46,54,54                | 0     |
| 1   | CXM  | O     | 1   | 11/12 | 0.95 | 0.06 | 45,47,54,58                | 0     |
| 1   | CXM  | E     | 1   | 11/12 | 0.95 | 0.06 | 41,46,48,50                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 1   | CXM  | I     | 1   | 11/12 | 0.97 | 0.05 | 38,45,51,52                 | 0     |

## 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | LDA  | K     | 1810 | 16/16 | 0.41 | 0.19 | 107,110,116,116             | 0     |
| 4   | LDA  | A     | 1816 | 16/16 | 0.49 | 0.17 | 86,87,91,93                 | 0     |
| 4   | LDA  | C     | 1815 | 16/16 | 0.53 | 0.15 | 79,96,103,103               | 0     |
| 4   | LDA  | M     | 1811 | 16/16 | 0.54 | 0.14 | 75,77,84,84                 | 0     |
| 4   | LDA  | E     | 1823 | 16/16 | 0.55 | 0.14 | 89,99,122,123               | 0     |
| 4   | LDA  | C     | 1821 | 16/16 | 0.57 | 0.12 | 82,90,101,103               | 0     |
| 4   | LDA  | G     | 1814 | 16/16 | 0.57 | 0.16 | 70,74,83,84                 | 0     |
| 4   | LDA  | R     | 1818 | 16/16 | 0.60 | 0.14 | 85,90,95,96                 | 0     |
| 4   | LDA  | I     | 1812 | 16/16 | 0.61 | 0.19 | 87,106,111,111              | 0     |
| 4   | LDA  | N     | 1807 | 16/16 | 0.62 | 0.16 | 61,66,76,78                 | 0     |
| 4   | LDA  | R     | 1819 | 16/16 | 0.62 | 0.12 | 80,83,85,87                 | 0     |
| 4   | LDA  | I     | 1825 | 16/16 | 0.63 | 0.13 | 95,101,108,108              | 0     |
| 4   | LDA  | E     | 1822 | 16/16 | 0.66 | 0.12 | 69,91,107,108               | 0     |
| 4   | LDA  | G     | 1824 | 16/16 | 0.67 | 0.12 | 89,105,120,121              | 0     |
| 4   | LDA  | M     | 1827 | 16/16 | 0.69 | 0.14 | 96,101,105,107              | 0     |
| 4   | LDA  | O     | 1820 | 16/16 | 0.71 | 0.10 | 71,80,92,95                 | 0     |
| 4   | LDA  | R     | 1809 | 16/16 | 0.72 | 0.11 | 57,63,71,73                 | 0     |
| 4   | LDA  | B     | 1801 | 16/16 | 0.72 | 0.13 | 49,62,76,78                 | 0     |
| 4   | LDA  | P     | 1808 | 16/16 | 0.72 | 0.14 | 53,61,84,86                 | 0     |
| 4   | LDA  | A     | 1817 | 16/16 | 0.74 | 0.11 | 67,69,87,87                 | 0     |
| 4   | LDA  | D     | 1802 | 16/16 | 0.77 | 0.10 | 53,57,75,77                 | 0     |
| 4   | LDA  | J     | 1805 | 16/16 | 0.78 | 0.11 | 44,54,67,68                 | 0     |
| 4   | LDA  | K     | 1826 | 16/16 | 0.79 | 0.10 | 83,88,103,104               | 0     |
| 4   | LDA  | I     | 1813 | 16/16 | 0.79 | 0.09 | 50,54,76,76                 | 0     |
| 4   | LDA  | H     | 1804 | 16/16 | 0.79 | 0.11 | 49,57,66,67                 | 0     |
| 4   | LDA  | F     | 1803 | 16/16 | 0.81 | 0.10 | 50,56,67,67                 | 0     |
| 4   | LDA  | L     | 1806 | 16/16 | 0.83 | 0.11 | 44,52,74,75                 | 0     |

*Continued on next page...*

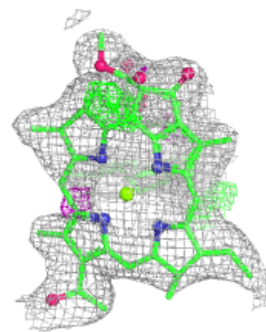
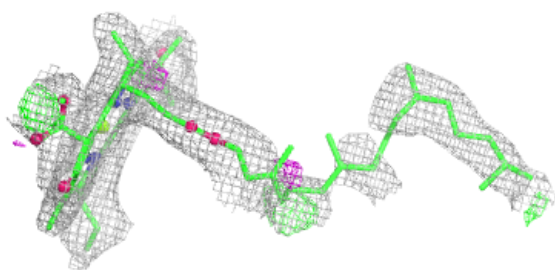
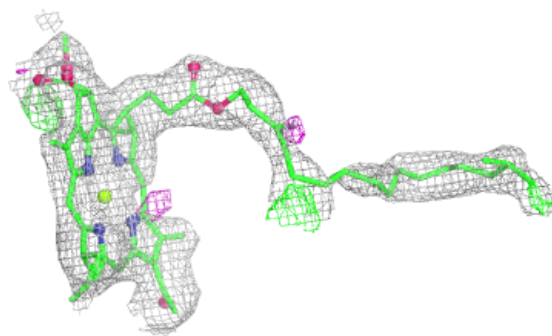
*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | BCL  | R     | 1709 | 66/66 | 0.84 | 0.09 | 43,53,78,82                 | 0     |
| 3   | BCL  | G     | 1704 | 66/66 | 0.86 | 0.09 | 32,45,73,76                 | 0     |
| 3   | BCL  | C     | 1702 | 66/66 | 0.87 | 0.08 | 41,48,78,80                 | 0     |
| 3   | BCL  | M     | 1707 | 66/66 | 0.89 | 0.08 | 29,44,74,76                 | 0     |
| 3   | BCL  | A     | 1701 | 66/66 | 0.90 | 0.07 | 42,49,80,83                 | 0     |
| 3   | BCL  | O     | 1708 | 66/66 | 0.90 | 0.08 | 42,50,79,81                 | 0     |
| 3   | BCL  | N     | 1607 | 66/66 | 0.91 | 0.08 | 31,41,63,65                 | 0     |
| 3   | BCL  | I     | 1705 | 66/66 | 0.91 | 0.07 | 34,41,73,75                 | 0     |
| 3   | BCL  | E     | 1703 | 66/66 | 0.91 | 0.07 | 29,37,69,72                 | 0     |
| 5   | RG1  | P     | 1408 | 52/52 | 0.91 | 0.07 | 32,42,75,78                 | 0     |
| 5   | RG1  | R     | 1401 | 52/52 | 0.91 | 0.07 | 30,40,74,77                 | 0     |
| 3   | BCL  | K     | 1706 | 66/66 | 0.92 | 0.07 | 27,36,78,82                 | 0     |
| 5   | RG1  | N     | 1407 | 52/52 | 0.92 | 0.06 | 29,37,69,73                 | 0     |
| 3   | BCL  | F     | 1603 | 66/66 | 0.93 | 0.07 | 26,35,62,64                 | 0     |
| 3   | BCL  | J     | 1605 | 66/66 | 0.93 | 0.07 | 31,39,64,66                 | 0     |
| 3   | BCL  | K     | 1506 | 66/66 | 0.93 | 0.06 | 28,35,47,51                 | 0     |
| 5   | RG1  | D     | 1402 | 52/52 | 0.93 | 0.06 | 30,44,77,81                 | 0     |
| 5   | RG1  | F     | 1403 | 52/52 | 0.93 | 0.07 | 28,38,77,82                 | 0     |
| 5   | RG1  | J     | 1405 | 52/52 | 0.93 | 0.07 | 28,37,76,80                 | 0     |
| 5   | RG1  | L     | 1406 | 52/52 | 0.93 | 0.06 | 26,35,74,77                 | 0     |
| 3   | BCL  | P     | 1608 | 66/66 | 0.93 | 0.07 | 34,42,66,68                 | 0     |
| 3   | BCL  | R     | 1509 | 66/66 | 0.93 | 0.06 | 31,38,49,57                 | 0     |
| 3   | BCL  | A     | 1501 | 66/66 | 0.93 | 0.06 | 33,42,51,65                 | 0     |
| 5   | RG1  | S     | 1409 | 52/52 | 0.93 | 0.06 | 29,40,77,78                 | 0     |
| 3   | BCL  | D     | 1602 | 66/66 | 0.94 | 0.07 | 30,37,64,67                 | 0     |
| 3   | BCL  | E     | 1503 | 66/66 | 0.94 | 0.05 | 28,35,46,49                 | 0     |
| 5   | RG1  | H     | 1404 | 52/52 | 0.94 | 0.07 | 27,37,78,80                 | 0     |
| 3   | BCL  | H     | 1604 | 66/66 | 0.94 | 0.07 | 29,39,63,64                 | 0     |
| 3   | BCL  | L     | 1606 | 66/66 | 0.94 | 0.06 | 27,36,66,69                 | 0     |
| 3   | BCL  | S     | 1609 | 66/66 | 0.94 | 0.07 | 31,41,69,72                 | 0     |
| 3   | BCL  | I     | 1505 | 66/66 | 0.94 | 0.06 | 28,36,42,48                 | 0     |
| 3   | BCL  | B     | 1601 | 66/66 | 0.94 | 0.07 | 33,42,67,68                 | 0     |
| 3   | BCL  | O     | 1508 | 66/66 | 0.94 | 0.05 | 30,37,46,54                 | 0     |
| 3   | BCL  | M     | 1507 | 66/66 | 0.95 | 0.05 | 27,35,41,48                 | 0     |
| 3   | BCL  | C     | 1502 | 66/66 | 0.95 | 0.05 | 33,38,50,57                 | 0     |
| 3   | BCL  | G     | 1504 | 66/66 | 0.95 | 0.05 | 26,34,44,49                 | 0     |

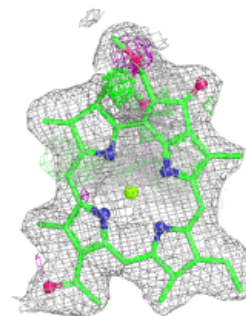
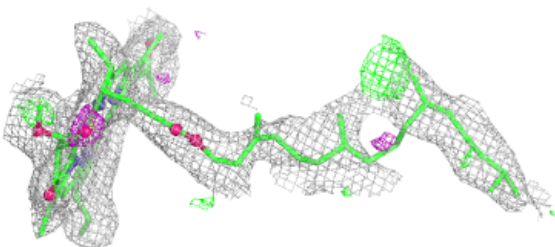
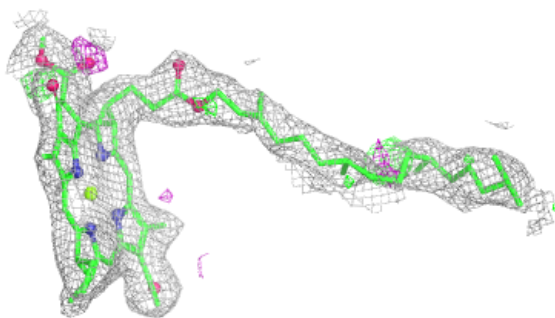
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BCL R 1709:**

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

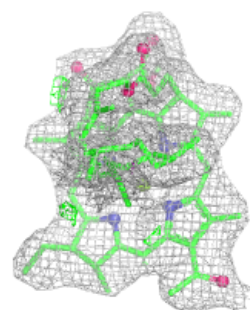
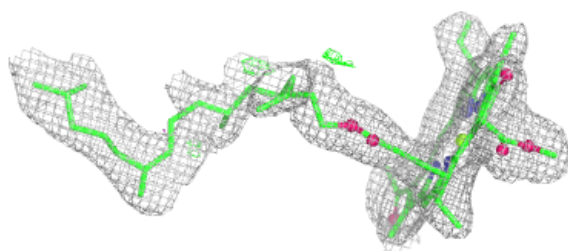
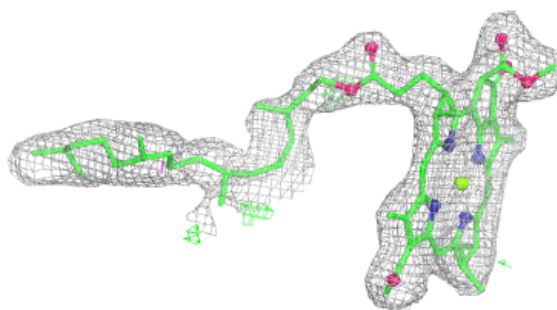
**Electron density around BCL G 1704:**

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

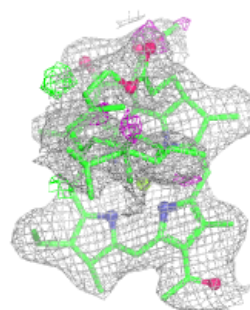
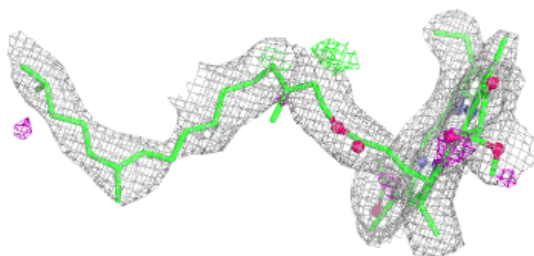
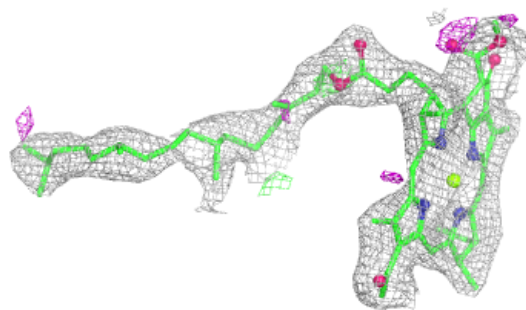


**Electron density around BCL C 1702:**

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

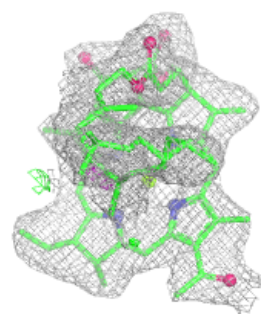
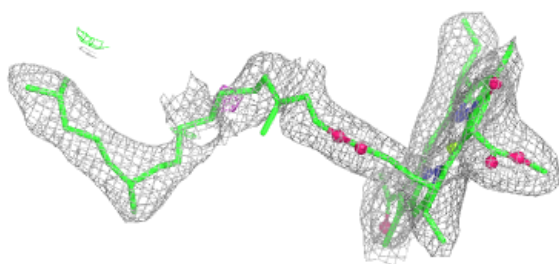
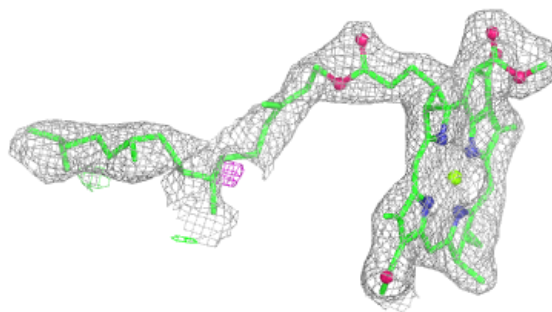
**Electron density around BCL M 1707:**

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

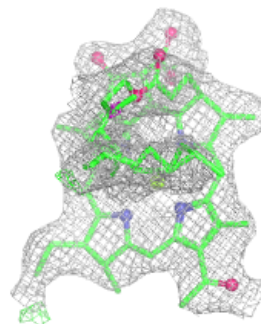
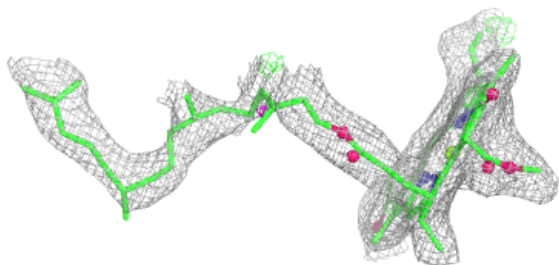
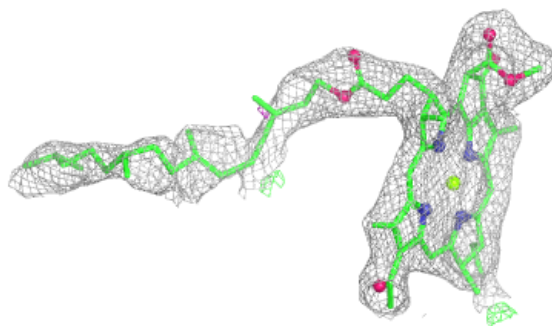


**Electron density around BCL A 1701:**

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

**Electron density around BCL O 1708:**

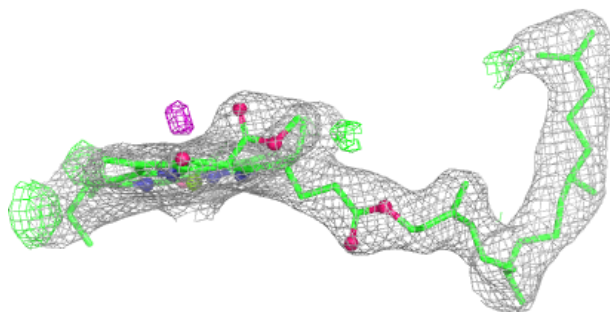
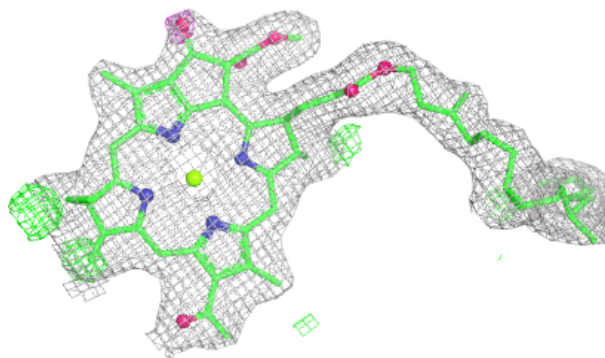
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



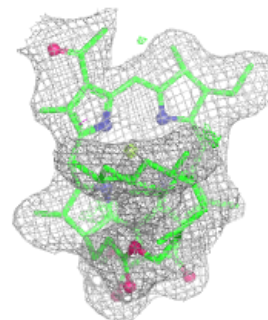
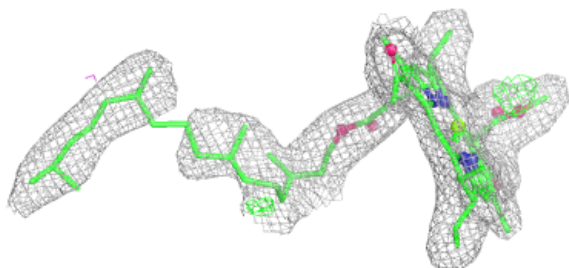
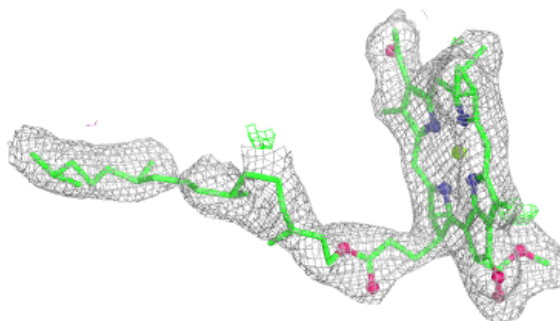


**Electron density around BCL N 1607:**

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

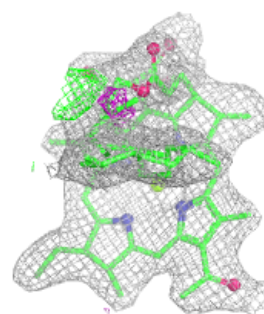
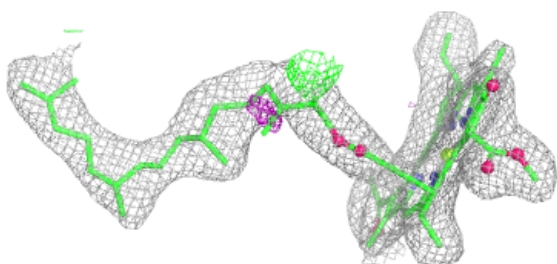
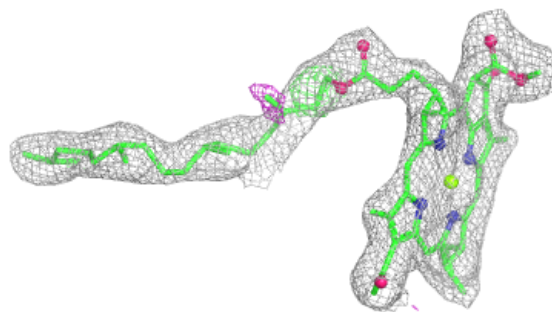
**Electron density around BCL I 1705:**

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

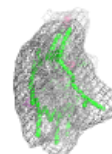
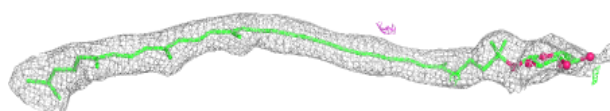
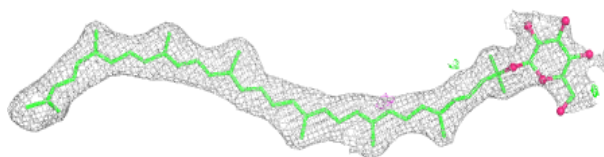


**Electron density around BCL E 1703:**

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

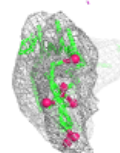
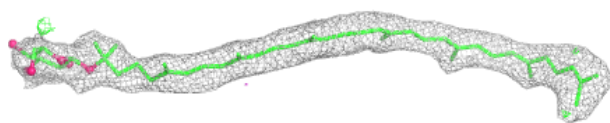
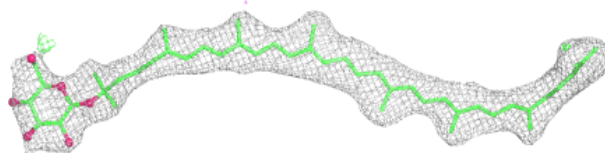
**Electron density around RG1 P 1408:**

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

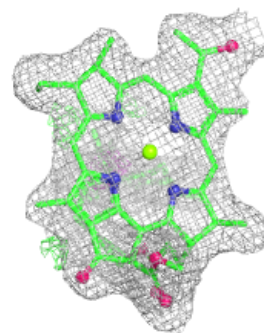
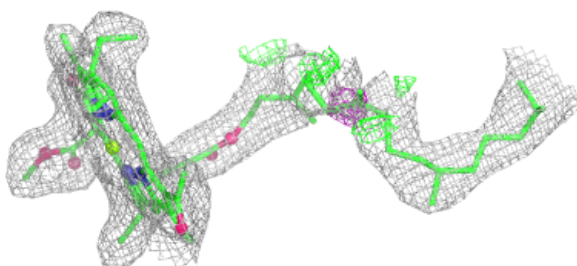
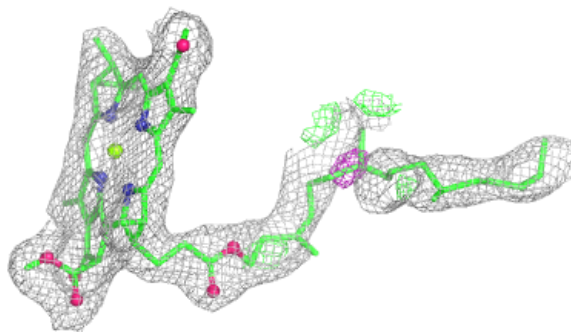


**Electron density around RG1 R 1401:**

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

**Electron density around BCL K 1706:**

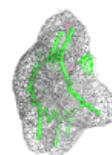
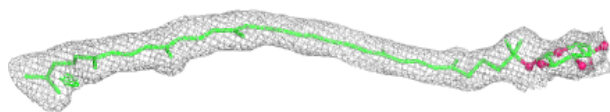
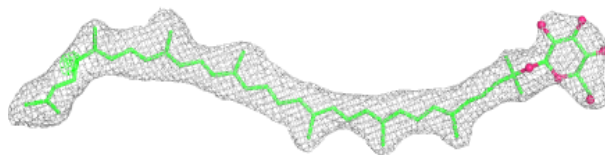
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



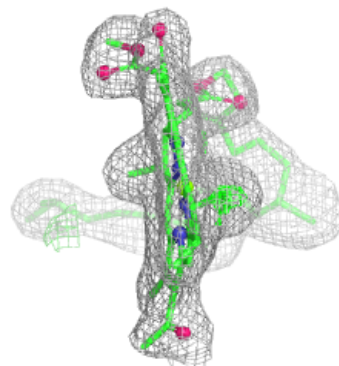
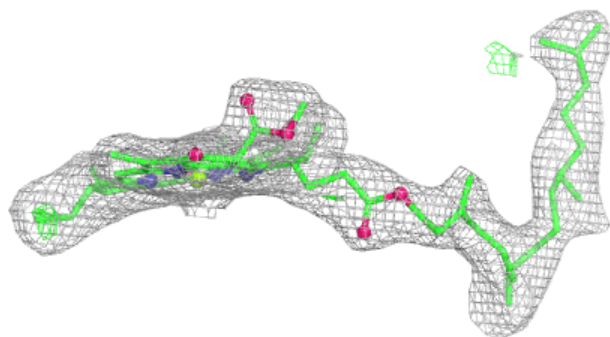
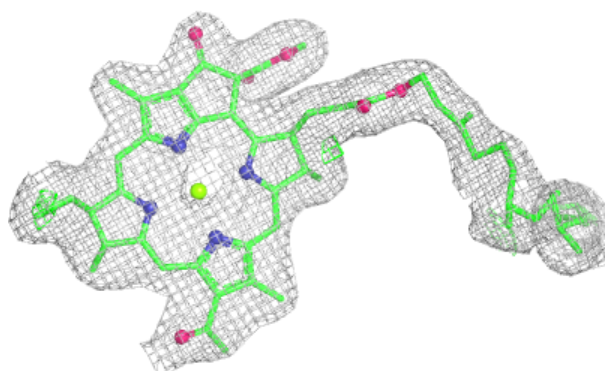


**Electron density around RG1 N 1407:**

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and green (positive)

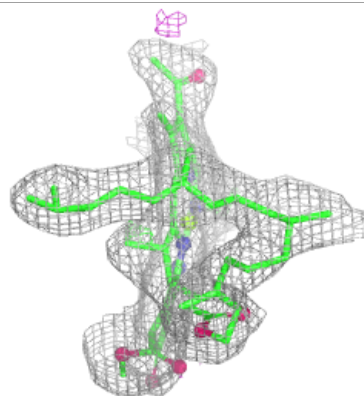
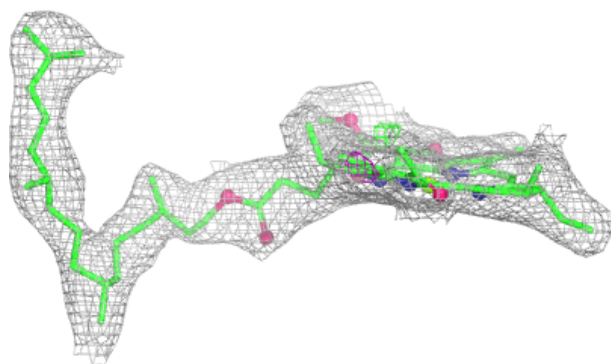
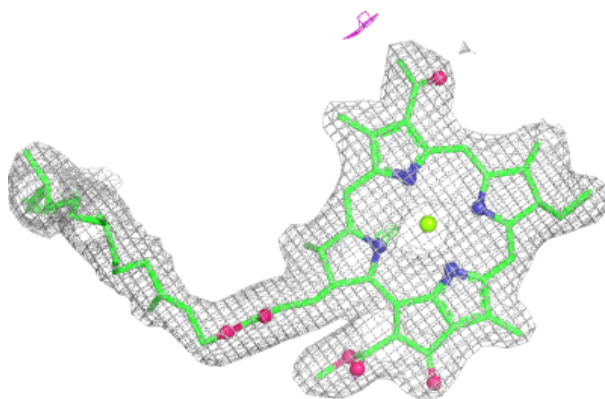
**Electron density around BCL F 1603:**

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

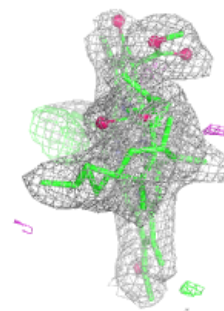
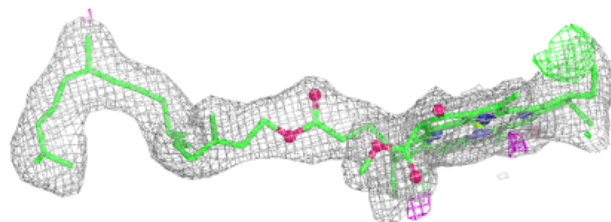
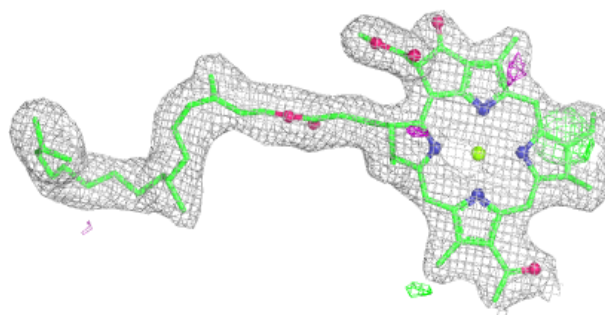


**Electron density around BCL J 1605:**

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

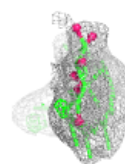
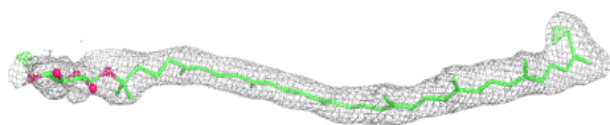
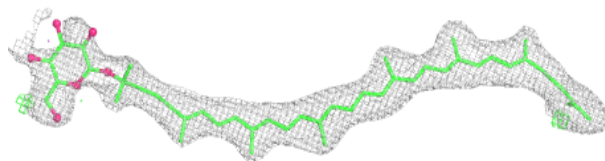
**Electron density around BCL K 1506:**

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

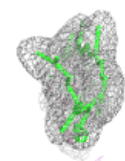
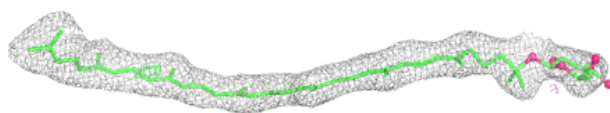
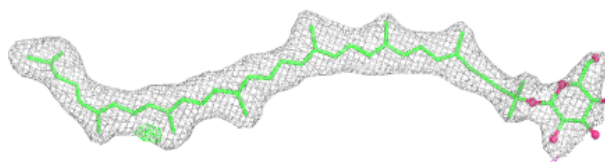


**Electron density around RG1 D 1402:**

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

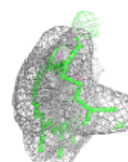
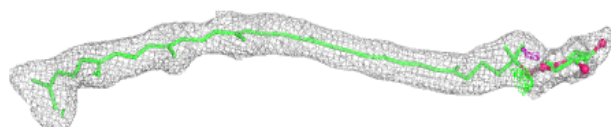
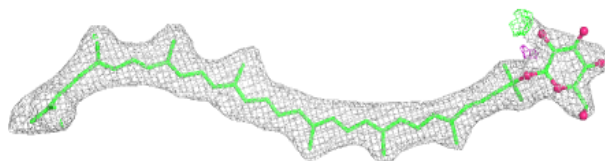
**Electron density around RG1 F 1403:**

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

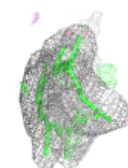
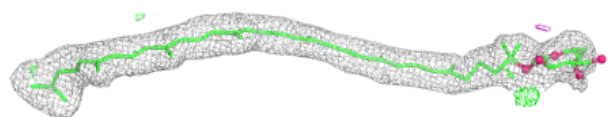
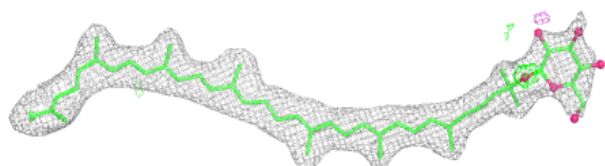


**Electron density around RG1 J 1405:**

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

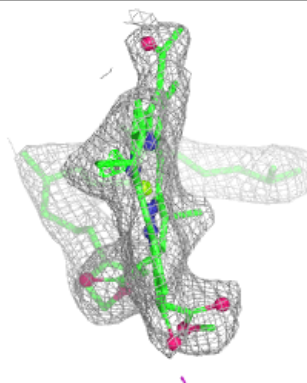
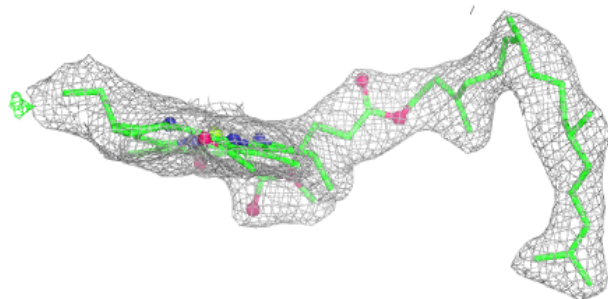
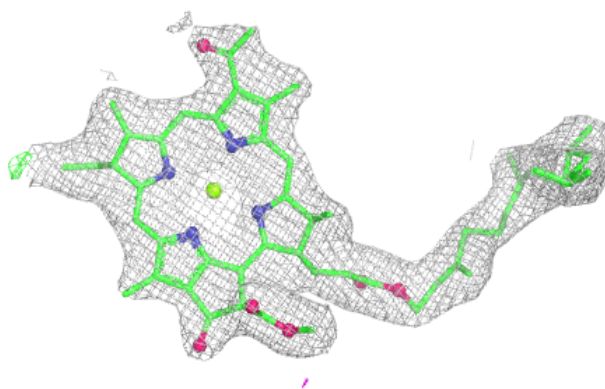
**Electron density around RG1 L 1406:**

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

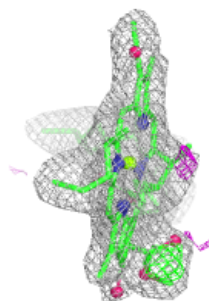
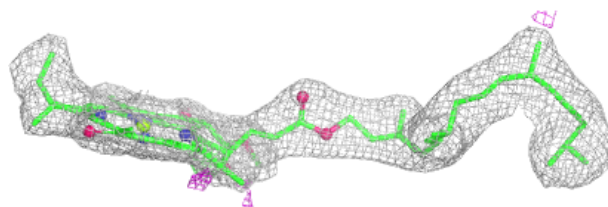


**Electron density around BCL P 1608:**

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

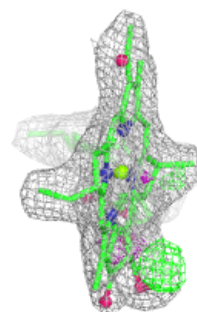
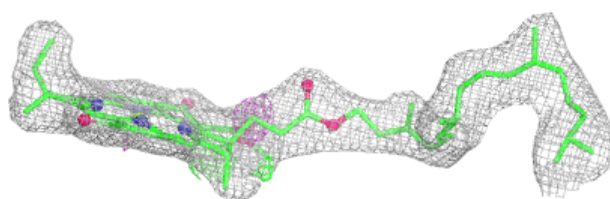
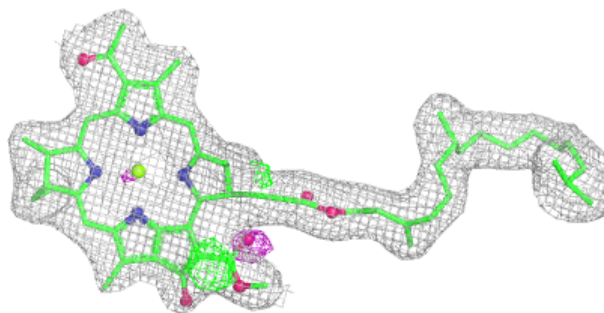
**Electron density around BCL R 1509:**

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

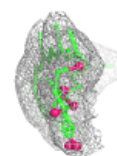
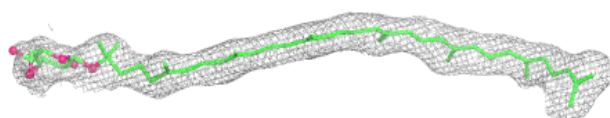
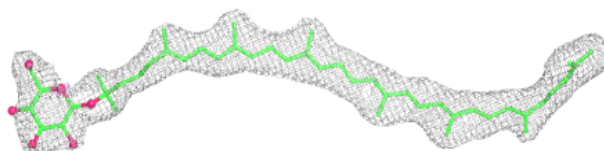


**Electron density around BCL A 1501:**

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

**Electron density around RG1 S 1409:**

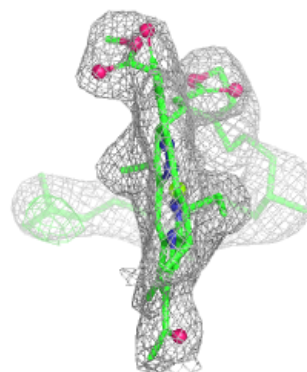
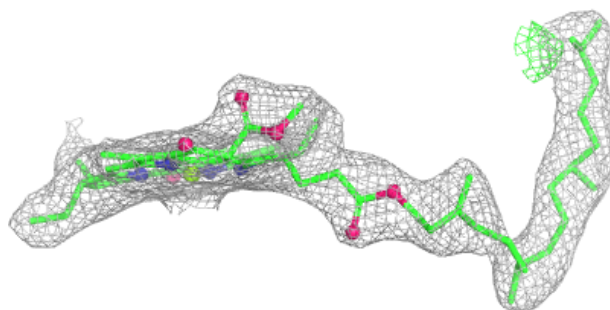
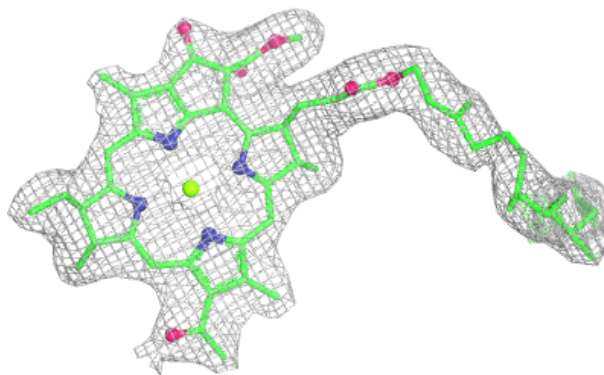
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



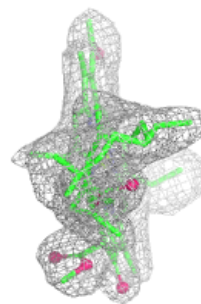
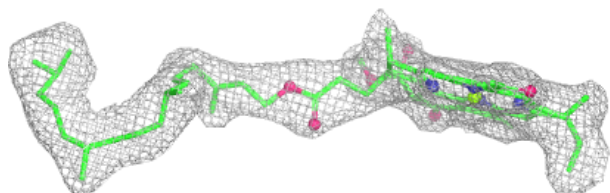
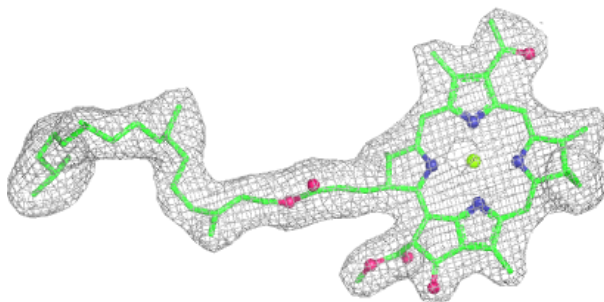


**Electron density around BCL D 1602:**

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

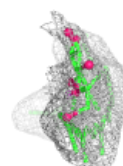
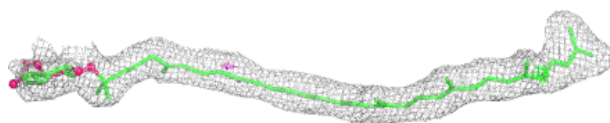
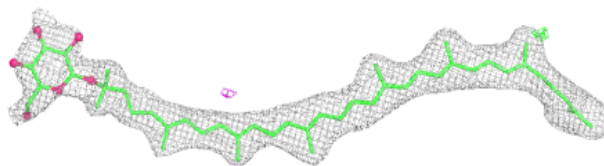
**Electron density around BCL E 1503:**

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

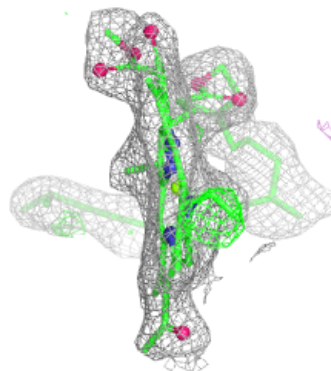
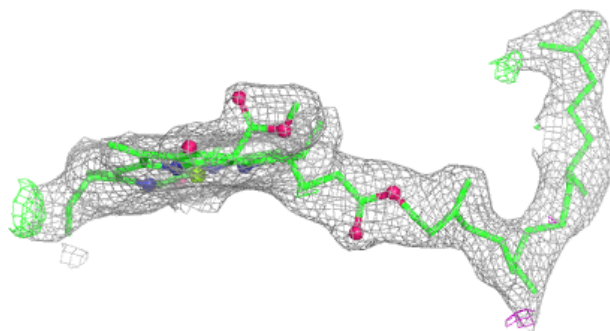
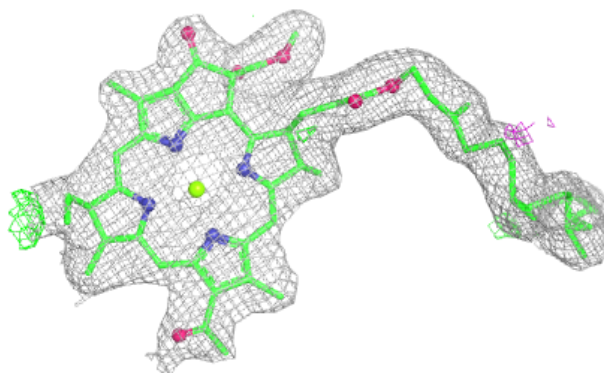


**Electron density around RG1 H 1404:**

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

**Electron density around BCL H 1604:**

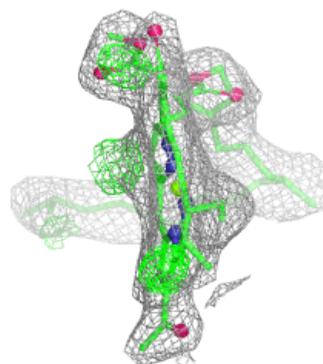
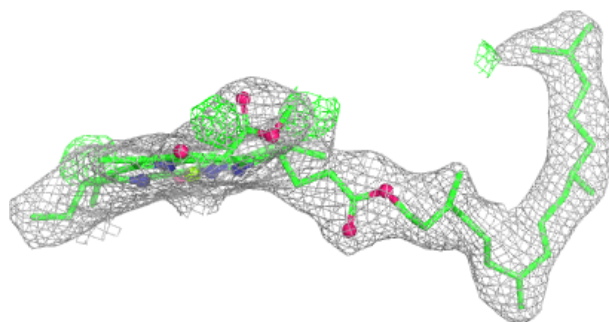
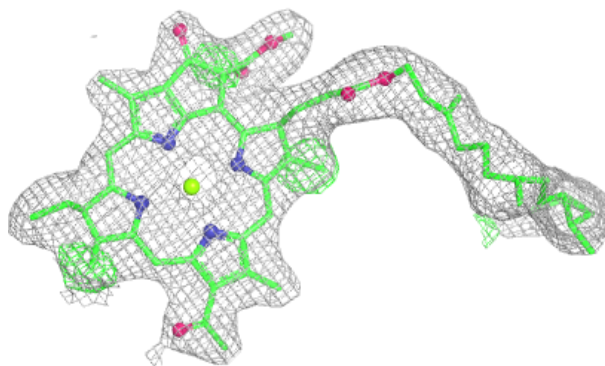
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



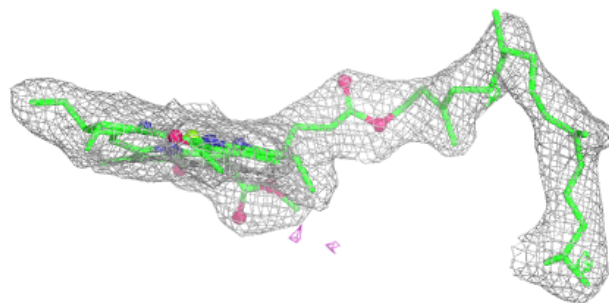
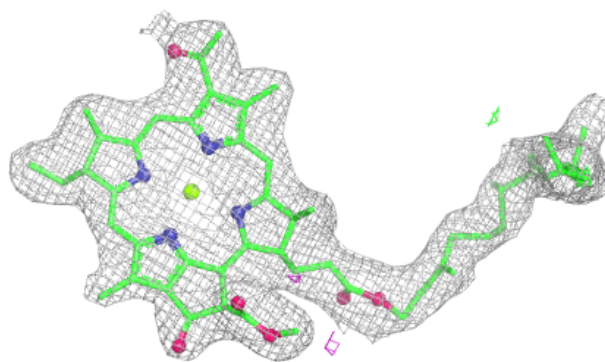


**Electron density around BCL L 1606:**

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

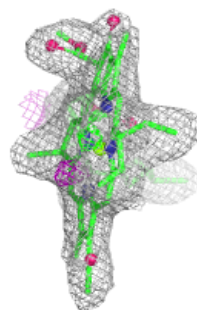
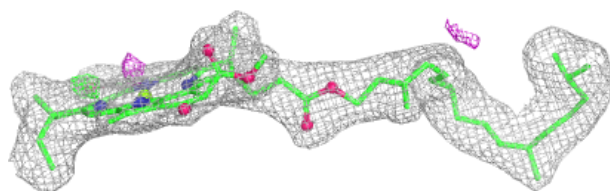
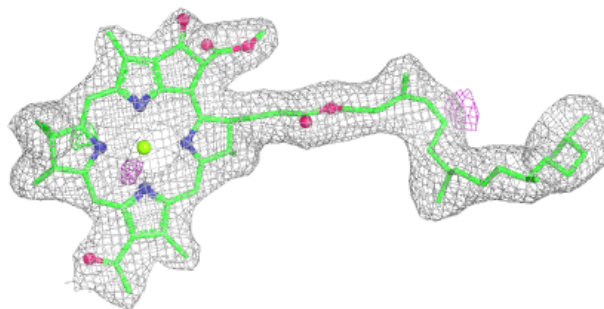
**Electron density around BCL S 1609:**

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

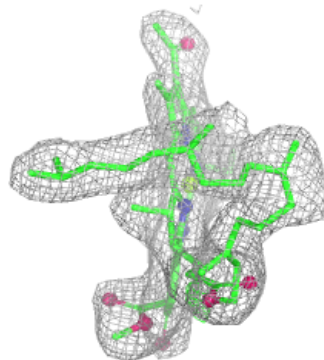
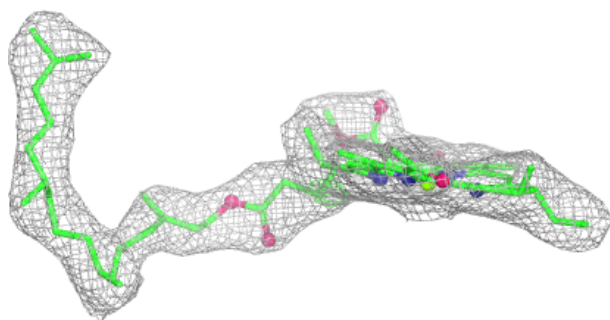
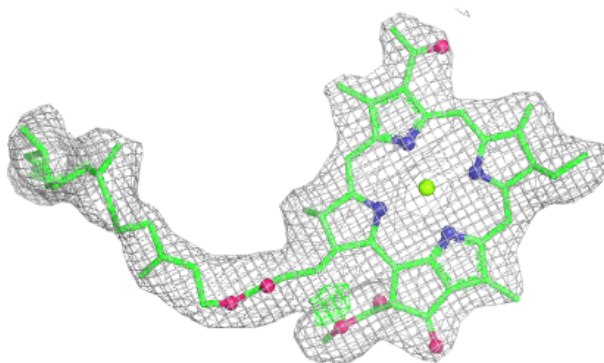


**Electron density around BCL I 1505:**

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

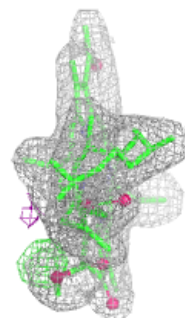
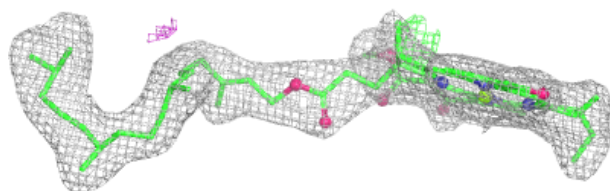
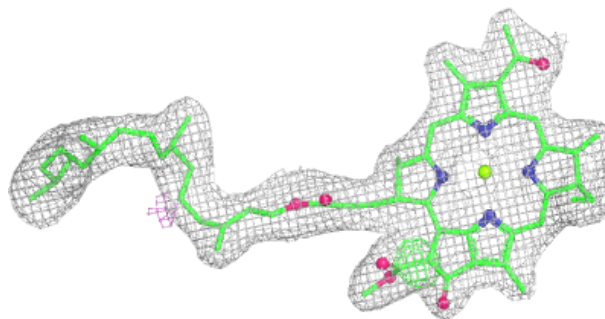
**Electron density around BCL B 1601:**

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

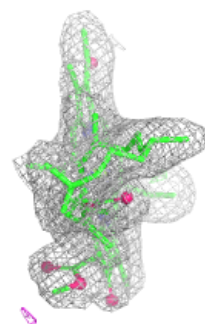
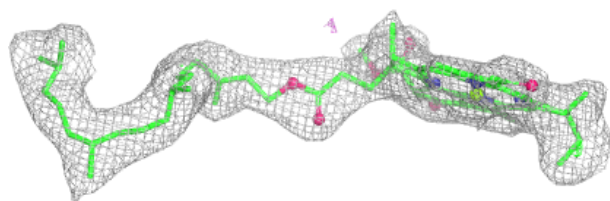
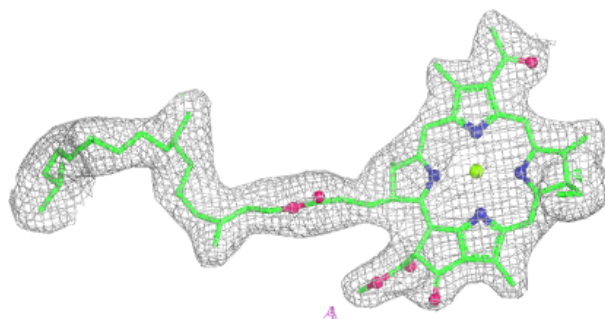


**Electron density around BCL O 1508:**

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

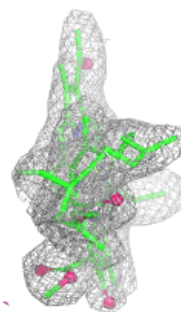
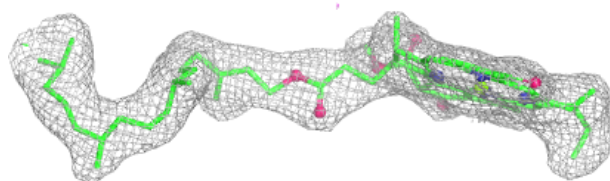
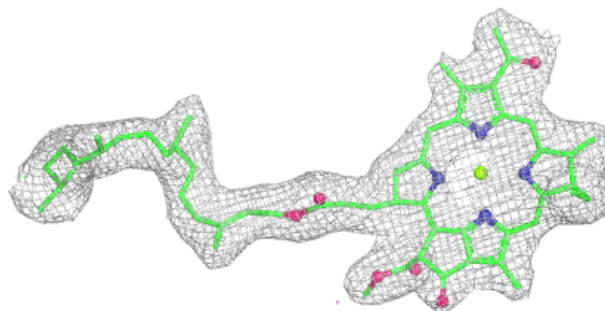
**Electron density around BCL M 1507:**

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

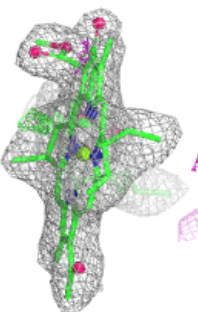
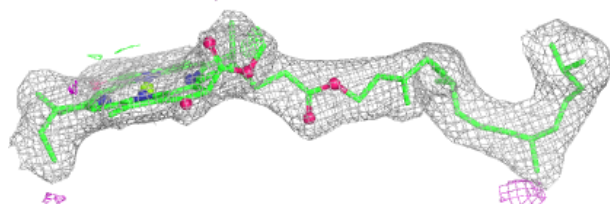
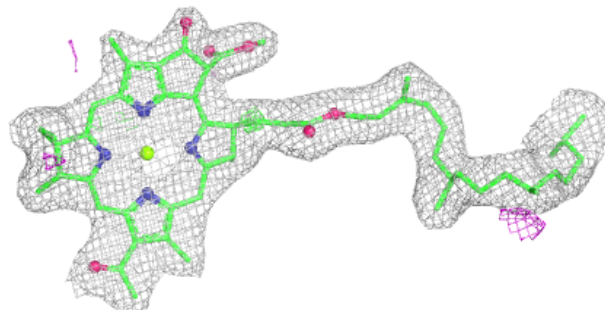


**Electron density around BCL C 1502:**

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

**Electron density around BCL G 1504:**

$2mF_o-DF_c$  (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.