



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:32 PM UTC

PDB ID : 7VZG / pdb\_00007vzg  
EMDB ID : EMD-32228  
Title : Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the larger form)  
Authors : Huang, G.Q.; Dong, S.S.; Qin, X.C.; Sui, S.F.  
Deposited on : 2021-11-16  
Resolution : 2.61 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>  
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:

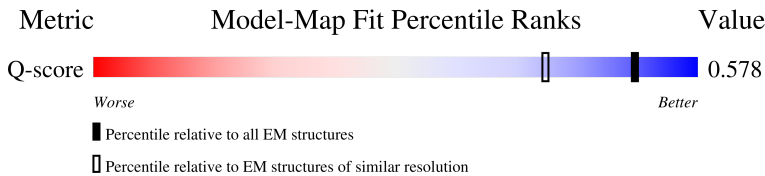
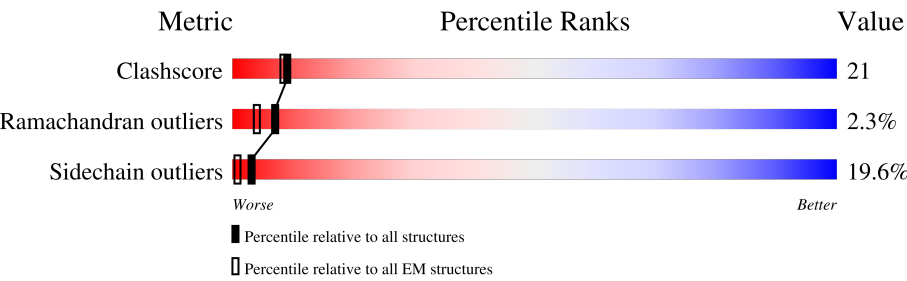
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.61 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.



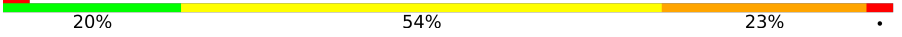
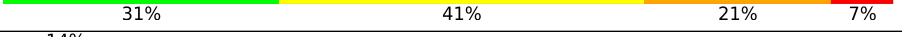
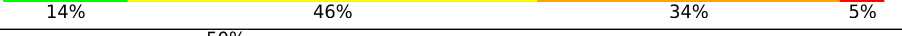
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8735 ( 2.11 - 3.11 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                |
|-----|-------|--------|---------------------------------------------------------------------------------|
| 1   | A     | 858    | <div><div>52%</div><div>31%</div><div>12%</div><div>.</div></div>               |
| 1   | a     | 858    | <div><div>58%</div><div>30%</div><div>9%</div><div>.</div></div>                |
| 2   | C     | 204    | <div><div>40%</div><div>36%</div><div>12%</div><div>7%</div><div>5%</div></div> |
| 3   | E     | 35     | <div><div>26%</div><div>57%</div><div>17%</div></div>                           |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | e     | 35     |  |
| 4   | F     | 35     |  |
| 4   | f     | 35     |  |
| 5   | G     | 38     |  |
| 5   | g     | 38     |  |
| 6   | H     | 19     |  |
| 6   | h     | 19     |  |
| 7   | c     | 145    |  |
| 8   | B     | 76     |  |
| 9   | D     | 70     |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 12  | CLA  | A     | 910 | X         | -        | -       | -                |
| 12  | CLA  | A     | 911 | X         | -        | -       | -                |
| 15  | 85I  | A     | 916 | X         | -        | -       | -                |
| 16  | UNL  | A     | 922 | -         | -        | X       | -                |
| 16  | UNL  | A     | 923 | -         | -        | X       | -                |
| 16  | UNL  | A     | 927 | -         | -        | X       | -                |
| 16  | UNL  | C     | 302 | -         | -        | X       | -                |
| 16  | UNL  | a     | 926 | -         | -        | X       | -                |
| 16  | UNL  | a     | 930 | -         | -        | X       | -                |
| 16  | UNL  | a     | 931 | -         | -        | X       | -                |
| 20  | SF4  | B     | 201 | -         | -        | X       | -                |
| 20  | SF4  | B     | 202 | -         | -        | X       | -                |
| 20  | SF4  | a     | 917 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 22458 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PscA.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 854      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6960  | 4602 | 1155 | 1170 | 33 |         |       |
| 1   | a     | 858      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6984  | 4616 | 1160 | 1175 | 33 |         |       |

- Molecule 2 is a protein called Cytochrome c, mono-and diheme variants.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1474  | 900 | 277 | 288 | 9 |         |       |

- Molecule 3 is a protein called PscE.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | E     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 258   | 174 | 40 | 42 | 2 |         |       |
| 3   | e     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 258   | 174 | 40 | 42 | 2 |         |       |

- Molecule 4 is a protein called PscF.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | F     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 273   | 185 | 43 | 43 | 2 |         |       |
| 4   | f     | 35       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 273   | 185 | 43 | 43 | 2 |         |       |

- Molecule 5 is a protein called PscG.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | G     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 210 | 45 | 44 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | g     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 302   | 210 | 45 | 44 | 3 |         |       |

- Molecule 6 is a protein called undefined polypeptide.

| Mol | Chain | Residues | Atoms |    |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|--|---------|-------|
| 6   | H     | 19       | Total | C  | N  | O  |  | 0       | 0     |
|     |       |          | 95    | 57 | 19 | 19 |  |         |       |
| 6   | h     | 19       | Total | C  | N  | O  |  | 0       | 0     |
|     |       |          | 95    | 57 | 19 | 19 |  |         |       |

- Molecule 7 is a protein called Cytochrome c domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | c     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1096  | 679 | 200 | 210 | 7 |         |       |

- Molecule 8 is a protein called Photosystem P840 reaction center iron-sulfur protein.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 8   | B     | 76       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 568   | 356 | 90 | 114 | 8 |         |       |

- Molecule 9 is a protein called PscD'.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | D     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 520   | 330 | 92 | 96 | 2 |         |       |

- Molecule 10 is [methyl 9-acetyl-14-ethyl-20-hydroxy-4,8,13,18-tetramethyl-3-{3-oxo-3-[(3,7,11,15-tetramethylhexadec-2-en-1-yl)oxy]propyl}-3,4,20,21-tetradehydrophorbine-21-carboxylato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26 ]zinc (CCD ID: 2GO) (formula: C<sub>55</sub>H<sub>70</sub>N<sub>4</sub>O<sub>6</sub>Zn) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |        |        |         | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 10  | A     | 1        | Total<br>66 | C<br>55 | N<br>4 | O<br>6 | Zn<br>1 | 0       |
| 10  | a     | 1        | Total<br>66 | C<br>55 | N<br>4 | O<br>6 | Zn<br>1 | 0       |

- Molecule 11 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula:  $\text{C}_{55}\text{H}_{74}\text{MgN}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).



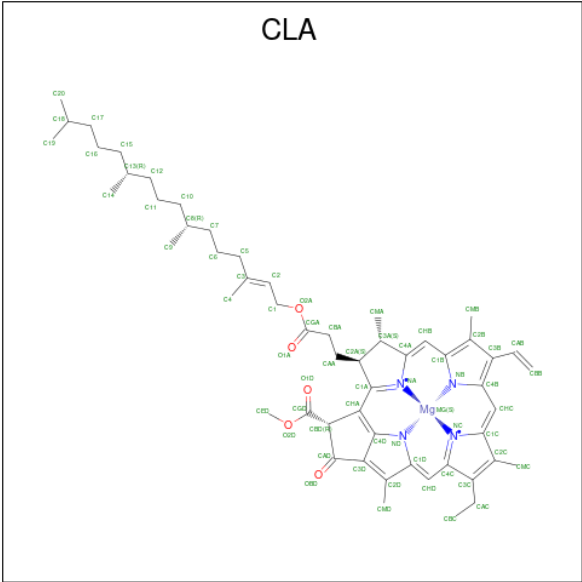
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 11  | A     | 1        | Total<br>66 | C<br>55 | Mg<br>1 | N<br>4 | O<br>6 | 0       |

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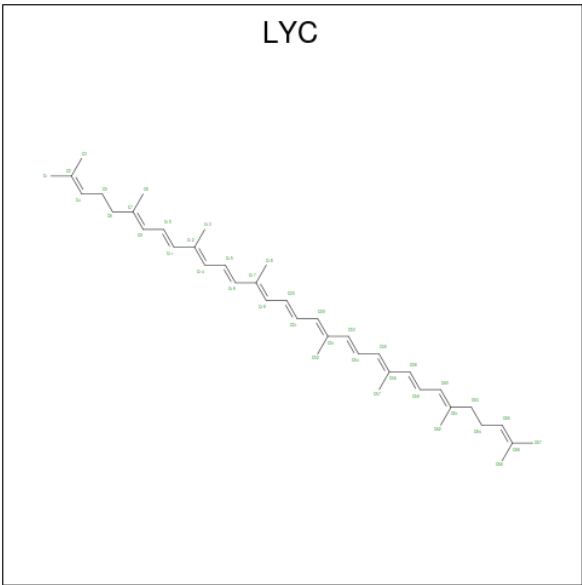
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 41 | 1  | 4 | 6 |         |
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 11  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 12  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 12  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 12  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 12  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 12  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 12  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 12  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 12  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 12  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 12  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |

- Molecule 13 is LYCOPENE (CCD ID: LYC) (formula: C<sub>40</sub>H<sub>56</sub>).

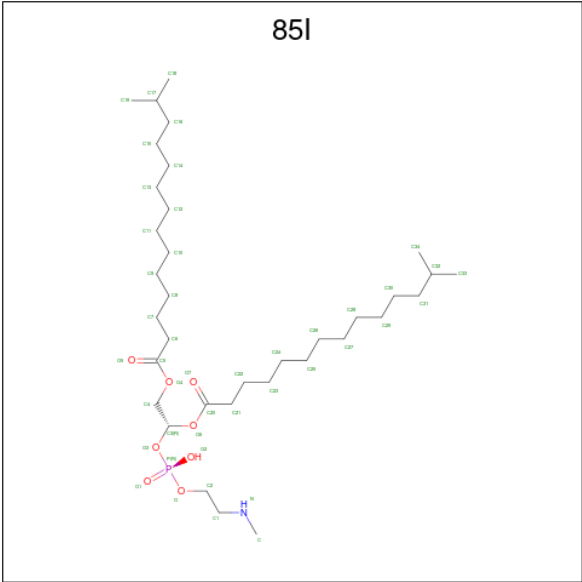


| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 13  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 13  | c     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

- Molecule 14 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 14  | A     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 14  | a     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 15 is [(2 {R})-2-[2-(methylamino)ethoxy-oxidanyl-phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (CCD ID: 85I) (formula: C<sub>35</sub>H<sub>70</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 15  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 15  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 15  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 15  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 15  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 15  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |

- Molecule 16 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

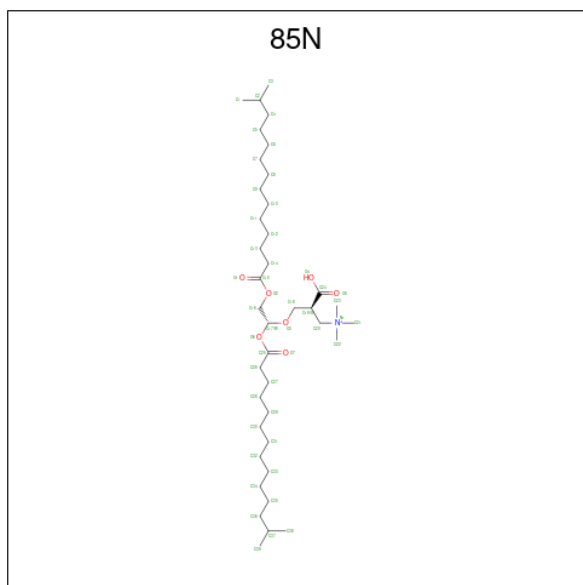
| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 16  | A     | 13       | Total | C   | 0       |
|     |       |          | 240   | 240 |         |
| 16  | C     | 1        | Total | C   | 0       |
|     |       |          | 18    | 18  |         |
| 16  | E     | 2        | Total | C   | 0       |
|     |       |          | 26    | 26  |         |
| 16  | a     | 13       | Total | C   | 0       |
|     |       |          | 243   | 243 |         |
| 16  | c     | 1        | Total | C   | 0       |
|     |       |          | 8     | 8   |         |

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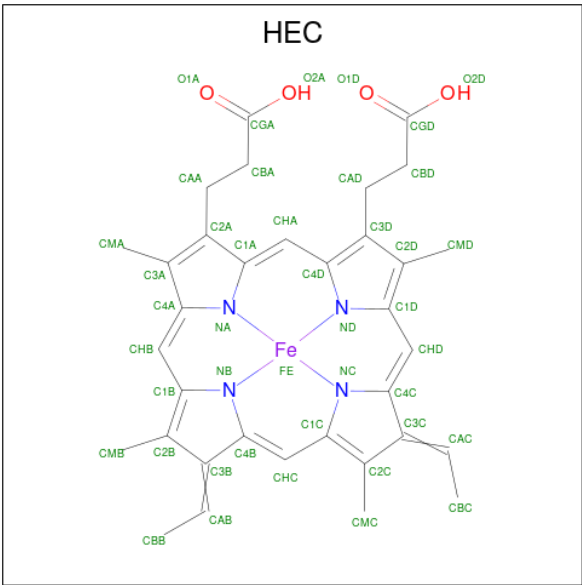
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 16  | e     | 2        | Total | C  | 0       |
|     |       |          | 26    | 26 |         |

- Molecule 17 is [(2 {S})-2-[[[(1 {R})-1,2-bis(13-methyltetradecanoyloxy)ethoxy]methyl]-3-oxidanyl-3-oxidanylidene-propyl]-trimethyl-azanium (CCD ID: 85N) (formula: C<sub>39</sub>H<sub>76</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



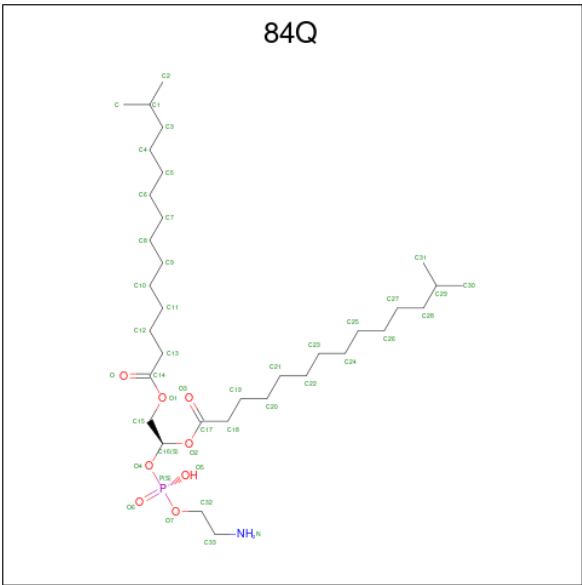
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 17  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 47    | 39 | 1 | 7 |         |
| 17  | G     | 1        | Total | C  | N | O | 0       |
|     |       |          | 38    | 30 | 1 | 7 |         |
| 17  | a     | 1        | Total | C  | N | O | 0       |
|     |       |          | 47    | 39 | 1 | 7 |         |
| 17  | g     | 1        | Total | C  | N | O | 0       |
|     |       |          | 38    | 30 | 1 | 7 |         |

- Molecule 18 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | C     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 18  | c     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

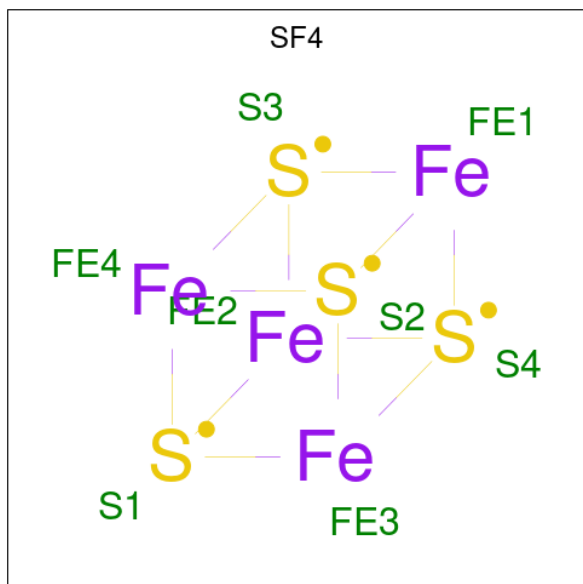
- Molecule 19 is [(2S)-2-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (CCD ID: 84Q) (formula: C<sub>34</sub>H<sub>68</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 19  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |

- Molecule 20 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 20  | a     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 20  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 20  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

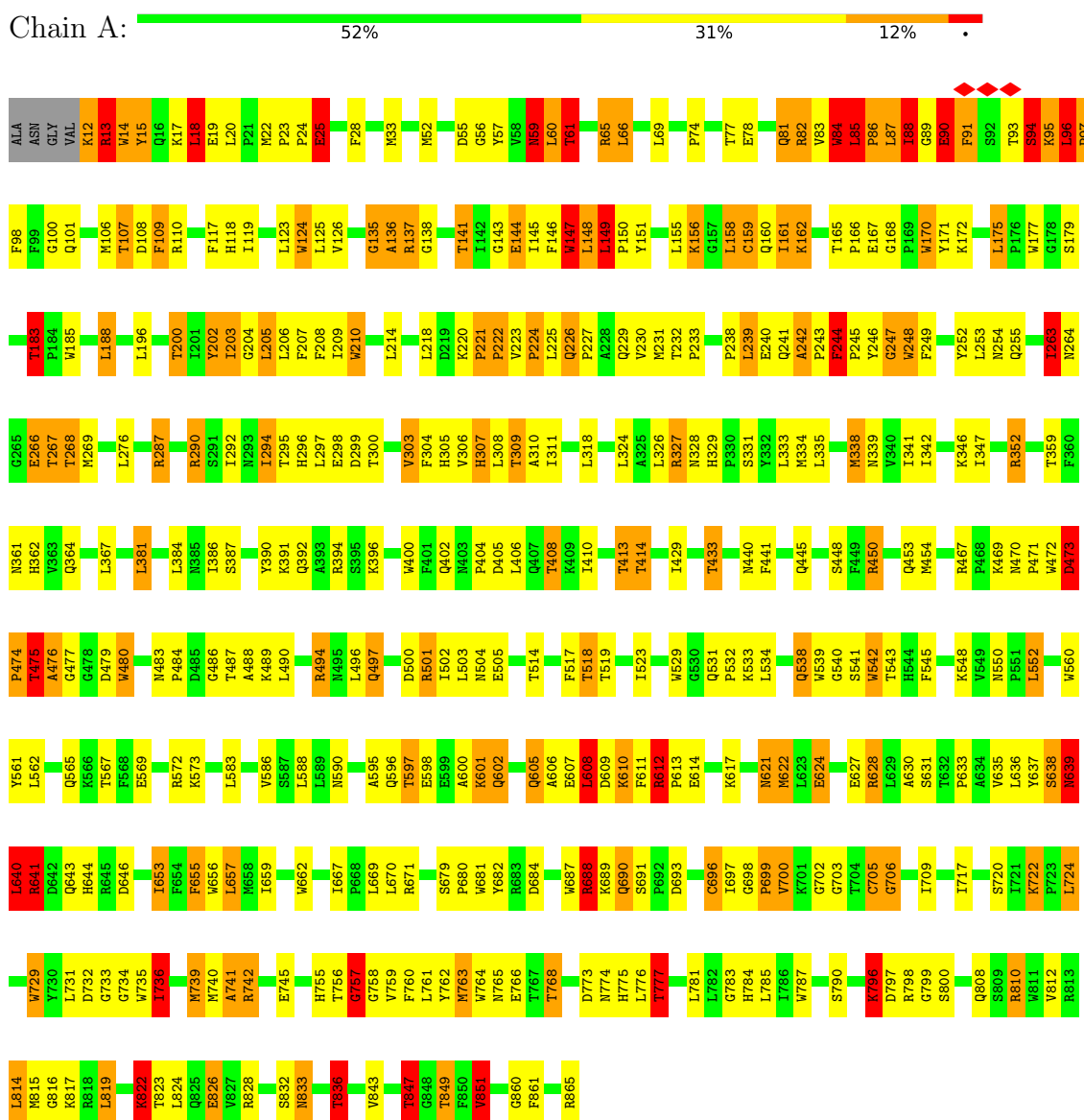
- Molecule 21 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 21  | A     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 21  | a     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |

### 3 Residue-property plots

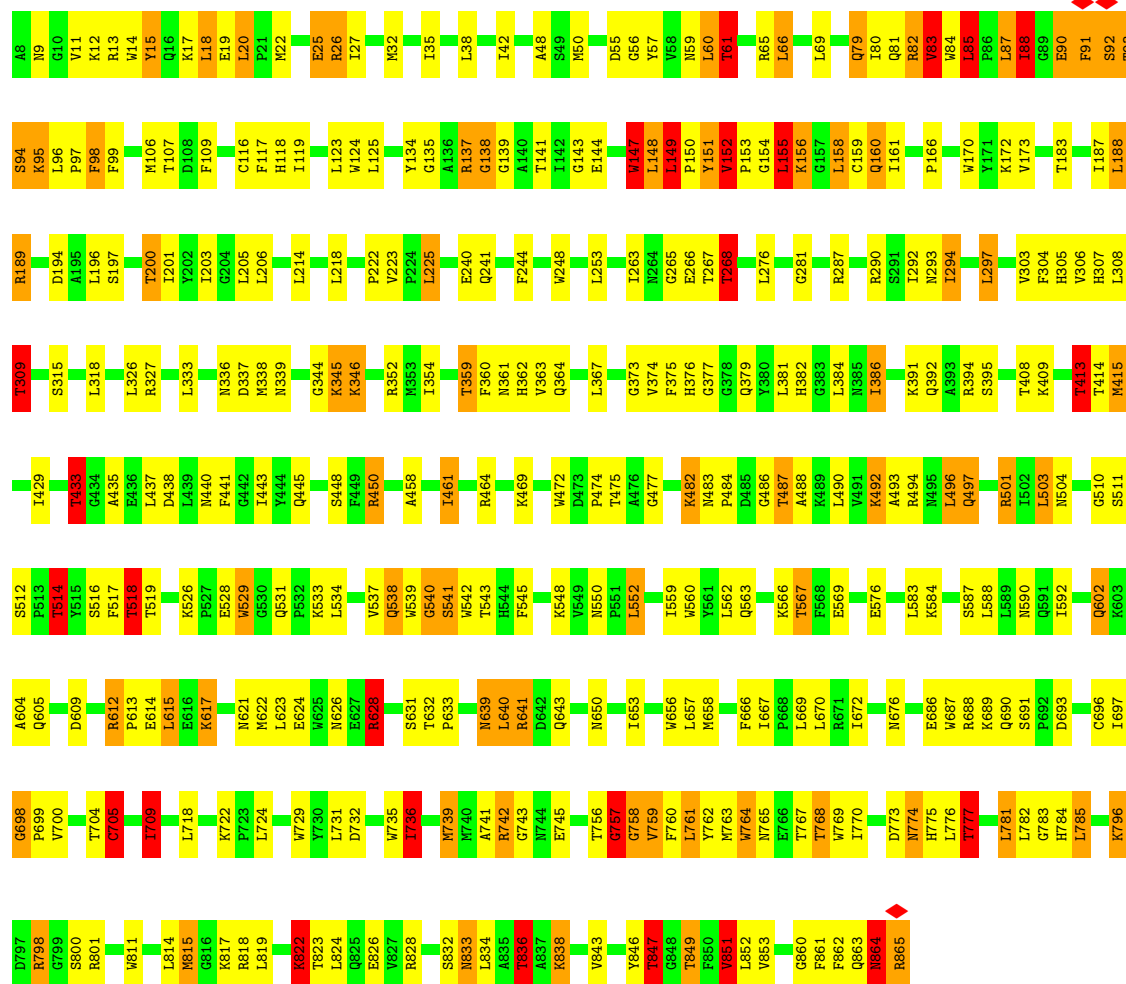
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: PscA



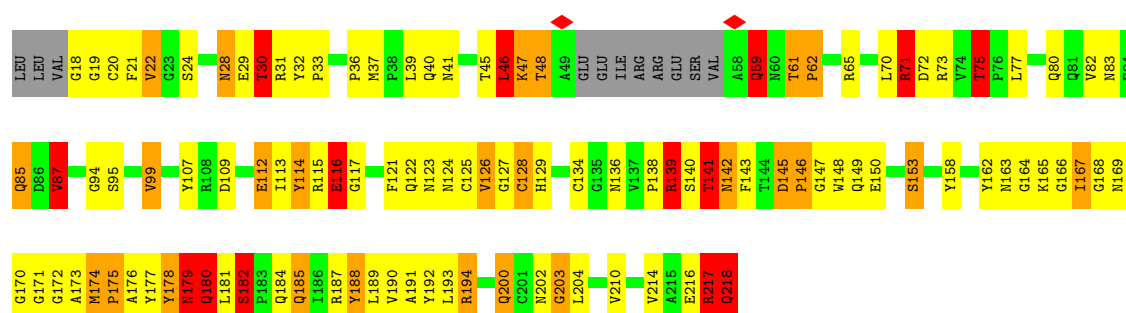
#### • Molecule 1: PscA

Chain a: 



• Molecule 2: Cytochrome c, mono- and di-heme variants

Chain C: 

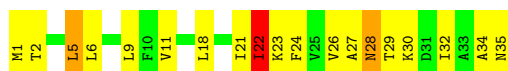


• Molecule 3: PscE

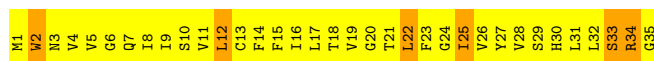
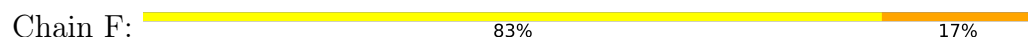
Chain E: 



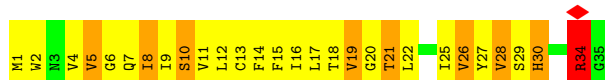
- Molecule 3: PscE



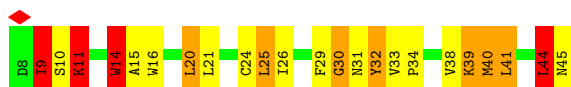
- Molecule 4: PscF



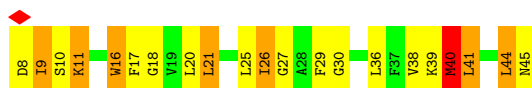
- Molecule 4: PscF



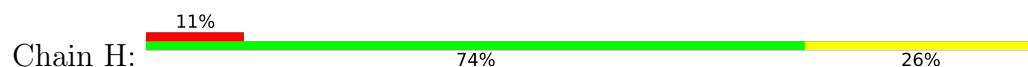
- Molecule 5: PscG



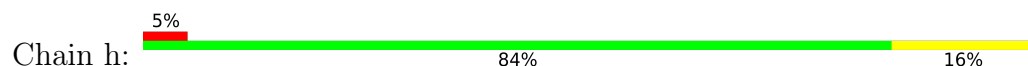
- Molecule 5: PscG



- Molecule 6: undefined polypeptide

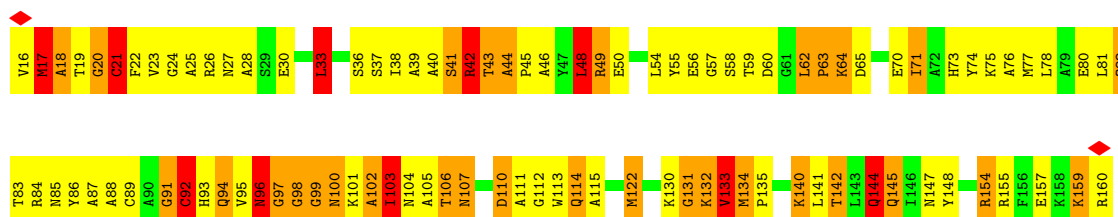
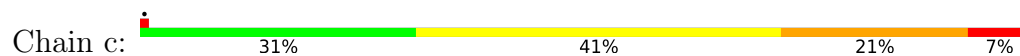


- Molecule 6: undefined polypeptide

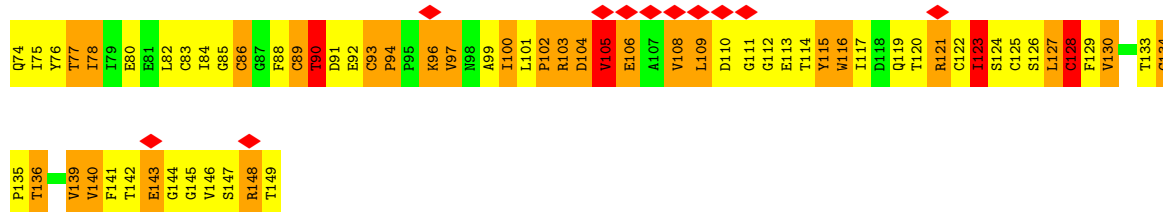
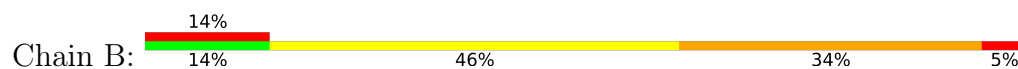




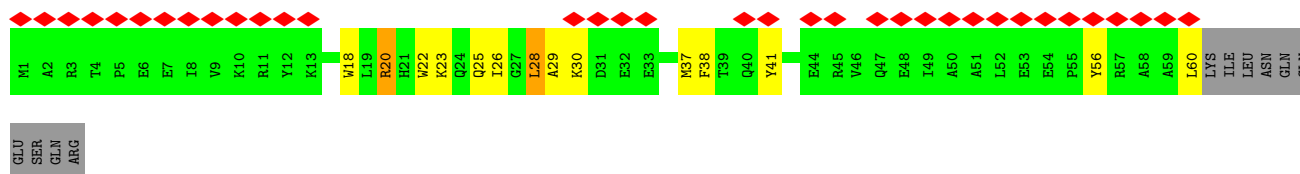
• Molecule 7: Cytochrome c domain-containing protein



• Molecule 8: Photosystem P840 reaction center iron-sulfur protein



• Molecule 9: PscD'



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 52612                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 2.381                                   | Depositor |
| Minimum map value                    | -1.010                                  | Depositor |
| Average map value                    | 0.008                                   | Depositor |
| Map value standard deviation         | 0.094                                   | Depositor |
| Recommended contour level            | 0.3                                     | Depositor |
| Map size (Å)                         | 238.15, 238.15, 238.15                  | wwPDB     |
| Map dimensions                       | 220, 220, 220                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.0825, 1.0825, 1.0825                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LYC, BCL, CA, 85I, SF4, 2GO, HEC, 84Q, UNL, 85N, CLA

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     | 2.28         | 246/7209 (3.4%)  | 1.57        | 111/9827 (1.1%)  |
| 1   | a     | 2.04         | 177/7233 (2.4%)  | 1.42        | 93/9860 (0.9%)   |
| 2   | C     | 3.01         | 111/1503 (7.4%)  | 2.06        | 65/2037 (3.2%)   |
| 3   | E     | 3.18         | 25/262 (9.5%)    | 1.95        | 7/356 (2.0%)     |
| 3   | e     | 2.23         | 9/262 (3.4%)     | 1.83        | 3/356 (0.8%)     |
| 4   | F     | 3.37         | 34/279 (12.2%)   | 1.79        | 8/379 (2.1%)     |
| 4   | f     | 2.88         | 22/279 (7.9%)    | 1.79        | 9/379 (2.4%)     |
| 5   | G     | 2.13         | 13/311 (4.2%)    | 1.93        | 9/421 (2.1%)     |
| 5   | g     | 1.68         | 1/311 (0.3%)     | 1.56        | 7/421 (1.7%)     |
| 7   | c     | 3.24         | 127/1115 (11.4%) | 2.20        | 53/1506 (3.5%)   |
| 8   | B     | 1.13         | 1/578 (0.2%)     | 1.72        | 18/789 (2.3%)    |
| 9   | D     | 0.74         | 0/531            | 1.24        | 2/714 (0.3%)     |
| All | All   | 2.30         | 766/19873 (3.9%) | 1.62        | 385/27045 (1.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | a     | 0                   | 4                   |
| 2   | C     | 0                   | 2                   |
| 7   | c     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (766) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | a     | 539 | TRP  | C-O   | -23.05 | 0.94        | 1.23     |
| 2   | C     | 141 | THR  | C-O   | -18.99 | 1.01        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | a     | 305 | HIS  | C-O    | -15.87 | 1.05        | 1.24     |
| 2   | C     | 179 | ASN  | C-O    | -15.84 | 1.04        | 1.24     |
| 1   | a     | 852 | LEU  | C-O    | -15.81 | 1.04        | 1.24     |
| 4   | F     | 4   | VAL  | C-O    | -15.43 | 1.06        | 1.24     |
| 7   | c     | 106 | THR  | C-O    | -15.40 | 1.05        | 1.23     |
| 1   | a     | 376 | HIS  | C-O    | -15.38 | 1.04        | 1.24     |
| 1   | A     | 731 | LEU  | C-O    | -15.26 | 1.06        | 1.24     |
| 3   | E     | 13  | GLY  | C-O    | -15.24 | 1.05        | 1.24     |
| 2   | C     | 140 | SER  | C-O    | -15.15 | 1.04        | 1.23     |
| 1   | a     | 759 | VAL  | C-O    | -15.13 | 1.06        | 1.24     |
| 1   | A     | 306 | VAL  | C-O    | -15.06 | 1.06        | 1.24     |
| 1   | A     | 758 | GLY  | C-O    | -14.88 | 1.03        | 1.23     |
| 1   | A     | 125 | LEU  | C-O    | -14.61 | 1.06        | 1.24     |
| 1   | A     | 709 | ILE  | C-O    | -14.43 | 1.06        | 1.24     |
| 1   | A     | 638 | SER  | C-O    | -14.39 | 1.05        | 1.23     |
| 1   | a     | 783 | GLY  | C-O    | -14.23 | 1.06        | 1.23     |
| 1   | a     | 346 | LYS  | C-O    | -14.07 | 1.06        | 1.24     |
| 2   | C     | 176 | ALA  | C-O    | -14.06 | 1.05        | 1.23     |
| 2   | C     | 178 | TYR  | C-O    | -14.03 | 1.06        | 1.24     |
| 2   | C     | 190 | VAL  | C-O    | -13.74 | 1.08        | 1.24     |
| 2   | C     | 126 | VAL  | C-O    | -13.61 | 1.07        | 1.24     |
| 1   | a     | 796 | LYS  | C-O    | -13.60 | 1.06        | 1.24     |
| 7   | c     | 130 | LYS  | C-O    | -13.46 | 1.08        | 1.23     |
| 1   | a     | 811 | TRP  | C-O    | -13.32 | 1.08        | 1.24     |
| 2   | C     | 123 | ASN  | C-O    | -13.27 | 1.08        | 1.24     |
| 2   | C     | 175 | PRO  | C-O    | -13.26 | 1.08        | 1.23     |
| 1   | A     | 764 | TRP  | C-O    | -13.18 | 1.08        | 1.24     |
| 1   | A     | 309 | THR  | CB-CG2 | -13.18 | 1.09        | 1.52     |
| 1   | A     | 245 | PRO  | C-O    | -13.17 | 1.08        | 1.24     |
| 1   | A     | 238 | PRO  | C-O    | -13.07 | 1.10        | 1.23     |
| 1   | A     | 796 | LYS  | C-O    | -13.07 | 1.09        | 1.23     |
| 1   | A     | 655 | PHE  | C-O    | -13.07 | 1.09        | 1.24     |
| 1   | a     | 537 | VAL  | C-O    | -13.04 | 1.11        | 1.24     |
| 1   | A     | 560 | TRP  | C-O    | -13.03 | 1.08        | 1.24     |
| 2   | C     | 121 | PHE  | C-O    | -12.93 | 1.09        | 1.24     |
| 1   | a     | 26  | ARG  | C-O    | -12.89 | 1.08        | 1.24     |
| 1   | A     | 362 | HIS  | C-O    | -12.88 | 1.08        | 1.24     |
| 1   | A     | 542 | TRP  | C-O    | -12.87 | 1.07        | 1.24     |
| 2   | C     | 30  | THR  | C-O    | -12.85 | 1.07        | 1.23     |
| 2   | C     | 188 | TYR  | C-O    | -12.84 | 1.08        | 1.24     |
| 7   | c     | 96  | ASN  | C-O    | -12.83 | 1.06        | 1.24     |
| 7   | c     | 112 | GLY  | C-O    | -12.73 | 1.08        | 1.23     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | a     | 731 | LEU  | C-O    | -12.66 | 1.09        | 1.24     |
| 1   | a     | 860 | GLY  | C-O    | -12.66 | 1.06        | 1.23     |
| 2   | C     | 147 | GLY  | C-O    | -12.63 | 1.08        | 1.23     |
| 1   | A     | 294 | ILE  | C-O    | -12.58 | 1.09        | 1.24     |
| 7   | c     | 26  | ARG  | C-O    | -12.52 | 1.08        | 1.23     |
| 1   | A     | 311 | ILE  | C-O    | -12.48 | 1.10        | 1.24     |
| 1   | a     | 758 | GLY  | C-O    | -12.43 | 1.07        | 1.23     |
| 2   | C     | 165 | LYS  | CA-C   | -12.42 | 1.38        | 1.52     |
| 1   | A     | 209 | ILE  | C-O    | -12.41 | 1.10        | 1.24     |
| 1   | a     | 763 | MET  | C-O    | -12.33 | 1.09        | 1.24     |
| 1   | A     | 543 | THR  | C-O    | -12.32 | 1.08        | 1.24     |
| 7   | c     | 20  | GLY  | C-O    | -12.26 | 1.07        | 1.23     |
| 1   | A     | 541 | SER  | C-O    | -12.24 | 1.07        | 1.24     |
| 1   | A     | 860 | GLY  | C-O    | -12.24 | 1.10        | 1.23     |
| 4   | F     | 25  | ILE  | C-O    | -12.22 | 1.09        | 1.24     |
| 2   | C     | 143 | PHE  | C-O    | -12.20 | 1.08        | 1.24     |
| 1   | A     | 297 | LEU  | C-O    | -12.12 | 1.08        | 1.24     |
| 7   | c     | 106 | THR  | CB-CG2 | -12.09 | 1.12        | 1.52     |
| 7   | c     | 56  | GLU  | C-O    | -12.08 | 1.08        | 1.24     |
| 4   | F     | 10  | SER  | C-O    | -12.06 | 1.10        | 1.24     |
| 1   | A     | 210 | TRP  | C-O    | -12.00 | 1.09        | 1.24     |
| 4   | f     | 17  | LEU  | C-O    | -11.98 | 1.10        | 1.24     |
| 1   | A     | 126 | VAL  | C-O    | -11.97 | 1.10        | 1.24     |
| 1   | a     | 757 | GLY  | C-O    | -11.91 | 1.07        | 1.23     |
| 1   | A     | 124 | TRP  | C-O    | -11.90 | 1.09        | 1.24     |
| 1   | A     | 640 | LEU  | C-O    | -11.90 | 1.08        | 1.24     |
| 1   | A     | 861 | PHE  | C-O    | -11.90 | 1.10        | 1.24     |
| 2   | C     | 189 | LEU  | C-O    | -11.87 | 1.10        | 1.24     |
| 2   | C     | 146 | PRO  | C-O    | -11.84 | 1.09        | 1.24     |
| 7   | c     | 18  | ALA  | CA-C   | -11.84 | 1.37        | 1.52     |
| 1   | a     | 765 | ASN  | C-O    | -11.83 | 1.10        | 1.24     |
| 2   | C     | 173 | ALA  | C-O    | -11.76 | 1.09        | 1.24     |
| 1   | A     | 776 | LEU  | C-O    | -11.73 | 1.09        | 1.24     |
| 1   | A     | 203 | ILE  | C-O    | -11.65 | 1.10        | 1.24     |
| 2   | C     | 148 | TRP  | C-O    | -11.59 | 1.10        | 1.24     |
| 1   | A     | 656 | TRP  | C-O    | -11.58 | 1.09        | 1.24     |
| 2   | C     | 180 | GLN  | C-O    | -11.54 | 1.09        | 1.24     |
| 3   | E     | 2   | THR  | C-O    | -11.51 | 1.10        | 1.24     |
| 1   | A     | 699 | PRO  | C-O    | -11.47 | 1.08        | 1.24     |
| 1   | A     | 741 | ALA  | C-O    | -11.45 | 1.09        | 1.23     |
| 7   | c     | 43  | THR  | C-O    | -11.35 | 1.10        | 1.23     |
| 7   | c     | 113 | TRP  | C-O    | -11.31 | 1.11        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 7   | c     | 46  | ALA  | C-O   | -11.30 | 1.10        | 1.23     |
| 7   | c     | 42  | ARG  | C-O   | -11.29 | 1.09        | 1.24     |
| 1   | A     | 742 | ARG  | C-O   | -11.26 | 1.10        | 1.23     |
| 2   | C     | 163 | ASN  | C-O   | -11.26 | 1.09        | 1.24     |
| 1   | a     | 116 | CYS  | C-O   | -11.16 | 1.11        | 1.24     |
| 2   | C     | 72  | ASP  | C-O   | -11.15 | 1.09        | 1.24     |
| 2   | C     | 167 | ILE  | C-O   | -11.13 | 1.09        | 1.24     |
| 2   | C     | 128 | CYS  | C-O   | -11.07 | 1.09        | 1.24     |
| 7   | c     | 93  | HIS  | C-O   | -11.03 | 1.09        | 1.24     |
| 1   | A     | 539 | TRP  | C-O   | -11.03 | 1.09        | 1.24     |
| 2   | C     | 181 | LEU  | C-O   | -11.02 | 1.09        | 1.23     |
| 2   | C     | 142 | ASN  | N-CA  | 11.02  | 1.61        | 1.46     |
| 1   | a     | 697 | ILE  | C-O   | -10.98 | 1.11        | 1.24     |
| 1   | a     | 375 | PHE  | C-O   | -10.96 | 1.11        | 1.24     |
| 1   | A     | 207 | PHE  | C-O   | -10.92 | 1.11        | 1.24     |
| 1   | a     | 631 | SER  | C-O   | -10.92 | 1.09        | 1.24     |
| 1   | A     | 740 | MET  | C-O   | -10.86 | 1.09        | 1.24     |
| 2   | C     | 165 | LYS  | C-O   | -10.86 | 1.11        | 1.23     |
| 2   | C     | 214 | VAL  | C-O   | -10.86 | 1.09        | 1.24     |
| 1   | A     | 307 | HIS  | C-O   | -10.81 | 1.10        | 1.24     |
| 7   | c     | 105 | ALA  | C-O   | -10.73 | 1.11        | 1.24     |
| 2   | C     | 19  | GLY  | C-O   | -10.72 | 1.09        | 1.23     |
| 1   | a     | 764 | TRP  | C-O   | -10.61 | 1.10        | 1.24     |
| 1   | A     | 361 | ASN  | C-O   | -10.58 | 1.11        | 1.24     |
| 7   | c     | 91  | GLY  | C-O   | -10.50 | 1.09        | 1.23     |
| 1   | A     | 308 | LEU  | C-O   | -10.49 | 1.11        | 1.24     |
| 7   | c     | 98  | GLY  | CA-C  | -10.49 | 1.37        | 1.51     |
| 1   | A     | 682 | TYR  | C-O   | -10.48 | 1.11        | 1.24     |
| 1   | A     | 480 | TRP  | C-O   | -10.42 | 1.10        | 1.23     |
| 1   | A     | 248 | TRP  | C-O   | -10.39 | 1.09        | 1.23     |
| 1   | A     | 119 | ILE  | C-O   | -10.37 | 1.11        | 1.24     |
| 1   | A     | 775 | HIS  | C-O   | -10.37 | 1.11        | 1.24     |
| 1   | A     | 208 | PHE  | C-O   | -10.36 | 1.12        | 1.24     |
| 1   | a     | 307 | HIS  | C-O   | -10.30 | 1.12        | 1.24     |
| 1   | A     | 118 | HIS  | C-O   | -10.28 | 1.11        | 1.24     |
| 1   | A     | 733 | GLY  | C-O   | -10.28 | 1.09        | 1.24     |
| 3   | e     | 28  | ASN  | C-O   | -10.27 | 1.10        | 1.24     |
| 1   | A     | 117 | PHE  | C-O   | -10.26 | 1.12        | 1.24     |
| 1   | A     | 756 | THR  | C-O   | -10.25 | 1.09        | 1.24     |
| 2   | C     | 124 | ASN  | C-O   | -10.24 | 1.10        | 1.24     |
| 3   | E     | 25  | VAL  | C-O   | -10.23 | 1.12        | 1.24     |
| 7   | c     | 21  | CYS  | C-O   | -10.23 | 1.11        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 305 | HIS  | C-O    | -10.21 | 1.12        | 1.24     |
| 4   | F     | 15  | PHE  | C-O    | -10.14 | 1.12        | 1.24     |
| 2   | C     | 177 | TYR  | C-O    | -10.11 | 1.10        | 1.24     |
| 2   | C     | 20  | CYS  | C-O    | -10.10 | 1.11        | 1.24     |
| 1   | A     | 561 | TYR  | C-O    | -10.09 | 1.12        | 1.24     |
| 1   | A     | 108 | ASP  | C-O    | -10.08 | 1.12        | 1.24     |
| 1   | A     | 739 | MET  | C-O    | -10.08 | 1.11        | 1.24     |
| 1   | A     | 338 | MET  | C-N    | -10.02 | 1.21        | 1.33     |
| 1   | A     | 538 | GLN  | CD-NE2 | -10.00 | 1.12        | 1.33     |
| 2   | C     | 182 | SER  | C-O    | -10.00 | 1.08        | 1.23     |
| 1   | A     | 774 | ASN  | C-O    | -9.98  | 1.11        | 1.24     |
| 1   | a     | 27  | ILE  | C-O    | -9.97  | 1.12        | 1.24     |
| 2   | C     | 142 | ASN  | CG-ND2 | -9.96  | 1.12        | 1.33     |
| 1   | a     | 560 | TRP  | C-O    | -9.95  | 1.12        | 1.24     |
| 1   | A     | 246 | TYR  | C-O    | -9.94  | 1.12        | 1.24     |
| 1   | A     | 299 | ASP  | C-O    | -9.89  | 1.11        | 1.24     |
| 2   | C     | 21  | PHE  | C-O    | -9.88  | 1.11        | 1.23     |
| 1   | A     | 109 | PHE  | C-O    | -9.77  | 1.12        | 1.24     |
| 4   | F     | 6   | GLY  | C-O    | -9.77  | 1.11        | 1.23     |
| 1   | a     | 756 | THR  | C-O    | -9.77  | 1.10        | 1.24     |
| 1   | A     | 249 | PHE  | C-O    | -9.76  | 1.12        | 1.24     |
| 1   | A     | 310 | ALA  | C-O    | -9.74  | 1.12        | 1.24     |
| 1   | a     | 134 | TYR  | C-O    | -9.74  | 1.11        | 1.24     |
| 2   | C     | 179 | ASN  | CG-OD1 | -9.71  | 1.05        | 1.23     |
| 2   | C     | 166 | GLY  | C-O    | -9.68  | 1.11        | 1.23     |
| 2   | C     | 185 | GLN  | C-O    | -9.67  | 1.12        | 1.24     |
| 7   | c     | 19  | THR  | CA-C   | -9.67  | 1.43        | 1.53     |
| 1   | A     | 501 | ARG  | C-O    | -9.66  | 1.12        | 1.24     |
| 1   | a     | 118 | HIS  | C-O    | -9.65  | 1.12        | 1.24     |
| 4   | f     | 20  | GLY  | C-O    | -9.64  | 1.12        | 1.23     |
| 2   | C     | 114 | TYR  | C-O    | -9.63  | 1.12        | 1.24     |
| 3   | E     | 17  | ALA  | C-O    | -9.63  | 1.13        | 1.24     |
| 7   | c     | 43  | THR  | CB-CG2 | -9.59  | 1.21        | 1.52     |
| 4   | f     | 15  | PHE  | C-O    | -9.55  | 1.12        | 1.24     |
| 3   | e     | 26  | VAL  | C-O    | -9.54  | 1.12        | 1.24     |
| 1   | A     | 810 | ARG  | C-O    | -9.53  | 1.13        | 1.24     |
| 7   | c     | 56  | GLU  | CA-C   | -9.49  | 1.40        | 1.52     |
| 2   | C     | 174 | MET  | C-O    | -9.47  | 1.12        | 1.24     |
| 1   | a     | 512 | SER  | C-O    | -9.41  | 1.12        | 1.24     |
| 2   | C     | 185 | GLN  | CD-NE2 | -9.39  | 1.13        | 1.33     |
| 1   | a     | 742 | ARG  | C-O    | -9.39  | 1.12        | 1.23     |
| 1   | a     | 696 | CYS  | C-O    | -9.38  | 1.12        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | a     | 864 | ASN  | CA-C   | -9.37 | 1.39        | 1.52     |
| 1   | A     | 231 | MET  | C-O    | -9.37 | 1.12        | 1.23     |
| 2   | C     | 31  | ARG  | C-O    | -9.37 | 1.11        | 1.23     |
| 4   | F     | 29  | SER  | C-O    | -9.36 | 1.13        | 1.24     |
| 1   | a     | 364 | GLN  | CD-NE2 | -9.34 | 1.13        | 1.33     |
| 7   | c     | 49  | ARG  | C-O    | -9.34 | 1.12        | 1.24     |
| 7   | c     | 135 | PRO  | C-O    | -9.32 | 1.13        | 1.23     |
| 1   | A     | 759 | VAL  | C-O    | -9.30 | 1.13        | 1.24     |
| 3   | E     | 10  | PHE  | C-O    | -9.30 | 1.12        | 1.24     |
| 1   | A     | 631 | SER  | C-O    | -9.28 | 1.11        | 1.24     |
| 4   | F     | 22  | LEU  | C-O    | -9.28 | 1.13        | 1.24     |
| 3   | E     | 15  | TYR  | C-O    | -9.24 | 1.12        | 1.24     |
| 2   | C     | 192 | TYR  | C-O    | -9.22 | 1.12        | 1.24     |
| 1   | A     | 137 | ARG  | C-O    | -9.18 | 1.11        | 1.24     |
| 1   | A     | 681 | TRP  | C-O    | -9.18 | 1.13        | 1.24     |
| 1   | A     | 812 | VAL  | C-O    | -9.17 | 1.13        | 1.24     |
| 4   | F     | 8   | ILE  | C-O    | -9.17 | 1.13        | 1.24     |
| 1   | a     | 541 | SER  | C-O    | -9.15 | 1.11        | 1.23     |
| 1   | A     | 222 | PRO  | C-O    | -9.13 | 1.13        | 1.23     |
| 2   | C     | 70  | LEU  | C-O    | -9.12 | 1.13        | 1.24     |
| 4   | F     | 21  | THR  | C-O    | -9.09 | 1.13        | 1.24     |
| 1   | A     | 828 | ARG  | C-O    | -9.09 | 1.13        | 1.24     |
| 1   | A     | 309 | THR  | C-O    | -9.05 | 1.13        | 1.24     |
| 4   | F     | 18  | THR  | C-O    | -9.04 | 1.13        | 1.24     |
| 7   | c     | 41  | SER  | C-O    | -9.02 | 1.11        | 1.24     |
| 3   | E     | 18  | LEU  | C-O    | -9.02 | 1.13        | 1.24     |
| 7   | c     | 74  | TYR  | C-O    | -9.02 | 1.13        | 1.24     |
| 7   | c     | 154 | ARG  | C-O    | -9.01 | 1.12        | 1.24     |
| 1   | A     | 202 | TYR  | C-O    | -9.00 | 1.13        | 1.24     |
| 1   | A     | 774 | ASN  | CG-ND2 | -8.96 | 1.14        | 1.33     |
| 1   | A     | 110 | ARG  | C-O    | -8.94 | 1.13        | 1.24     |
| 1   | A     | 680 | PRO  | C-O    | -8.94 | 1.13        | 1.24     |
| 1   | A     | 679 | SER  | C-O    | -8.93 | 1.16        | 1.24     |
| 1   | a     | 612 | ARG  | N-CA   | -8.93 | 1.38        | 1.46     |
| 4   | f     | 14  | PHE  | C-O    | -8.92 | 1.13        | 1.24     |
| 1   | a     | 633 | PRO  | C-O    | -8.90 | 1.13        | 1.23     |
| 4   | f     | 12  | LEU  | C-O    | -8.89 | 1.13        | 1.24     |
| 1   | a     | 542 | TRP  | C-O    | -8.89 | 1.13        | 1.24     |
| 1   | A     | 23  | PRO  | C-O    | -8.88 | 1.14        | 1.24     |
| 1   | A     | 688 | ARG  | C-O    | -8.85 | 1.12        | 1.24     |
| 1   | a     | 18  | LEU  | C-O    | -8.83 | 1.11        | 1.23     |
| 7   | c     | 75  | LYS  | C-O    | -8.83 | 1.13        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | a     | 225 | LEU  | C-O    | -8.82 | 1.12        | 1.24     |
| 1   | a     | 339 | ASN  | C-O    | -8.80 | 1.12        | 1.24     |
| 7   | c     | 99  | GLY  | C-O    | -8.77 | 1.12        | 1.23     |
| 7   | c     | 145 | GLN  | C-O    | -8.75 | 1.13        | 1.24     |
| 1   | a     | 79  | GLN  | C-O    | -8.74 | 1.13        | 1.23     |
| 7   | c     | 76  | ALA  | C-O    | -8.74 | 1.13        | 1.24     |
| 7   | c     | 87  | ALA  | C-O    | -8.72 | 1.13        | 1.24     |
| 1   | a     | 338 | MET  | C-O    | -8.72 | 1.12        | 1.24     |
| 2   | C     | 115 | ARG  | C-O    | -8.71 | 1.14        | 1.24     |
| 7   | c     | 74  | TYR  | CA-C   | -8.71 | 1.41        | 1.52     |
| 1   | A     | 123 | LEU  | C-O    | -8.69 | 1.13        | 1.24     |
| 1   | A     | 630 | ALA  | C-O    | -8.66 | 1.11        | 1.24     |
| 1   | a     | 19  | GLU  | C-O    | -8.65 | 1.12        | 1.23     |
| 1   | A     | 20  | LEU  | C-O    | -8.64 | 1.12        | 1.23     |
| 1   | A     | 61  | THR  | CB-CG2 | -8.61 | 1.24        | 1.52     |
| 1   | A     | 538 | GLN  | C-O    | -8.61 | 1.13        | 1.24     |
| 1   | a     | 632 | THR  | C-O    | -8.59 | 1.13        | 1.23     |
| 1   | A     | 734 | GLY  | C-O    | -8.57 | 1.11        | 1.23     |
| 1   | a     | 528 | GLU  | C-O    | -8.56 | 1.13        | 1.24     |
| 3   | E     | 12  | LEU  | C-O    | -8.56 | 1.13        | 1.24     |
| 7   | c     | 97  | GLY  | N-CA   | 8.56  | 1.54        | 1.45     |
| 1   | a     | 777 | THR  | CB-CG2 | -8.55 | 1.24        | 1.52     |
| 4   | f     | 13  | CYS  | C-O    | -8.54 | 1.14        | 1.24     |
| 1   | a     | 222 | PRO  | C-O    | -8.52 | 1.14        | 1.23     |
| 1   | A     | 205 | LEU  | C-O    | -8.51 | 1.14        | 1.24     |
| 7   | c     | 89  | CYS  | C-O    | -8.50 | 1.13        | 1.24     |
| 1   | A     | 501 | ARG  | CA-C   | -8.49 | 1.42        | 1.52     |
| 1   | A     | 242 | ALA  | C-O    | -8.49 | 1.13        | 1.24     |
| 4   | F     | 20  | GLY  | C-O    | -8.47 | 1.13        | 1.23     |
| 2   | C     | 191 | ALA  | C-O    | -8.45 | 1.13        | 1.24     |
| 7   | c     | 77  | MET  | C-O    | -8.45 | 1.14        | 1.24     |
| 1   | A     | 639 | ASN  | CG-OD1 | -8.45 | 1.07        | 1.23     |
| 2   | C     | 122 | GLN  | C-O    | -8.45 | 1.13        | 1.24     |
| 1   | A     | 479 | ASP  | CA-C   | -8.43 | 1.41        | 1.52     |
| 4   | F     | 9   | ILE  | C-O    | -8.41 | 1.14        | 1.24     |
| 4   | F     | 27  | TYR  | C-O    | -8.39 | 1.14        | 1.24     |
| 1   | A     | 735 | TRP  | C-O    | -8.38 | 1.13        | 1.24     |
| 3   | E     | 15  | TYR  | CA-C   | -8.36 | 1.41        | 1.52     |
| 1   | A     | 233 | PRO  | C-O    | -8.36 | 1.13        | 1.24     |
| 7   | c     | 100 | ASN  | N-CA   | -8.30 | 1.36        | 1.46     |
| 1   | A     | 639 | ASN  | C-O    | -8.30 | 1.12        | 1.23     |
| 1   | A     | 266 | GLU  | C-O    | -8.28 | 1.13        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 123 | ASN  | CG-ND2  | -8.27 | 1.15        | 1.33     |
| 1   | a     | 377 | GLY  | C-O     | -8.27 | 1.14        | 1.23     |
| 2   | C     | 125 | CYS  | C-O     | -8.27 | 1.13        | 1.24     |
| 1   | A     | 611 | PHE  | C-O     | -8.24 | 1.13        | 1.24     |
| 1   | A     | 165 | THR  | C-O     | -8.24 | 1.12        | 1.24     |
| 1   | a     | 20  | LEU  | C-O     | -8.23 | 1.12        | 1.24     |
| 4   | F     | 26  | VAL  | C-O     | -8.21 | 1.14        | 1.24     |
| 1   | a     | 61  | THR  | CB-CG2  | -8.21 | 1.25        | 1.52     |
| 7   | c     | 44  | ALA  | C-O     | -8.19 | 1.13        | 1.24     |
| 2   | C     | 169 | ASN  | CG-OD1  | -8.18 | 1.08        | 1.23     |
| 2   | C     | 140 | SER  | CA-C    | -8.18 | 1.42        | 1.52     |
| 3   | E     | 9   | LEU  | C-O     | -8.15 | 1.13        | 1.24     |
| 4   | F     | 5   | VAL  | C-O     | -8.15 | 1.14        | 1.24     |
| 1   | A     | 241 | GLN  | C-O     | -8.12 | 1.13        | 1.24     |
| 4   | F     | 7   | GLN  | C-O     | -8.11 | 1.14        | 1.24     |
| 2   | C     | 164 | GLY  | C-O     | -8.11 | 1.11        | 1.23     |
| 7   | c     | 144 | GLN  | C-O     | -8.11 | 1.14        | 1.24     |
| 1   | a     | 364 | GLN  | CD-OE1  | -8.10 | 1.08        | 1.23     |
| 1   | A     | 690 | GLN  | C-O     | -8.09 | 1.13        | 1.24     |
| 2   | C     | 71  | ARG  | C-O     | -8.09 | 1.13        | 1.24     |
| 1   | a     | 25  | GLU  | C-O     | -8.06 | 1.13        | 1.24     |
| 1   | a     | 488 | ALA  | C-O     | -8.04 | 1.13        | 1.23     |
| 7   | c     | 80  | GLU  | C-O     | -8.03 | 1.13        | 1.24     |
| 1   | a     | 119 | ILE  | C-O     | -8.03 | 1.14        | 1.24     |
| 1   | a     | 346 | LYS  | N-CA    | 8.02  | 1.56        | 1.46     |
| 7   | c     | 45  | PRO  | C-O     | -8.01 | 1.13        | 1.24     |
| 7   | c     | 40  | ALA  | C-O     | -7.99 | 1.14        | 1.24     |
| 1   | A     | 849 | THR  | CB-CG2  | -7.99 | 1.26        | 1.52     |
| 7   | c     | 26  | ARG  | CZ-NH1  | -7.97 | 1.21        | 1.32     |
| 4   | F     | 24  | GLY  | C-O     | -7.96 | 1.14        | 1.23     |
| 1   | A     | 540 | GLY  | C-O     | -7.95 | 1.12        | 1.24     |
| 1   | a     | 709 | ILE  | CG1-CD1 | -7.92 | 1.20        | 1.51     |
| 1   | a     | 765 | ASN  | CG-OD1  | -7.92 | 1.08        | 1.23     |
| 1   | a     | 863 | GLN  | C-O     | -7.92 | 1.14        | 1.24     |
| 7   | c     | 39  | ALA  | C-O     | -7.89 | 1.15        | 1.24     |
| 1   | a     | 656 | TRP  | C-O     | -7.88 | 1.14        | 1.24     |
| 1   | A     | 22  | MET  | C-O     | -7.88 | 1.14        | 1.24     |
| 1   | a     | 511 | SER  | C-O     | -7.88 | 1.13        | 1.24     |
| 7   | c     | 105 | ALA  | CA-C    | -7.87 | 1.42        | 1.52     |
| 1   | a     | 757 | GLY  | CA-C    | -7.86 | 1.40        | 1.51     |
| 7   | c     | 38  | ILE  | C-O     | -7.86 | 1.14        | 1.24     |
| 1   | A     | 204 | GLY  | C-O     | -7.85 | 1.14        | 1.23     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | a     | 776 | LEU  | C-O    | -7.84 | 1.14        | 1.24     |
| 1   | a     | 732 | ASP  | CB-CG  | -7.84 | 1.32        | 1.52     |
| 1   | a     | 864 | ASN  | C-O    | -7.83 | 1.13        | 1.23     |
| 1   | A     | 783 | GLY  | C-O    | -7.83 | 1.14        | 1.24     |
| 4   | f     | 10  | SER  | C-O    | -7.83 | 1.15        | 1.24     |
| 2   | C     | 162 | TYR  | C-O    | -7.83 | 1.15        | 1.24     |
| 1   | a     | 613 | PRO  | C-O    | -7.83 | 1.13        | 1.24     |
| 5   | G     | 20  | LEU  | C-O    | -7.81 | 1.13        | 1.24     |
| 1   | A     | 298 | GLU  | C-O    | -7.80 | 1.14        | 1.24     |
| 7   | c     | 140 | LYS  | C-O    | -7.80 | 1.11        | 1.23     |
| 4   | F     | 17  | LEU  | C-O    | -7.79 | 1.14        | 1.24     |
| 1   | A     | 244 | PHE  | CA-C   | -7.79 | 1.43        | 1.52     |
| 1   | A     | 784 | HIS  | C-O    | -7.78 | 1.13        | 1.24     |
| 7   | c     | 111 | ALA  | C-O    | -7.75 | 1.14        | 1.24     |
| 1   | a     | 784 | HIS  | C-O    | -7.75 | 1.14        | 1.24     |
| 1   | A     | 221 | PRO  | C-O    | -7.74 | 1.15        | 1.24     |
| 1   | A     | 657 | LEU  | C-O    | -7.74 | 1.14        | 1.24     |
| 1   | A     | 697 | ILE  | C-O    | -7.74 | 1.14        | 1.24     |
| 2   | C     | 182 | SER  | CA-C   | 7.73  | 1.61        | 1.52     |
| 1   | A     | 488 | ALA  | C-O    | -7.70 | 1.15        | 1.24     |
| 7   | c     | 25  | ALA  | C-O    | -7.68 | 1.14        | 1.23     |
| 1   | A     | 243 | PRO  | C-O    | -7.67 | 1.14        | 1.23     |
| 1   | a     | 117 | PHE  | C-O    | -7.66 | 1.15        | 1.24     |
| 7   | c     | 99  | GLY  | CA-C   | -7.66 | 1.41        | 1.51     |
| 1   | a     | 765 | ASN  | CG-ND2 | -7.64 | 1.17        | 1.33     |
| 7   | c     | 83  | THR  | C-O    | -7.64 | 1.13        | 1.24     |
| 2   | C     | 192 | TYR  | CA-C   | -7.63 | 1.42        | 1.52     |
| 7   | c     | 130 | LYS  | CA-C   | -7.63 | 1.43        | 1.52     |
| 3   | E     | 8   | CYS  | C-O    | -7.63 | 1.15        | 1.24     |
| 1   | a     | 769 | TRP  | C-O    | -7.62 | 1.14        | 1.24     |
| 2   | C     | 114 | TYR  | N-CA   | -7.60 | 1.37        | 1.46     |
| 2   | C     | 170 | GLY  | C-O    | -7.60 | 1.12        | 1.24     |
| 5   | G     | 44  | LEU  | CA-CB  | -7.60 | 1.41        | 1.53     |
| 1   | A     | 364 | GLN  | N-CA   | -7.59 | 1.37        | 1.46     |
| 1   | a     | 732 | ASP  | C-O    | -7.59 | 1.13        | 1.24     |
| 2   | C     | 149 | GLN  | C-O    | -7.59 | 1.15        | 1.24     |
| 3   | E     | 22  | ILE  | C-O    | -7.58 | 1.15        | 1.24     |
| 1   | a     | 739 | MET  | C-O    | -7.56 | 1.14        | 1.24     |
| 4   | f     | 22  | LEU  | C-O    | -7.56 | 1.15        | 1.24     |
| 1   | A     | 639 | ASN  | CG-ND2 | -7.56 | 1.17        | 1.33     |
| 1   | A     | 327 | ARG  | C-O    | -7.55 | 1.15        | 1.24     |
| 1   | a     | 363 | VAL  | C-O    | -7.55 | 1.15        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | f     | 7   | GLN  | C-O     | -7.54 | 1.15        | 1.24     |
| 4   | F     | 16  | ILE  | C-O     | -7.51 | 1.14        | 1.24     |
| 7   | c     | 142 | THR  | C-O     | -7.50 | 1.13        | 1.23     |
| 7   | c     | 114 | GLN  | C-O     | -7.47 | 1.15        | 1.24     |
| 1   | A     | 732 | ASP  | CG-OD2  | -7.47 | 1.11        | 1.25     |
| 1   | a     | 433 | THR  | CB-CG2  | -7.46 | 1.27        | 1.52     |
| 1   | a     | 548 | LYS  | C-O     | -7.46 | 1.14        | 1.24     |
| 7   | c     | 23  | VAL  | C-O     | -7.45 | 1.15        | 1.24     |
| 1   | a     | 22  | MET  | C-O     | -7.43 | 1.16        | 1.24     |
| 3   | E     | 29  | THR  | C-O     | -7.43 | 1.14        | 1.24     |
| 4   | f     | 21  | THR  | C-O     | -7.43 | 1.15        | 1.24     |
| 1   | a     | 639 | ASN  | CB-CG   | -7.42 | 1.33        | 1.52     |
| 7   | c     | 134 | MET  | C-O     | -7.42 | 1.14        | 1.24     |
| 3   | E     | 16  | ALA  | C-O     | -7.40 | 1.14        | 1.24     |
| 1   | A     | 239 | LEU  | C-O     | -7.40 | 1.15        | 1.24     |
| 1   | A     | 745 | GLU  | CB-CG   | -7.37 | 1.30        | 1.52     |
| 1   | a     | 698 | GLY  | CA-C    | -7.35 | 1.41        | 1.51     |
| 3   | E     | 34  | ALA  | N-CA    | 7.33  | 1.55        | 1.46     |
| 1   | A     | 653 | ILE  | CG1-CD1 | -7.33 | 1.23        | 1.51     |
| 1   | a     | 615 | LEU  | C-O     | -7.31 | 1.14        | 1.24     |
| 1   | a     | 362 | HIS  | C-O     | -7.31 | 1.14        | 1.24     |
| 7   | c     | 141 | LEU  | C-O     | -7.29 | 1.14        | 1.23     |
| 1   | A     | 20  | LEU  | CA-C    | -7.28 | 1.44        | 1.53     |
| 7   | c     | 28  | ALA  | C-O     | -7.27 | 1.14        | 1.24     |
| 1   | A     | 814 | LEU  | C-O     | -7.26 | 1.15        | 1.24     |
| 1   | a     | 139 | GLY  | C-O     | -7.26 | 1.16        | 1.23     |
| 1   | a     | 414 | THR  | CB-CG2  | -7.25 | 1.28        | 1.52     |
| 1   | A     | 166 | PRO  | C-O     | -7.22 | 1.15        | 1.24     |
| 1   | A     | 329 | HIS  | C-O     | -7.22 | 1.14        | 1.24     |
| 7   | c     | 110 | ASP  | CG-OD2  | -7.22 | 1.11        | 1.25     |
| 7   | c     | 107 | ASN  | CG-ND2  | -7.22 | 1.18        | 1.33     |
| 7   | c     | 133 | VAL  | C-O     | -7.22 | 1.15        | 1.23     |
| 1   | a     | 487 | THR  | C-O     | -7.21 | 1.15        | 1.23     |
| 2   | C     | 179 | ASN  | C-N     | -7.21 | 1.23        | 1.33     |
| 1   | a     | 852 | LEU  | N-CA    | -7.20 | 1.37        | 1.46     |
| 1   | A     | 785 | LEU  | C-O     | -7.19 | 1.15        | 1.24     |
| 2   | C     | 217 | ARG  | CA-C    | -7.19 | 1.43        | 1.52     |
| 7   | c     | 37  | SER  | C-O     | -7.18 | 1.14        | 1.24     |
| 4   | F     | 30  | HIS  | C-O     | -7.15 | 1.15        | 1.24     |
| 2   | C     | 172 | GLY  | C-O     | -7.15 | 1.14        | 1.23     |
| 4   | F     | 17  | LEU  | N-CA    | -7.14 | 1.37        | 1.46     |
| 2   | C     | 124 | ASN  | CA-C    | -7.12 | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | a     | 364 | GLN  | N-CA    | -7.10 | 1.37        | 1.46     |
| 2   | C     | 216 | GLU  | CA-CB   | -7.08 | 1.42        | 1.53     |
| 1   | A     | 640 | LEU  | CA-C    | -7.07 | 1.43        | 1.52     |
| 1   | A     | 700 | VAL  | CA-C    | -7.06 | 1.44        | 1.52     |
| 1   | A     | 304 | PHE  | C-O     | -7.05 | 1.15        | 1.24     |
| 1   | A     | 328 | ASN  | CG-OD1  | -7.04 | 1.10        | 1.23     |
| 1   | a     | 514 | THR  | CB-CG2  | -7.04 | 1.29        | 1.52     |
| 1   | a     | 394 | ARG  | CA-C    | -7.04 | 1.43        | 1.52     |
| 2   | C     | 112 | GLU  | N-CA    | -7.04 | 1.37        | 1.46     |
| 7   | c     | 103 | ILE  | C-O     | -7.03 | 1.14        | 1.24     |
| 7   | c     | 26  | ARG  | CZ-NH2  | -7.03 | 1.24        | 1.33     |
| 1   | a     | 518 | THR  | CB-CG2  | -7.02 | 1.29        | 1.52     |
| 1   | a     | 699 | PRO  | C-O     | -7.02 | 1.09        | 1.23     |
| 1   | a     | 847 | THR  | CB-CG2  | -7.02 | 1.29        | 1.52     |
| 3   | e     | 11  | VAL  | C-O     | 6.99  | 1.32        | 1.24     |
| 3   | E     | 23  | LYS  | C-O     | -6.98 | 1.15        | 1.24     |
| 4   | f     | 11  | VAL  | C-O     | -6.98 | 1.16        | 1.24     |
| 4   | F     | 14  | PHE  | C-O     | -6.96 | 1.16        | 1.24     |
| 1   | A     | 836 | THR  | CB-CG2  | -6.96 | 1.29        | 1.52     |
| 1   | A     | 742 | ARG  | CZ-NH1  | -6.93 | 1.23        | 1.32     |
| 4   | f     | 5   | VAL  | C-O     | -6.93 | 1.15        | 1.24     |
| 1   | a     | 764 | TRP  | N-CA    | -6.93 | 1.37        | 1.46     |
| 1   | a     | 266 | GLU  | CD-OE2  | -6.92 | 1.12        | 1.25     |
| 1   | A     | 136 | ALA  | C-O     | -6.91 | 1.15        | 1.24     |
| 7   | c     | 36  | SER  | C-O     | -6.90 | 1.15        | 1.24     |
| 7   | c     | 18  | ALA  | C-O     | -6.89 | 1.16        | 1.24     |
| 3   | E     | 21  | ILE  | C-O     | -6.86 | 1.16        | 1.24     |
| 1   | a     | 413 | THR  | CB-CG2  | -6.86 | 1.29        | 1.52     |
| 2   | C     | 129 | HIS  | C-O     | -6.85 | 1.14        | 1.24     |
| 1   | a     | 666 | PHE  | C-O     | -6.85 | 1.14        | 1.24     |
| 7   | c     | 82  | GLN  | C-O     | -6.83 | 1.15        | 1.24     |
| 2   | C     | 171 | GLY  | C-O     | -6.81 | 1.15        | 1.23     |
| 7   | c     | 73  | HIS  | C-O     | -6.80 | 1.15        | 1.24     |
| 1   | a     | 732 | ASP  | C-N     | -6.79 | 1.24        | 1.33     |
| 1   | A     | 541 | SER  | CB-OG   | -6.79 | 1.28        | 1.42     |
| 2   | C     | 142 | ASN  | CG-OD1  | -6.78 | 1.10        | 1.23     |
| 2   | C     | 187 | ARG  | C-O     | -6.78 | 1.15        | 1.24     |
| 1   | a     | 689 | LYS  | C-O     | -6.78 | 1.16        | 1.24     |
| 7   | c     | 55  | TYR  | CD1-CE1 | -6.76 | 1.18        | 1.38     |
| 7   | c     | 88  | ALA  | C-O     | -6.74 | 1.14        | 1.23     |
| 2   | C     | 29  | GLU  | C-O     | -6.71 | 1.14        | 1.23     |
| 3   | e     | 22  | ILE  | C-O     | -6.71 | 1.16        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | E     | 28  | ASN  | C-O    | -6.70 | 1.15        | 1.24     |
| 1   | A     | 232 | THR  | C-O    | -6.68 | 1.15        | 1.24     |
| 5   | G     | 14  | TRP  | CA-C   | -6.68 | 1.44        | 1.52     |
| 1   | a     | 308 | LEU  | N-CA   | -6.68 | 1.38        | 1.46     |
| 1   | a     | 775 | HIS  | C-O    | -6.68 | 1.15        | 1.24     |
| 4   | F     | 3   | ASN  | CA-C   | -6.67 | 1.44        | 1.52     |
| 1   | A     | 328 | ASN  | C-O    | -6.66 | 1.14        | 1.23     |
| 7   | c     | 48  | LEU  | C-O    | -6.66 | 1.15        | 1.24     |
| 1   | a     | 134 | TYR  | CA-C   | -6.63 | 1.43        | 1.52     |
| 1   | a     | 732 | ASP  | N-CA   | -6.61 | 1.37        | 1.46     |
| 2   | C     | 163 | ASN  | CG-OD1 | -6.61 | 1.10        | 1.23     |
| 7   | c     | 122 | MET  | SD-CE  | -6.61 | 1.63        | 1.79     |
| 2   | C     | 124 | ASN  | CG-OD1 | -6.60 | 1.11        | 1.23     |
| 1   | a     | 364 | GLN  | C-O    | -6.59 | 1.15        | 1.24     |
| 5   | G     | 25  | LEU  | C-O    | -6.59 | 1.16        | 1.24     |
| 2   | C     | 149 | GLN  | CD-NE2 | -6.58 | 1.19        | 1.33     |
| 1   | A     | 487 | THR  | C-O    | -6.56 | 1.15        | 1.23     |
| 1   | a     | 759 | VAL  | CA-CB  | 6.56  | 1.63        | 1.54     |
| 2   | C     | 162 | TYR  | CZ-OH  | -6.56 | 1.24        | 1.38     |
| 4   | F     | 19  | VAL  | C-O    | -6.56 | 1.16        | 1.24     |
| 1   | A     | 268 | THR  | CB-CG2 | -6.54 | 1.30        | 1.52     |
| 7   | c     | 131 | GLY  | C-O    | -6.54 | 1.15        | 1.23     |
| 1   | a     | 541 | SER  | N-CA   | -6.52 | 1.37        | 1.46     |
| 7   | c     | 81  | LEU  | C-O    | -6.50 | 1.15        | 1.24     |
| 1   | A     | 810 | ARG  | CZ-NH1 | -6.50 | 1.23        | 1.32     |
| 3   | E     | 24  | PHE  | C-O    | -6.49 | 1.16        | 1.24     |
| 7   | c     | 107 | ASN  | CG-OD1 | -6.48 | 1.11        | 1.23     |
| 4   | f     | 26  | VAL  | C-O    | -6.48 | 1.16        | 1.24     |
| 1   | A     | 135 | GLY  | C-O    | -6.47 | 1.15        | 1.23     |
| 1   | a     | 394 | ARG  | CA-CB  | -6.47 | 1.44        | 1.54     |
| 1   | a     | 811 | TRP  | N-CA   | -6.46 | 1.38        | 1.46     |
| 1   | A     | 224 | PRO  | C-O    | -6.46 | 1.10        | 1.23     |
| 2   | C     | 31  | ARG  | CZ-NH2 | -6.46 | 1.25        | 1.33     |
| 1   | A     | 702 | GLY  | C-O    | -6.46 | 1.15        | 1.24     |
| 1   | A     | 691 | SER  | C-N    | -6.45 | 1.28        | 1.33     |
| 7   | c     | 141 | LEU  | CA-C   | -6.45 | 1.45        | 1.52     |
| 1   | a     | 785 | LEU  | C-O    | -6.44 | 1.15        | 1.24     |
| 1   | A     | 25  | GLU  | C-O    | -6.44 | 1.15        | 1.24     |
| 1   | a     | 225 | LEU  | N-CA   | -6.43 | 1.39        | 1.46     |
| 1   | a     | 612 | ARG  | CA-CB  | -6.42 | 1.46        | 1.53     |
| 1   | A     | 732 | ASP  | N-CA   | -6.42 | 1.37        | 1.46     |
| 2   | C     | 28  | ASN  | C-O    | -6.42 | 1.15        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | a     | 529 | TRP  | CB-CG   | -6.42 | 1.30        | 1.50     |
| 1   | A     | 223 | VAL  | C-O     | -6.41 | 1.16        | 1.24     |
| 1   | A     | 226 | GLN  | C-O     | -6.41 | 1.15        | 1.23     |
| 7   | c     | 55  | TYR  | CD2-CE2 | -6.41 | 1.19        | 1.38     |
| 1   | a     | 308 | LEU  | C-O     | -6.39 | 1.16        | 1.24     |
| 1   | A     | 732 | ASP  | CG-OD1  | -6.38 | 1.13        | 1.25     |
| 1   | a     | 50  | MET  | SD-CE   | -6.38 | 1.63        | 1.79     |
| 1   | A     | 763 | MET  | SD-CE   | -6.35 | 1.63        | 1.79     |
| 1   | a     | 339 | ASN  | CG-ND2  | -6.35 | 1.20        | 1.33     |
| 1   | A     | 299 | ASP  | N-CA    | -6.34 | 1.38        | 1.46     |
| 7   | c     | 142 | THR  | CB-CG2  | -6.34 | 1.31        | 1.52     |
| 1   | a     | 137 | ARG  | C-O     | -6.33 | 1.16        | 1.24     |
| 7   | c     | 97  | GLY  | C-O     | -6.33 | 1.16        | 1.23     |
| 1   | A     | 91  | PHE  | N-CA    | 6.32  | 1.54        | 1.46     |
| 1   | A     | 628 | ARG  | CB-CG   | -6.31 | 1.33        | 1.52     |
| 1   | a     | 248 | TRP  | C-O     | -6.31 | 1.15        | 1.24     |
| 7   | c     | 55  | TYR  | CZ-OH   | -6.30 | 1.24        | 1.38     |
| 1   | A     | 364 | GLN  | C-O     | -6.30 | 1.16        | 1.24     |
| 2   | C     | 46  | LEU  | C-O     | -6.29 | 1.16        | 1.24     |
| 5   | G     | 26  | ILE  | C-O     | -6.28 | 1.17        | 1.24     |
| 7   | c     | 154 | ARG  | CZ-NH2  | -6.27 | 1.25        | 1.33     |
| 2   | C     | 178 | TYR  | CZ-OH   | -6.27 | 1.24        | 1.38     |
| 5   | G     | 31  | ASN  | C-O     | -6.26 | 1.16        | 1.24     |
| 1   | A     | 689 | LYS  | C-O     | -6.26 | 1.16        | 1.24     |
| 1   | a     | 540 | GLY  | N-CA    | 6.25  | 1.54        | 1.45     |
| 1   | A     | 700 | VAL  | C-O     | -6.25 | 1.16        | 1.24     |
| 1   | a     | 768 | THR  | CB-CG2  | -6.25 | 1.31        | 1.52     |
| 3   | e     | 26  | VAL  | N-CA    | -6.24 | 1.38        | 1.46     |
| 1   | A     | 172 | LYS  | C-O     | -6.24 | 1.17        | 1.24     |
| 1   | a     | 732 | ASP  | CG-OD2  | -6.23 | 1.13        | 1.25     |
| 7   | c     | 103 | ILE  | N-CA    | -6.22 | 1.37        | 1.46     |
| 1   | a     | 756 | THR  | CA-C    | -6.22 | 1.44        | 1.52     |
| 1   | a     | 815 | MET  | C-O     | -6.21 | 1.16        | 1.24     |
| 7   | c     | 71  | ILE  | C-O     | -6.21 | 1.16        | 1.24     |
| 4   | f     | 8   | ILE  | C-O     | -6.21 | 1.17        | 1.24     |
| 1   | A     | 706 | GLY  | C-O     | -6.20 | 1.16        | 1.24     |
| 2   | C     | 116 | GLU  | C-O     | -6.20 | 1.16        | 1.24     |
| 1   | a     | 309 | THR  | CB-CG2  | -6.19 | 1.32        | 1.52     |
| 1   | a     | 742 | ARG  | CA-C    | -6.19 | 1.44        | 1.52     |
| 1   | A     | 225 | LEU  | C-O     | -6.18 | 1.15        | 1.23     |
| 2   | C     | 123 | ASN  | N-CA    | -6.18 | 1.39        | 1.46     |
| 1   | A     | 659 | ILE  | CG1-CD1 | -6.17 | 1.27        | 1.51     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | F     | 7   | GLN  | N-CA   | -6.16 | 1.38        | 1.46     |
| 7   | c     | 58  | SER  | CA-C   | -6.16 | 1.45        | 1.52     |
| 2   | C     | 115 | ARG  | CD-NE  | -6.16 | 1.37        | 1.46     |
| 7   | c     | 59  | THR  | C-O    | -6.16 | 1.15        | 1.23     |
| 1   | a     | 742 | ARG  | CZ-NH1 | -6.15 | 1.24        | 1.32     |
| 1   | a     | 268 | THR  | CB-CG2 | -6.15 | 1.32        | 1.52     |
| 1   | A     | 18  | LEU  | C-O    | -6.14 | 1.16        | 1.23     |
| 7   | c     | 93  | HIS  | CA-C   | -6.14 | 1.44        | 1.52     |
| 1   | A     | 633 | PRO  | C-O    | -6.14 | 1.16        | 1.23     |
| 7   | c     | 98  | GLY  | C-O    | -6.13 | 1.15        | 1.23     |
| 1   | A     | 705 | CYS  | C-O    | -6.13 | 1.16        | 1.23     |
| 1   | A     | 657 | LEU  | N-CA   | -6.13 | 1.38        | 1.46     |
| 1   | A     | 246 | TYR  | CA-C   | -6.12 | 1.45        | 1.52     |
| 7   | c     | 27  | ASN  | C-O    | -6.12 | 1.16        | 1.23     |
| 1   | A     | 144 | GLU  | C-O    | -6.12 | 1.16        | 1.23     |
| 1   | a     | 529 | TRP  | C-O    | -6.12 | 1.16        | 1.24     |
| 1   | A     | 638 | SER  | CB-OG  | -6.11 | 1.29        | 1.42     |
| 1   | a     | 861 | PHE  | C-O    | -6.09 | 1.16        | 1.24     |
| 3   | e     | 27  | ALA  | C-O    | -6.09 | 1.16        | 1.24     |
| 1   | a     | 376 | HIS  | CA-C   | -6.09 | 1.44        | 1.52     |
| 1   | A     | 471 | PRO  | C-O    | -6.09 | 1.16        | 1.24     |
| 7   | c     | 20  | GLY  | N-CA   | -6.09 | 1.36        | 1.45     |
| 1   | a     | 697 | ILE  | N-CA   | -6.08 | 1.38        | 1.46     |
| 5   | G     | 15  | ALA  | C-O    | -6.08 | 1.16        | 1.24     |
| 1   | A     | 172 | LYS  | N-CA   | -6.07 | 1.40        | 1.46     |
| 7   | c     | 39  | ALA  | CA-C   | -6.07 | 1.45        | 1.52     |
| 4   | f     | 6   | GLY  | C-O    | -6.06 | 1.16        | 1.23     |
| 1   | A     | 639 | ASN  | CB-CG  | -6.05 | 1.36        | 1.52     |
| 1   | A     | 470 | ASN  | CA-C   | -6.05 | 1.45        | 1.52     |
| 2   | C     | 127 | GLY  | C-O    | -6.05 | 1.15        | 1.23     |
| 3   | E     | 11  | VAL  | C-O    | -6.05 | 1.16        | 1.24     |
| 1   | A     | 816 | GLY  | C-O    | -6.04 | 1.16        | 1.23     |
| 1   | A     | 170 | TRP  | C-O    | -6.04 | 1.16        | 1.24     |
| 7   | c     | 94  | GLN  | C-O    | -6.03 | 1.16        | 1.24     |
| 1   | a     | 223 | VAL  | C-O    | -6.03 | 1.17        | 1.25     |
| 1   | A     | 637 | TYR  | C-O    | -6.03 | 1.16        | 1.24     |
| 1   | A     | 479 | ASP  | C-O    | -6.02 | 1.16        | 1.23     |
| 1   | a     | 538 | GLN  | CD-NE2 | -6.02 | 1.20        | 1.33     |
| 2   | C     | 115 | ARG  | N-CA   | -6.01 | 1.39        | 1.46     |
| 1   | a     | 352 | ARG  | CZ-NH2 | -6.01 | 1.25        | 1.33     |
| 2   | C     | 181 | LEU  | CA-C   | -6.01 | 1.45        | 1.52     |
| 1   | A     | 671 | ARG  | CZ-NH2 | -5.99 | 1.25        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | a     | 497 | GLN  | CB-CG  | -5.99 | 1.34        | 1.52     |
| 1   | a     | 732 | ASP  | CA-CB  | -5.99 | 1.43        | 1.53     |
| 1   | A     | 817 | LYS  | C-O    | -5.98 | 1.17        | 1.24     |
| 1   | A     | 295 | THR  | CB-CG2 | -5.98 | 1.32        | 1.52     |
| 1   | A     | 497 | GLN  | CB-CG  | -5.98 | 1.34        | 1.52     |
| 1   | a     | 541 | SER  | CB-OG  | -5.98 | 1.30        | 1.42     |
| 1   | A     | 295 | THR  | C-O    | -5.98 | 1.16        | 1.24     |
| 1   | A     | 606 | ALA  | C-O    | -5.97 | 1.16        | 1.24     |
| 1   | A     | 610 | LYS  | C-O    | -5.97 | 1.16        | 1.24     |
| 5   | G     | 31  | ASN  | CG-OD1 | -5.96 | 1.12        | 1.23     |
| 5   | G     | 24  | CYS  | C-O    | -5.96 | 1.17        | 1.24     |
| 1   | A     | 470 | ASN  | C-O    | -5.96 | 1.16        | 1.24     |
| 5   | G     | 33  | VAL  | C-O    | -5.94 | 1.17        | 1.24     |
| 4   | F     | 13  | CYS  | C-O    | -5.93 | 1.17        | 1.24     |
| 1   | a     | 306 | VAL  | C-O    | -5.93 | 1.17        | 1.24     |
| 1   | A     | 502 | ILE  | C-O    | -5.93 | 1.17        | 1.24     |
| 7   | c     | 49  | ARG  | N-CA   | -5.92 | 1.39        | 1.46     |
| 4   | F     | 7   | GLN  | CD-OE1 | -5.91 | 1.12        | 1.23     |
| 1   | A     | 183 | THR  | CB-CG2 | -5.90 | 1.33        | 1.52     |
| 1   | A     | 266 | GLU  | CD-OE2 | -5.90 | 1.14        | 1.25     |
| 1   | a     | 361 | ASN  | C-O    | -5.89 | 1.16        | 1.24     |
| 1   | A     | 732 | ASP  | C-O    | -5.89 | 1.16        | 1.24     |
| 4   | f     | 10  | SER  | CB-OG  | -5.89 | 1.30        | 1.42     |
| 1   | a     | 200 | THR  | CB-CG2 | -5.88 | 1.33        | 1.52     |
| 7   | c     | 95  | VAL  | C-O    | -5.87 | 1.16        | 1.24     |
| 1   | A     | 249 | PHE  | N-CA   | -5.85 | 1.39        | 1.46     |
| 1   | a     | 538 | GLN  | C-O    | -5.85 | 1.17        | 1.24     |
| 5   | g     | 41  | LEU  | C-O    | -5.84 | 1.16        | 1.24     |
| 1   | A     | 202 | TYR  | N-CA   | -5.83 | 1.39        | 1.46     |
| 2   | C     | 71  | ARG  | CA-C   | -5.83 | 1.44        | 1.52     |
| 2   | C     | 116 | GLU  | CA-CB  | -5.83 | 1.44        | 1.53     |
| 4   | f     | 16  | ILE  | C-O    | -5.83 | 1.17        | 1.24     |
| 1   | A     | 777 | THR  | CB-CG2 | -5.82 | 1.33        | 1.52     |
| 7   | c     | 78  | LEU  | C-O    | -5.82 | 1.17        | 1.24     |
| 1   | a     | 705 | CYS  | CB-SG  | 5.81  | 2.00        | 1.81     |
| 4   | f     | 19  | VAL  | C-O    | -5.80 | 1.16        | 1.24     |
| 1   | A     | 774 | ASN  | CG-OD1 | -5.80 | 1.12        | 1.23     |
| 2   | C     | 31  | ARG  | CZ-NH1 | -5.79 | 1.24        | 1.32     |
| 2   | C     | 168 | GLY  | C-O    | -5.79 | 1.15        | 1.23     |
| 4   | F     | 8   | ILE  | N-CA   | -5.79 | 1.39        | 1.46     |
| 1   | A     | 860 | GLY  | C-N    | -5.78 | 1.25        | 1.33     |
| 7   | c     | 96  | ASN  | CG-OD1 | -5.78 | 1.12        | 1.23     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | G     | 41  | LEU  | C-O    | -5.77 | 1.15        | 1.24     |
| 2   | C     | 182 | SER  | CB-OG  | -5.77 | 1.30        | 1.42     |
| 1   | A     | 414 | THR  | CB-CG2 | -5.75 | 1.33        | 1.52     |
| 1   | A     | 763 | MET  | C-N    | -5.75 | 1.26        | 1.33     |
| 1   | A     | 759 | VAL  | C-N    | -5.74 | 1.26        | 1.33     |
| 1   | a     | 836 | THR  | CB-CG2 | -5.74 | 1.33        | 1.52     |
| 1   | a     | 415 | MET  | SD-CE  | -5.72 | 1.65        | 1.79     |
| 1   | a     | 759 | VAL  | C-N    | -5.71 | 1.26        | 1.33     |
| 4   | f     | 28  | VAL  | C-O    | -5.71 | 1.17        | 1.24     |
| 1   | A     | 107 | THR  | CB-CG2 | -5.70 | 1.33        | 1.52     |
| 1   | A     | 476 | ALA  | C-O    | -5.70 | 1.16        | 1.24     |
| 3   | E     | 17  | ALA  | CA-C   | -5.70 | 1.45        | 1.52     |
| 1   | a     | 732 | ASP  | CG-OD1 | -5.70 | 1.14        | 1.25     |
| 1   | A     | 822 | LYS  | C-O    | -5.69 | 1.17        | 1.24     |
| 1   | A     | 145 | ILE  | N-CA   | -5.68 | 1.39        | 1.46     |
| 1   | A     | 548 | LYS  | C-O    | -5.68 | 1.16        | 1.24     |
| 3   | E     | 21  | ILE  | N-CA   | -5.68 | 1.40        | 1.46     |
| 7   | c     | 85  | ASN  | C-O    | -5.68 | 1.16        | 1.23     |
| 3   | e     | 26  | VAL  | CA-C   | -5.67 | 1.45        | 1.52     |
| 2   | C     | 112 | GLU  | CA-CB  | -5.66 | 1.44        | 1.53     |
| 5   | G     | 30  | GLY  | C-O    | -5.66 | 1.17        | 1.23     |
| 1   | A     | 560 | TRP  | N-CA   | -5.65 | 1.39        | 1.46     |
| 1   | A     | 847 | THR  | CB-CG2 | -5.65 | 1.33        | 1.52     |
| 7   | c     | 114 | GLN  | CD-NE2 | -5.65 | 1.21        | 1.33     |
| 1   | A     | 766 | GLU  | CD-OE2 | -5.64 | 1.14        | 1.25     |
| 2   | C     | 164 | GLY  | C-N    | -5.64 | 1.26        | 1.33     |
| 1   | a     | 621 | ASN  | CB-CG  | -5.62 | 1.38        | 1.52     |
| 7   | c     | 97  | GLY  | C-N    | -5.62 | 1.25        | 1.33     |
| 1   | A     | 230 | VAL  | CA-C   | -5.61 | 1.45        | 1.52     |
| 7   | c     | 38  | ILE  | CA-C   | -5.61 | 1.45        | 1.52     |
| 1   | A     | 606 | ALA  | CA-C   | -5.60 | 1.45        | 1.52     |
| 1   | a     | 379 | GLN  | CG-CD  | -5.60 | 1.38        | 1.52     |
| 7   | c     | 114 | GLN  | CD-OE1 | -5.58 | 1.12        | 1.23     |
| 2   | C     | 71  | ARG  | CZ-NH1 | -5.58 | 1.25        | 1.32     |
| 1   | a     | 394 | ARG  | C-O    | -5.58 | 1.17        | 1.23     |
| 1   | A     | 361 | ASN  | CG-ND2 | -5.56 | 1.21        | 1.33     |
| 1   | a     | 537 | VAL  | CA-C   | -5.56 | 1.45        | 1.52     |
| 2   | C     | 73  | ARG  | C-O    | -5.56 | 1.16        | 1.24     |
| 4   | F     | 23  | PHE  | C-O    | -5.55 | 1.16        | 1.24     |
| 1   | a     | 486 | GLY  | C-O    | -5.55 | 1.16        | 1.24     |
| 2   | C     | 139 | ARG  | C-O    | -5.55 | 1.14        | 1.24     |
| 1   | a     | 15  | TYR  | C-O    | -5.55 | 1.16        | 1.24     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 631 | SER  | CA-C   | -5.55 | 1.45        | 1.52     |
| 7   | c     | 75  | LYS  | N-CA   | -5.55 | 1.39        | 1.46     |
| 4   | F     | 11  | VAL  | C-O    | -5.54 | 1.17        | 1.24     |
| 1   | A     | 810 | ARG  | CA-CB  | -5.54 | 1.44        | 1.53     |
| 7   | c     | 107 | ASN  | C-O    | -5.53 | 1.16        | 1.23     |
| 1   | a     | 757 | GLY  | C-N    | -5.52 | 1.25        | 1.33     |
| 7   | c     | 100 | ASN  | C-O    | -5.52 | 1.17        | 1.24     |
| 3   | e     | 9   | LEU  | C-O    | -5.52 | 1.17        | 1.24     |
| 1   | a     | 438 | ASP  | CB-CG  | -5.52 | 1.38        | 1.52     |
| 1   | A     | 328 | ASN  | N-CA   | -5.50 | 1.39        | 1.46     |
| 7   | c     | 104 | ASN  | C-O    | -5.50 | 1.15        | 1.23     |
| 1   | a     | 337 | ASP  | C-O    | -5.50 | 1.16        | 1.24     |
| 1   | a     | 363 | VAL  | N-CA   | -5.50 | 1.39        | 1.46     |
| 2   | C     | 142 | ASN  | C-O    | -5.50 | 1.15        | 1.23     |
| 1   | A     | 703 | GLY  | C-O    | -5.49 | 1.16        | 1.23     |
| 1   | A     | 138 | GLY  | C-O    | -5.49 | 1.17        | 1.24     |
| 1   | A     | 657 | LEU  | CA-C   | -5.49 | 1.45        | 1.52     |
| 7   | c     | 107 | ASN  | N-CA   | 5.48  | 1.53        | 1.46     |
| 1   | a     | 18  | LEU  | CA-C   | -5.47 | 1.44        | 1.53     |
| 7   | c     | 132 | LYS  | C-O    | -5.47 | 1.17        | 1.24     |
| 1   | A     | 757 | GLY  | CA-C   | -5.47 | 1.44        | 1.51     |
| 7   | c     | 22  | PHE  | C-O    | -5.47 | 1.16        | 1.23     |
| 2   | C     | 147 | GLY  | N-CA   | -5.47 | 1.39        | 1.45     |
| 1   | A     | 538 | GLN  | CD-OE1 | -5.46 | 1.13        | 1.23     |
| 7   | c     | 154 | ARG  | CZ-NH1 | -5.45 | 1.25        | 1.32     |
| 7   | c     | 110 | ASP  | C-O    | -5.45 | 1.17        | 1.24     |
| 7   | c     | 58  | SER  | C-O    | -5.44 | 1.17        | 1.23     |
| 4   | f     | 29  | SER  | C-O    | -5.44 | 1.16        | 1.24     |
| 1   | A     | 24  | PRO  | C-O    | -5.44 | 1.17        | 1.24     |
| 1   | A     | 740 | MET  | CA-C   | -5.44 | 1.45        | 1.52     |
| 1   | A     | 294 | ILE  | CB-CG1 | -5.43 | 1.42        | 1.53     |
| 7   | c     | 57  | GLY  | C-O    | -5.43 | 1.16        | 1.23     |
| 7   | c     | 63  | PRO  | C-O    | -5.42 | 1.17        | 1.24     |
| 7   | c     | 145 | GLN  | CA-C   | 5.42  | 1.60        | 1.52     |
| 1   | A     | 311 | ILE  | N-CA   | -5.42 | 1.40        | 1.46     |
| 1   | A     | 22  | MET  | C-N    | -5.42 | 1.26        | 1.33     |
| 3   | E     | 32  | ILE  | C-O    | -5.41 | 1.18        | 1.24     |
| 1   | a     | 359 | THR  | CB-CG2 | -5.41 | 1.34        | 1.52     |
| 1   | A     | 143 | GLY  | C-O    | -5.40 | 1.18        | 1.24     |
| 2   | C     | 189 | LEU  | N-CA   | -5.40 | 1.40        | 1.46     |
| 1   | A     | 609 | ASP  | C-O    | -5.38 | 1.17        | 1.24     |
| 1   | A     | 622 | MET  | CB-CG  | -5.38 | 1.36        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | a     | 757 | GLY  | N-CA    | -5.38 | 1.37        | 1.45     |
| 1   | a     | 364 | GLN  | C-N     | -5.38 | 1.27        | 1.33     |
| 1   | a     | 774 | ASN  | C-O     | -5.38 | 1.17        | 1.24     |
| 1   | A     | 230 | VAL  | C-O     | -5.37 | 1.18        | 1.23     |
| 1   | A     | 202 | TYR  | CZ-OH   | -5.37 | 1.26        | 1.38     |
| 1   | A     | 341 | ILE  | CG1-CD1 | -5.35 | 1.30        | 1.51     |
| 2   | C     | 187 | ARG  | CZ-NH2  | -5.34 | 1.26        | 1.33     |
| 5   | G     | 29  | PHE  | C-O     | -5.33 | 1.18        | 1.24     |
| 1   | a     | 482 | LYS  | C-O     | -5.33 | 1.16        | 1.23     |
| 1   | a     | 482 | LYS  | CA-CB   | -5.33 | 1.46        | 1.53     |
| 1   | a     | 305 | HIS  | CD2-NE2 | -5.33 | 1.31        | 1.37     |
| 1   | a     | 691 | SER  | C-O     | -5.33 | 1.17        | 1.24     |
| 7   | c     | 100 | ASN  | CG-ND2  | -5.32 | 1.22        | 1.33     |
| 1   | A     | 177 | TRP  | C-O     | -5.32 | 1.16        | 1.23     |
| 7   | c     | 80  | GLU  | CA-C    | -5.32 | 1.45        | 1.52     |
| 7   | c     | 86  | TYR  | C-O     | -5.32 | 1.17        | 1.23     |
| 4   | f     | 9   | ILE  | C-O     | -5.32 | 1.18        | 1.24     |
| 2   | C     | 169 | ASN  | C-O     | -5.31 | 1.17        | 1.24     |
| 2   | C     | 180 | GLN  | CD-NE2  | -5.31 | 1.22        | 1.33     |
| 3   | E     | 24  | PHE  | N-CA    | -5.30 | 1.39        | 1.46     |
| 3   | E     | 20  | GLY  | C-N     | -5.30 | 1.27        | 1.33     |
| 7   | c     | 42  | ARG  | CZ-NH2  | -5.30 | 1.26        | 1.33     |
| 1   | a     | 542 | TRP  | CD1-NE1 | -5.29 | 1.26        | 1.37     |
| 1   | A     | 742 | ARG  | CZ-NH2  | -5.29 | 1.26        | 1.33     |
| 2   | C     | 109 | ASP  | C-N     | -5.28 | 1.27        | 1.34     |
| 1   | A     | 108 | ASP  | N-CA    | -5.28 | 1.40        | 1.46     |
| 4   | F     | 28  | VAL  | C-O     | -5.27 | 1.17        | 1.24     |
| 1   | A     | 631 | SER  | CB-OG   | -5.27 | 1.31        | 1.42     |
| 4   | F     | 10  | SER  | CB-OG   | -5.26 | 1.31        | 1.42     |
| 1   | A     | 200 | THR  | CB-CG2  | -5.26 | 1.35        | 1.52     |
| 2   | C     | 124 | ASN  | CA-CB   | -5.26 | 1.45        | 1.53     |
| 7   | c     | 48  | LEU  | CB-CG   | -5.26 | 1.43        | 1.53     |
| 1   | A     | 757 | GLY  | C-O     | -5.25 | 1.16        | 1.23     |
| 2   | C     | 48  | THR  | C-O     | -5.25 | 1.17        | 1.24     |
| 1   | a     | 612 | ARG  | C-O     | -5.25 | 1.19        | 1.24     |
| 1   | A     | 612 | ARG  | C-O     | -5.24 | 1.19        | 1.24     |
| 7   | c     | 97  | GLY  | CA-C    | 5.24  | 1.59        | 1.52     |
| 7   | c     | 24  | GLY  | C-O     | -5.24 | 1.15        | 1.23     |
| 1   | A     | 606 | ALA  | N-CA    | -5.23 | 1.39        | 1.46     |
| 2   | C     | 113 | ILE  | C-O     | -5.22 | 1.18        | 1.24     |
| 1   | A     | 679 | SER  | CA-CB   | -5.22 | 1.46        | 1.53     |
| 1   | a     | 135 | GLY  | C-O     | -5.22 | 1.17        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | F     | 12  | LEU  | C-O     | -5.22 | 1.18        | 1.24     |
| 1   | A     | 542 | TRP  | C-N     | -5.19 | 1.26        | 1.33     |
| 1   | a     | 614 | GLU  | C-O     | -5.19 | 1.17        | 1.24     |
| 1   | A     | 764 | TRP  | N-CA    | -5.19 | 1.40        | 1.46     |
| 1   | a     | 116 | CYS  | CA-C    | -5.18 | 1.46        | 1.52     |
| 1   | a     | 510 | GLY  | C-O     | -5.18 | 1.17        | 1.23     |
| 7   | c     | 21  | CYS  | CA-C    | -5.18 | 1.45        | 1.52     |
| 1   | A     | 247 | GLY  | C-O     | -5.17 | 1.13        | 1.23     |
| 1   | A     | 735 | TRP  | C-N     | -5.17 | 1.27        | 1.33     |
| 2   | C     | 184 | GLN  | CB-CG   | -5.16 | 1.36        | 1.52     |
| 1   | a     | 307 | HIS  | CA-C    | -5.16 | 1.46        | 1.52     |
| 2   | C     | 188 | TYR  | CB-CG   | -5.14 | 1.40        | 1.51     |
| 1   | a     | 315 | SER  | CB-OG   | -5.14 | 1.31        | 1.42     |
| 2   | C     | 149 | GLN  | CD-OE1  | -5.14 | 1.13        | 1.23     |
| 7   | c     | 84  | ARG  | CA-CB   | -5.13 | 1.46        | 1.53     |
| 1   | A     | 177 | TRP  | CA-C    | -5.13 | 1.45        | 1.52     |
| 1   | A     | 19  | GLU  | C-O     | -5.13 | 1.17        | 1.23     |
| 1   | a     | 838 | LYS  | CB-CG   | -5.12 | 1.37        | 1.52     |
| 2   | C     | 31  | ARG  | NE-CZ   | -5.12 | 1.27        | 1.33     |
| 1   | a     | 774 | ASN  | CA-C    | -5.11 | 1.45        | 1.52     |
| 1   | A     | 655 | PHE  | N-CA    | -5.11 | 1.40        | 1.46     |
| 2   | C     | 162 | TYR  | N-CA    | -5.10 | 1.40        | 1.46     |
| 1   | a     | 138 | GLY  | C-O     | -5.09 | 1.16        | 1.24     |
| 7   | c     | 155 | ARG  | C-O     | -5.09 | 1.17        | 1.24     |
| 7   | c     | 19  | THR  | CB-CG2  | -5.08 | 1.35        | 1.52     |
| 4   | F     | 31  | LEU  | C-O     | -5.08 | 1.18        | 1.24     |
| 1   | a     | 346 | LYS  | CA-C    | -5.08 | 1.46        | 1.52     |
| 3   | e     | 29  | THR  | N-CA    | -5.07 | 1.39        | 1.46     |
| 4   | f     | 18  | THR  | CA-C    | -5.07 | 1.46        | 1.52     |
| 1   | a     | 628 | ARG  | CB-CG   | -5.06 | 1.37        | 1.52     |
| 2   | C     | 122 | GLN  | C-N     | -5.06 | 1.27        | 1.33     |
| 1   | A     | 448 | SER  | CB-OG   | -5.05 | 1.32        | 1.42     |
| 7   | c     | 41  | SER  | CB-OG   | -5.04 | 1.32        | 1.42     |
| 7   | c     | 94  | GLN  | N-CA    | 5.04  | 1.52        | 1.46     |
| 1   | A     | 25  | GLU  | CA-C    | -5.03 | 1.45        | 1.52     |
| 1   | a     | 764 | TRP  | CZ3-CH2 | -5.03 | 1.27        | 1.40     |
| 1   | A     | 136 | ALA  | CA-C    | -5.03 | 1.46        | 1.52     |
| 2   | C     | 114 | TYR  | CZ-OH   | -5.03 | 1.27        | 1.38     |
| 1   | a     | 567 | THR  | CB-CG2  | -5.03 | 1.35        | 1.52     |
| 1   | A     | 621 | ASN  | CB-CG   | -5.03 | 1.39        | 1.52     |
| 1   | A     | 605 | GLN  | C-O     | -5.03 | 1.17        | 1.24     |
| 1   | a     | 828 | ARG  | CA-C    | -5.03 | 1.47        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 227 | PRO  | C-O   | -5.02 | 1.17        | 1.23     |
| 8   | B     | 86  | CYS  | CA-C  | -5.02 | 1.46        | 1.53     |
| 1   | A     | 246 | TYR  | CZ-OH | -5.02 | 1.27        | 1.38     |
| 1   | A     | 328 | ASN  | CA-CB | 5.01  | 1.60        | 1.53     |
| 1   | A     | 762 | TYR  | CZ-OH | -5.01 | 1.27        | 1.38     |
| 1   | a     | 134 | TYR  | CB-CG | -5.00 | 1.40        | 1.51     |
| 7   | c     | 41  | SER  | CA-CB | -5.00 | 1.45        | 1.53     |
| 7   | c     | 102 | ALA  | C-O   | -5.00 | 1.17        | 1.24     |

All (385) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 96  | LEU  | CA-C-N  | 22.17  | 147.55      | 119.84   |
| 1   | A     | 96  | LEU  | C-N-CA  | 22.17  | 147.55      | 119.84   |
| 1   | A     | 473 | ASP  | CA-C-N  | 17.02  | 136.88      | 120.03   |
| 1   | A     | 473 | ASP  | C-N-CA  | 17.02  | 136.88      | 120.03   |
| 2   | C     | 141 | THR  | CA-C-O  | -14.92 | 104.52      | 120.63   |
| 2   | C     | 141 | THR  | N-CA-C  | 14.45  | 128.81      | 111.33   |
| 8   | B     | 140 | VAL  | N-CA-C  | 14.09  | 124.89      | 110.23   |
| 3   | e     | 24  | PHE  | N-CA-C  | -13.79 | 96.92       | 113.88   |
| 7   | c     | 133 | VAL  | N-CA-C  | 12.97  | 122.71      | 111.56   |
| 1   | A     | 13  | ARG  | N-CA-C  | 12.73  | 130.93      | 113.37   |
| 7   | c     | 106 | THR  | CA-C-O  | 12.61  | 134.70      | 120.96   |
| 2   | C     | 179 | ASN  | O-C-N   | -11.50 | 107.30      | 122.59   |
| 1   | A     | 757 | GLY  | N-CA-C  | 11.24  | 139.81      | 113.18   |
| 1   | A     | 244 | PHE  | CA-C-N  | -11.11 | 107.41      | 119.19   |
| 1   | A     | 244 | PHE  | C-N-CA  | -11.11 | 107.41      | 119.19   |
| 7   | c     | 106 | THR  | O-C-N   | -10.86 | 110.03      | 123.06   |
| 2   | C     | 142 | ASN  | N-CA-C  | 10.64  | 123.36      | 110.91   |
| 1   | a     | 85  | LEU  | CA-C-N  | 10.60  | 133.09      | 119.84   |
| 1   | a     | 85  | LEU  | C-N-CA  | 10.60  | 133.09      | 119.84   |
| 1   | a     | 539 | TRP  | O-C-N   | -10.43 | 109.43      | 122.68   |
| 7   | c     | 60  | ASP  | N-CA-C  | 10.35  | 123.61      | 111.71   |
| 1   | A     | 700 | VAL  | CB-CA-C | -10.02 | 97.46       | 111.28   |
| 1   | A     | 221 | PRO  | CA-C-N  | 9.93   | 129.69      | 119.76   |
| 1   | A     | 221 | PRO  | C-N-CA  | 9.93   | 129.69      | 119.76   |
| 1   | a     | 346 | LYS  | N-CA-CB | 9.80   | 127.06      | 110.49   |
| 1   | A     | 687 | TRP  | N-CA-C  | 9.55   | 125.39      | 112.68   |
| 1   | A     | 88  | ILE  | N-CA-C  | 9.46   | 129.02      | 109.34   |
| 7   | c     | 91  | GLY  | CA-C-N  | 9.45   | 139.59      | 121.54   |
| 7   | c     | 91  | GLY  | C-N-CA  | 9.45   | 139.59      | 121.54   |
| 3   | E     | 33  | ALA  | N-CA-C  | 9.35   | 124.01      | 112.23   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | a     | 537 | VAL  | N-CA-C    | 9.32  | 122.35      | 108.46   |
| 2   | C     | 22  | VAL  | CA-C-N    | -9.28 | 113.08      | 122.27   |
| 2   | C     | 22  | VAL  | C-N-CA    | -9.28 | 113.08      | 122.27   |
| 7   | c     | 19  | THR  | N-CA-C    | -9.07 | 96.93       | 109.71   |
| 1   | a     | 327 | ARG  | CA-C-N    | -9.06 | 108.02      | 122.79   |
| 1   | a     | 327 | ARG  | C-N-CA    | -9.06 | 108.02      | 122.79   |
| 1   | A     | 706 | GLY  | N-CA-C    | 8.97  | 127.77      | 115.30   |
| 2   | C     | 116 | GLU  | N-CA-C    | 8.85  | 122.19      | 111.40   |
| 1   | a     | 757 | GLY  | N-CA-C    | 8.81  | 134.07      | 113.18   |
| 7   | c     | 159 | LYS  | CA-C-O    | -8.77 | 111.85      | 121.94   |
| 7   | c     | 96  | ASN  | N-CA-C    | 8.75  | 123.68      | 112.92   |
| 1   | A     | 96  | LEU  | C-N-CD    | -8.75 | 89.14       | 125.00   |
| 1   | A     | 475 | THR  | N-CA-C    | -8.64 | 99.42       | 111.52   |
| 1   | A     | 85  | LEU  | CA-C-N    | 8.63  | 130.62      | 119.84   |
| 1   | A     | 85  | LEU  | C-N-CA    | 8.63  | 130.62      | 119.84   |
| 2   | C     | 124 | ASN  | N-CA-C    | 8.57  | 124.13      | 112.90   |
| 1   | A     | 338 | MET  | CA-C-N    | -8.57 | 109.32      | 123.37   |
| 1   | A     | 338 | MET  | C-N-CA    | -8.57 | 109.32      | 123.37   |
| 1   | a     | 344 | GLY  | CA-C-N    | -8.54 | 109.02      | 122.17   |
| 1   | a     | 344 | GLY  | C-N-CA    | -8.54 | 109.02      | 122.17   |
| 5   | g     | 16  | TRP  | N-CA-C    | -8.46 | 101.43      | 112.68   |
| 8   | B     | 90  | THR  | N-CA-C    | -8.44 | 102.08      | 112.38   |
| 1   | A     | 501 | ARG  | NE-CZ-NH2 | 8.40  | 126.76      | 119.20   |
| 1   | a     | 705 | CYS  | N-CA-C    | 8.39  | 121.24      | 109.15   |
| 2   | C     | 202 | ASN  | CB-CA-C   | 8.30  | 125.68      | 109.33   |
| 4   | f     | 2   | TRP  | N-CA-C    | -8.30 | 103.17      | 113.38   |
| 1   | A     | 167 | GLU  | N-CA-CB   | -8.26 | 98.41       | 110.47   |
| 1   | A     | 135 | GLY  | N-CA-C    | -8.25 | 93.62       | 113.18   |
| 7   | c     | 21  | CYS  | N-CA-CB   | 8.24  | 124.41      | 110.49   |
| 1   | a     | 364 | GLN  | N-CA-CB   | -8.24 | 97.62       | 110.30   |
| 1   | A     | 639 | ASN  | CB-CA-C   | -8.23 | 92.94       | 111.30   |
| 1   | a     | 861 | PHE  | CB-CA-C   | 8.21  | 124.17      | 110.79   |
| 7   | c     | 92  | CYS  | N-CA-C    | -8.20 | 93.34       | 110.80   |
| 8   | B     | 105 | VAL  | N-CA-C    | 8.09  | 126.16      | 109.34   |
| 7   | c     | 98  | GLY  | O-C-N     | 8.08  | 133.20      | 122.70   |
| 7   | c     | 106 | THR  | N-CA-CB   | 8.03  | 121.93      | 109.48   |
| 2   | C     | 142 | ASN  | N-CA-CB   | 8.03  | 124.85      | 111.53   |
| 1   | A     | 156 | LYS  | N-CA-C    | -7.98 | 102.07      | 112.68   |
| 1   | a     | 18  | LEU  | CA-CB-CG  | 7.94  | 144.09      | 116.30   |
| 1   | a     | 528 | GLU  | N-CA-C    | -7.89 | 98.20       | 109.96   |
| 1   | a     | 482 | LYS  | N-CA-C    | 7.87  | 120.36      | 109.18   |
| 7   | c     | 101 | LYS  | N-CA-C    | -7.85 | 97.23       | 109.25   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | C     | 178 | TYR  | N-CA-C   | 7.84  | 122.53      | 112.34   |
| 7   | c     | 98  | GLY  | CA-C-N   | 7.79  | 136.68      | 121.41   |
| 7   | c     | 98  | GLY  | C-N-CA   | 7.79  | 136.68      | 121.41   |
| 1   | A     | 167 | GLU  | N-CA-C   | 7.78  | 122.91      | 113.41   |
| 7   | c     | 131 | GLY  | N-CA-C   | 7.78  | 131.62      | 113.18   |
| 4   | f     | 18  | THR  | N-CA-C   | 7.77  | 119.83      | 111.36   |
| 1   | A     | 295 | THR  | N-CA-C   | 7.77  | 122.44      | 112.34   |
| 7   | c     | 111 | ALA  | CA-C-N   | 7.75  | 128.39      | 119.94   |
| 7   | c     | 111 | ALA  | C-N-CA   | 7.75  | 128.39      | 119.94   |
| 8   | B     | 109 | LEU  | N-CA-C   | -7.68 | 94.45       | 110.80   |
| 1   | a     | 345 | LYS  | N-CA-C   | 7.66  | 122.38      | 112.12   |
| 1   | a     | 22  | MET  | CA-C-N   | 7.66  | 125.25      | 119.66   |
| 1   | a     | 22  | MET  | C-N-CA   | 7.66  | 125.25      | 119.66   |
| 8   | B     | 134 | CYS  | CA-C-N   | 7.61  | 129.35      | 119.84   |
| 8   | B     | 134 | CYS  | C-N-CA   | 7.61  | 129.35      | 119.84   |
| 1   | A     | 638 | SER  | CA-C-N   | 7.59  | 134.50      | 121.29   |
| 1   | A     | 638 | SER  | C-N-CA   | 7.59  | 134.50      | 121.29   |
| 1   | A     | 361 | ASN  | CA-C-N   | 7.56  | 131.03      | 120.29   |
| 1   | A     | 361 | ASN  | C-N-CA   | 7.56  | 131.03      | 120.29   |
| 7   | c     | 134 | MET  | CA-C-N   | 7.48  | 127.41      | 119.85   |
| 7   | c     | 134 | MET  | C-N-CA   | 7.48  | 127.41      | 119.85   |
| 1   | A     | 475 | THR  | N-CA-CB  | 7.47  | 123.27      | 111.91   |
| 8   | B     | 109 | LEU  | CA-C-N   | 7.45  | 133.18      | 121.56   |
| 8   | B     | 109 | LEU  | C-N-CA   | 7.45  | 133.18      | 121.56   |
| 7   | c     | 133 | VAL  | CA-C-O   | -7.44 | 113.59      | 120.73   |
| 7   | c     | 62  | LEU  | CA-C-N   | 7.43  | 129.12      | 119.84   |
| 7   | c     | 62  | LEU  | C-N-CA   | 7.43  | 129.12      | 119.84   |
| 1   | a     | 759 | VAL  | N-CA-C   | 7.38  | 124.70      | 109.34   |
| 7   | c     | 26  | ARG  | CG-CD-NE | -7.38 | 95.76       | 112.00   |
| 7   | c     | 96  | ASN  | CA-C-O   | -7.38 | 110.93      | 119.56   |
| 5   | g     | 44  | LEU  | N-CA-C   | 7.37  | 120.91      | 110.23   |
| 5   | G     | 11  | LYS  | N-CA-C   | -7.34 | 103.21      | 111.14   |
| 3   | E     | 32  | ILE  | N-CA-C   | -7.32 | 96.88       | 107.78   |
| 1   | A     | 245 | PRO  | CA-C-O   | -7.26 | 108.67      | 119.34   |
| 5   | G     | 44  | LEU  | N-CA-CB  | -7.22 | 99.15       | 110.06   |
| 1   | a     | 154 | GLY  | N-CA-C   | -7.21 | 96.09       | 113.18   |
| 2   | C     | 180 | GLN  | N-CA-C   | 7.20  | 126.12      | 110.80   |
| 1   | a     | 690 | GLN  | N-CA-C   | 7.19  | 121.88      | 113.18   |
| 1   | A     | 641 | ARG  | CA-C-N   | -7.18 | 110.92      | 122.62   |
| 1   | A     | 641 | ARG  | C-N-CA   | -7.18 | 110.92      | 122.62   |
| 1   | a     | 782 | LEU  | CA-C-N   | 7.09  | 127.67      | 119.94   |
| 1   | a     | 782 | LEU  | C-N-CA   | 7.09  | 127.67      | 119.94   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | a     | 732 | ASP  | CA-C-N    | 7.09  | 131.33      | 121.26   |
| 1   | a     | 732 | ASP  | C-N-CA    | 7.09  | 131.33      | 121.26   |
| 2   | C     | 202 | ASN  | N-CA-C    | -7.09 | 98.38       | 109.72   |
| 9   | D     | 29  | ALA  | CA-C-N    | 7.07  | 134.10      | 121.66   |
| 9   | D     | 29  | ALA  | C-N-CA    | 7.07  | 134.10      | 121.66   |
| 1   | A     | 91  | PHE  | CA-CB-CG  | 7.05  | 120.85      | 113.80   |
| 1   | a     | 612 | ARG  | N-CA-C    | 7.05  | 122.41      | 113.25   |
| 1   | A     | 145 | ILE  | N-CA-C    | -7.02 | 103.82      | 110.42   |
| 1   | a     | 88  | ILE  | N-CA-C    | 6.96  | 123.82      | 109.34   |
| 4   | F     | 10  | SER  | CA-C-N    | 6.95  | 130.28      | 120.42   |
| 4   | F     | 10  | SER  | C-N-CA    | 6.95  | 130.28      | 120.42   |
| 1   | a     | 18  | LEU  | CB-CG-CD1 | -6.95 | 89.86       | 110.70   |
| 2   | C     | 141 | THR  | O-C-N     | -6.92 | 114.78      | 122.12   |
| 1   | A     | 166 | PRO  | CA-C-N    | 6.91  | 134.46      | 122.09   |
| 1   | A     | 166 | PRO  | C-N-CA    | 6.91  | 134.46      | 122.09   |
| 5   | g     | 26  | ILE  | N-CA-C    | -6.87 | 95.05       | 109.34   |
| 1   | A     | 682 | TYR  | N-CA-C    | 6.87  | 119.64      | 111.33   |
| 1   | A     | 732 | ASP  | N-CA-C    | 6.86  | 121.50      | 113.20   |
| 1   | A     | 698 | GLY  | N-CA-C    | 6.84  | 126.30      | 112.34   |
| 7   | c     | 92  | CYS  | N-CA-CB   | 6.81  | 122.00      | 110.49   |
| 7   | c     | 106 | THR  | N-CA-C    | 6.81  | 120.25      | 110.24   |
| 7   | c     | 20  | GLY  | N-CA-C    | -6.79 | 97.09       | 113.18   |
| 1   | A     | 147 | TRP  | N-CA-C    | 6.77  | 125.21      | 110.80   |
| 7   | c     | 132 | LYS  | N-CA-CB   | 6.76  | 121.92      | 110.49   |
| 2   | C     | 141 | THR  | N-CA-CB   | 6.75  | 120.19      | 110.06   |
| 1   | A     | 501 | ARG  | CD-NE-CZ  | 6.74  | 133.84      | 124.40   |
| 1   | A     | 736 | ILE  | CA-CB-CG2 | 6.73  | 121.93      | 110.50   |
| 3   | e     | 28  | ASN  | N-CA-C    | 6.70  | 120.76      | 112.59   |
| 5   | G     | 40  | MET  | N-CA-C    | -6.65 | 102.30      | 111.28   |
| 1   | A     | 709 | ILE  | CA-C-O    | -6.64 | 113.81      | 120.85   |
| 1   | A     | 90  | GLU  | O-C-N     | -6.62 | 114.62      | 122.96   |
| 1   | a     | 83  | VAL  | N-CA-C    | 6.61  | 123.08      | 109.34   |
| 1   | A     | 327 | ARG  | N-CA-C    | 6.60  | 119.32      | 111.33   |
| 1   | a     | 759 | VAL  | CA-C-N    | 6.58  | 129.39      | 120.44   |
| 1   | a     | 759 | VAL  | C-N-CA    | 6.58  | 129.39      | 120.44   |
| 8   | B     | 115 | TYR  | N-CA-C    | 6.58  | 119.34      | 108.49   |
| 2   | C     | 190 | VAL  | CA-C-O    | -6.57 | 114.26      | 121.29   |
| 2   | C     | 48  | THR  | N-CA-C    | 6.57  | 124.79      | 110.80   |
| 1   | a     | 732 | ASP  | N-CA-CB   | -6.53 | 101.03      | 110.56   |
| 1   | A     | 170 | TRP  | N-CA-C    | 6.52  | 124.69      | 110.80   |
| 1   | A     | 688 | ARG  | CB-CG-CD  | -6.51 | 96.33       | 111.30   |
| 2   | C     | 202 | ASN  | CA-C-O    | -6.50 | 113.76      | 121.11   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 739 | MET  | CA-CB-CG  | 6.49  | 127.07      | 114.10   |
| 1   | a     | 14  | TRP  | N-CA-C    | -6.48 | 105.39      | 113.55   |
| 1   | A     | 608 | LEU  | N-CA-C    | -6.47 | 104.07      | 112.23   |
| 1   | a     | 147 | TRP  | N-CA-C    | 6.46  | 124.56      | 110.80   |
| 1   | a     | 197 | SER  | N-CA-C    | 6.45  | 121.00      | 112.35   |
| 2   | C     | 218 | GLN  | N-CA-CB   | -6.43 | 99.57       | 110.50   |
| 2   | C     | 216 | GLU  | CB-CA-C   | -6.42 | 99.70       | 110.81   |
| 1   | A     | 690 | GLN  | N-CA-C    | 6.42  | 120.37      | 112.54   |
| 1   | a     | 336 | ASN  | O-C-N     | -6.41 | 113.90      | 122.43   |
| 1   | A     | 638 | SER  | CB-CA-C   | -6.40 | 96.67       | 109.79   |
| 1   | A     | 741 | ALA  | N-CA-C    | 6.39  | 119.64      | 110.24   |
| 1   | a     | 686 | GLU  | CA-C-N    | -6.39 | 111.93      | 122.79   |
| 1   | a     | 686 | GLU  | C-N-CA    | -6.39 | 111.93      | 122.79   |
| 1   | a     | 137 | ARG  | CB-CG-CD  | -6.37 | 96.66       | 111.30   |
| 2   | C     | 179 | ASN  | N-CA-C    | -6.33 | 97.31       | 110.80   |
| 1   | A     | 244 | PHE  | N-CA-C    | 6.33  | 123.79      | 109.81   |
| 2   | C     | 117 | GLY  | CA-C-O    | -6.32 | 113.96      | 120.66   |
| 2   | C     | 71  | ARG  | CG-CD-NE  | -6.29 | 98.17       | 112.00   |
| 1   | a     | 852 | LEU  | CA-C-O    | -6.28 | 113.00      | 120.10   |
| 1   | a     | 851 | VAL  | CA-CB-CG2 | 6.27  | 121.06      | 110.40   |
| 2   | C     | 125 | CYS  | CA-C-N    | 6.26  | 129.30      | 120.42   |
| 2   | C     | 125 | CYS  | C-N-CA    | 6.26  | 129.30      | 120.42   |
| 1   | A     | 734 | GLY  | N-CA-C    | 6.25  | 120.54      | 112.54   |
| 1   | a     | 822 | LYS  | N-CA-C    | 6.25  | 120.00      | 112.38   |
| 1   | a     | 537 | VAL  | CB-CA-C   | -6.24 | 100.89      | 110.50   |
| 2   | C     | 121 | PHE  | CA-C-N    | 6.23  | 129.26      | 120.28   |
| 2   | C     | 121 | PHE  | C-N-CA    | 6.23  | 129.26      | 120.28   |
| 1   | A     | 94  | SER  | N-CA-C    | 6.23  | 124.07      | 110.80   |
| 1   | a     | 698 | GLY  | CA-C-O    | -6.21 | 116.44      | 122.46   |
| 5   | g     | 36  | LEU  | N-CA-C    | 6.19  | 119.30      | 111.69   |
| 4   | f     | 5   | VAL  | CA-C-N    | 6.16  | 126.65      | 119.94   |
| 4   | f     | 5   | VAL  | C-N-CA    | 6.16  | 126.65      | 119.94   |
| 1   | a     | 731 | LEU  | N-CA-C    | 6.15  | 117.98      | 111.28   |
| 1   | a     | 762 | TYR  | CA-C-N    | 6.15  | 128.44      | 120.44   |
| 1   | a     | 762 | TYR  | C-N-CA    | 6.15  | 128.44      | 120.44   |
| 1   | a     | 394 | ARG  | CB-CA-C   | -6.15 | 98.75       | 109.07   |
| 1   | A     | 310 | ALA  | CA-C-N    | 6.13  | 128.29      | 120.56   |
| 1   | A     | 310 | ALA  | C-N-CA    | 6.13  | 128.29      | 120.56   |
| 2   | C     | 191 | ALA  | N-CA-C    | 6.12  | 118.75      | 111.71   |
| 2   | C     | 129 | HIS  | CA-C-N    | 6.11  | 131.90      | 121.87   |
| 2   | C     | 129 | HIS  | C-N-CA    | 6.11  | 131.90      | 121.87   |
| 1   | A     | 65  | ARG  | NE-CZ-NH1 | 6.08  | 127.58      | 121.50   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | a     | 539 | TRP  | CA-C-O    | -6.07 | 114.61      | 120.92   |
| 1   | A     | 59  | ASN  | CA-CB-CG  | 6.07  | 118.67      | 112.60   |
| 1   | A     | 501 | ARG  | NE-CZ-NH1 | -6.06 | 115.44      | 121.50   |
| 1   | A     | 136 | ALA  | N-CA-C    | -6.06 | 97.90       | 110.80   |
| 1   | a     | 633 | PRO  | N-CA-C    | 6.05  | 120.58      | 111.14   |
| 1   | A     | 548 | LYS  | CA-C-O    | 6.05  | 126.64      | 119.56   |
| 8   | B     | 104 | ASP  | N-CA-C    | 6.04  | 119.51      | 110.14   |
| 2   | C     | 216 | GLU  | N-CA-CB   | -6.04 | 102.23      | 110.56   |
| 7   | c     | 26  | ARG  | CD-NE-CZ  | 6.04  | 132.85      | 124.40   |
| 7   | c     | 48  | LEU  | CA-CB-CG  | 6.02  | 137.37      | 116.30   |
| 1   | a     | 160 | GLN  | N-CA-C    | -6.01 | 105.50      | 114.64   |
| 8   | B     | 136 | THR  | N-CA-C    | 6.01  | 119.44      | 111.75   |
| 1   | a     | 196 | LEU  | CA-C-N    | -5.99 | 112.35      | 119.78   |
| 1   | a     | 196 | LEU  | C-N-CA    | -5.99 | 112.35      | 119.78   |
| 1   | A     | 640 | LEU  | CA-C-N    | 5.99  | 132.99      | 121.54   |
| 1   | A     | 640 | LEU  | C-N-CA    | 5.99  | 132.99      | 121.54   |
| 2   | C     | 146 | PRO  | CA-C-N    | 5.98  | 126.58      | 120.00   |
| 2   | C     | 146 | PRO  | C-N-CA    | 5.98  | 126.58      | 120.00   |
| 1   | A     | 239 | LEU  | N-CA-C    | 5.98  | 121.24      | 111.37   |
| 1   | A     | 763 | MET  | CB-CG-SD  | -5.98 | 94.77       | 112.70   |
| 2   | C     | 47  | LYS  | CA-C-N    | 5.96  | 132.93      | 121.54   |
| 2   | C     | 47  | LYS  | C-N-CA    | 5.96  | 132.93      | 121.54   |
| 1   | A     | 633 | PRO  | N-CA-C    | 5.92  | 120.37      | 111.14   |
| 2   | C     | 75  | THR  | N-CA-CB   | 5.92  | 118.64      | 110.01   |
| 1   | a     | 377 | GLY  | CA-C-N    | 5.90  | 127.51      | 120.14   |
| 1   | a     | 377 | GLY  | C-N-CA    | 5.90  | 127.51      | 120.14   |
| 1   | a     | 736 | ILE  | CA-CB-CG2 | 5.89  | 120.52      | 110.50   |
| 1   | a     | 339 | ASN  | CB-CA-C   | 5.88  | 122.13      | 110.42   |
| 7   | c     | 100 | ASN  | N-CA-CB   | -5.88 | 101.72      | 110.90   |
| 1   | A     | 167 | GLU  | CB-CA-C   | -5.88 | 98.96       | 109.24   |
| 8   | B     | 94  | PRO  | CA-C-N    | 5.87  | 127.17      | 119.84   |
| 8   | B     | 94  | PRO  | C-N-CA    | 5.87  | 127.17      | 119.84   |
| 2   | C     | 22  | VAL  | O-C-N     | -5.86 | 115.24      | 122.57   |
| 2   | C     | 141 | THR  | CA-C-N    | -5.84 | 114.11      | 122.93   |
| 2   | C     | 141 | THR  | C-N-CA    | -5.84 | 114.11      | 122.93   |
| 2   | C     | 218 | GLN  | N-CA-C    | 5.83  | 127.33      | 111.00   |
| 2   | C     | 163 | ASN  | N-CA-C    | 5.83  | 119.57      | 112.23   |
| 1   | A     | 413 | THR  | CA-C-N    | -5.82 | 110.78      | 120.68   |
| 1   | A     | 413 | THR  | C-N-CA    | -5.82 | 110.78      | 120.68   |
| 1   | A     | 196 | LEU  | CA-C-N    | -5.81 | 107.63      | 121.80   |
| 1   | A     | 196 | LEU  | C-N-CA    | -5.81 | 107.63      | 121.80   |
| 1   | A     | 294 | ILE  | CA-CB-CG2 | 5.81  | 120.37      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 309 | THR  | OG1-CB-CG2 | -5.80 | 97.69       | 109.30   |
| 8   | B     | 136 | THR  | O-C-N      | 5.80  | 128.82      | 122.20   |
| 1   | a     | 852 | LEU  | CA-C-N     | 5.79  | 129.80      | 120.30   |
| 1   | a     | 852 | LEU  | C-N-CA     | 5.79  | 129.80      | 120.30   |
| 5   | G     | 16  | TRP  | N-CA-C     | -5.77 | 105.07      | 111.36   |
| 5   | G     | 32  | TYR  | N-CA-C     | 5.75  | 120.41      | 113.17   |
| 1   | A     | 851 | VAL  | CA-CB-CG1  | 5.74  | 120.16      | 110.40   |
| 1   | a     | 374 | VAL  | CA-C-N     | 5.74  | 128.24      | 120.38   |
| 1   | a     | 374 | VAL  | C-N-CA     | 5.74  | 128.24      | 120.38   |
| 5   | g     | 40  | MET  | CA-C-N     | 5.72  | 128.74      | 120.38   |
| 5   | g     | 40  | MET  | C-N-CA     | 5.72  | 128.74      | 120.38   |
| 2   | C     | 145 | ASP  | CA-C-N     | 5.72  | 125.40      | 119.05   |
| 2   | C     | 145 | ASP  | C-N-CA     | 5.72  | 125.40      | 119.05   |
| 7   | c     | 106 | THR  | CA-CB-OG1  | 5.71  | 118.17      | 109.60   |
| 1   | A     | 486 | GLY  | N-CA-C     | 5.71  | 124.14      | 115.63   |
| 1   | a     | 437 | LEU  | CA-C-N     | 5.71  | 130.23      | 122.07   |
| 1   | a     | 437 | LEU  | C-N-CA     | 5.71  | 130.23      | 122.07   |
| 1   | a     | 362 | HIS  | CA-C-N     | 5.71  | 128.52      | 120.42   |
| 1   | a     | 362 | HIS  | C-N-CA     | 5.71  | 128.52      | 120.42   |
| 1   | a     | 472 | TRP  | CA-C-N     | -5.70 | 114.22      | 121.74   |
| 1   | a     | 472 | TRP  | C-N-CA     | -5.70 | 114.22      | 121.74   |
| 1   | a     | 757 | GLY  | CA-C-O     | -5.69 | 110.67      | 120.57   |
| 2   | C     | 112 | GLU  | N-CA-C     | 5.68  | 117.55      | 111.36   |
| 7   | c     | 43  | THR  | OG1-CB-CG2 | -5.67 | 97.97       | 109.30   |
| 7   | c     | 115 | ALA  | CA-C-N     | -5.66 | 113.61      | 122.73   |
| 7   | c     | 115 | ALA  | C-N-CA     | -5.66 | 113.61      | 122.73   |
| 1   | A     | 501 | ARG  | CG-CD-NE   | -5.66 | 99.56       | 112.00   |
| 1   | a     | 698 | GLY  | CA-C-N     | 5.65  | 140.56      | 127.00   |
| 1   | a     | 698 | GLY  | C-N-CA     | 5.65  | 140.56      | 127.00   |
| 2   | C     | 45  | THR  | N-CA-C     | -5.64 | 105.75      | 113.30   |
| 1   | a     | 709 | ILE  | CA-CB-CG2  | 5.64  | 120.08      | 110.50   |
| 7   | c     | 48  | LEU  | CB-CG-CD2  | -5.63 | 93.80       | 110.70   |
| 1   | A     | 611 | PHE  | N-CA-C     | -5.63 | 106.41      | 113.72   |
| 5   | G     | 44  | LEU  | CB-CG-CD1  | 5.62  | 127.57      | 110.70   |
| 1   | A     | 722 | LYS  | N-CA-C     | 5.62  | 120.39      | 112.75   |
| 7   | c     | 26  | ARG  | N-CA-C     | 5.62  | 118.39      | 109.96   |
| 2   | C     | 71  | ARG  | N-CA-CB    | 5.61  | 118.98      | 110.28   |
| 7   | c     | 102 | ALA  | N-CA-CB    | 5.61  | 119.97      | 110.49   |
| 7   | c     | 130 | LYS  | CA-C-N     | 5.61  | 132.41      | 121.41   |
| 7   | c     | 130 | LYS  | C-N-CA     | 5.61  | 132.41      | 121.41   |
| 3   | E     | 11  | VAL  | N-CA-C     | -5.60 | 104.90      | 111.00   |
| 1   | A     | 729 | TRP  | CA-CB-CG   | 5.60  | 124.24      | 113.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 5   | g     | 11  | LYS  | N-CA-C    | -5.59 | 105.09      | 111.07   |
| 2   | C     | 20  | CYS  | N-CA-CB   | 5.58  | 119.92      | 110.49   |
| 7   | c     | 26  | ARG  | NE-CZ-NH2 | -5.58 | 114.18      | 119.20   |
| 2   | C     | 129 | HIS  | N-CA-C    | 5.57  | 119.77      | 112.92   |
| 1   | a     | 801 | ARG  | NE-CZ-NH2 | -5.56 | 114.20      | 119.20   |
| 1   | A     | 539 | TRP  | CA-C-N    | 5.55  | 129.62      | 120.25   |
| 1   | A     | 539 | TRP  | C-N-CA    | 5.55  | 129.62      | 120.25   |
| 5   | G     | 9   | ILE  | N-CA-C    | 5.53  | 120.83      | 109.34   |
| 1   | A     | 263 | ILE  | CB-CA-C   | -5.51 | 103.33      | 112.26   |
| 1   | a     | 308 | LEU  | CA-C-O    | -5.51 | 115.02      | 120.70   |
| 4   | F     | 29  | SER  | N-CA-C    | -5.50 | 105.19      | 111.07   |
| 1   | A     | 244 | PHE  | N-CA-CB   | 5.50  | 120.16      | 110.37   |
| 2   | C     | 30  | THR  | N-CA-CB   | 5.50  | 118.08      | 110.17   |
| 1   | A     | 238 | PRO  | CA-C-O    | -5.49 | 115.23      | 121.98   |
| 1   | a     | 364 | GLN  | CB-CA-C   | 5.46  | 121.52      | 110.38   |
| 1   | a     | 764 | TRP  | CA-C-N    | 5.45  | 128.03      | 120.29   |
| 1   | a     | 764 | TRP  | C-N-CA    | 5.45  | 128.03      | 120.29   |
| 2   | C     | 164 | GLY  | O-C-N     | -5.43 | 116.86      | 122.68   |
| 1   | A     | 759 | VAL  | N-CA-C    | 5.43  | 120.63      | 109.34   |
| 1   | A     | 641 | ARG  | NE-CZ-NH2 | -5.41 | 114.33      | 119.20   |
| 7   | c     | 81  | LEU  | CA-CB-CG  | 5.38  | 135.15      | 116.30   |
| 1   | A     | 822 | LYS  | N-CA-C    | 5.37  | 118.63      | 111.75   |
| 4   | f     | 14  | PHE  | CA-C-N    | 5.37  | 127.92      | 120.29   |
| 4   | f     | 14  | PHE  | C-N-CA    | 5.37  | 127.92      | 120.29   |
| 7   | c     | 112 | GLY  | CA-C-O    | -5.37 | 114.89      | 120.90   |
| 1   | A     | 287 | ARG  | CA-C-N    | 5.37  | 125.91      | 120.38   |
| 1   | A     | 287 | ARG  | C-N-CA    | 5.37  | 125.91      | 120.38   |
| 8   | B     | 123 | ILE  | CB-CA-C   | -5.36 | 102.50      | 111.29   |
| 3   | e     | 29  | THR  | N-CA-C    | -5.35 | 104.04      | 110.88   |
| 1   | A     | 474 | PRO  | N-CA-C    | -5.34 | 103.40      | 111.41   |
| 3   | E     | 33  | ALA  | CA-C-O    | -5.34 | 113.49      | 119.79   |
| 1   | a     | 19  | GLU  | N-CA-C    | 5.34  | 118.69      | 110.42   |
| 1   | a     | 367 | LEU  | CA-CB-CG  | -5.34 | 97.62       | 116.30   |
| 4   | f     | 15  | PHE  | CA-C-N    | 5.33  | 128.00      | 120.42   |
| 4   | f     | 15  | PHE  | C-N-CA    | 5.33  | 128.00      | 120.42   |
| 2   | C     | 174 | MET  | N-CA-C    | -5.33 | 98.02       | 109.81   |
| 1   | A     | 785 | LEU  | CA-C-N    | 5.33  | 127.27      | 120.56   |
| 1   | A     | 785 | LEU  | C-N-CA    | 5.33  | 127.27      | 120.56   |
| 7   | c     | 33  | LEU  | N-CA-C    | 5.33  | 118.04      | 110.10   |
| 1   | a     | 152 | VAL  | N-CA-C    | -5.31 | 97.41       | 108.88   |
| 7   | c     | 26  | ARG  | CB-CG-CD  | 5.31  | 123.50      | 111.30   |
| 2   | C     | 216 | GLU  | CA-C-N    | 5.30  | 131.67      | 121.54   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | C     | 216 | GLU  | C-N-CA    | 5.30  | 131.67      | 121.54   |
| 2   | C     | 73  | ARG  | CB-CA-C   | -5.30 | 99.97       | 109.24   |
| 1   | a     | 305 | HIS  | CA-C-O    | -5.30 | 114.81      | 120.42   |
| 2   | C     | 30  | THR  | CB-CA-C   | -5.29 | 99.80       | 109.54   |
| 4   | F     | 5   | VAL  | CA-C-N    | 5.28  | 126.75      | 120.14   |
| 4   | F     | 5   | VAL  | C-N-CA    | 5.28  | 126.75      | 120.14   |
| 1   | A     | 91  | PHE  | CA-C-N    | 5.28  | 128.35      | 120.90   |
| 1   | A     | 91  | PHE  | C-N-CA    | 5.28  | 128.35      | 120.90   |
| 2   | C     | 194 | ARG  | NE-CZ-NH2 | -5.28 | 114.45      | 119.20   |
| 1   | A     | 709 | ILE  | N-CA-CB   | 5.27  | 118.49      | 110.58   |
| 3   | E     | 34  | ALA  | N-CA-CB   | 5.27  | 119.39      | 110.49   |
| 1   | a     | 851 | VAL  | CA-CB-CG1 | 5.24  | 119.31      | 110.40   |
| 3   | E     | 27  | ALA  | N-CA-C    | 5.23  | 116.98      | 111.28   |
| 2   | C     | 179 | ASN  | CB-CA-C   | 5.23  | 120.83      | 110.42   |
| 2   | C     | 48  | THR  | N-CA-CB   | 5.22  | 119.32      | 110.49   |
| 2   | C     | 71  | ARG  | N-CA-C    | 5.22  | 117.88      | 111.82   |
| 8   | B     | 103 | ARG  | N-CA-C    | -5.22 | 101.91      | 109.59   |
| 2   | C     | 19  | GLY  | CA-C-N    | 5.22  | 131.52      | 121.54   |
| 2   | C     | 19  | GLY  | C-N-CA    | 5.22  | 131.52      | 121.54   |
| 1   | A     | 242 | ALA  | CA-C-N    | 5.21  | 125.15      | 119.78   |
| 1   | A     | 242 | ALA  | C-N-CA    | 5.21  | 125.15      | 119.78   |
| 1   | A     | 500 | ASP  | N-CA-C    | 5.20  | 117.83      | 110.50   |
| 1   | A     | 65  | ARG  | CG-CD-NE  | 5.20  | 123.43      | 112.00   |
| 7   | c     | 131 | GLY  | CA-C-O    | -5.18 | 111.56      | 120.57   |
| 1   | A     | 84  | TRP  | N-CA-C    | -5.18 | 107.03      | 113.55   |
| 2   | C     | 174 | MET  | CG-SD-CE  | 5.18  | 112.29      | 100.90   |
| 7   | c     | 103 | ILE  | N-CA-CB   | -5.17 | 103.39      | 112.08   |
| 8   | B     | 116 | TRP  | N-CA-C    | 5.17  | 117.93      | 110.28   |
| 4   | F     | 25  | ILE  | CA-C-N    | 5.16  | 127.06      | 120.56   |
| 4   | F     | 25  | ILE  | C-N-CA    | 5.16  | 127.06      | 120.56   |
| 1   | a     | 768 | THR  | CA-CB-OG1 | 5.16  | 117.34      | 109.60   |
| 7   | c     | 41  | SER  | N-CA-C    | 5.16  | 119.44      | 113.20   |
| 1   | a     | 528 | GLU  | CA-C-O    | -5.15 | 114.77      | 120.70   |
| 1   | a     | 698 | GLY  | C-N-CD    | -5.15 | 109.28      | 120.60   |
| 2   | C     | 87  | VAL  | CA-CB-CG1 | 5.14  | 119.15      | 110.40   |
| 1   | a     | 188 | LEU  | CA-CB-CG  | 5.13  | 134.25      | 116.30   |
| 2   | C     | 203 | GLY  | N-CA-C    | 5.12  | 125.31      | 113.18   |
| 1   | a     | 742 | ARG  | NE-CZ-NH2 | 5.11  | 123.80      | 119.20   |
| 8   | B     | 106 | GLU  | N-CA-C    | -5.11 | 100.15      | 109.56   |
| 1   | a     | 798 | ARG  | CG-CD-NE  | -5.09 | 100.80      | 112.00   |
| 4   | f     | 13  | CYS  | N-CA-C    | -5.09 | 105.81      | 111.36   |
| 4   | F     | 3   | ASN  | N-CA-C    | -5.08 | 105.44      | 111.69   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 860 | GLY  | O-C-N      | -5.08 | 117.17      | 123.21   |
| 2   | C     | 59  | GLN  | CB-CA-C    | -5.07 | 100.33      | 110.42   |
| 1   | A     | 168 | GLY  | N-CA-C     | 5.07  | 122.67      | 112.34   |
| 7   | c     | 26  | ARG  | NE-CZ-NH1  | 5.07  | 126.57      | 121.50   |
| 1   | a     | 775 | HIS  | N-CA-C     | -5.06 | 105.41      | 112.45   |
| 1   | A     | 472 | TRP  | N-CA-C     | 5.06  | 118.55      | 112.38   |
| 1   | a     | 65  | ARG  | CG-CD-NE   | 5.05  | 123.12      | 112.00   |
| 1   | A     | 529 | TRP  | N-CA-C     | 5.05  | 121.55      | 110.80   |
| 5   | G     | 41  | LEU  | N-CA-C     | 5.04  | 119.19      | 113.19   |
| 7   | c     | 135 | PRO  | N-CA-C     | 5.04  | 119.39      | 111.38   |
| 1   | a     | 697 | ILE  | CA-C-N     | 5.04  | 129.35      | 121.64   |
| 1   | a     | 697 | ILE  | C-N-CA     | 5.04  | 129.35      | 121.64   |
| 3   | E     | 31  | ASP  | N-CA-C     | 5.03  | 119.37      | 113.23   |
| 1   | A     | 736 | ILE  | CB-CG1-CD1 | -5.03 | 103.24      | 113.80   |
| 1   | A     | 706 | GLY  | CA-C-N     | 5.02  | 128.87      | 120.64   |
| 1   | A     | 706 | GLY  | C-N-CA     | 5.02  | 128.87      | 120.64   |
| 7   | c     | 48  | LEU  | CB-CG-CD1  | -5.01 | 95.67       | 110.70   |
| 1   | a     | 170 | TRP  | N-CA-C     | 5.01  | 121.47      | 110.80   |
| 5   | G     | 40  | MET  | CB-CA-C    | 5.01  | 119.42      | 112.11   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 639 | ASN  | Mainchain |
| 2   | C     | 141 | THR  | Mainchain |
| 2   | C     | 179 | ASN  | Mainchain |
| 1   | a     | 360 | PHE  | Mainchain |
| 1   | a     | 698 | GLY  | Peptide   |
| 1   | a     | 92  | SER  | Peptide   |
| 1   | a     | 93  | THR  | Peptide   |
| 7   | c     | 97  | GLY  | Mainchain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6960  | 0        | 6807     | 271     | 0            |
| 1   | a     | 6984  | 0        | 6830     | 241     | 0            |
| 2   | C     | 1474  | 0        | 1403     | 55      | 0            |
| 3   | E     | 258   | 0        | 279      | 6       | 0            |
| 3   | e     | 258   | 0        | 279      | 14      | 0            |
| 4   | F     | 273   | 0        | 290      | 8       | 0            |
| 4   | f     | 273   | 0        | 290      | 12      | 0            |
| 5   | G     | 302   | 0        | 318      | 23      | 0            |
| 5   | g     | 302   | 0        | 318      | 27      | 0            |
| 6   | H     | 95    | 0        | 23       | 8       | 0            |
| 6   | h     | 95    | 0        | 24       | 6       | 0            |
| 7   | c     | 1096  | 0        | 1079     | 51      | 0            |
| 8   | B     | 568   | 0        | 543      | 132     | 0            |
| 9   | D     | 520   | 0        | 510      | 22      | 0            |
| 10  | A     | 66    | 0        | 68       | 3       | 0            |
| 10  | a     | 66    | 0        | 69       | 1       | 0            |
| 11  | A     | 489   | 0        | 507      | 44      | 0            |
| 11  | a     | 508   | 0        | 553      | 42      | 0            |
| 12  | A     | 292   | 0        | 285      | 30      | 0            |
| 12  | a     | 292   | 0        | 284      | 16      | 0            |
| 13  | A     | 40    | 0        | 56       | 7       | 0            |
| 13  | c     | 40    | 0        | 55       | 5       | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| 14  | a     | 1     | 0        | 0        | 0       | 0            |
| 15  | A     | 135   | 0        | 0        | 5       | 0            |
| 15  | a     | 135   | 0        | 0        | 5       | 0            |
| 16  | A     | 240   | 0        | 0        | 15      | 0            |
| 16  | C     | 18    | 0        | 0        | 2       | 0            |
| 16  | E     | 26    | 0        | 0        | 0       | 0            |
| 16  | a     | 243   | 0        | 0        | 10      | 0            |
| 16  | c     | 8     | 0        | 0        | 1       | 0            |
| 16  | e     | 26    | 0        | 0        | 1       | 0            |
| 17  | A     | 47    | 0        | 0        | 8       | 0            |
| 17  | G     | 38    | 0        | 0        | 7       | 0            |
| 17  | a     | 47    | 0        | 0        | 3       | 0            |
| 17  | g     | 38    | 0        | 0        | 1       | 0            |
| 18  | C     | 43    | 0        | 31       | 9       | 0            |
| 18  | c     | 43    | 0        | 31       | 5       | 0            |
| 19  | E     | 44    | 0        | 0        | 0       | 0            |
| 19  | a     | 44    | 0        | 0        | 0       | 0            |
| 20  | B     | 16    | 0        | 0        | 13      | 0            |
| 20  | a     | 8     | 0        | 0        | 5       | 0            |
| 21  | A     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | a     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 22458 | 0        | 20932    | 893     | 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 21.

All (893) 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:A:85:LEU:HD12   | 1:A:86:PRO:CD    | 1.38                     | 1.46              |
| 5:G:40:MET:HE1    | 17:G:101:85N:C22 | 1.47                     | 1.41              |
| 5:G:40:MET:CE     | 17:G:101:85N:C22 | 1.95                     | 1.41              |
| 1:a:150:PRO:HA    | 1:a:156:LYS:NZ   | 1.27                     | 1.40              |
| 1:a:150:PRO:CA    | 1:a:156:LYS:NZ   | 1.84                     | 1.40              |
| 2:C:128:CYS:SG    | 18:C:301:HEC:CAC | 2.09                     | 1.39              |
| 1:a:150:PRO:CA    | 1:a:156:LYS:HZ1  | 1.34                     | 1.39              |
| 8:B:90:THR:HG21   | 8:B:115:TYR:CE2  | 1.56                     | 1.38              |
| 1:A:826:GLU:OE1   | 17:A:932:85N:C22 | 1.78                     | 1.32              |
| 8:B:97:VAL:HG11   | 8:B:123:ILE:CD1  | 1.59                     | 1.30              |
| 1:a:700:VAL:HG12  | 8:B:111:GLY:N    | 1.43                     | 1.30              |
| 8:B:89:CYS:SG     | 20:B:201:SF4:FE4 | 1.25                     | 1.28              |
| 1:a:150:PRO:C     | 1:a:156:LYS:HZ1  | 1.39                     | 1.27              |
| 1:a:700:VAL:HG12  | 8:B:111:GLY:CA   | 1.63                     | 1.26              |
| 8:B:97:VAL:CG1    | 8:B:123:ILE:HD11 | 1.65                     | 1.26              |
| 1:A:85:LEU:CD1    | 1:A:86:PRO:HD2   | 1.66                     | 1.25              |
| 8:B:90:THR:HG21   | 8:B:115:TYR:CD2  | 1.70                     | 1.25              |
| 7:c:98:GLY:HA2    | 7:c:107:ASN:CA   | 1.66                     | 1.24              |
| 1:a:12:LYS:NZ     | 1:a:693:ASP:OD2  | 1.69                     | 1.24              |
| 8:B:140:VAL:CG1   | 8:B:146:VAL:CG1  | 2.16                     | 1.23              |
| 2:C:128:CYS:SG    | 18:C:301:HEC:HAC | 1.76                     | 1.21              |
| 8:B:80:GLU:OE2    | 8:B:116:TRP:HB3  | 1.34                     | 1.20              |
| 1:a:149:LEU:O     | 1:a:156:LYS:NZ   | 1.75                     | 1.19              |
| 8:B:140:VAL:CG1   | 8:B:146:VAL:HG11 | 1.73                     | 1.19              |
| 1:a:700:VAL:CG1   | 8:B:111:GLY:HA2  | 1.74                     | 1.18              |
| 11:A:908:BCL:HBA1 | 11:A:908:BCL:HBD | 1.21                     | 1.17              |
| 12:A:910:CLA:HED3 | 1:a:760:PHE:CZ   | 1.79                     | 1.17              |
| 8:B:140:VAL:HG12  | 8:B:146:VAL:CG1  | 1.73                     | 1.17              |
| 1:A:94:SER:HB2    | 1:A:97:PRO:HA    | 1.19                     | 1.16              |
| 11:a:904:BCL:H203 | 7:c:16:VAL:CG2   | 1.77                     | 1.15              |
| 1:A:88:ILE:HA     | 1:A:95:LYS:NZ    | 1.62                     | 1.12              |
| 8:B:97:VAL:HG11   | 8:B:123:ILE:HD11 | 1.14                     | 1.12              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:G:34:PRO:HB3    | 5:G:44:LEU:HD22   | 1.22                     | 1.11              |
| 1:A:88:ILE:HA     | 1:A:95:LYS:HZ3    | 1.09                     | 1.11              |
| 1:A:85:LEU:CD1    | 1:A:86:PRO:CD     | 2.25                     | 1.10              |
| 7:c:49:ARG:HH11   | 7:c:63:PRO:HG2    | 1.06                     | 1.10              |
| 1:a:700:VAL:CG1   | 8:B:111:GLY:CA    | 2.29                     | 1.09              |
| 8:B:90:THR:CG2    | 8:B:115:TYR:CD2   | 2.35                     | 1.09              |
| 7:c:98:GLY:CA     | 7:c:107:ASN:HA    | 1.83                     | 1.09              |
| 8:B:140:VAL:HG12  | 8:B:146:VAL:HG13  | 1.36                     | 1.07              |
| 8:B:89:CYS:SG     | 20:B:201:SF4:S3   | 2.55                     | 1.05              |
| 7:c:98:GLY:HA3    | 7:c:107:ASN:OD1   | 1.57                     | 1.05              |
| 1:A:66:LEU:HD13   | 12:A:911:CLA:CED  | 1.85                     | 1.05              |
| 1:A:83:VAL:HG21   | 1:A:106:MET:HE1   | 1.37                     | 1.02              |
| 8:B:97:VAL:HG21   | 8:B:123:ILE:HD12  | 1.36                     | 1.02              |
| 1:a:152:VAL:HB    | 1:a:155:LEU:HD21  | 1.39                     | 1.02              |
| 1:a:640:LEU:H     | 1:a:865:ARG:HG3   | 1.25                     | 1.01              |
| 8:B:77:THR:CG2    | 9:D:25:GLN:OE1    | 2.09                     | 1.01              |
| 11:a:904:BCL:H203 | 7:c:16:VAL:HG21   | 1.42                     | 1.01              |
| 8:B:77:THR:HG21   | 9:D:25:GLN:OE1    | 1.61                     | 1.00              |
| 8:B:97:VAL:CB     | 8:B:123:ILE:HD11  | 1.91                     | 1.00              |
| 4:f:4:VAL:O       | 4:f:8:ILE:HD12    | 1.62                     | 0.99              |
| 11:A:903:BCL:HAA1 | 11:A:903:BCL:HBD  | 1.42                     | 0.99              |
| 1:A:865:ARG:NH1   | 2:C:83:ASN:OD1    | 1.95                     | 0.98              |
| 7:c:18:ALA:HB2    | 13:c:201:LYC:H622 | 1.42                     | 0.98              |
| 8:B:83:CYS:HG     | 20:B:201:SF4:FE2  | 0.72                     | 0.98              |
| 1:A:639:ASN:HD22  | 1:A:643:GLN:HB2   | 1.29                     | 0.97              |
| 11:A:902:BCL:HBB3 | 13:A:913:LYC:H62  | 1.43                     | 0.97              |
| 1:A:91:PHE:HB3    | 1:A:95:LYS:HB3    | 1.46                     | 0.97              |
| 1:a:445:GLN:HE22  | 1:a:514:THR:HG22  | 1.28                     | 0.96              |
| 1:A:28:PHE:CE2    | 11:A:905:BCL:HED2 | 2.01                     | 0.95              |
| 1:a:475:THR:HA    | 5:g:39:LYS:HG2    | 1.46                     | 0.95              |
| 8:B:134:CYS:HG    | 20:B:201:SF4:FE3  | 0.70                     | 0.95              |
| 5:G:40:MET:HE2    | 17:G:101:85N:C22  | 1.93                     | 0.94              |
| 8:B:140:VAL:HG11  | 8:B:146:VAL:HG11  | 1.45                     | 0.94              |
| 8:B:97:VAL:HG11   | 8:B:123:ILE:HD13  | 1.49                     | 0.94              |
| 1:A:85:LEU:HD12   | 1:A:86:PRO:HD3    | 1.50                     | 0.93              |
| 11:A:906:BCL:HMB1 | 11:A:906:BCL:HBB3 | 1.49                     | 0.93              |
| 12:A:910:CLA:HED3 | 1:a:760:PHE:CE2   | 2.04                     | 0.92              |
| 1:A:699:PRO:HD2   | 8:B:86:CYS:O      | 1.70                     | 0.92              |
| 1:A:149:LEU:H     | 1:A:150:PRO:CD    | 1.82                     | 0.92              |
| 8:B:128:CYS:SG    | 20:B:202:SF4:S4   | 2.67                     | 0.92              |
| 5:G:41:LEU:HG     | 5:G:44:LEU:HD23   | 1.52                     | 0.92              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:a:700:VAL:HG11  | 8:B:111:GLY:HA2  | 1.51                     | 0.91              |
| 11:A:908:BCL:HBA1 | 11:A:908:BCL:CBD | 1.99                     | 0.91              |
| 5:G:34:PRO:HB3    | 5:G:44:LEU:CD2   | 2.00                     | 0.91              |
| 1:a:700:VAL:HG12  | 8:B:111:GLY:H    | 1.14                     | 0.91              |
| 1:A:483:ASN:HB3   | 1:A:484:PRO:HD2  | 1.51                     | 0.91              |
| 8:B:76:TYR:CE1    | 8:B:141:PHE:CD1  | 2.58                     | 0.91              |
| 8:B:128:CYS:SG    | 20:B:202:SF4:FE3 | 1.62                     | 0.91              |
| 5:G:34:PRO:CB     | 5:G:44:LEU:HD22  | 2.01                     | 0.90              |
| 5:g:30:GLY:HA3    | 17:g:101:85N:O4  | 1.70                     | 0.90              |
| 1:A:66:LEU:CD1    | 12:A:911:CLA:CED | 2.50                     | 0.90              |
| 1:A:88:ILE:CA     | 1:A:95:LYS:NZ    | 2.36                     | 0.89              |
| 7:c:98:GLY:HA2    | 7:c:107:ASN:HA   | 0.93                     | 0.89              |
| 1:A:477:GLY:H     | 5:G:41:LEU:HD13  | 1.38                     | 0.88              |
| 1:A:696:CYS:HG    | 20:a:917:SF4:FE4 | 0.84                     | 0.88              |
| 5:G:32:TYR:OH     | 6:H:6:UNK:O      | 1.91                     | 0.88              |
| 7:c:98:GLY:HA2    | 7:c:107:ASN:CB   | 2.05                     | 0.87              |
| 1:A:13:ARG:HH11   | 1:A:13:ARG:HB2   | 1.38                     | 0.87              |
| 11:a:908:BCL:H193 | 3:e:5:LEU:HD21   | 1.55                     | 0.87              |
| 7:c:49:ARG:NH1    | 7:c:63:PRO:HG2   | 1.89                     | 0.87              |
| 11:a:908:BCL:C19  | 3:e:5:LEU:HD21   | 2.04                     | 0.86              |
| 1:A:94:SER:CB     | 1:A:97:PRO:HA    | 2.06                     | 0.86              |
| 1:A:85:LEU:CD1    | 1:A:86:PRO:HD3   | 2.04                     | 0.86              |
| 1:A:109:PHE:CD1   | 16:A:922:UNL:C16 | 2.59                     | 0.86              |
| 1:A:94:SER:HB2    | 1:A:97:PRO:CA    | 2.03                     | 0.85              |
| 7:c:33:LEU:O      | 7:c:33:LEU:HD23  | 1.76                     | 0.85              |
| 1:a:149:LEU:C     | 1:a:156:LYS:HZ3  | 1.84                     | 0.85              |
| 1:A:88:ILE:CA     | 1:A:95:LYS:HZ3   | 1.89                     | 0.85              |
| 11:a:904:BCL:H203 | 7:c:16:VAL:HG23  | 1.59                     | 0.84              |
| 8:B:104:ASP:OD1   | 8:B:113:GLU:HB3  | 1.77                     | 0.84              |
| 7:c:98:GLY:CA     | 7:c:107:ASN:OD1  | 2.24                     | 0.84              |
| 1:A:433:THR:HG21  | 1:A:739:MET:HG2  | 1.59                     | 0.84              |
| 4:F:34:ARG:HA     | 4:F:34:ARG:NE    | 1.93                     | 0.84              |
| 8:B:97:VAL:HG21   | 8:B:123:ILE:CD1  | 2.07                     | 0.83              |
| 1:A:613:PRO:O     | 1:A:614:GLU:HB3  | 1.79                     | 0.83              |
| 8:B:75:ILE:HG13   | 9:D:37:MET:HE1   | 1.58                     | 0.83              |
| 1:A:156:LYS:HD2   | 1:A:156:LYS:O    | 1.79                     | 0.82              |
| 1:a:149:LEU:C     | 1:a:156:LYS:NZ   | 2.36                     | 0.82              |
| 1:a:501:ARG:HD2   | 5:g:44:LEU:HD23  | 1.59                     | 0.82              |
| 1:A:149:LEU:N     | 1:A:150:PRO:CD   | 2.41                     | 0.82              |
| 1:A:158:LEU:HD22  | 1:A:158:LEU:O    | 1.78                     | 0.82              |
| 1:a:445:GLN:HE22  | 1:a:514:THR:CG2  | 1.91                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:88:ILE:C      | 1:A:95:LYS:NZ     | 2.38                     | 0.82              |
| 12:A:910:CLA:CED  | 1:a:760:PHE:CE2   | 2.62                     | 0.82              |
| 1:A:765:ASN:O     | 1:A:768:THR:HG23  | 1.79                     | 0.81              |
| 11:A:907:BCL:HBB3 | 11:A:907:BCL:HMB1 | 1.61                     | 0.81              |
| 8:B:146:VAL:HG21  | 9:D:22:TRP:HZ2    | 1.45                     | 0.81              |
| 1:a:150:PRO:HA    | 1:a:156:LYS:HZ2   | 0.99                     | 0.81              |
| 1:a:150:PRO:CA    | 1:a:156:LYS:HZ2   | 1.74                     | 0.81              |
| 1:a:149:LEU:N     | 1:a:150:PRO:CD    | 2.44                     | 0.81              |
| 1:a:641:ARG:HD3   | 1:a:865:ARG:HH11  | 1.46                     | 0.81              |
| 8:B:104:ASP:OD1   | 8:B:113:GLU:CB    | 2.29                     | 0.80              |
| 1:a:149:LEU:H     | 1:a:150:PRO:CD    | 1.93                     | 0.80              |
| 1:A:66:LEU:HD13   | 12:A:911:CLA:HED1 | 1.62                     | 0.80              |
| 1:A:83:VAL:HG12   | 1:A:88:ILE:HD12   | 1.63                     | 0.80              |
| 1:A:307:HIS:ND1   | 11:A:902:BCL:HBB1 | 1.96                     | 0.80              |
| 7:c:18:ALA:CB     | 13:c:201:LYC:H622 | 2.11                     | 0.80              |
| 1:a:641:ARG:CG    | 1:a:865:ARG:HH11  | 1.94                     | 0.80              |
| 11:A:903:BCL:HAA1 | 11:A:903:BCL:CBD  | 2.04                     | 0.79              |
| 8:B:101:LEU:O     | 8:B:115:TYR:CD2   | 2.35                     | 0.79              |
| 1:a:641:ARG:CD    | 1:a:865:ARG:HH11  | 1.94                     | 0.79              |
| 5:G:34:PRO:CB     | 5:G:44:LEU:CD2    | 2.61                     | 0.79              |
| 1:a:641:ARG:HD3   | 1:a:865:ARG:NH1   | 1.96                     | 0.79              |
| 1:a:12:LYS:HZ1    | 1:a:693:ASP:CG    | 1.88                     | 0.79              |
| 1:a:150:PRO:C     | 1:a:156:LYS:NZ    | 2.26                     | 0.78              |
| 8:B:77:THR:HG22   | 9:D:25:GLN:OE1    | 1.83                     | 0.78              |
| 8:B:97:VAL:CG1    | 8:B:123:ILE:CD1   | 2.39                     | 0.78              |
| 1:A:141:THR:HG22  | 1:A:162:LYS:HG2   | 1.64                     | 0.78              |
| 1:A:78:GLU:CD     | 2:C:62:PRO:HG2    | 2.09                     | 0.78              |
| 1:a:641:ARG:CD    | 1:a:865:ARG:NH1   | 2.46                     | 0.78              |
| 1:A:82:ARG:HA     | 1:A:88:ILE:HG13   | 1.66                     | 0.77              |
| 16:A:926:UNL:C2   | 16:A:927:UNL:C    | 2.63                     | 0.77              |
| 8:B:75:ILE:CG1    | 9:D:37:MET:HE1    | 2.14                     | 0.77              |
| 1:A:641:ARG:HG2   | 2:C:39:LEU:CD1    | 2.14                     | 0.77              |
| 1:a:501:ARG:CD    | 5:g:44:LEU:HD23   | 2.15                     | 0.77              |
| 1:a:440:ASN:HB2   | 1:a:514:THR:HG21  | 1.67                     | 0.77              |
| 1:A:760:PHE:CE2   | 12:A:931:CLA:HED3 | 2.20                     | 0.76              |
| 8:B:90:THR:CG2    | 8:B:115:TYR:CE2   | 2.53                     | 0.76              |
| 1:a:700:VAL:CG1   | 8:B:111:GLY:H     | 1.97                     | 0.76              |
| 1:A:13:ARG:HB2    | 1:A:13:ARG:NH1    | 2.00                     | 0.75              |
| 1:a:639:ASN:HB3   | 1:a:641:ARG:H     | 1.51                     | 0.75              |
| 2:C:128:CYS:SG    | 18:C:301:HEC:CBC  | 2.75                     | 0.74              |
| 1:A:149:LEU:H     | 1:A:150:PRO:HD3   | 1.51                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:129:PHE:HA    | 8:B:139:VAL:HG21  | 1.70                     | 0.74              |
| 8:B:86:CYS:SG     | 20:B:201:SF4:FE1  | 1.78                     | 0.74              |
| 5:g:40:MET:HG3    | 5:g:40:MET:O      | 1.88                     | 0.73              |
| 1:A:85:LEU:HD12   | 1:A:86:PRO:HD2    | 0.73                     | 0.73              |
| 1:A:833:ASN:C     | 1:A:833:ASN:HD22  | 1.97                     | 0.73              |
| 1:a:493:ALA:HA    | 1:a:496:LEU:HD22  | 1.71                     | 0.73              |
| 1:A:429:ILE:O     | 1:A:433:THR:HG23  | 1.89                     | 0.73              |
| 8:B:90:THR:HG22   | 8:B:115:TYR:CD2   | 2.24                     | 0.72              |
| 1:a:158:LEU:HD13  | 1:a:158:LEU:C     | 2.14                     | 0.72              |
| 4:F:2:TRP:HA      | 4:F:2:TRP:CE3     | 2.24                     | 0.72              |
| 7:c:33:LEU:HD23   | 7:c:33:LEU:C      | 2.12                     | 0.72              |
| 12:A:910:CLA:O1A  | 12:A:910:CLA:H3A  | 1.90                     | 0.72              |
| 1:a:475:THR:HA    | 5:g:39:LYS:CG     | 2.19                     | 0.72              |
| 1:a:705:CYS:HB3   | 20:a:917:SF4:S4   | 2.29                     | 0.72              |
| 2:C:87:VAL:HG22   | 2:C:179:ASN:O     | 1.89                     | 0.72              |
| 1:A:826:GLU:OE1   | 17:A:932:85N:C19  | 2.38                     | 0.71              |
| 1:A:627:GLU:HB3   | 2:C:46:LEU:HD22   | 1.72                     | 0.71              |
| 11:a:909:BCL:HBB3 | 11:a:909:BCL:HMB1 | 1.72                     | 0.71              |
| 1:A:148:LEU:H     | 1:A:148:LEU:HD23  | 1.55                     | 0.71              |
| 2:C:87:VAL:CG2    | 2:C:179:ASN:O     | 2.39                     | 0.71              |
| 8:B:80:GLU:HG2    | 8:B:114:THR:HG21  | 1.72                     | 0.71              |
| 8:B:97:VAL:HB     | 8:B:123:ILE:HD11  | 1.73                     | 0.71              |
| 7:c:133:VAL:HG22  | 18:c:202:HEC:HMD2 | 1.72                     | 0.71              |
| 11:A:904:BCL:HMB1 | 11:A:904:BCL:HBB3 | 1.72                     | 0.70              |
| 11:a:905:BCL:H92  | 16:a:931:UNL:C    | 2.22                     | 0.70              |
| 8:B:97:VAL:CB     | 8:B:123:ILE:CD1   | 2.67                     | 0.70              |
| 1:a:55:ASP:OD1    | 7:c:42:ARG:NH2    | 2.23                     | 0.70              |
| 2:C:107:TYR:CG    | 2:C:218:GLN:HB2   | 2.27                     | 0.70              |
| 1:a:13:ARG:O      | 1:a:17:LYS:HE2    | 1.91                     | 0.70              |
| 1:a:149:LEU:H     | 1:a:150:PRO:HD3   | 1.55                     | 0.70              |
| 16:a:932:UNL:C16  | 16:a:933:UNL:C17  | 2.69                     | 0.70              |
| 8:B:92:GLU:OE2    | 8:B:92:GLU:HA     | 1.91                     | 0.70              |
| 1:a:155:LEU:HD23  | 1:a:155:LEU:O     | 1.91                     | 0.70              |
| 1:a:294:ILE:HG13  | 1:a:297:LEU:HD23  | 1.74                     | 0.69              |
| 1:A:627:GLU:HB3   | 2:C:46:LEU:CD2    | 2.22                     | 0.69              |
| 1:a:641:ARG:HG3   | 1:a:865:ARG:NH1   | 2.07                     | 0.69              |
| 1:A:87:LEU:O      | 1:A:87:LEU:HD12   | 1.93                     | 0.69              |
| 1:a:152:VAL:CG1   | 1:a:155:LEU:HD11  | 2.23                     | 0.69              |
| 1:A:57:TYR:O      | 1:A:61:THR:HG22   | 1.92                     | 0.69              |
| 1:A:88:ILE:C      | 1:A:95:LYS:HZ1    | 1.99                     | 0.69              |
| 1:A:741:ALA:O     | 1:A:757:GLY:O     | 2.10                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:494:ARG:HD2   | 1:A:586:VAL:HG13  | 1.75                     | 0.69              |
| 4:F:2:TRP:HA      | 4:F:2:TRP:HE3     | 1.57                     | 0.69              |
| 8:B:76:TYR:HE1    | 8:B:141:PHE:CG    | 2.11                     | 0.69              |
| 11:A:905:BCL:HBB2 | 11:A:905:BCL:HMB3 | 1.74                     | 0.69              |
| 1:A:287:ARG:NH1   | 1:A:287:ARG:HG3   | 2.06                     | 0.68              |
| 11:a:904:BCL:C20  | 7:c:16:VAL:HG23   | 2.22                     | 0.68              |
| 7:c:98:GLY:HA3    | 7:c:107:ASN:CG    | 2.16                     | 0.68              |
| 1:a:12:LYS:NZ     | 1:a:693:ASP:CG    | 2.49                     | 0.68              |
| 1:a:640:LEU:HD22  | 1:a:865:ARG:HB2   | 1.76                     | 0.68              |
| 1:A:641:ARG:HG2   | 2:C:39:LEU:HD12   | 1.75                     | 0.68              |
| 8:B:124:SER:HA    | 20:B:202:SF4:S2   | 2.33                     | 0.68              |
| 2:C:59:GLN:CD     | 2:C:59:GLN:H      | 2.02                     | 0.68              |
| 8:B:82:LEU:O      | 8:B:136:THR:HG21  | 1.94                     | 0.68              |
| 1:A:141:THR:HB    | 1:A:161:ILE:O     | 1.94                     | 0.68              |
| 1:a:88:ILE:O      | 1:a:95:LYS:HD2    | 1.94                     | 0.67              |
| 11:A:902:BCL:CBB  | 13:A:913:LYC:H62  | 2.19                     | 0.67              |
| 1:a:150:PRO:N     | 1:a:156:LYS:NZ    | 2.43                     | 0.67              |
| 8:B:129:PHE:HA    | 8:B:139:VAL:CG2   | 2.25                     | 0.67              |
| 1:a:705:CYS:CB    | 20:a:917:SF4:S4   | 2.83                     | 0.67              |
| 8:B:75:ILE:HG13   | 9:D:37:MET:CE     | 2.24                     | 0.67              |
| 1:A:135:GLY:O     | 1:A:175:LEU:HD22  | 1.94                     | 0.67              |
| 1:A:597:THR:HG22  | 1:A:600:ALA:H     | 1.60                     | 0.67              |
| 1:A:84:TRP:HE3    | 1:A:84:TRP:O      | 1.78                     | 0.66              |
| 1:A:763:MET:HE1   | 12:A:931:CLA:HED2 | 1.77                     | 0.66              |
| 11:A:906:BCL:HBB3 | 11:A:906:BCL:CMB  | 2.23                     | 0.66              |
| 8:B:146:VAL:HG21  | 9:D:22:TRP:CZ2    | 2.29                     | 0.66              |
| 7:c:98:GLY:CA     | 7:c:107:ASN:CG    | 2.69                     | 0.66              |
| 4:f:34:ARG:HG3    | 4:f:34:ARG:O      | 1.94                     | 0.66              |
| 1:A:109:PHE:HD1   | 16:A:922:UNL:C16  | 2.05                     | 0.66              |
| 1:A:810:ARG:HG2   | 3:e:35:ASN:HA     | 1.75                     | 0.66              |
| 1:A:66:LEU:CD1    | 12:A:911:CLA:HED3 | 2.23                     | 0.66              |
| 1:A:88:ILE:C      | 1:A:95:LYS:HZ3    | 2.01                     | 0.66              |
| 2:C:107:TYR:CD1   | 2:C:218:GLN:HB2   | 2.31                     | 0.66              |
| 18:c:202:HEC:HMB3 | 18:c:202:HEC:HBB3 | 1.77                     | 0.66              |
| 1:a:152:VAL:HB    | 1:a:155:LEU:CD2   | 2.23                     | 0.66              |
| 1:a:440:ASN:O     | 6:h:5:UNK:CB      | 2.44                     | 0.66              |
| 8:B:76:TYR:HE1    | 8:B:141:PHE:CD1   | 2.14                     | 0.66              |
| 6:H:2:UNK:CB      | 16:c:203:UNL:C4   | 2.73                     | 0.65              |
| 8:B:89:CYS:SG     | 20:B:201:SF4:S2   | 2.85                     | 0.65              |
| 1:A:441:PHE:CE2   | 6:H:3:UNK:CB      | 2.80                     | 0.65              |
| 11:a:905:BCL:CHB  | 11:a:905:BCL:H11  | 2.26                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:487:THR:HB    | 6:h:17:UNK:O      | 1.97                     | 0.65              |
| 1:a:658:MET:HE2   | 1:a:658:MET:HA    | 1.77                     | 0.65              |
| 1:A:826:GLU:CD    | 17:A:932:85N:C22  | 2.69                     | 0.65              |
| 1:A:149:LEU:N     | 1:A:150:PRO:HD2   | 2.09                     | 0.65              |
| 2:C:134:CYS:HA    | 2:C:142:ASN:OD1   | 1.97                     | 0.65              |
| 8:B:97:VAL:CG2    | 8:B:123:ILE:CD1   | 2.74                     | 0.65              |
| 1:A:342:ILE:HD12  | 1:A:347:ILE:HG13  | 1.79                     | 0.64              |
| 1:A:135:GLY:O     | 1:A:175:LEU:CD2   | 2.45                     | 0.64              |
| 1:A:28:PHE:CD2    | 11:A:905:BCL:HED2 | 2.32                     | 0.64              |
| 1:A:531:GLN:HE21  | 1:A:533:LYS:HE3   | 1.61                     | 0.64              |
| 1:a:864:ASN:C     | 1:a:864:ASN:HD22  | 2.06                     | 0.64              |
| 7:c:144:GLN:NE2   | 7:c:147:ASN:HD22  | 1.95                     | 0.64              |
| 11:A:902:BCL:HHC  | 11:A:902:BCL:HBB2 | 1.79                     | 0.64              |
| 1:a:155:LEU:HD22  | 1:a:155:LEU:N     | 2.11                     | 0.64              |
| 7:c:96:ASN:C      | 7:c:96:ASN:HD22   | 2.06                     | 0.64              |
| 8:B:80:GLU:OE2    | 8:B:116:TRP:CB    | 2.29                     | 0.64              |
| 1:A:158:LEU:HD22  | 1:A:158:LEU:C     | 2.20                     | 0.63              |
| 2:C:71:ARG:HB2    | 2:C:75:THR:HG23   | 1.79                     | 0.63              |
| 1:a:700:VAL:CG1   | 8:B:111:GLY:N     | 2.39                     | 0.63              |
| 8:B:129:PHE:HD1   | 8:B:139:VAL:HG22  | 1.62                     | 0.63              |
| 1:a:641:ARG:CG    | 1:a:865:ARG:NH1   | 2.58                     | 0.63              |
| 3:e:18:LEU:HD23   | 16:e:101:UNL:C4   | 2.29                     | 0.63              |
| 1:A:696:CYS:SG    | 20:a:917:SF4:FE4  | 1.89                     | 0.63              |
| 1:a:150:PRO:O     | 1:a:156:LYS:NZ    | 2.30                     | 0.63              |
| 1:A:392:GLN:O     | 1:A:394:ARG:NH1   | 2.31                     | 0.63              |
| 2:C:128:CYS:SG    | 18:C:301:HEC:C3C  | 2.86                     | 0.63              |
| 1:A:109:PHE:CD1   | 16:A:922:UNL:C15  | 2.81                     | 0.63              |
| 8:B:97:VAL:CG2    | 8:B:123:ILE:HD12  | 2.22                     | 0.63              |
| 1:A:13:ARG:HH11   | 1:A:13:ARG:CB     | 2.09                     | 0.62              |
| 11:a:905:BCL:CBB  | 11:a:905:BCL:HMB3 | 2.30                     | 0.62              |
| 1:A:843:VAL:O     | 1:A:847:THR:HG23  | 1.99                     | 0.62              |
| 1:a:109:PHE:HD1   | 16:a:926:UNL:C7   | 2.12                     | 0.62              |
| 12:A:910:CLA:HED3 | 1:a:760:PHE:CE1   | 2.33                     | 0.62              |
| 5:G:34:PRO:HB2    | 5:G:44:LEU:CG     | 2.30                     | 0.62              |
| 1:a:158:LEU:HD22  | 1:a:158:LEU:O     | 2.00                     | 0.62              |
| 15:A:917:85I:C33  | 12:a:901:CLA:H141 | 2.30                     | 0.62              |
| 1:A:160:GLN:O     | 1:A:160:GLN:HG3   | 2.00                     | 0.62              |
| 1:A:156:LYS:HD2   | 1:A:156:LYS:C     | 2.21                     | 0.61              |
| 1:A:220:LYS:O     | 1:A:267:THR:HG21  | 2.00                     | 0.61              |
| 5:G:30:GLY:CA     | 17:G:101:85N:O5   | 2.48                     | 0.61              |
| 8:B:80:GLU:HG2    | 8:B:114:THR:CG2   | 2.31                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:85:LEU:H      | 1:a:85:LEU:CD2    | 2.13                     | 0.61              |
| 1:a:773:ASP:O     | 1:a:777:THR:HG22  | 2.00                     | 0.61              |
| 1:A:94:SER:CB     | 1:A:97:PRO:CA     | 2.73                     | 0.61              |
| 1:a:158:LEU:HD13  | 1:a:158:LEU:O     | 2.00                     | 0.61              |
| 1:a:309:THR:HG22  | 1:a:373:GLY:HA3   | 1.80                     | 0.61              |
| 8:B:89:CYS:HG     | 20:B:201:SF4:FE4  | 1.03                     | 0.61              |
| 1:A:66:LEU:HD13   | 12:A:911:CLA:HED2 | 1.77                     | 0.61              |
| 1:A:83:VAL:CG2    | 1:A:106:MET:HE1   | 2.23                     | 0.61              |
| 1:a:415:MET:HG2   | 1:a:667:ILE:HD13  | 1.82                     | 0.61              |
| 1:a:615:LEU:HG    | 1:a:615:LEU:O     | 1.99                     | 0.61              |
| 4:f:4:VAL:O       | 4:f:4:VAL:HG12    | 2.01                     | 0.60              |
| 1:A:87:LEU:HD12   | 1:A:95:LYS:HG3    | 1.81                     | 0.60              |
| 1:A:729:TRP:HB3   | 1:A:736:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:78:GLU:OE2    | 2:C:62:PRO:HG2    | 2.01                     | 0.60              |
| 1:a:501:ARG:NH1   | 5:g:44:LEU:O      | 2.34                     | 0.60              |
| 8:B:142:THR:OG1   | 8:B:145:GLY:C     | 2.45                     | 0.60              |
| 1:A:33:MET:HB3    | 11:A:902:BCL:C9   | 2.31                     | 0.60              |
| 1:a:155:LEU:HD22  | 1:a:155:LEU:H     | 1.65                     | 0.60              |
| 1:a:474:PRO:O     | 1:a:475:THR:OG1   | 2.15                     | 0.60              |
| 1:A:252:TYR:CE1   | 2:C:36:PRO:HB3    | 2.37                     | 0.59              |
| 1:A:445:GLN:NE2   | 1:A:514:THR:OG1   | 2.34                     | 0.59              |
| 1:A:550:ASN:HD21  | 1:A:552:LEU:HB2   | 1.67                     | 0.59              |
| 11:a:904:BCL:C20  | 7:c:16:VAL:CG2    | 2.66                     | 0.59              |
| 1:A:532:PRO:HB2   | 1:A:622:MET:HE1   | 1.83                     | 0.59              |
| 1:a:93:THR:O      | 1:a:97:PRO:HA     | 2.01                     | 0.59              |
| 1:a:445:GLN:NE2   | 1:a:514:THR:HG22  | 2.08                     | 0.59              |
| 5:g:38:VAL:HG12   | 5:g:38:VAL:O      | 2.01                     | 0.59              |
| 8:B:76:TYR:CD1    | 8:B:141:PHE:HA    | 2.37                     | 0.59              |
| 1:A:242:ALA:HB3   | 1:A:247:GLY:HA3   | 1.82                     | 0.59              |
| 16:A:923:UNL:C10  | 2:C:22:VAL:O      | 2.50                     | 0.59              |
| 8:B:76:TYR:CE1    | 8:B:141:PHE:CG    | 2.89                     | 0.59              |
| 1:A:148:LEU:H     | 1:A:148:LEU:CD2   | 2.14                     | 0.59              |
| 1:A:156:LYS:NZ    | 1:A:160:GLN:HB3   | 2.17                     | 0.59              |
| 1:a:487:THR:CB    | 6:h:17:UNK:O      | 2.50                     | 0.59              |
| 8:B:76:TYR:CE1    | 8:B:141:PHE:HB2   | 2.38                     | 0.59              |
| 11:A:908:BCL:HBA1 | 11:A:908:BCL:CHA  | 2.31                     | 0.58              |
| 2:C:116:GLU:HG2   | 2:C:188:TYR:CD2   | 2.38                     | 0.58              |
| 1:a:458:ALA:HA    | 1:a:461:ILE:HD12  | 1.85                     | 0.58              |
| 1:A:88:ILE:O      | 1:A:88:ILE:HG22   | 2.03                     | 0.58              |
| 8:B:142:THR:OG1   | 8:B:145:GLY:O     | 2.19                     | 0.58              |
| 1:A:826:GLU:O     | 17:A:932:85N:C18  | 2.52                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:c:133:VAL:HG22  | 18:c:202:HEC:CMD  | 2.34                     | 0.58              |
| 1:A:610:LYS:O     | 1:A:610:LYS:HG2   | 2.04                     | 0.58              |
| 1:a:94:SER:C      | 1:a:96:LEU:H      | 2.12                     | 0.58              |
| 1:a:61:THR:HG21   | 11:a:910:BCL:HAA2 | 1.86                     | 0.58              |
| 1:A:82:ARG:HG3    | 1:A:82:ARG:O      | 1.99                     | 0.58              |
| 1:a:149:LEU:HA    | 1:a:152:VAL:HG23  | 1.85                     | 0.58              |
| 1:A:696:CYS:SG    | 20:a:917:SF4:S1   | 3.01                     | 0.58              |
| 8:B:94:PRO:HB2    | 8:B:97:VAL:HG13   | 1.84                     | 0.57              |
| 11:A:907:BCL:HBB3 | 11:A:907:BCL:CMB  | 2.33                     | 0.57              |
| 7:c:44:ALA:O      | 7:c:48:LEU:HD22   | 2.04                     | 0.57              |
| 11:a:905:BCL:HHD  | 11:a:909:BCL:HBB2 | 1.85                     | 0.57              |
| 12:a:913:CLA:HBD  | 12:a:913:CLA:HAA1 | 1.85                     | 0.57              |
| 1:a:203:ILE:HD12  | 11:a:909:BCL:HED2 | 1.86                     | 0.57              |
| 12:A:910:CLA:HAA2 | 12:A:910:CLA:HBD  | 1.87                     | 0.57              |
| 5:G:34:PRO:HB2    | 5:G:44:LEU:CD1    | 2.35                     | 0.57              |
| 1:a:843:VAL:O     | 1:a:847:THR:HG23  | 2.04                     | 0.57              |
| 1:A:85:LEU:HD13   | 1:A:86:PRO:HD3    | 1.86                     | 0.56              |
| 11:a:904:BCL:HED3 | 12:a:914:CLA:HMB1 | 1.87                     | 0.56              |
| 16:a:930:UNL:C    | 16:a:931:UNL:C8   | 2.83                     | 0.56              |
| 8:B:140:VAL:HG13  | 8:B:146:VAL:CG1   | 2.27                     | 0.56              |
| 12:A:910:CLA:HED1 | 1:a:760:PHE:CE2   | 2.39                     | 0.56              |
| 11:A:908:BCL:HMB1 | 11:A:908:BCL:HBB3 | 1.87                     | 0.56              |
| 8:B:129:PHE:HD1   | 8:B:139:VAL:O     | 1.88                     | 0.56              |
| 2:C:107:TYR:CG    | 2:C:218:GLN:CB    | 2.89                     | 0.56              |
| 1:a:143:GLY:O     | 1:a:147:TRP:HA    | 2.04                     | 0.56              |
| 1:a:531:GLN:HE21  | 1:a:533:LYS:HE2   | 1.70                     | 0.56              |
| 5:g:9:ILE:CD1     | 5:g:9:ILE:H       | 2.18                     | 0.56              |
| 1:a:443:ILE:O     | 5:g:27:GLY:C      | 2.49                     | 0.56              |
| 1:a:818:ARG:HG3   | 1:a:818:ARG:HH11  | 1.71                     | 0.56              |
| 1:A:595:ALA:HB3   | 1:A:601:LYS:HG2   | 1.88                     | 0.56              |
| 11:A:907:BCL:CMB  | 11:A:907:BCL:CBB  | 2.83                     | 0.56              |
| 1:A:147:TRP:CD1   | 1:A:147:TRP:C     | 2.83                     | 0.56              |
| 5:G:9:ILE:HD12    | 5:G:9:ILE:H       | 1.70                     | 0.56              |
| 16:a:929:UNL:C9   | 16:a:929:UNL:C13  | 2.83                     | 0.56              |
| 4:f:30:HIS:C      | 4:f:30:HIS:CD2    | 2.84                     | 0.56              |
| 8:B:93:CYS:SG     | 8:B:99:ALA:HB3    | 2.46                     | 0.55              |
| 1:A:88:ILE:CG2    | 1:A:109:PHE:HZ    | 2.18                     | 0.55              |
| 12:A:910:CLA:CED  | 1:a:760:PHE:CZ    | 2.69                     | 0.55              |
| 1:a:640:LEU:H     | 1:a:865:ARG:CG    | 2.10                     | 0.55              |
| 8:B:121:ARG:HD2   | 8:B:121:ARG:O     | 2.05                     | 0.55              |
| 1:a:672:ILE:HG12  | 1:a:709:ILE:HG13  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:149:LEU:H    | 1:A:150:PRO:HD2   | 1.64                     | 0.55              |
| 17:A:932:85N:C8  | 17:A:932:85N:C4   | 2.85                     | 0.55              |
| 16:C:302:UNL:C19 | 16:C:302:UNL:C14  | 2.84                     | 0.55              |
| 1:a:494:ARG:NH1  | 1:a:590:ASN:OD1   | 2.39                     | 0.55              |
| 1:A:185:TRP:HB2  | 1:A:188:LEU:HD22  | 1.89                     | 0.55              |
| 1:A:441:PHE:CD2  | 6:H:3:UNK:CB      | 2.90                     | 0.55              |
| 17:A:932:85N:C18 | 17:A:932:85N:C21  | 2.85                     | 0.55              |
| 1:A:309:THR:HG23 | 11:A:903:BCL:HMC1 | 1.88                     | 0.55              |
| 1:A:450:ARG:HH21 | 1:A:518:THR:HG22  | 1.72                     | 0.55              |
| 1:a:441:PHE:CE2  | 6:h:3:UNK:CB      | 2.89                     | 0.55              |
| 1:A:826:GLU:OE1  | 17:A:932:85N:C21  | 2.53                     | 0.55              |
| 2:C:59:GLN:H     | 2:C:59:GLN:NE2    | 2.05                     | 0.55              |
| 8:B:90:THR:CG2   | 8:B:115:TYR:HD2   | 2.14                     | 0.55              |
| 9:D:25:GLN:HE21  | 9:D:25:GLN:N      | 2.03                     | 0.55              |
| 11:A:906:BCL:CMB | 11:A:906:BCL:CBB  | 2.85                     | 0.55              |
| 16:a:931:UNL:C   | 16:a:931:UNL:C5   | 2.85                     | 0.55              |
| 8:B:76:TYR:CE1   | 8:B:141:PHE:HD1   | 2.24                     | 0.55              |
| 8:B:96:LYS:NZ    | 8:B:96:LYS:HB3    | 2.18                     | 0.55              |
| 15:A:915:85I:C4  | 15:A:915:85I:C21  | 2.85                     | 0.55              |
| 1:a:559:ILE:O    | 1:a:563:GLN:HG3   | 2.07                     | 0.55              |
| 1:a:735:TRP:O    | 1:a:758:GLY:HA2   | 2.06                     | 0.55              |
| 1:A:89:GLY:O     | 1:A:95:LYS:HE2    | 2.07                     | 0.55              |
| 1:A:156:LYS:HZ2  | 1:A:160:GLN:HB3   | 1.71                     | 0.55              |
| 1:A:636:LEU:HD21 | 15:A:915:85I:O7   | 2.07                     | 0.55              |
| 1:A:14:TRP:CD1   | 1:A:14:TRP:C      | 2.85                     | 0.54              |
| 1:A:847:THR:O    | 1:A:851:VAL:HG13  | 2.06                     | 0.54              |
| 2:C:37:MET:HE1   | 2:C:80:GLN:HB3    | 1.89                     | 0.54              |
| 8:B:148:ARG:NH2  | 9:D:18:TRP:HZ2    | 2.05                     | 0.54              |
| 1:a:433:THR:HG21 | 1:a:739:MET:HG2   | 1.89                     | 0.54              |
| 4:f:25:ILE:HG22  | 4:f:25:ILE:O      | 2.07                     | 0.54              |
| 8:B:108:VAL:HG21 | 8:B:112:GLY:O     | 2.06                     | 0.54              |
| 1:A:755:HIS:HD2  | 1:A:757:GLY:H     | 1.55                     | 0.54              |
| 17:G:101:85N:C22 | 17:G:101:85N:C24  | 2.85                     | 0.54              |
| 1:a:147:TRP:CD1  | 1:a:147:TRP:C     | 2.85                     | 0.54              |
| 8:B:141:PHE:CD1  | 8:B:141:PHE:C     | 2.86                     | 0.54              |
| 1:A:826:GLU:OE1  | 17:A:932:85N:N1   | 2.39                     | 0.54              |
| 5:G:30:GLY:HA3   | 17:G:101:85N:O5   | 2.07                     | 0.54              |
| 1:a:85:LEU:N     | 1:a:85:LEU:HD23   | 2.22                     | 0.54              |
| 1:a:409:LYS:O    | 1:a:413:THR:HG23  | 2.07                     | 0.54              |
| 8:B:129:PHE:CD1  | 8:B:139:VAL:O     | 2.61                     | 0.54              |
| 1:A:501:ARG:HB3  | 1:A:517:PHE:HB3   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:639:ASN:ND2   | 1:A:643:GLN:HE21  | 2.04                     | 0.54              |
| 16:A:918:UNL:C8   | 16:A:918:UNL:C12  | 2.86                     | 0.54              |
| 1:A:158:LEU:C     | 1:A:158:LEU:HD13  | 2.33                     | 0.54              |
| 1:A:814:LEU:HD13  | 3:e:34:ALA:HA     | 1.89                     | 0.54              |
| 2:C:182:SER:H     | 2:C:185:GLN:HE21  | 1.56                     | 0.54              |
| 1:A:519:THR:H     | 1:A:538:GLN:HE21  | 1.55                     | 0.54              |
| 1:a:382:HIS:CE1   | 1:a:386:ILE:HD13  | 2.43                     | 0.54              |
| 8:B:146:VAL:CG2   | 9:D:22:TRP:HZ2    | 2.19                     | 0.54              |
| 12:A:911:CLA:HAA1 | 12:A:911:CLA:HBD  | 1.90                     | 0.54              |
| 1:a:151:TYR:N     | 1:a:151:TYR:CD1   | 2.72                     | 0.54              |
| 17:a:902:85N:C27  | 17:a:902:85N:C16  | 2.86                     | 0.54              |
| 16:A:919:UNL:C10  | 16:A:919:UNL:C6   | 2.85                     | 0.53              |
| 1:a:48:ALA:HB2    | 7:c:20:GLY:CA     | 2.38                     | 0.53              |
| 2:C:116:GLU:HG2   | 2:C:188:TYR:CE2   | 2.43                     | 0.53              |
| 12:A:910:CLA:C1C  | 1:a:722:LYS:HD3   | 2.38                     | 0.53              |
| 1:A:720:SER:O     | 1:A:724:LEU:HD22  | 2.09                     | 0.53              |
| 9:D:25:GLN:HB3    | 9:D:38:PHE:CE2    | 2.44                     | 0.53              |
| 1:a:641:ARG:HG3   | 1:a:865:ARG:HH11  | 1.67                     | 0.53              |
| 1:a:676:ASN:HA    | 1:a:709:ILE:CD1   | 2.38                     | 0.53              |
| 1:A:13:ARG:HG3    | 1:A:13:ARG:O      | 2.09                     | 0.53              |
| 11:a:905:BCL:HMB3 | 11:a:905:BCL:HBB2 | 1.90                     | 0.53              |
| 7:c:98:GLY:HA2    | 7:c:107:ASN:CG    | 2.34                     | 0.53              |
| 1:A:94:SER:CB     | 1:A:98:PHE:N      | 2.72                     | 0.53              |
| 1:a:849:THR:O     | 1:a:853:VAL:HG23  | 2.08                     | 0.53              |
| 4:F:33:SER:HB2    | 15:a:920:85I:O3   | 2.09                     | 0.53              |
| 1:a:832:SER:HA    | 15:a:920:85I:O2   | 2.09                     | 0.53              |
| 8:B:76:TYR:CE1    | 8:B:141:PHE:CB    | 2.92                     | 0.53              |
| 8:B:101:LEU:O     | 8:B:115:TYR:CG    | 2.61                     | 0.53              |
| 11:a:908:BCL:H191 | 3:e:5:LEU:HD21    | 1.91                     | 0.53              |
| 1:a:526:LYS:NZ    | 1:a:626:ASN:HD21  | 2.07                     | 0.53              |
| 1:A:148:LEU:HD23  | 1:A:148:LEU:N     | 2.24                     | 0.52              |
| 1:A:287:ARG:HG3   | 1:A:287:ARG:HH11  | 1.73                     | 0.52              |
| 1:A:612:ARG:HB3   | 1:A:613:PRO:HD3   | 1.91                     | 0.52              |
| 11:A:908:BCL:HHC  | 11:A:908:BCL:OBB  | 2.10                     | 0.52              |
| 3:e:21:ILE:C      | 3:e:23:LYS:H      | 2.16                     | 0.52              |
| 5:G:14:TRP:HA     | 5:G:14:TRP:CE3    | 2.43                     | 0.52              |
| 4:f:26:VAL:HG12   | 4:f:26:VAL:O      | 2.08                     | 0.52              |
| 7:c:114:GLN:HG3   | 7:c:157:GLU:HG3   | 1.91                     | 0.52              |
| 5:g:9:ILE:CD1     | 5:g:9:ILE:N       | 2.72                     | 0.52              |
| 8:B:101:LEU:HD22  | 8:B:102:PRO:HD3   | 1.91                     | 0.52              |
| 8:B:103:ARG:HH21  | 8:B:116:TRP:CD1   | 2.26                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:33:MET:HB3   | 11:A:902:BCL:H92  | 1.92                     | 0.52              |
| 1:A:151:TYR:N    | 1:A:151:TYR:CD1   | 2.74                     | 0.52              |
| 1:A:287:ARG:HH11 | 1:A:287:ARG:CG    | 2.23                     | 0.52              |
| 7:c:100:ASN:C    | 7:c:100:ASN:HD22  | 2.16                     | 0.52              |
| 5:g:16:TRP:C     | 5:g:18:GLY:H      | 2.17                     | 0.52              |
| 8:B:101:LEU:HB3  | 8:B:102:PRO:CD    | 2.39                     | 0.52              |
| 1:A:148:LEU:CD2  | 1:A:148:LEU:N     | 2.73                     | 0.52              |
| 1:A:612:ARG:HB3  | 1:A:613:PRO:CD    | 2.39                     | 0.52              |
| 1:a:609:ASP:HA   | 1:a:612:ARG:NH1   | 2.24                     | 0.52              |
| 7:c:98:GLY:CA    | 7:c:107:ASN:CB    | 2.81                     | 0.52              |
| 8:B:84:ILE:O     | 8:B:111:GLY:O     | 2.26                     | 0.52              |
| 1:A:269:MET:HB2  | 11:A:906:BCL:HED2 | 1.90                     | 0.52              |
| 1:A:688:ARG:CG   | 1:A:688:ARG:HH11  | 2.21                     | 0.52              |
| 10:a:903:2GO:H21 | 10:a:903:2GO:H25  | 1.91                     | 0.52              |
| 2:C:59:GLN:HB2   | 2:C:61:THR:HG22   | 1.90                     | 0.52              |
| 1:a:85:LEU:CD2   | 1:a:85:LEU:N      | 2.73                     | 0.52              |
| 1:a:149:LEU:N    | 1:a:150:PRO:HD2   | 2.21                     | 0.52              |
| 1:a:155:LEU:CD2  | 1:a:155:LEU:N     | 2.72                     | 0.52              |
| 9:D:22:TRP:HA    | 9:D:22:TRP:CE3    | 2.45                     | 0.52              |
| 1:a:293:ASN:HA   | 1:a:395:SER:HB2   | 1.91                     | 0.52              |
| 1:A:171:TYR:CD1  | 1:A:171:TYR:C     | 2.86                     | 0.52              |
| 5:G:40:MET:HE3   | 17:G:101:85N:C22  | 2.24                     | 0.51              |
| 7:c:49:ARG:HD3   | 7:c:70:GLU:OE2    | 2.10                     | 0.51              |
| 9:D:20:ARG:HG2   | 9:D:20:ARG:HH11   | 1.75                     | 0.51              |
| 2:C:167:ILE:HB   | 1:a:345:LYS:HE3   | 1.92                     | 0.51              |
| 1:A:25:GLU:CD    | 1:A:25:GLU:H      | 2.19                     | 0.51              |
| 1:A:640:LEU:HB2  | 1:A:865:ARG:HA    | 1.91                     | 0.51              |
| 1:a:687:TRP:O    | 1:a:688:ARG:HB2   | 2.10                     | 0.51              |
| 1:a:729:TRP:HB2  | 1:a:736:ILE:HD11  | 1.92                     | 0.51              |
| 1:A:151:TYR:N    | 1:A:151:TYR:HD1   | 2.06                     | 0.51              |
| 1:A:639:ASN:ND2  | 1:A:643:GLN:HB2   | 2.11                     | 0.51              |
| 12:A:933:CLA:HAB | 6:h:3:UNK:CB      | 2.41                     | 0.51              |
| 2:C:136:ASN:HD22 | 1:a:743:GLY:H     | 1.59                     | 0.51              |
| 1:A:89:GLY:C     | 1:A:95:LYS:HE2    | 2.36                     | 0.51              |
| 1:A:612:ARG:HH11 | 1:A:612:ARG:CG    | 2.24                     | 0.51              |
| 1:A:624:GLU:OE2  | 1:A:628:ARG:NH1   | 2.38                     | 0.51              |
| 1:A:742:ARG:HG3  | 1:A:761:LEU:CD2   | 2.40                     | 0.51              |
| 1:A:440:ASN:O    | 6:H:5:UNK:CB      | 2.58                     | 0.51              |
| 1:A:483:ASN:HB3  | 1:A:484:PRO:CD    | 2.33                     | 0.51              |
| 1:A:639:ASN:HB3  | 1:A:641:ARG:H     | 1.74                     | 0.51              |
| 15:A:916:85I:C11 | 15:A:917:85I:C14  | 2.88                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:676:ASN:HA    | 1:a:709:ILE:HD13  | 1.93                     | 0.51              |
| 7:c:63:PRO:C      | 7:c:65:ASP:H      | 2.18                     | 0.51              |
| 8:B:85:GLY:HA3    | 8:B:113:GLU:O     | 2.11                     | 0.51              |
| 1:A:440:ASN:ND2   | 6:H:5:UNK:CB      | 2.74                     | 0.51              |
| 2:C:87:VAL:HG21   | 2:C:179:ASN:O     | 2.11                     | 0.51              |
| 1:a:93:THR:HB     | 1:a:98:PHE:N      | 2.26                     | 0.51              |
| 3:e:23:LYS:O      | 3:e:23:LYS:HG2    | 2.10                     | 0.50              |
| 1:a:141:THR:OG1   | 1:a:144:GLU:HG3   | 2.10                     | 0.50              |
| 8:B:89:CYS:C      | 8:B:91:ASP:N      | 2.64                     | 0.50              |
| 1:A:693:ASP:OD1   | 1:A:693:ASP:N     | 2.44                     | 0.50              |
| 7:c:48:LEU:HD22   | 7:c:48:LEU:H      | 1.76                     | 0.50              |
| 8:B:148:ARG:HH21  | 9:D:18:TRP:HZ2    | 1.60                     | 0.50              |
| 1:A:244:PHE:CD1   | 1:A:244:PHE:O     | 2.63                     | 0.50              |
| 12:A:910:CLA:NC   | 1:a:722:LYS:HD3   | 2.27                     | 0.50              |
| 8:B:103:ARG:NH2   | 8:B:116:TRP:CD1   | 2.80                     | 0.50              |
| 16:C:302:UNL:C14  | 16:C:302:UNL:C18  | 2.85                     | 0.50              |
| 1:a:57:TYR:O      | 1:a:61:THR:CG2    | 2.59                     | 0.50              |
| 1:a:150:PRO:HA    | 1:a:156:LYS:CE    | 2.33                     | 0.50              |
| 12:a:901:CLA:H191 | 4:f:21:THR:HG22   | 1.93                     | 0.50              |
| 1:A:179:SER:O     | 1:A:183:THR:HG22  | 2.12                     | 0.50              |
| 1:A:221:PRO:CB    | 1:A:222:PRO:HD2   | 2.42                     | 0.50              |
| 8:B:130:VAL:O     | 8:B:130:VAL:HG13  | 2.11                     | 0.50              |
| 15:A:917:85I:C25  | 4:f:26:VAL:HG22   | 2.42                     | 0.49              |
| 1:a:38:LEU:HD23   | 12:a:913:CLA:HBC1 | 1.93                     | 0.49              |
| 1:a:94:SER:O      | 1:a:96:LEU:N      | 2.40                     | 0.49              |
| 1:A:381:LEU:HD21  | 11:A:903:BCL:HAA2 | 1.94                     | 0.49              |
| 1:A:226:GLN:O     | 1:A:226:GLN:HG2   | 2.12                     | 0.49              |
| 7:c:41:SER:HB2    | 7:c:148:TYR:OH    | 2.12                     | 0.49              |
| 7:c:142:THR:H     | 7:c:145:GLN:HE21  | 1.60                     | 0.49              |
| 1:A:441:PHE:HE2   | 6:H:3:UNK:CB      | 2.26                     | 0.49              |
| 1:a:833:ASN:C     | 1:a:833:ASN:HD22  | 2.19                     | 0.49              |
| 12:A:931:CLA:H142 | 12:A:931:CLA:H12  | 1.93                     | 0.49              |
| 5:g:29:PHE:CD1    | 5:g:29:PHE:C      | 2.90                     | 0.49              |
| 13:A:913:LYC:H10  | 13:A:913:LYC:H81  | 1.54                     | 0.49              |
| 1:a:152:VAL:HB    | 1:a:155:LEU:HD11  | 1.94                     | 0.49              |
| 1:a:592:ILE:HD11  | 1:a:605:GLN:HA    | 1.95                     | 0.49              |
| 8:B:76:TYR:HE1    | 8:B:141:PHE:CB    | 2.25                     | 0.49              |
| 1:a:94:SER:C      | 1:a:96:LEU:N      | 2.71                     | 0.49              |
| 9:D:25:GLN:NE2    | 9:D:25:GLN:HA     | 2.28                     | 0.49              |
| 1:A:15:TYR:CD1    | 1:A:15:TYR:N      | 2.80                     | 0.49              |
| 1:A:56:GLY:H      | 1:A:59:ASN:ND2    | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:156:LYS:NZ    | 1:A:160:GLN:OE1   | 2.44                     | 0.49              |
| 1:A:605:GLN:O     | 1:A:605:GLN:HG3   | 2.13                     | 0.49              |
| 1:a:158:LEU:C     | 1:a:158:LEU:CD1   | 2.85                     | 0.49              |
| 11:a:911:BCL:H3A  | 11:a:911:BCL:H12  | 1.94                     | 0.49              |
| 1:A:597:THR:O     | 1:A:600:ALA:N     | 2.46                     | 0.48              |
| 1:a:592:ILE:HG13  | 1:a:604:ALA:HB1   | 1.95                     | 0.48              |
| 1:A:148:LEU:HG    | 1:A:148:LEU:O     | 2.12                     | 0.48              |
| 1:A:706:GLY:O     | 1:a:800:SER:HB2   | 2.14                     | 0.48              |
| 1:a:109:PHE:CD1   | 16:a:926:UNL:C7   | 2.94                     | 0.48              |
| 8:B:129:PHE:CD1   | 8:B:139:VAL:HG22  | 2.47                     | 0.48              |
| 1:A:81:GLN:HG3    | 1:A:89:GLY:HA2    | 1.93                     | 0.48              |
| 3:E:32:ILE:CD1    | 1:a:818:ARG:HD3   | 2.44                     | 0.48              |
| 1:a:25:GLU:CD     | 1:a:25:GLU:H      | 2.22                     | 0.48              |
| 3:e:21:ILE:C      | 3:e:23:LYS:N      | 2.70                     | 0.48              |
| 8:B:125:CYS:SG    | 8:B:127:LEU:HB2   | 2.53                     | 0.48              |
| 9:D:25:GLN:NE2    | 9:D:25:GLN:CA     | 2.77                     | 0.48              |
| 16:A:927:UNL:C9   | 16:A:927:UNL:C5   | 2.85                     | 0.48              |
| 2:C:178:TYR:CD1   | 2:C:178:TYR:C     | 2.91                     | 0.48              |
| 1:a:450:ARG:NH2   | 1:a:504:ASN:OD1   | 2.47                     | 0.48              |
| 8:B:140:VAL:O     | 8:B:147:SER:O     | 2.31                     | 0.48              |
| 1:A:74:PRO:HB3    | 1:A:338:MET:HE3   | 1.96                     | 0.48              |
| 2:C:128:CYS:HG    | 1:a:764:TRP:HH2   | 1.61                     | 0.48              |
| 8:B:139:VAL:HG22  | 8:B:139:VAL:O     | 2.12                     | 0.48              |
| 1:A:324:LEU:O     | 1:A:327:ARG:HG2   | 2.13                     | 0.48              |
| 2:C:217:ARG:HA    | 2:C:217:ARG:NE    | 2.29                     | 0.48              |
| 1:a:42:ILE:HG13   | 12:a:913:CLA:HMD3 | 1.95                     | 0.48              |
| 1:a:98:PHE:CD1    | 1:a:98:PHE:C      | 2.92                     | 0.48              |
| 1:A:94:SER:CB     | 1:A:98:PHE:H      | 2.27                     | 0.48              |
| 1:a:152:VAL:HG11  | 1:a:155:LEU:HD11  | 1.96                     | 0.48              |
| 1:a:152:VAL:CB    | 1:a:155:LEU:HD21  | 2.21                     | 0.48              |
| 1:a:440:ASN:CB    | 1:a:514:THR:HG21  | 2.42                     | 0.48              |
| 1:a:440:ASN:HB2   | 1:a:514:THR:CG2   | 2.40                     | 0.48              |
| 1:A:635:VAL:O     | 3:E:3:ALA:HB2     | 2.13                     | 0.48              |
| 2:C:30:THR:HB     | 2:C:32:TYR:H      | 1.79                     | 0.48              |
| 1:a:156:LYS:HA    | 1:a:156:LYS:HD3   | 1.46                     | 0.48              |
| 8:B:113:GLU:CD    | 8:B:113:GLU:N     | 2.72                     | 0.48              |
| 1:A:253:LEU:HD23  | 1:A:255:GLN:HE22  | 1.79                     | 0.47              |
| 1:A:255:GLN:HE21  | 1:A:255:GLN:HB2   | 1.32                     | 0.47              |
| 11:a:909:BCL:HAA1 | 11:a:909:BCL:HBD  | 1.95                     | 0.47              |
| 1:A:729:TRP:CB    | 1:A:736:ILE:HD11  | 2.44                     | 0.47              |
| 4:f:27:TYR:O      | 4:f:27:TYR:CG     | 2.68                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:97:VAL:O      | 8:B:121:ARG:HD3   | 2.13                     | 0.47              |
| 1:A:66:LEU:CD1    | 12:A:911:CLA:HED2 | 2.40                     | 0.47              |
| 11:a:911:BCL:O1A  | 12:a:913:CLA:HMD1 | 2.14                     | 0.47              |
| 1:a:85:LEU:H      | 1:a:85:LEU:HD23   | 1.79                     | 0.47              |
| 8:B:76:TYR:HE1    | 8:B:141:PHE:HB2   | 1.77                     | 0.47              |
| 9:D:56:TYR:CZ     | 9:D:60:LEU:HD11   | 2.49                     | 0.47              |
| 1:A:454:MET:HE1   | 1:A:523:ILE:HB    | 1.96                     | 0.47              |
| 1:A:655:PHE:C     | 1:A:655:PHE:CD2   | 2.93                     | 0.47              |
| 1:a:304:PHE:HA    | 11:a:904:BCL:HBB3 | 1.97                     | 0.47              |
| 11:a:905:BCL:H12  | 16:a:931:UNL:C1   | 2.45                     | 0.47              |
| 5:g:16:TRP:C      | 5:g:18:GLY:N      | 2.70                     | 0.47              |
| 1:A:221:PRO:CB    | 1:A:222:PRO:CD    | 2.90                     | 0.47              |
| 1:A:300:THR:HA    | 1:A:303:VAL:HG23  | 1.97                     | 0.47              |
| 1:A:799:GLY:HA3   | 1:a:704:THR:C     | 2.39                     | 0.47              |
| 2:C:175:PRO:HD3   | 18:C:301:HEC:HBC2 | 1.96                     | 0.47              |
| 1:a:35:ILE:HD11   | 13:c:201:LYC:H131 | 1.97                     | 0.47              |
| 1:a:501:ARG:HD3   | 5:g:44:LEU:HD23   | 1.93                     | 0.47              |
| 7:c:103:ILE:HD13  | 7:c:103:ILE:HA    | 1.55                     | 0.47              |
| 8:B:123:ILE:HG22  | 8:B:123:ILE:O     | 2.14                     | 0.47              |
| 1:A:612:ARG:NH1   | 1:A:612:ARG:HG3   | 2.30                     | 0.47              |
| 1:A:644:HIS:HE1   | 1:A:646:ASP:OD1   | 1.98                     | 0.47              |
| 4:f:5:VAL:O       | 4:f:5:VAL:HG12    | 2.15                     | 0.47              |
| 1:A:88:ILE:HA     | 1:A:95:LYS:HZ2    | 1.71                     | 0.47              |
| 1:a:543:THR:HB    | 1:a:545:PHE:CE2   | 2.50                     | 0.47              |
| 1:A:85:LEU:HD13   | 1:A:85:LEU:HA     | 1.54                     | 0.47              |
| 11:a:910:BCL:H43  | 11:a:910:BCL:H12  | 1.72                     | 0.47              |
| 1:A:202:TYR:HE2   | 11:A:905:BCL:H192 | 1.80                     | 0.46              |
| 1:A:473:ASP:HA    | 1:A:474:PRO:HD2   | 1.40                     | 0.46              |
| 1:A:480:TRP:CE2   | 6:H:15:UNK:HA     | 2.51                     | 0.46              |
| 1:A:815:MET:O     | 1:A:819:LEU:HB2   | 2.14                     | 0.46              |
| 11:A:904:BCL:HMB1 | 11:A:904:BCL:CBB  | 2.43                     | 0.46              |
| 1:a:818:ARG:HG3   | 1:a:818:ARG:NH1   | 2.27                     | 0.46              |
| 17:a:902:85N:C3   | 15:a:920:85I:C33  | 2.93                     | 0.46              |
| 1:A:612:ARG:CG    | 1:A:612:ARG:NH1   | 2.77                     | 0.46              |
| 1:A:688:ARG:CG    | 1:A:688:ARG:NH1   | 2.72                     | 0.46              |
| 16:A:918:UNL:C17  | 16:A:918:UNL:C6   | 2.94                     | 0.46              |
| 7:c:144:GLN:HA    | 7:c:144:GLN:HE21  | 1.79                     | 0.46              |
| 8:B:101:LEU:HD23  | 8:B:101:LEU:HA    | 1.62                     | 0.46              |
| 1:A:405:ASP:OD1   | 3:E:33:ALA:O      | 2.33                     | 0.46              |
| 1:A:595:ALA:CB    | 1:A:601:LYS:HG2   | 2.46                     | 0.46              |
| 1:a:429:ILE:O     | 1:a:433:THR:HG22  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:639:ASN:HB2   | 1:a:643:GLN:H     | 1.79                     | 0.46              |
| 1:A:96:LEU:HA     | 1:A:97:PRO:HD2    | 1.52                     | 0.46              |
| 1:A:696:CYS:HB3   | 1:A:705:CYS:HA    | 1.98                     | 0.46              |
| 1:a:477:GLY:HA2   | 5:g:41:LEU:HD11   | 1.98                     | 0.46              |
| 7:c:144:GLN:HE21  | 7:c:147:ASN:HD22  | 1.62                     | 0.46              |
| 13:c:201:LYC:H54  | 13:c:201:LYC:H521 | 1.64                     | 0.46              |
| 1:A:264:ASN:HA    | 1:A:267:THR:HG23  | 1.98                     | 0.46              |
| 16:A:923:UNL:C7   | 16:A:923:UNL:C11  | 2.94                     | 0.46              |
| 2:C:94:GLY:HA2    | 2:C:99:VAL:HG13   | 1.97                     | 0.46              |
| 1:a:503:LEU:HD13  | 1:a:517:PHE:CE1   | 2.50                     | 0.46              |
| 1:a:550:ASN:HD21  | 1:a:552:LEU:HB2   | 1.80                     | 0.46              |
| 1:a:640:LEU:HB2   | 1:a:865:ARG:CB    | 2.46                     | 0.46              |
| 1:A:12:LYS:HE2    | 1:A:12:LYS:HB3    | 1.69                     | 0.46              |
| 1:A:220:LYS:HD2   | 1:A:263:ILE:HD13  | 1.97                     | 0.46              |
| 5:G:34:PRO:HB2    | 5:G:44:LEU:CD2    | 2.41                     | 0.46              |
| 4:F:34:ARG:NE     | 4:F:34:ARG:CA     | 2.71                     | 0.46              |
| 1:a:147:TRP:CD1   | 1:a:147:TRP:O     | 2.69                     | 0.46              |
| 11:a:907:BCL:H172 | 11:a:907:BCL:H13  | 1.73                     | 0.46              |
| 5:g:9:ILE:N       | 5:g:9:ILE:HD12    | 2.29                     | 0.46              |
| 8:B:90:THR:HG22   | 8:B:100:ILE:HG21  | 1.98                     | 0.46              |
| 1:A:760:PHE:CD2   | 12:A:931:CLA:HED3 | 2.51                     | 0.46              |
| 3:e:22:ILE:HG21   | 3:e:22:ILE:HD13   | 1.61                     | 0.46              |
| 4:f:19:VAL:O      | 4:f:19:VAL:HG12   | 2.16                     | 0.46              |
| 8:B:142:THR:HG21  | 8:B:146:VAL:HG22  | 1.98                     | 0.46              |
| 9:D:28:LEU:N      | 9:D:28:LEU:HD23   | 2.31                     | 0.46              |
| 1:A:773:ASP:O     | 1:A:777:THR:HG23  | 2.15                     | 0.46              |
| 8:B:104:ASP:CG    | 8:B:113:GLU:HB3   | 2.40                     | 0.46              |
| 1:A:90:GLU:HB2    | 1:A:100:GLY:O     | 2.16                     | 0.45              |
| 2:C:41:ASN:ND2    | 2:C:85:GLN:HG3    | 2.31                     | 0.45              |
| 1:a:639:ASN:ND2   | 1:a:643:GLN:HE21  | 2.14                     | 0.45              |
| 1:a:847:THR:O     | 1:a:851:VAL:HG13  | 2.15                     | 0.45              |
| 1:A:55:ASP:HA     | 1:A:59:ASN:HD21   | 1.80                     | 0.45              |
| 1:A:406:LEU:O     | 1:A:410:ILE:HG13  | 2.15                     | 0.45              |
| 5:G:10:SER:OG     | 17:a:902:85N:C18  | 2.65                     | 0.45              |
| 1:a:90:GLU:HB2    | 1:a:94:SER:HB2    | 1.97                     | 0.45              |
| 1:A:14:TRP:CD1    | 1:A:14:TRP:O      | 2.69                     | 0.45              |
| 1:A:796:LYS:HE2   | 1:a:838:LYS:HE2   | 1.99                     | 0.45              |
| 2:C:114:TYR:HB2   | 2:C:210:VAL:HG21  | 1.98                     | 0.45              |
| 1:A:722:LYS:HE2   | 12:A:931:CLA:NB   | 2.31                     | 0.45              |
| 1:a:150:PRO:O     | 1:a:156:LYS:CE    | 2.65                     | 0.45              |
| 1:a:519:THR:H     | 1:a:538:GLN:HE21  | 1.65                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:832:SER:HA    | 15:a:920:85I:C4   | 2.46                     | 0.45              |
| 1:a:15:TYR:O      | 1:a:15:TYR:CD2    | 2.69                     | 0.45              |
| 1:A:688:ARG:HH11  | 1:A:688:ARG:HG2   | 1.82                     | 0.45              |
| 1:A:742:ARG:HG3   | 1:A:761:LEU:HD21  | 1.98                     | 0.45              |
| 1:a:189:ARG:CG    | 1:a:194:ASP:HB3   | 2.46                     | 0.45              |
| 5:g:29:PHE:CD1    | 5:g:29:PHE:O      | 2.69                     | 0.45              |
| 8:B:113:GLU:CD    | 8:B:113:GLU:H     | 2.25                     | 0.45              |
| 1:A:98:PHE:CG     | 1:A:98:PHE:O      | 2.70                     | 0.45              |
| 1:A:475:THR:HA    | 5:G:39:LYS:HG2    | 1.98                     | 0.45              |
| 13:A:913:LYC:H20  | 13:A:913:LYC:H181 | 1.57                     | 0.45              |
| 12:a:912:CLA:H92  | 12:a:912:CLA:H52  | 1.98                     | 0.45              |
| 12:a:915:CLA:C6   | 7:c:17:MET:HG2    | 2.47                     | 0.45              |
| 7:c:134:MET:HB2   | 18:c:202:HEC:C4D  | 2.47                     | 0.45              |
| 8:B:78:ILE:HD13   | 20:B:201:SF4:S1   | 2.56                     | 0.45              |
| 8:B:129:PHE:CA    | 8:B:139:VAL:HG21  | 2.42                     | 0.45              |
| 1:A:171:TYR:CD1   | 1:A:171:TYR:O     | 2.70                     | 0.45              |
| 1:A:819:LEU:HA    | 1:A:819:LEU:HD12  | 1.69                     | 0.45              |
| 1:A:833:ASN:C     | 1:A:833:ASN:ND2   | 2.70                     | 0.45              |
| 1:a:189:ARG:HG2   | 1:a:194:ASP:HB3   | 1.98                     | 0.45              |
| 11:a:908:BCL:H171 | 3:e:1:MET:HE2     | 1.99                     | 0.45              |
| 5:g:17:PHE:O      | 5:g:17:PHE:CG     | 2.69                     | 0.45              |
| 1:A:94:SER:C      | 1:A:96:LEU:H      | 2.26                     | 0.45              |
| 1:A:504:ASN:OD1   | 1:A:518:THR:HG22  | 2.17                     | 0.45              |
| 1:a:602:GLN:HE21  | 1:a:602:GLN:N     | 2.15                     | 0.45              |
| 1:a:822:LYS:H     | 1:a:822:LYS:HG2   | 1.33                     | 0.45              |
| 7:c:18:ALA:HB2    | 13:c:201:LYC:C62  | 2.30                     | 0.45              |
| 5:g:17:PHE:O      | 5:g:17:PHE:CD2    | 2.70                     | 0.45              |
| 1:A:109:PHE:CE1   | 16:A:922:UNL:C16  | 2.97                     | 0.44              |
| 1:A:610:LYS:HB3   | 1:A:610:LYS:HE3   | 1.44                     | 0.44              |
| 1:a:152:VAL:CB    | 1:a:155:LEU:HD11  | 2.46                     | 0.44              |
| 1:a:818:ARG:HA    | 1:a:818:ARG:HD2   | 1.63                     | 0.44              |
| 2:C:145:ASP:HA    | 2:C:146:PRO:HD3   | 1.78                     | 0.44              |
| 1:a:201:ILE:HG13  | 1:a:281:GLY:HA3   | 1.98                     | 0.44              |
| 1:A:396:LYS:HE3   | 1:A:400:TRP:CZ2   | 2.53                     | 0.44              |
| 1:A:729:TRP:HB3   | 1:A:736:ILE:CD1   | 2.46                     | 0.44              |
| 11:A:909:BCL:H162 | 11:A:909:BCL:H141 | 1.62                     | 0.44              |
| 5:G:34:PRO:HB2    | 5:G:44:LEU:HD13   | 1.99                     | 0.44              |
| 1:a:38:LEU:HD23   | 12:a:913:CLA:CBC  | 2.47                     | 0.44              |
| 11:a:911:BCL:CBB  | 11:a:911:BCL:HMB1 | 2.47                     | 0.44              |
| 7:c:63:PRO:C      | 7:c:65:ASP:N      | 2.74                     | 0.44              |
| 1:A:98:PHE:O      | 1:A:98:PHE:CD1    | 2.70                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:220:LYS:HD2   | 1:A:263:ILE:CD1   | 2.47                     | 0.44              |
| 1:A:644:HIS:CE1   | 1:A:646:ASP:OD1   | 2.70                     | 0.44              |
| 1:A:822:LYS:HB3   | 1:A:822:LYS:HE2   | 1.62                     | 0.44              |
| 1:a:628:ARG:HH11  | 1:a:628:ARG:HB2   | 1.83                     | 0.44              |
| 12:a:915:CLA:C5   | 7:c:17:MET:HG2    | 2.48                     | 0.44              |
| 8:B:90:THR:HG22   | 8:B:115:TYR:HD2   | 1.79                     | 0.44              |
| 1:A:85:LEU:HA     | 1:A:86:PRO:HD3    | 1.75                     | 0.44              |
| 12:A:933:CLA:ND   | 2:C:18:GLY:HA3    | 2.33                     | 0.44              |
| 11:a:907:BCL:HBB2 | 11:a:907:BCL:HMB3 | 1.99                     | 0.44              |
| 8:B:121:ARG:HE    | 8:B:121:ARG:HB3   | 1.57                     | 0.44              |
| 1:A:643:GLN:HB2   | 1:A:643:GLN:HE21  | 1.55                     | 0.44              |
| 1:A:833:ASN:ND2   | 1:A:836:THR:CG2   | 2.81                     | 0.44              |
| 1:a:700:VAL:HG11  | 8:B:84:ILE:HB     | 1.99                     | 0.44              |
| 1:A:28:PHE:CZ     | 11:A:905:BCL:HED2 | 2.49                     | 0.44              |
| 1:A:88:ILE:HG21   | 1:A:109:PHE:CZ    | 2.53                     | 0.44              |
| 1:A:494:ARG:NH1   | 1:A:590:ASN:OD1   | 2.51                     | 0.44              |
| 11:a:908:BCL:H41  | 11:a:908:BCL:H62  | 1.29                     | 0.44              |
| 11:a:909:BCL:HBB3 | 11:a:909:BCL:CMB  | 2.43                     | 0.44              |
| 8:B:134:CYS:HB2   | 20:B:201:SF4:S2   | 2.58                     | 0.44              |
| 1:A:607:GLU:O     | 1:A:607:GLU:HG2   | 2.17                     | 0.44              |
| 1:a:609:ASP:HA    | 1:a:612:ARG:HH12  | 1.81                     | 0.44              |
| 12:a:912:CLA:H162 | 12:a:912:CLA:H202 | 1.67                     | 0.44              |
| 12:a:914:CLA:HAA1 | 12:a:914:CLA:HBD  | 2.00                     | 0.44              |
| 8:B:133:THR:O     | 8:B:133:THR:OG1   | 2.24                     | 0.44              |
| 2:C:138:PRO:HB3   | 1:a:862:PHE:HB3   | 2.00                     | 0.43              |
| 4:F:22:LEU:HD13   | 12:a:912:CLA:H172 | 2.00                     | 0.43              |
| 11:a:908:BCL:H71  | 16:a:930:UNL:C21  | 2.48                     | 0.43              |
| 7:c:82:GLN:O      | 7:c:82:GLN:HG3    | 2.17                     | 0.43              |
| 7:c:98:GLY:CA     | 7:c:107:ASN:CA    | 2.62                     | 0.43              |
| 8:B:109:LEU:HB3   | 8:B:110:ASP:H     | 1.64                     | 0.43              |
| 1:A:57:TYR:O      | 1:A:61:THR:CG2    | 2.64                     | 0.43              |
| 11:A:905:BCL:HBB2 | 11:A:905:BCL:CMB  | 2.47                     | 0.43              |
| 1:a:155:LEU:HD23  | 1:a:155:LEU:C     | 2.43                     | 0.43              |
| 1:a:475:THR:HG22  | 5:g:39:LYS:HD3    | 2.01                     | 0.43              |
| 8:B:140:VAL:HG13  | 8:B:146:VAL:HG11  | 1.84                     | 0.43              |
| 1:A:266:GLU:HB2   | 11:A:906:BCL:C1D  | 2.49                     | 0.43              |
| 3:E:32:ILE:HG22   | 1:a:814:LEU:HD12  | 2.00                     | 0.43              |
| 1:a:640:LEU:HB2   | 1:a:865:ARG:CG    | 2.48                     | 0.43              |
| 1:a:761:LEU:HD23  | 1:a:761:LEU:HA    | 1.85                     | 0.43              |
| 1:A:367:LEU:HD13  | 1:A:662:TRP:HZ3   | 1.82                     | 0.43              |
| 11:A:908:BCL:HHD  | 11:A:908:BCL:HAC1 | 1.68                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:95:SER:O      | 2:C:99:VAL:HG22   | 2.18                     | 0.43              |
| 3:E:32:ILE:CG2    | 1:a:817:LYS:HE3   | 2.48                     | 0.43              |
| 1:a:409:LYS:O     | 1:a:413:THR:CG2   | 2.67                     | 0.43              |
| 8:B:122:CYS:C     | 8:B:124:SER:H     | 2.26                     | 0.43              |
| 1:A:87:LEU:O      | 1:A:95:LYS:HG3    | 2.19                     | 0.43              |
| 1:A:239:LEU:HD21  | 1:A:248:TRP:CE2   | 2.53                     | 0.43              |
| 1:A:787:TRP:CG    | 10:A:901:2GO:H27  | 2.53                     | 0.43              |
| 1:a:822:LYS:HE3   | 1:a:822:LYS:HB3   | 1.87                     | 0.43              |
| 1:a:152:VAL:N     | 1:a:153:PRO:HD3   | 2.34                     | 0.43              |
| 18:C:301:HEC:CMB  | 18:C:301:HEC:HBB3 | 2.48                     | 0.43              |
| 1:a:244:PHE:CD1   | 1:a:244:PHE:C     | 2.90                     | 0.43              |
| 1:a:475:THR:HA    | 5:g:39:LYS:CD     | 2.48                     | 0.43              |
| 1:a:700:VAL:CG1   | 8:B:111:GLY:C     | 2.92                     | 0.43              |
| 1:a:833:ASN:ND2   | 1:a:836:THR:HG23  | 2.33                     | 0.43              |
| 8:B:144:GLY:HA2   | 9:D:41:TYR:OH     | 2.19                     | 0.43              |
| 1:A:59:ASN:HD22   | 1:A:60:LEU:N      | 2.16                     | 0.43              |
| 2:C:153:SER:HB2   | 18:c:202:HEC:O2D  | 2.18                     | 0.43              |
| 1:a:93:THR:HB     | 1:a:98:PHE:H      | 1.83                     | 0.43              |
| 1:a:138:GLY:O     | 1:a:166:PRO:HD3   | 2.18                     | 0.43              |
| 1:A:808:GLN:HG3   | 1:a:415:MET:HE1   | 2.00                     | 0.43              |
| 1:a:48:ALA:HB2    | 7:c:20:GLY:HA3    | 2.00                     | 0.43              |
| 1:a:143:GLY:HA3   | 1:a:159:CYS:SG    | 2.59                     | 0.43              |
| 1:a:150:PRO:HB2   | 1:a:151:TYR:CE1   | 2.53                     | 0.43              |
| 11:a:907:BCL:H141 | 11:a:907:BCL:H161 | 1.50                     | 0.43              |
| 1:A:202:TYR:CE2   | 11:A:905:BCL:H192 | 2.54                     | 0.43              |
| 1:A:494:ARG:CD    | 1:A:586:VAL:HG13  | 2.48                     | 0.43              |
| 1:A:797:ASP:HA    | 1:a:705:CYS:O     | 2.19                     | 0.43              |
| 5:g:9:ILE:H       | 5:g:9:ILE:HD13    | 1.84                     | 0.43              |
| 8:B:110:ASP:C     | 8:B:112:GLY:H     | 2.26                     | 0.43              |
| 8:B:119:GLN:C     | 8:B:121:ARG:H     | 2.27                     | 0.43              |
| 1:A:290:ARG:H     | 16:A:920:UNL:C21  | 2.32                     | 0.42              |
| 11:A:903:BCL:HAC1 | 11:A:903:BCL:HHD  | 1.78                     | 0.42              |
| 11:a:910:BCL:HHD  | 11:a:910:BCL:HAC1 | 1.81                     | 0.42              |
| 8:B:108:VAL:HG12  | 8:B:110:ASP:OD1   | 2.19                     | 0.42              |
| 1:a:435:ALA:HB2   | 1:a:541:SER:HB2   | 2.01                     | 0.42              |
| 11:a:905:BCL:CBB  | 11:a:905:BCL:CMB  | 2.93                     | 0.42              |
| 1:A:78:GLU:HG3    | 2:C:62:PRO:HB2    | 2.02                     | 0.42              |
| 1:A:159:CYS:SG    | 1:A:159:CYS:O     | 2.77                     | 0.42              |
| 1:a:48:ALA:HB2    | 7:c:20:GLY:HA2    | 2.01                     | 0.42              |
| 1:a:265:GLY:O     | 1:a:268:THR:HG23  | 2.19                     | 0.42              |
| 1:a:718:LEU:H     | 1:a:718:LEU:HG    | 1.79                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:a:847:THR:HB    | 11:a:910:BCL:H91 | 2.01                     | 0.42              |
| 12:a:901:CLA:C19  | 4:f:21:THR:HG22  | 2.49                     | 0.42              |
| 1:A:124:TRP:NE1   | 16:A:924:UNL:C10 | 2.83                     | 0.42              |
| 2:C:139:ARG:HA    | 2:C:139:ARG:HD2  | 1.84                     | 0.42              |
| 8:B:129:PHE:CA    | 8:B:139:VAL:CG2  | 2.96                     | 0.42              |
| 9:D:23:LYS:HA     | 9:D:26:ILE:HD12  | 2.02                     | 0.42              |
| 1:A:390:TYR:CZ    | 1:A:402:GLN:HG2  | 2.54                     | 0.42              |
| 10:A:901:2GO:H52  | 10:A:901:2GO:H47 | 1.74                     | 0.42              |
| 12:A:931:CLA:H62  | 12:A:931:CLA:H41 | 1.82                     | 0.42              |
| 2:C:128:CYS:CB    | 18:C:301:HEC:CAC | 2.94                     | 0.42              |
| 1:a:477:GLY:C     | 5:g:41:LEU:HD12  | 2.44                     | 0.42              |
| 3:e:22:ILE:O      | 3:e:22:ILE:CG2   | 2.67                     | 0.42              |
| 1:A:292:ILE:HD12  | 1:A:292:ILE:H    | 1.84                     | 0.42              |
| 1:A:352:ARG:HA    | 1:A:352:ARG:HD3  | 1.88                     | 0.42              |
| 13:A:913:LYC:H131 | 13:A:913:LYC:H15 | 1.60                     | 0.42              |
| 1:a:742:ARG:HB2   | 1:a:745:GLU:HG3  | 2.01                     | 0.42              |
| 7:c:71:ILE:HG23   | 7:c:71:ILE:HD12  | 1.72                     | 0.42              |
| 1:A:88:ILE:HG21   | 1:A:109:PHE:HZ   | 1.85                     | 0.42              |
| 1:A:137:ARG:HH21  | 1:A:137:ARG:HD2  | 1.72                     | 0.42              |
| 1:A:469:LYS:HE2   | 1:A:477:GLY:C    | 2.45                     | 0.42              |
| 1:a:96:LEU:HB2    | 1:a:99:PHE:HB2   | 2.00                     | 0.42              |
| 7:c:48:LEU:HD22   | 7:c:48:LEU:N     | 2.33                     | 0.42              |
| 8:B:116:TRP:CD1   | 8:B:116:TRP:H    | 2.37                     | 0.42              |
| 1:A:146:PHE:O     | 1:A:148:LEU:HD22 | 2.19                     | 0.42              |
| 1:A:595:ALA:O     | 1:A:596:GLN:HB2  | 2.20                     | 0.42              |
| 12:A:910:CLA:H41  | 12:A:910:CLA:H62 | 1.47                     | 0.42              |
| 12:A:910:CLA:HBA2 | 1:a:760:PHE:CZ   | 2.54                     | 0.42              |
| 5:G:11:LYS:HA     | 5:G:11:LYS:HD2   | 1.63                     | 0.42              |
| 1:a:149:LEU:H     | 1:a:150:PRO:HD2  | 1.80                     | 0.42              |
| 1:a:475:THR:CA    | 5:g:39:LYS:HG2   | 2.33                     | 0.42              |
| 9:D:20:ARG:HG2    | 9:D:20:ARG:NH1   | 2.35                     | 0.42              |
| 1:A:573:LYS:HE3   | 1:A:573:LYS:HB2  | 1.42                     | 0.42              |
| 12:A:931:CLA:H52  | 1:a:781:LEU:HD23 | 2.02                     | 0.42              |
| 2:C:141:THR:O     | 2:C:141:THR:CG2  | 2.66                     | 0.42              |
| 4:F:25:ILE:HD13   | 15:a:919:85I:C29 | 2.50                     | 0.42              |
| 1:a:150:PRO:HB2   | 1:a:151:TYR:CD1  | 2.55                     | 0.42              |
| 1:a:617:LYS:HZ3   | 1:a:617:LYS:HG2  | 1.60                     | 0.42              |
| 1:A:221:PRO:HA    | 1:A:222:PRO:HD3  | 1.81                     | 0.41              |
| 1:A:608:LEU:HD11  | 1:A:612:ARG:HH21 | 1.83                     | 0.41              |
| 2:C:85:GLN:H      | 2:C:85:GLN:HG2   | 1.51                     | 0.41              |
| 2:C:99:VAL:HG11   | 2:C:158:TYR:CZ   | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:32:MET:HB2    | 11:a:907:BCL:HED1 | 2.02                     | 0.41              |
| 1:a:475:THR:HA    | 5:g:39:LYS:HD3    | 2.01                     | 0.41              |
| 11:a:904:BCL:HBC3 | 11:a:911:BCL:H91  | 2.02                     | 0.41              |
| 11:a:908:BCL:O1D  | 11:a:908:BCL:H12  | 2.20                     | 0.41              |
| 11:a:908:BCL:H161 | 11:a:908:BCL:H141 | 1.49                     | 0.41              |
| 1:A:266:GLU:HG3   | 11:A:906:BCL:HED3 | 2.02                     | 0.41              |
| 11:A:908:BCL:H41  | 11:A:908:BCL:H61  | 1.73                     | 0.41              |
| 11:A:909:BCL:C2B  | 11:A:909:BCL:H52  | 2.51                     | 0.41              |
| 2:C:71:ARG:HB2    | 2:C:75:THR:CG2    | 2.48                     | 0.41              |
| 4:F:34:ARG:HB3    | 4:F:35:GLY:H      | 1.52                     | 0.41              |
| 1:a:85:LEU:H      | 1:a:85:LEU:HD22   | 1.85                     | 0.41              |
| 1:a:147:TRP:NE1   | 1:a:148:LEU:HD22  | 2.34                     | 0.41              |
| 8:B:140:VAL:CG1   | 8:B:146:VAL:HG12  | 2.33                     | 0.41              |
| 10:A:901:2GO:H21  | 10:A:901:2GO:H25  | 2.03                     | 0.41              |
| 11:A:902:BCL:H43  | 11:A:902:BCL:H12  | 1.89                     | 0.41              |
| 2:C:174:MET:HB2   | 18:C:301:HEC:C4D  | 2.50                     | 0.41              |
| 1:a:56:GLY:O      | 1:a:60:LEU:HB2    | 2.20                     | 0.41              |
| 1:a:57:TYR:O      | 1:a:61:THR:HG23   | 2.20                     | 0.41              |
| 1:a:492:LYS:H     | 1:a:492:LYS:HG2   | 1.53                     | 0.41              |
| 1:a:741:ALA:O     | 1:a:757:GLY:O     | 2.39                     | 0.41              |
| 1:A:91:PHE:HB3    | 1:A:95:LYS:CB     | 2.33                     | 0.41              |
| 1:a:66:LEU:HD13   | 12:a:913:CLA:HED1 | 2.03                     | 0.41              |
| 8:B:134:CYS:CB    | 20:B:201:SF4:S2   | 3.08                     | 0.41              |
| 1:A:296:HIS:H     | 1:A:296:HIS:CD2   | 2.39                     | 0.41              |
| 1:A:404:PRO:O     | 1:A:408:THR:HG22  | 2.20                     | 0.41              |
| 2:C:128:CYS:CB    | 18:C:301:HEC:HAC  | 2.48                     | 0.41              |
| 1:a:91:PHE:H      | 1:a:94:SER:CB     | 2.33                     | 0.41              |
| 1:a:354:ILE:HD13  | 1:a:354:ILE:HA    | 1.89                     | 0.41              |
| 1:a:487:THR:HG22  | 6:h:17:UNK:O      | 2.21                     | 0.41              |
| 1:a:729:TRP:CB    | 1:a:736:ILE:HD11  | 2.51                     | 0.41              |
| 8:B:121:ARG:O     | 8:B:121:ARG:CG    | 2.68                     | 0.41              |
| 1:A:171:TYR:O     | 1:A:171:TYR:HD1   | 2.03                     | 0.41              |
| 8:B:76:TYR:CD1    | 8:B:141:PHE:HB2   | 2.54                     | 0.41              |
| 1:A:545:PHE:HB2   | 16:A:928:UNL:C17  | 2.51                     | 0.41              |
| 1:A:640:LEU:HB3   | 1:A:865:ARG:HG3   | 2.02                     | 0.41              |
| 11:A:907:BCL:HAA1 | 11:A:907:BCL:HBD  | 2.02                     | 0.41              |
| 13:A:913:LYC:H59  | 13:A:913:LYC:H571 | 1.45                     | 0.41              |
| 1:a:483:ASN:HB3   | 1:a:484:PRO:CD    | 2.51                     | 0.41              |
| 1:a:92:SER:O      | 1:a:93:THR:C      | 2.63                     | 0.41              |
| 1:a:159:CYS:SG    | 1:a:159:CYS:O     | 2.78                     | 0.41              |
| 7:c:91:GLY:H      | 7:c:94:GLN:H      | 1.69                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:110:ASP:O     | 8:B:112:GLY:N     | 2.54                     | 0.41              |
| 1:A:146:PHE:O     | 1:A:148:LEU:CD2   | 2.69                     | 0.41              |
| 1:A:429:ILE:O     | 1:A:433:THR:CG2   | 2.65                     | 0.41              |
| 1:A:453:GLN:NE2   | 1:A:533:LYS:HD3   | 2.36                     | 0.41              |
| 1:A:477:GLY:H     | 5:G:41:LEU:CD1    | 2.20                     | 0.41              |
| 1:A:610:LYS:O     | 1:A:610:LYS:CG    | 2.68                     | 0.41              |
| 1:A:796:LYS:HG3   | 1:a:796:LYS:CG    | 2.50                     | 0.41              |
| 11:A:902:BCL:HAA1 | 11:A:902:BCL:HBD  | 2.03                     | 0.41              |
| 1:a:91:PHE:HB2    | 1:a:95:LYS:H      | 1.85                     | 0.41              |
| 1:a:526:LYS:HZ3   | 1:a:626:ASN:HD21  | 1.68                     | 0.41              |
| 1:a:774:ASN:HA    | 1:a:777:THR:HG23  | 2.03                     | 0.41              |
| 7:c:160:ARG:HD3   | 7:c:160:ARG:HA    | 1.89                     | 0.41              |
| 3:e:23:LYS:O      | 3:e:23:LYS:CG     | 2.69                     | 0.41              |
| 8:B:119:GLN:C     | 8:B:121:ARG:N     | 2.79                     | 0.41              |
| 1:a:504:ASN:OD1   | 1:a:518:THR:HG22  | 2.21                     | 0.41              |
| 1:A:210:TRP:CH2   | 12:A:911:CLA:HBA1 | 2.55                     | 0.40              |
| 13:A:913:LYC:H54  | 13:A:913:LYC:H521 | 1.82                     | 0.40              |
| 1:a:846:TYR:CD1   | 11:a:910:BCL:H162 | 2.55                     | 0.40              |
| 3:E:32:ILE:CG2    | 1:a:814:LEU:HD12  | 2.52                     | 0.40              |
| 11:a:909:BCL:H192 | 11:a:909:BCL:H162 | 1.53                     | 0.40              |
| 8:B:90:THR:HG21   | 8:B:115:TYR:HE2   | 1.56                     | 0.40              |
| 8:B:122:CYS:C     | 8:B:124:SER:N     | 2.79                     | 0.40              |
| 1:A:602:GLN:HE21  | 1:A:602:GLN:HB3   | 1.40                     | 0.40              |
| 11:A:908:BCL:HBD  | 11:A:908:BCL:CBA  | 2.15                     | 0.40              |
| 2:C:32:TYR:HA     | 2:C:33:PRO:HD3    | 1.86                     | 0.40              |
| 2:C:200:GLN:HE21  | 2:C:200:GLN:HB2   | 1.39                     | 0.40              |
| 1:a:82:ARG:O      | 1:a:82:ARG:HG2    | 2.12                     | 0.40              |
| 1:a:639:ASN:HD22  | 1:a:643:GLN:HE21  | 1.69                     | 0.40              |
| 1:a:767:THR:HA    | 1:a:770:ILE:HB    | 2.04                     | 0.40              |
| 11:a:906:BCL:HAC1 | 11:a:906:BCL:HHD  | 1.78                     | 0.40              |
| 1:A:18:LEU:O      | 12:A:912:CLA:HAA2 | 2.21                     | 0.40              |
| 11:A:903:BCL:H2   | 16:A:927:UNL:C9   | 2.51                     | 0.40              |
| 11:A:905:BCL:CMB  | 11:A:905:BCL:CBB  | 2.98                     | 0.40              |
| 3:e:5:LEU:HD12    | 3:e:5:LEU:HA      | 1.84                     | 0.40              |
| 1:A:742:ARG:HG3   | 1:A:761:LEU:HD22  | 2.04                     | 0.40              |
| 1:A:796:LYS:HE3   | 1:a:834:LEU:HD22  | 2.03                     | 0.40              |
| 2:C:37:MET:HE1    | 2:C:80:GLN:CB     | 2.50                     | 0.40              |
| 1:a:650:ASN:HB2   | 1:a:735:TRP:CE3   | 2.57                     | 0.40              |
| 11:a:908:BCL:H12  | 11:a:908:BCL:HBA1 | 1.85                     | 0.40              |
| 16:a:922:UNL:C1   | 16:a:922:UNL:C18  | 3.00                     | 0.40              |
| 5:g:21:LEU:HA     | 5:g:21:LEU:HD12   | 1.65                     | 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 PDB entries followed by that with respect to all EM entries.

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     | 852/858 (99%)   | 792 (93%)  | 42 (5%)  | 18 (2%)  | 5           | 10  |
| 1   | a     | 856/858 (100%)  | 798 (93%)  | 46 (5%)  | 12 (1%)  | 9           | 17  |
| 2   | C     | 189/204 (93%)   | 174 (92%)  | 9 (5%)   | 6 (3%)   | 3           | 4   |
| 3   | E     | 33/35 (94%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 3   | e     | 33/35 (94%)     | 32 (97%)   | 0        | 1 (3%)   | 3           | 5   |
| 4   | F     | 33/35 (94%)     | 31 (94%)   | 2 (6%)   | 0        | 100         | 100 |
| 4   | f     | 33/35 (94%)     | 30 (91%)   | 2 (6%)   | 1 (3%)   | 3           | 5   |
| 5   | G     | 36/38 (95%)     | 32 (89%)   | 3 (8%)   | 1 (3%)   | 4           | 6   |
| 5   | g     | 36/38 (95%)     | 32 (89%)   | 4 (11%)  | 0        | 100         | 100 |
| 7   | c     | 143/145 (99%)   | 127 (89%)  | 8 (6%)   | 8 (6%)   | 1           | 1   |
| 8   | B     | 74/76 (97%)     | 43 (58%)   | 24 (32%) | 7 (10%)  | 0           | 0   |
| 9   | D     | 58/70 (83%)     | 58 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 2376/2427 (98%) | 2180 (92%) | 142 (6%) | 54 (2%)  | 7           | 8   |

All (54) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 86  | PRO  |
| 1   | A     | 97  | PRO  |
| 1   | A     | 147 | TRP  |
| 1   | A     | 170 | TRP  |
| 1   | A     | 346 | LYS  |
| 2   | C     | 48  | THR  |
| 2   | C     | 62  | PRO  |
| 2   | C     | 180 | GLN  |
| 2   | C     | 203 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 83  | VAL  |
| 1   | a     | 759 | VAL  |
| 7   | c     | 99  | GLY  |
| 7   | c     | 102 | ALA  |
| 7   | c     | 132 | LYS  |
| 8   | B     | 102 | PRO  |
| 8   | B     | 105 | VAL  |
| 1   | A     | 87  | LEU  |
| 1   | A     | 136 | ALA  |
| 1   | a     | 137 | ARG  |
| 1   | a     | 155 | LEU  |
| 1   | a     | 346 | LYS  |
| 7   | c     | 17  | MET  |
| 7   | c     | 21  | CYS  |
| 7   | c     | 131 | GLY  |
| 8   | B     | 128 | CYS  |
| 1   | A     | 688 | ARG  |
| 1   | a     | 9   | ASN  |
| 1   | a     | 87  | LEU  |
| 7   | c     | 92  | CYS  |
| 8   | B     | 123 | ILE  |
| 1   | A     | 94  | SER  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 244 | PHE  |
| 1   | A     | 476 | ALA  |
| 1   | A     | 542 | TRP  |
| 5   | G     | 9   | ILE  |
| 1   | a     | 147 | TRP  |
| 4   | f     | 34  | ARG  |
| 8   | B     | 88  | PHE  |
| 1   | A     | 13  | ARG  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 757 | GLY  |
| 2   | C     | 59  | GLN  |
| 2   | C     | 217 | ARG  |
| 7   | c     | 64  | LYS  |
| 8   | B     | 143 | GLU  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 696 | CYS  |
| 1   | a     | 529 | TRP  |
| 8   | B     | 135 | PRO  |
| 1   | a     | 540 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 757 | GLY  |
| 1   | a     | 149 | LEU  |
| 3   | e     | 22  | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 718/720 (100%)  | 582 (81%)  | 136 (19%) | 1           | 2  |
| 1   | a     | 720/720 (100%)  | 583 (81%)  | 137 (19%) | 1           | 2  |
| 2   | C     | 155/166 (93%)   | 126 (81%)  | 29 (19%)  | 1           | 2  |
| 3   | E     | 25/25 (100%)    | 20 (80%)   | 5 (20%)   | 1           | 2  |
| 3   | e     | 25/25 (100%)    | 18 (72%)   | 7 (28%)   | 0           | 1  |
| 4   | F     | 31/31 (100%)    | 25 (81%)   | 6 (19%)   | 1           | 2  |
| 4   | f     | 31/31 (100%)    | 26 (84%)   | 5 (16%)   | 2           | 4  |
| 5   | G     | 31/31 (100%)    | 22 (71%)   | 9 (29%)   | 0           | 0  |
| 5   | g     | 31/31 (100%)    | 21 (68%)   | 10 (32%)  | 0           | 0  |
| 7   | c     | 112/112 (100%)  | 90 (80%)   | 22 (20%)  | 1           | 2  |
| 8   | B     | 65/65 (100%)    | 42 (65%)   | 23 (35%)  | 0           | 0  |
| 9   | D     | 52/62 (84%)     | 49 (94%)   | 3 (6%)    | 18          | 37 |
| All | All   | 1996/2019 (99%) | 1604 (80%) | 392 (20%) | 3           | 2  |

All (392) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | LYS  |
| 1   | A     | 13  | ARG  |
| 1   | A     | 14  | TRP  |
| 1   | A     | 15  | TYR  |
| 1   | A     | 17  | LYS  |
| 1   | A     | 18  | LEU  |
| 1   | A     | 25  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | MET  |
| 1   | A     | 59  | ASN  |
| 1   | A     | 60  | LEU  |
| 1   | A     | 61  | THR  |
| 1   | A     | 65  | ARG  |
| 1   | A     | 66  | LEU  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 77  | THR  |
| 1   | A     | 81  | GLN  |
| 1   | A     | 82  | ARG  |
| 1   | A     | 84  | TRP  |
| 1   | A     | 85  | LEU  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 90  | GLU  |
| 1   | A     | 93  | THR  |
| 1   | A     | 95  | LYS  |
| 1   | A     | 96  | LEU  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 107 | THR  |
| 1   | A     | 141 | THR  |
| 1   | A     | 144 | GLU  |
| 1   | A     | 147 | TRP  |
| 1   | A     | 148 | LEU  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 159 | CYS  |
| 1   | A     | 161 | ILE  |
| 1   | A     | 162 | LYS  |
| 1   | A     | 175 | LEU  |
| 1   | A     | 183 | THR  |
| 1   | A     | 188 | LEU  |
| 1   | A     | 200 | THR  |
| 1   | A     | 203 | ILE  |
| 1   | A     | 205 | LEU  |
| 1   | A     | 206 | LEU  |
| 1   | A     | 214 | LEU  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 224 | PRO  |
| 1   | A     | 229 | GLN  |
| 1   | A     | 240 | GLU  |
| 1   | A     | 254 | ASN  |
| 1   | A     | 263 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 267 | THR  |
| 1   | A     | 268 | THR  |
| 1   | A     | 276 | LEU  |
| 1   | A     | 290 | ARG  |
| 1   | A     | 294 | ILE  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 318 | LEU  |
| 1   | A     | 326 | LEU  |
| 1   | A     | 331 | SER  |
| 1   | A     | 333 | LEU  |
| 1   | A     | 334 | MET  |
| 1   | A     | 335 | LEU  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 352 | ARG  |
| 1   | A     | 359 | THR  |
| 1   | A     | 381 | LEU  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 386 | ILE  |
| 1   | A     | 387 | SER  |
| 1   | A     | 391 | LYS  |
| 1   | A     | 408 | THR  |
| 1   | A     | 413 | THR  |
| 1   | A     | 414 | THR  |
| 1   | A     | 433 | THR  |
| 1   | A     | 450 | ARG  |
| 1   | A     | 467 | ARG  |
| 1   | A     | 473 | ASP  |
| 1   | A     | 475 | THR  |
| 1   | A     | 489 | LYS  |
| 1   | A     | 490 | LEU  |
| 1   | A     | 494 | ARG  |
| 1   | A     | 496 | LEU  |
| 1   | A     | 497 | GLN  |
| 1   | A     | 503 | LEU  |
| 1   | A     | 505 | GLU  |
| 1   | A     | 518 | THR  |
| 1   | A     | 534 | LEU  |
| 1   | A     | 552 | LEU  |
| 1   | A     | 562 | LEU  |
| 1   | A     | 565 | GLN  |
| 1   | A     | 567 | THR  |
| 1   | A     | 569 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 572 | ARG  |
| 1   | A     | 583 | LEU  |
| 1   | A     | 588 | LEU  |
| 1   | A     | 597 | THR  |
| 1   | A     | 598 | GLU  |
| 1   | A     | 601 | LYS  |
| 1   | A     | 602 | GLN  |
| 1   | A     | 608 | LEU  |
| 1   | A     | 612 | ARG  |
| 1   | A     | 617 | LYS  |
| 1   | A     | 621 | ASN  |
| 1   | A     | 624 | GLU  |
| 1   | A     | 638 | SER  |
| 1   | A     | 640 | LEU  |
| 1   | A     | 641 | ARG  |
| 1   | A     | 653 | ILE  |
| 1   | A     | 657 | LEU  |
| 1   | A     | 667 | ILE  |
| 1   | A     | 669 | LEU  |
| 1   | A     | 670 | LEU  |
| 1   | A     | 684 | ASP  |
| 1   | A     | 688 | ARG  |
| 1   | A     | 690 | GLN  |
| 1   | A     | 700 | VAL  |
| 1   | A     | 717 | ILE  |
| 1   | A     | 724 | LEU  |
| 1   | A     | 736 | ILE  |
| 1   | A     | 768 | THR  |
| 1   | A     | 777 | THR  |
| 1   | A     | 781 | LEU  |
| 1   | A     | 790 | SER  |
| 1   | A     | 796 | LYS  |
| 1   | A     | 798 | ARG  |
| 1   | A     | 800 | SER  |
| 1   | A     | 819 | LEU  |
| 1   | A     | 822 | LYS  |
| 1   | A     | 823 | THR  |
| 1   | A     | 824 | LEU  |
| 1   | A     | 826 | GLU  |
| 1   | A     | 832 | SER  |
| 1   | A     | 833 | ASN  |
| 1   | A     | 836 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 847 | THR  |
| 1   | A     | 849 | THR  |
| 1   | A     | 851 | VAL  |
| 2   | C     | 24  | SER  |
| 2   | C     | 28  | ASN  |
| 2   | C     | 30  | THR  |
| 2   | C     | 40  | GLN  |
| 2   | C     | 46  | LEU  |
| 2   | C     | 47  | LYS  |
| 2   | C     | 61  | THR  |
| 2   | C     | 65  | ARG  |
| 2   | C     | 71  | ARG  |
| 2   | C     | 75  | THR  |
| 2   | C     | 77  | LEU  |
| 2   | C     | 82  | VAL  |
| 2   | C     | 85  | GLN  |
| 2   | C     | 87  | VAL  |
| 2   | C     | 99  | VAL  |
| 2   | C     | 112 | GLU  |
| 2   | C     | 116 | GLU  |
| 2   | C     | 126 | VAL  |
| 2   | C     | 139 | ARG  |
| 2   | C     | 150 | GLU  |
| 2   | C     | 153 | SER  |
| 2   | C     | 180 | GLN  |
| 2   | C     | 182 | SER  |
| 2   | C     | 193 | LEU  |
| 2   | C     | 194 | ARG  |
| 2   | C     | 200 | GLN  |
| 2   | C     | 204 | LEU  |
| 2   | C     | 217 | ARG  |
| 2   | C     | 218 | GLN  |
| 3   | E     | 9   | LEU  |
| 3   | E     | 18  | LEU  |
| 3   | E     | 23  | LYS  |
| 3   | E     | 30  | LYS  |
| 3   | E     | 31  | ASP  |
| 4   | F     | 1   | MET  |
| 4   | F     | 2   | TRP  |
| 4   | F     | 12  | LEU  |
| 4   | F     | 32  | LEU  |
| 4   | F     | 33  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | F     | 34  | ARG  |
| 5   | G     | 11  | LYS  |
| 5   | G     | 14  | TRP  |
| 5   | G     | 20  | LEU  |
| 5   | G     | 21  | LEU  |
| 5   | G     | 25  | LEU  |
| 5   | G     | 38  | VAL  |
| 5   | G     | 39  | LYS  |
| 5   | G     | 44  | LEU  |
| 5   | G     | 45  | ASN  |
| 1   | a     | 11  | VAL  |
| 1   | a     | 18  | LEU  |
| 1   | a     | 20  | LEU  |
| 1   | a     | 26  | ARG  |
| 1   | a     | 59  | ASN  |
| 1   | a     | 60  | LEU  |
| 1   | a     | 61  | THR  |
| 1   | a     | 66  | LEU  |
| 1   | a     | 69  | LEU  |
| 1   | a     | 79  | GLN  |
| 1   | a     | 80  | ILE  |
| 1   | a     | 81  | GLN  |
| 1   | a     | 82  | ARG  |
| 1   | a     | 83  | VAL  |
| 1   | a     | 84  | TRP  |
| 1   | a     | 85  | LEU  |
| 1   | a     | 87  | LEU  |
| 1   | a     | 88  | ILE  |
| 1   | a     | 90  | GLU  |
| 1   | a     | 91  | PHE  |
| 1   | a     | 94  | SER  |
| 1   | a     | 95  | LYS  |
| 1   | a     | 98  | PHE  |
| 1   | a     | 106 | MET  |
| 1   | a     | 107 | THR  |
| 1   | a     | 123 | LEU  |
| 1   | a     | 124 | TRP  |
| 1   | a     | 125 | LEU  |
| 1   | a     | 147 | TRP  |
| 1   | a     | 148 | LEU  |
| 1   | a     | 149 | LEU  |
| 1   | a     | 151 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 152 | VAL  |
| 1   | a     | 155 | LEU  |
| 1   | a     | 156 | LYS  |
| 1   | a     | 158 | LEU  |
| 1   | a     | 160 | GLN  |
| 1   | a     | 161 | ILE  |
| 1   | a     | 172 | LYS  |
| 1   | a     | 173 | VAL  |
| 1   | a     | 183 | THR  |
| 1   | a     | 187 | ILE  |
| 1   | a     | 188 | LEU  |
| 1   | a     | 189 | ARG  |
| 1   | a     | 200 | THR  |
| 1   | a     | 205 | LEU  |
| 1   | a     | 206 | LEU  |
| 1   | a     | 214 | LEU  |
| 1   | a     | 218 | LEU  |
| 1   | a     | 225 | LEU  |
| 1   | a     | 240 | GLU  |
| 1   | a     | 241 | GLN  |
| 1   | a     | 253 | LEU  |
| 1   | a     | 263 | ILE  |
| 1   | a     | 267 | THR  |
| 1   | a     | 268 | THR  |
| 1   | a     | 276 | LEU  |
| 1   | a     | 287 | ARG  |
| 1   | a     | 290 | ARG  |
| 1   | a     | 292 | ILE  |
| 1   | a     | 294 | ILE  |
| 1   | a     | 297 | LEU  |
| 1   | a     | 303 | VAL  |
| 1   | a     | 309 | THR  |
| 1   | a     | 318 | LEU  |
| 1   | a     | 326 | LEU  |
| 1   | a     | 333 | LEU  |
| 1   | a     | 359 | THR  |
| 1   | a     | 381 | LEU  |
| 1   | a     | 384 | LEU  |
| 1   | a     | 386 | ILE  |
| 1   | a     | 391 | LYS  |
| 1   | a     | 392 | GLN  |
| 1   | a     | 408 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 413 | THR  |
| 1   | a     | 433 | THR  |
| 1   | a     | 448 | SER  |
| 1   | a     | 450 | ARG  |
| 1   | a     | 461 | ILE  |
| 1   | a     | 464 | ARG  |
| 1   | a     | 469 | LYS  |
| 1   | a     | 482 | LYS  |
| 1   | a     | 490 | LEU  |
| 1   | a     | 492 | LYS  |
| 1   | a     | 496 | LEU  |
| 1   | a     | 497 | GLN  |
| 1   | a     | 501 | ARG  |
| 1   | a     | 503 | LEU  |
| 1   | a     | 514 | THR  |
| 1   | a     | 516 | SER  |
| 1   | a     | 518 | THR  |
| 1   | a     | 534 | LEU  |
| 1   | a     | 552 | LEU  |
| 1   | a     | 562 | LEU  |
| 1   | a     | 566 | LYS  |
| 1   | a     | 567 | THR  |
| 1   | a     | 569 | GLU  |
| 1   | a     | 576 | GLU  |
| 1   | a     | 583 | LEU  |
| 1   | a     | 584 | LYS  |
| 1   | a     | 587 | SER  |
| 1   | a     | 588 | LEU  |
| 1   | a     | 602 | GLN  |
| 1   | a     | 617 | LYS  |
| 1   | a     | 622 | MET  |
| 1   | a     | 623 | LEU  |
| 1   | a     | 624 | GLU  |
| 1   | a     | 628 | ARG  |
| 1   | a     | 640 | LEU  |
| 1   | a     | 641 | ARG  |
| 1   | a     | 653 | ILE  |
| 1   | a     | 657 | LEU  |
| 1   | a     | 669 | LEU  |
| 1   | a     | 670 | LEU  |
| 1   | a     | 705 | CYS  |
| 1   | a     | 709 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 724 | LEU  |
| 1   | a     | 736 | ILE  |
| 1   | a     | 761 | LEU  |
| 1   | a     | 768 | THR  |
| 1   | a     | 777 | THR  |
| 1   | a     | 781 | LEU  |
| 1   | a     | 785 | LEU  |
| 1   | a     | 798 | ARG  |
| 1   | a     | 815 | MET  |
| 1   | a     | 819 | LEU  |
| 1   | a     | 822 | LYS  |
| 1   | a     | 823 | THR  |
| 1   | a     | 824 | LEU  |
| 1   | a     | 826 | GLU  |
| 1   | a     | 833 | ASN  |
| 1   | a     | 836 | THR  |
| 1   | a     | 847 | THR  |
| 1   | a     | 849 | THR  |
| 1   | a     | 851 | VAL  |
| 1   | a     | 864 | ASN  |
| 1   | a     | 865 | ARG  |
| 7   | c     | 17  | MET  |
| 7   | c     | 21  | CYS  |
| 7   | c     | 30  | GLU  |
| 7   | c     | 33  | LEU  |
| 7   | c     | 42  | ARG  |
| 7   | c     | 43  | THR  |
| 7   | c     | 48  | LEU  |
| 7   | c     | 50  | GLU  |
| 7   | c     | 54  | LEU  |
| 7   | c     | 62  | LEU  |
| 7   | c     | 64  | LYS  |
| 7   | c     | 92  | CYS  |
| 7   | c     | 96  | ASN  |
| 7   | c     | 103 | ILE  |
| 7   | c     | 106 | THR  |
| 7   | c     | 110 | ASP  |
| 7   | c     | 122 | MET  |
| 7   | c     | 133 | VAL  |
| 7   | c     | 140 | LYS  |
| 7   | c     | 144 | GLN  |
| 7   | c     | 154 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | c     | 159 | LYS  |
| 3   | e     | 2   | THR  |
| 3   | e     | 5   | LEU  |
| 3   | e     | 6   | LEU  |
| 3   | e     | 22  | ILE  |
| 3   | e     | 28  | ASN  |
| 3   | e     | 30  | LYS  |
| 3   | e     | 32  | ILE  |
| 4   | f     | 1   | MET  |
| 4   | f     | 10  | SER  |
| 4   | f     | 28  | VAL  |
| 4   | f     | 30  | HIS  |
| 4   | f     | 34  | ARG  |
| 5   | g     | 8   | ASP  |
| 5   | g     | 9   | ILE  |
| 5   | g     | 10  | SER  |
| 5   | g     | 11  | LYS  |
| 5   | g     | 20  | LEU  |
| 5   | g     | 21  | LEU  |
| 5   | g     | 25  | LEU  |
| 5   | g     | 26  | ILE  |
| 5   | g     | 40  | MET  |
| 5   | g     | 45  | ASN  |
| 8   | B     | 74  | GLN  |
| 8   | B     | 77  | THR  |
| 8   | B     | 78  | ILE  |
| 8   | B     | 89  | CYS  |
| 8   | B     | 90  | THR  |
| 8   | B     | 93  | CYS  |
| 8   | B     | 96  | LYS  |
| 8   | B     | 97  | VAL  |
| 8   | B     | 100 | ILE  |
| 8   | B     | 105 | VAL  |
| 8   | B     | 106 | GLU  |
| 8   | B     | 108 | VAL  |
| 8   | B     | 117 | ILE  |
| 8   | B     | 120 | THR  |
| 8   | B     | 121 | ARG  |
| 8   | B     | 126 | SER  |
| 8   | B     | 127 | LEU  |
| 8   | B     | 128 | CYS  |
| 8   | B     | 130 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | B     | 139 | VAL  |
| 8   | B     | 143 | GLU  |
| 8   | B     | 148 | ARG  |
| 8   | B     | 149 | THR  |
| 9   | D     | 20  | ARG  |
| 9   | D     | 28  | LEU  |
| 9   | D     | 30  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | ASN  |
| 1   | A     | 79  | GLN  |
| 1   | A     | 81  | GLN  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 241 | GLN  |
| 1   | A     | 255 | GLN  |
| 1   | A     | 261 | ASN  |
| 1   | A     | 296 | HIS  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 362 | HIS  |
| 1   | A     | 364 | GLN  |
| 1   | A     | 379 | GLN  |
| 1   | A     | 392 | GLN  |
| 1   | A     | 445 | GLN  |
| 1   | A     | 460 | ASN  |
| 1   | A     | 470 | ASN  |
| 1   | A     | 531 | GLN  |
| 1   | A     | 538 | GLN  |
| 1   | A     | 550 | ASN  |
| 1   | A     | 565 | GLN  |
| 1   | A     | 602 | GLN  |
| 1   | A     | 639 | ASN  |
| 1   | A     | 643 | GLN  |
| 1   | A     | 644 | HIS  |
| 1   | A     | 675 | HIS  |
| 1   | A     | 755 | HIS  |
| 1   | A     | 808 | GLN  |
| 1   | A     | 825 | GLN  |
| 1   | A     | 833 | ASN  |
| 2   | C     | 40  | GLN  |
| 2   | C     | 59  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 78  | ASN  |
| 2   | C     | 81  | GLN  |
| 2   | C     | 85  | GLN  |
| 2   | C     | 122 | GLN  |
| 2   | C     | 123 | ASN  |
| 2   | C     | 136 | ASN  |
| 2   | C     | 149 | GLN  |
| 2   | C     | 169 | ASN  |
| 2   | C     | 180 | GLN  |
| 2   | C     | 185 | GLN  |
| 2   | C     | 200 | GLN  |
| 2   | C     | 202 | ASN  |
| 3   | E     | 28  | ASN  |
| 5   | G     | 45  | ASN  |
| 1   | a     | 16  | GLN  |
| 1   | a     | 59  | ASN  |
| 1   | a     | 81  | GLN  |
| 1   | a     | 160 | GLN  |
| 1   | a     | 254 | ASN  |
| 1   | a     | 296 | HIS  |
| 1   | a     | 329 | HIS  |
| 1   | a     | 362 | HIS  |
| 1   | a     | 364 | GLN  |
| 1   | a     | 382 | HIS  |
| 1   | a     | 445 | GLN  |
| 1   | a     | 531 | GLN  |
| 1   | a     | 538 | GLN  |
| 1   | a     | 550 | ASN  |
| 1   | a     | 602 | GLN  |
| 1   | a     | 619 | HIS  |
| 1   | a     | 621 | ASN  |
| 1   | a     | 626 | ASN  |
| 1   | a     | 643 | GLN  |
| 1   | a     | 644 | HIS  |
| 1   | a     | 744 | ASN  |
| 1   | a     | 755 | HIS  |
| 1   | a     | 765 | ASN  |
| 1   | a     | 825 | GLN  |
| 1   | a     | 833 | ASN  |
| 1   | a     | 864 | ASN  |
| 7   | c     | 52  | GLN  |
| 7   | c     | 82  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | c     | 94  | GLN  |
| 7   | c     | 96  | ASN  |
| 7   | c     | 100 | ASN  |
| 7   | c     | 109 | GLN  |
| 7   | c     | 144 | GLN  |
| 7   | c     | 145 | GLN  |
| 4   | f     | 30  | HIS  |
| 5   | g     | 45  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 2 are monoatomic and 32 are unknown - leaving 47 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 12  | CLA  | a     | 913 | -    | 69,73,73     | 2.43 | 21 (30%)    | 82,113,113  | 3.95 | 37 (45%)    |
| 11  | BCL  | A     | 907 | -    | 64,69,74     | 3.20 | 30 (46%)    | 73,109,115  | 4.63 | 40 (54%)    |
| 11  | BCL  | A     | 903 | -    | 69,74,74     | 2.83 | 22 (31%)    | 79,115,115  | 3.75 | 35 (44%)    |
| 15  | 85I  | A     | 915 | -    | 43,44,44     | 2.32 | 11 (25%)    | 46,51,51    | 2.54 | 9 (19%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | BCL  | a     | 905 | -    | 69,74,74     | 2.72 | 21 (30%) | 79,115,115  | 3.68 | 36 (45%) |
| 11  | BCL  | a     | 911 | -    | 69,74,74     | 2.76 | 28 (40%) | 79,115,115  | 3.29 | 33 (41%) |
| 12  | CLA  | a     | 914 | -    | 50,54,73     | 2.88 | 22 (44%) | 59,90,113   | 3.73 | 32 (54%) |
| 17  | 85N  | g     | 101 | -    | 36,37,46     | 0.83 | 1 (2%)   | 39,45,55    | 0.55 | 0        |
| 20  | SF4  | a     | 917 | 1    | 0,12,12      | -    | -        | -           | -    | -        |
| 11  | BCL  | A     | 906 | 1    | 55,60,74     | 2.89 | 19 (34%) | 61,98,115   | 4.66 | 26 (42%) |
| 12  | CLA  | a     | 915 | -    | 55,59,73     | 2.80 | 21 (38%) | 64,96,113   | 3.55 | 38 (59%) |
| 18  | HEC  | c     | 202 | 7    | 46,50,50     | 3.44 | 21 (45%) | 58,82,82    | 2.91 | 26 (44%) |
| 11  | BCL  | A     | 904 | -    | 49,54,74     | 2.52 | 22 (44%) | 55,91,115   | 3.01 | 21 (38%) |
| 15  | 85I  | A     | 916 | -    | 43,44,44     | 2.07 | 3 (6%)   | 46,51,51    | 2.38 | 7 (15%)  |
| 20  | SF4  | B     | 201 | -    | 0,12,12      | -    | -        | -           | -    | -        |
| 19  | 84Q  | E     | 101 | -    | 42,43,43     | 2.12 | 11 (26%) | 47,50,50    | 1.93 | 8 (17%)  |
| 11  | BCL  | a     | 907 | -    | 69,74,74     | 2.54 | 27 (39%) | 79,115,115  | 3.76 | 30 (37%) |
| 17  | 85N  | a     | 902 | -    | 45,46,46     | 0.61 | 0        | 49,55,55    | 0.40 | 0        |
| 15  | 85I  | a     | 918 | -    | 43,44,44     | 1.05 | 2 (4%)   | 46,51,51    | 1.72 | 4 (8%)   |
| 12  | CLA  | A     | 910 | -    | 69,73,73     | 2.11 | 22 (31%) | 82,113,113  | 3.10 | 36 (43%) |
| 12  | CLA  | A     | 911 | -    | 69,73,73     | 2.56 | 23 (33%) | 82,113,113  | 3.28 | 33 (40%) |
| 15  | 85I  | A     | 917 | -    | 43,44,44     | 1.57 | 2 (4%)   | 46,51,51    | 2.51 | 3 (6%)   |
| 10  | 2GO  | a     | 903 | 1    | 73,74,74     | 3.17 | 22 (30%) | 91,115,115  | 2.91 | 32 (35%) |
| 10  | 2GO  | A     | 901 | 1    | 73,74,74     | 3.36 | 25 (34%) | 91,115,115  | 3.32 | 31 (34%) |
| 11  | BCL  | a     | 904 | -    | 69,74,74     | 2.61 | 21 (30%) | 79,115,115  | 3.33 | 27 (34%) |
| 13  | LYC  | A     | 913 | -    | 39,39,39     | 1.64 | 9 (23%)  | 46,46,46    | 2.71 | 19 (41%) |
| 11  | BCL  | a     | 906 | -    | 49,54,74     | 2.77 | 21 (42%) | 55,91,115   | 3.23 | 27 (49%) |
| 19  | 84Q  | a     | 921 | -    | 42,43,43     | 1.35 | 2 (4%)   | 47,50,50    | 1.05 | 2 (4%)   |
| 11  | BCL  | A     | 902 | -    | 69,74,74     | 2.74 | 24 (34%) | 79,115,115  | 3.26 | 34 (43%) |
| 11  | BCL  | A     | 909 | -    | 69,74,74     | 3.16 | 29 (42%) | 79,115,115  | 4.29 | 36 (45%) |
| 15  | 85I  | a     | 919 | -    | 43,44,44     | 1.39 | 2 (4%)   | 46,51,51    | 1.72 | 3 (6%)   |
| 11  | BCL  | a     | 908 | 1    | 69,74,74     | 2.83 | 26 (37%) | 79,115,115  | 4.35 | 38 (48%) |
| 11  | BCL  | A     | 908 | -    | 69,74,74     | 2.47 | 30 (43%) | 79,115,115  | 2.74 | 32 (40%) |
| 17  | 85N  | G     | 101 | -    | 36,37,46     | 0.76 | 0        | 39,45,55    | 0.78 | 2 (5%)   |
| 11  | BCL  | A     | 905 | -    | 69,74,74     | 2.64 | 22 (31%) | 79,115,115  | 3.79 | 36 (45%) |
| 12  | CLA  | A     | 912 | -    | 50,54,73     | 2.62 | 16 (32%) | 59,90,113   | 4.01 | 31 (52%) |
| 12  | CLA  | A     | 931 | -    | 69,73,73     | 2.88 | 26 (37%) | 82,113,113  | 4.32 | 43 (52%) |
| 15  | 85I  | a     | 920 | -    | 43,44,44     | 2.21 | 2 (4%)   | 46,51,51    | 2.09 | 3 (6%)   |
| 12  | CLA  | a     | 901 | 21   | 69,73,73     | 2.60 | 23 (33%) | 82,113,113  | 3.55 | 35 (42%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | HEC  | C     | 301 | 2    | 46,50,50     | 3.58 | 29 (63%) | 58,82,82    | 3.13 | 30 (51%) |
| 12  | CLA  | a     | 912 | 21   | 69,73,73     | 2.76 | 20 (28%) | 82,113,113  | 3.41 | 41 (50%) |
| 11  | BCL  | a     | 910 | -    | 69,74,74     | 3.12 | 22 (31%) | 79,115,115  | 4.02 | 36 (45%) |
| 12  | CLA  | A     | 933 | -    | 55,59,73     | 2.58 | 21 (38%) | 64,96,113   | 4.07 | 33 (51%) |
| 17  | 85N  | A     | 932 | -    | 45,46,46     | 1.07 | 1 (2%)   | 49,55,55    | 1.73 | 4 (8%)   |
| 20  | SF4  | B     | 202 | 8    | 0,12,12      | -    | -        | -           | -    | -        |
| 11  | BCL  | a     | 909 | -    | 69,74,74     | 2.49 | 25 (36%) | 79,115,115  | 3.79 | 32 (40%) |
| 13  | LYC  | c     | 201 | -    | 39,39,39     | 1.51 | 9 (23%)  | 46,46,46    | 5.59 | 27 (58%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 12  | CLA  | a     | 913 | -    | -         | 10/39/115/115 | -       |
| 11  | BCL  | A     | 907 | -    | -         | 15/35/131/137 | -       |
| 11  | BCL  | A     | 903 | -    | -         | 20/41/137/137 | -       |
| 15  | 85I  | A     | 915 | -    | -         | 18/47/48/48   | -       |
| 11  | BCL  | a     | 905 | -    | -         | 16/41/137/137 | -       |
| 11  | BCL  | a     | 911 | -    | -         | 5/41/137/137  | -       |
| 12  | CLA  | a     | 914 | -    | -         | 4/17/93/115   | -       |
| 17  | 85N  | g     | 101 | -    | -         | 18/42/42/51   | -       |
| 20  | SF4  | a     | 917 | 1    | -         | -             | 0/6/5/5 |
| 11  | BCL  | A     | 906 | 1    | -         | 4/25/121/137  | -       |
| 12  | CLA  | a     | 915 | -    | -         | 8/23/99/115   | -       |
| 18  | HEC  | c     | 202 | 7    | -         | 7/14/54/54    | -       |
| 11  | BCL  | A     | 904 | -    | -         | 4/17/113/137  | -       |
| 15  | 85I  | A     | 916 | -    | 1/1/6/7   | 27/47/48/48   | -       |
| 20  | SF4  | B     | 201 | -    | -         | -             | 0/6/5/5 |
| 19  | 84Q  | E     | 101 | -    | -         | 26/46/47/47   | -       |
| 11  | BCL  | a     | 907 | -    | -         | 10/41/137/137 | -       |
| 17  | 85N  | a     | 902 | -    | -         | 24/51/51/51   | -       |
| 15  | 85I  | a     | 918 | -    | -         | 21/47/48/48   | -       |
| 12  | CLA  | A     | 910 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 12  | CLA  | A     | 911 | -    | 1/1/15/20 | 11/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 15  | 85I  | A     | 917 | -    | -       | 29/47/48/48   | -       |
| 10  | 2GO  | a     | 903 | 1    | -       | 11/41/97/97   | -       |
| 10  | 2GO  | A     | 901 | 1    | -       | 4/41/97/97    | -       |
| 11  | BCL  | a     | 904 | -    | -       | 12/41/137/137 | -       |
| 13  | LYC  | A     | 913 | -    | -       | 1/43/43/43    | -       |
| 11  | BCL  | a     | 906 | -    | -       | 4/17/113/137  | -       |
| 19  | 84Q  | a     | 921 | -    | -       | 31/46/47/47   | -       |
| 11  | BCL  | A     | 902 | -    | -       | 18/41/137/137 | -       |
| 11  | BCL  | A     | 909 | -    | -       | 12/41/137/137 | -       |
| 15  | 85I  | a     | 919 | -    | -       | 37/47/48/48   | -       |
| 11  | BCL  | a     | 908 | 1    | -       | 20/41/137/137 | -       |
| 11  | BCL  | A     | 908 | -    | -       | 13/41/137/137 | -       |
| 17  | 85N  | G     | 101 | -    | -       | 18/42/42/51   | -       |
| 11  | BCL  | A     | 905 | -    | -       | 15/41/137/137 | -       |
| 12  | CLA  | A     | 912 | -    | -       | 2/17/93/115   | -       |
| 12  | CLA  | A     | 931 | -    | -       | 17/39/115/115 | -       |
| 15  | 85I  | a     | 920 | -    | -       | 29/47/48/48   | -       |
| 12  | CLA  | a     | 901 | 21   | -       | 24/39/115/115 | -       |
| 18  | HEC  | C     | 301 | 2    | -       | 7/14/54/54    | -       |
| 12  | CLA  | a     | 912 | 21   | -       | 12/39/115/115 | -       |
| 11  | BCL  | a     | 910 | -    | -       | 11/41/137/137 | -       |
| 12  | CLA  | A     | 933 | -    | -       | 5/23/99/115   | -       |
| 17  | 85N  | A     | 932 | -    | -       | 20/51/51/51   | -       |
| 20  | SF4  | B     | 202 | 8    | -       | -             | 0/6/5/5 |
| 11  | BCL  | a     | 909 | -    | -       | 12/41/137/137 | -       |
| 13  | LYC  | c     | 201 | -    | -       | 15/43/43/43   | -       |

All (756) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 10  | A     | 901 | 2GO  | C2A-C3A | 14.40  | 1.67        | 1.36     |
| 15  | a     | 920 | 85I  | O6-C3   | -13.94 | 1.20        | 1.44     |
| 11  | a     | 910 | BCL  | C4B-NB  | -12.65 | 1.21        | 1.37     |
| 10  | a     | 903 | 2GO  | C3C-C2C | 11.75  | 1.62        | 1.36     |
| 12  | a     | 912 | CLA  | C3D-C4D | -10.31 | 1.21        | 1.44     |
| 12  | A     | 931 | CLA  | C4B-NB  | -9.98  | 1.24        | 1.37     |
| 15  | A     | 915 | 85I  | C4-C3   | -9.77  | 1.29        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | a     | 904 | BCL  | C3D-C4D | -9.74 | 1.22        | 1.44     |
| 11  | a     | 910 | BCL  | C3D-C4D | -9.70 | 1.22        | 1.44     |
| 11  | A     | 909 | BCL  | C4B-NB  | -9.37 | 1.25        | 1.37     |
| 12  | a     | 914 | CLA  | C3D-C4D | -9.02 | 1.23        | 1.44     |
| 11  | A     | 903 | BCL  | C4B-NB  | -9.01 | 1.26        | 1.37     |
| 12  | A     | 931 | CLA  | C3D-C4D | -8.91 | 1.24        | 1.44     |
| 11  | a     | 905 | BCL  | C3D-C4D | -8.84 | 1.24        | 1.44     |
| 11  | A     | 907 | BCL  | O2A-CGA | 8.64  | 1.58        | 1.33     |
| 11  | A     | 909 | BCL  | OBB-CAB | -8.55 | 1.03        | 1.23     |
| 11  | a     | 907 | BCL  | C1D-ND  | -8.53 | 1.26        | 1.37     |
| 10  | A     | 901 | 2GO  | C4D-ND  | -8.53 | 1.18        | 1.38     |
| 11  | A     | 903 | BCL  | OBB-CAB | -8.50 | 1.03        | 1.23     |
| 11  | a     | 908 | BCL  | C3D-C4D | -8.49 | 1.25        | 1.44     |
| 15  | A     | 916 | 85I  | P-O3    | 8.49  | 1.85        | 1.59     |
| 10  | a     | 903 | 2GO  | OBB-CAB | -8.47 | 1.04        | 1.23     |
| 11  | A     | 903 | BCL  | C3D-C4D | -8.47 | 1.25        | 1.44     |
| 12  | A     | 912 | CLA  | C3D-C4D | -8.47 | 1.25        | 1.44     |
| 11  | A     | 907 | BCL  | C1B-NB  | -8.43 | 1.26        | 1.37     |
| 11  | a     | 910 | BCL  | C1B-NB  | -8.41 | 1.26        | 1.37     |
| 12  | A     | 933 | CLA  | C3D-C4D | -8.38 | 1.25        | 1.44     |
| 12  | A     | 933 | CLA  | C4B-NB  | -8.37 | 1.26        | 1.37     |
| 12  | A     | 912 | CLA  | C4B-NB  | -8.35 | 1.26        | 1.37     |
| 11  | a     | 907 | BCL  | C3D-C4D | -8.34 | 1.25        | 1.44     |
| 11  | A     | 902 | BCL  | C3D-C4D | -8.30 | 1.25        | 1.44     |
| 12  | a     | 913 | CLA  | C4B-NB  | -8.30 | 1.27        | 1.37     |
| 10  | A     | 901 | 2GO  | C3C-C2C | 8.28  | 1.54        | 1.36     |
| 11  | A     | 909 | BCL  | C3D-C4D | -8.27 | 1.25        | 1.44     |
| 11  | a     | 910 | BCL  | OBB-CAB | -8.27 | 1.04        | 1.23     |
| 12  | A     | 911 | CLA  | C1D-ND  | 8.17  | 1.48        | 1.37     |
| 12  | A     | 931 | CLA  | O1D-CGD | -8.15 | 1.00        | 1.21     |
| 11  | A     | 905 | BCL  | CAA-C2A | -8.15 | 1.39        | 1.54     |
| 12  | a     | 915 | CLA  | C1B-NB  | -8.04 | 1.27        | 1.37     |
| 11  | A     | 906 | BCL  | C3D-C4D | -7.91 | 1.26        | 1.44     |
| 10  | a     | 903 | 2GO  | C2A-C3A | 7.89  | 1.53        | 1.36     |
| 19  | a     | 921 | 84Q  | O2-C16  | -7.87 | 1.31        | 1.44     |
| 12  | a     | 915 | CLA  | C3D-C4D | -7.86 | 1.26        | 1.44     |
| 19  | E     | 101 | 84Q  | P-O4    | 7.85  | 1.83        | 1.59     |
| 18  | C     | 301 | HEC  | C4C-NC  | -7.82 | 1.24        | 1.39     |
| 11  | a     | 905 | BCL  | C4B-NB  | -7.80 | 1.27        | 1.37     |
| 12  | a     | 901 | CLA  | C1C-NC  | -7.78 | 1.25        | 1.37     |
| 12  | a     | 901 | CLA  | C3D-C4D | -7.72 | 1.26        | 1.44     |
| 11  | a     | 909 | BCL  | C3D-C4D | -7.72 | 1.26        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | a     | 906 | BCL  | C3D-C4D | -7.70 | 1.26        | 1.44     |
| 15  | a     | 919 | 85I  | O6-C3   | 7.67  | 1.57        | 1.44     |
| 11  | a     | 911 | BCL  | C4B-NB  | -7.60 | 1.27        | 1.37     |
| 11  | A     | 905 | BCL  | C3D-C4D | -7.50 | 1.27        | 1.44     |
| 11  | a     | 911 | BCL  | C1B-NB  | -7.48 | 1.28        | 1.37     |
| 18  | c     | 202 | HEC  | C4A-NA  | -7.48 | 1.25        | 1.39     |
| 12  | a     | 913 | CLA  | C1B-NB  | -7.42 | 1.28        | 1.37     |
| 11  | A     | 904 | BCL  | C3D-C4D | -7.42 | 1.27        | 1.44     |
| 11  | A     | 909 | BCL  | C1B-NB  | -7.41 | 1.28        | 1.37     |
| 11  | A     | 907 | BCL  | C4B-NB  | -7.38 | 1.28        | 1.37     |
| 11  | a     | 908 | BCL  | CAA-C2A | -7.37 | 1.40        | 1.54     |
| 11  | a     | 904 | BCL  | C3C-C4C | -7.32 | 1.42        | 1.51     |
| 12  | a     | 915 | CLA  | CHC-C1C | 7.31  | 1.53        | 1.38     |
| 11  | A     | 908 | BCL  | C4B-NB  | -7.31 | 1.28        | 1.37     |
| 11  | a     | 911 | BCL  | C3D-C4D | -7.29 | 1.27        | 1.44     |
| 10  | A     | 901 | 2GO  | C1A-NA  | -7.28 | 1.22        | 1.38     |
| 12  | a     | 901 | CLA  | C1B-NB  | -7.24 | 1.28        | 1.37     |
| 15  | A     | 916 | 85I  | C4-C3   | 7.23  | 1.68        | 1.51     |
| 11  | A     | 906 | BCL  | CBB-CAB | -7.22 | 1.36        | 1.50     |
| 18  | c     | 202 | HEC  | C4B-NB  | -7.19 | 1.26        | 1.39     |
| 11  | A     | 902 | BCL  | C1D-ND  | -7.19 | 1.28        | 1.37     |
| 11  | A     | 906 | BCL  | C1D-ND  | -7.19 | 1.28        | 1.37     |
| 11  | a     | 908 | BCL  | CBB-CAB | -7.18 | 1.36        | 1.50     |
| 12  | a     | 914 | CLA  | C1B-NB  | -7.14 | 1.28        | 1.37     |
| 12  | A     | 911 | CLA  | C1C-NC  | -7.13 | 1.26        | 1.37     |
| 15  | A     | 917 | 85I  | C4-C3   | 7.11  | 1.68        | 1.51     |
| 10  | A     | 901 | 2GO  | C1D-C2D | -7.10 | 1.31        | 1.45     |
| 12  | a     | 914 | CLA  | C4B-NB  | -7.10 | 1.28        | 1.37     |
| 12  | a     | 912 | CLA  | C9-C8   | -7.07 | 1.30        | 1.52     |
| 10  | a     | 903 | 2GO  | OBD-CAD | -7.06 | 1.09        | 1.33     |
| 18  | C     | 301 | HEC  | C1B-NB  | -7.01 | 1.26        | 1.39     |
| 11  | a     | 911 | BCL  | OBB-CAB | -6.98 | 1.07        | 1.23     |
| 12  | a     | 901 | CLA  | C4B-NB  | -6.95 | 1.28        | 1.37     |
| 10  | a     | 903 | 2GO  | C1A-NA  | -6.94 | 1.23        | 1.38     |
| 18  | c     | 202 | HEC  | O2A-CGA | -6.93 | 1.07        | 1.30     |
| 11  | A     | 907 | BCL  | C3D-C4D | -6.91 | 1.28        | 1.44     |
| 11  | A     | 902 | BCL  | C1B-NB  | -6.86 | 1.28        | 1.37     |
| 11  | A     | 908 | BCL  | C3D-C4D | -6.85 | 1.28        | 1.44     |
| 18  | c     | 202 | HEC  | C3B-C4B | -6.85 | 1.34        | 1.46     |
| 12  | A     | 911 | CLA  | C3D-C4D | -6.83 | 1.28        | 1.44     |
| 15  | A     | 917 | 85I  | O6-C3   | -6.82 | 1.33        | 1.44     |
| 11  | a     | 910 | BCL  | C3C-C4C | -6.78 | 1.43        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | A     | 902 | BCL  | C4B-NB  | -6.78 | 1.29        | 1.37     |
| 11  | a     | 908 | BCL  | C1D-ND  | -6.75 | 1.29        | 1.37     |
| 12  | a     | 913 | CLA  | C3D-C4D | -6.71 | 1.29        | 1.44     |
| 12  | a     | 912 | CLA  | C1C-NC  | -6.71 | 1.27        | 1.37     |
| 10  | A     | 901 | 2GO  | ZN-NC   | 6.62  | 2.25        | 2.03     |
| 12  | A     | 910 | CLA  | C3D-C4D | -6.62 | 1.29        | 1.44     |
| 11  | A     | 909 | BCL  | O1A-CGA | -6.54 | 1.03        | 1.22     |
| 10  | A     | 901 | 2GO  | ZN-NA   | 6.53  | 2.24        | 2.03     |
| 10  | A     | 901 | 2GO  | OBD-CAD | -6.50 | 1.11        | 1.33     |
| 10  | A     | 901 | 2GO  | C3D-C4D | -6.50 | 1.29        | 1.44     |
| 11  | A     | 907 | BCL  | O1D-CGD | -6.48 | 1.04        | 1.21     |
| 11  | a     | 905 | BCL  | C1D-ND  | -6.43 | 1.29        | 1.37     |
| 18  | c     | 202 | HEC  | C4D-ND  | -6.41 | 1.27        | 1.39     |
| 11  | a     | 911 | BCL  | C1D-ND  | -6.34 | 1.29        | 1.37     |
| 11  | a     | 906 | BCL  | C4B-NB  | -6.34 | 1.29        | 1.37     |
| 12  | a     | 915 | CLA  | C4B-NB  | -6.31 | 1.29        | 1.37     |
| 12  | a     | 912 | CLA  | C4B-NB  | -6.30 | 1.29        | 1.37     |
| 11  | a     | 908 | BCL  | C2A-C1A | -6.29 | 1.38        | 1.52     |
| 18  | C     | 301 | HEC  | C3B-C4B | -6.28 | 1.35        | 1.46     |
| 11  | a     | 905 | BCL  | OBB-CAB | -6.24 | 1.09        | 1.23     |
| 10  | a     | 903 | 2GO  | C3D-C4D | -6.19 | 1.30        | 1.44     |
| 11  | a     | 904 | BCL  | C1B-NB  | -6.14 | 1.29        | 1.37     |
| 11  | A     | 909 | BCL  | C3C-C4C | -6.12 | 1.43        | 1.51     |
| 18  | c     | 202 | HEC  | C1B-NB  | -6.12 | 1.28        | 1.39     |
| 11  | A     | 907 | BCL  | C1D-ND  | -6.12 | 1.29        | 1.37     |
| 11  | A     | 906 | BCL  | C4B-NB  | -6.12 | 1.29        | 1.37     |
| 12  | A     | 933 | CLA  | O1D-CGD | -6.11 | 1.05        | 1.21     |
| 12  | A     | 931 | CLA  | C1D-ND  | 6.08  | 1.45        | 1.37     |
| 11  | a     | 908 | BCL  | C4B-NB  | -6.06 | 1.29        | 1.37     |
| 11  | a     | 904 | BCL  | C1D-ND  | -6.05 | 1.29        | 1.37     |
| 12  | a     | 914 | CLA  | MG-NB   | 6.05  | 2.17        | 2.05     |
| 11  | A     | 906 | BCL  | O2D-CED | -6.05 | 1.31        | 1.45     |
| 12  | a     | 912 | CLA  | OBD-CAD | -6.02 | 1.12        | 1.22     |
| 11  | A     | 905 | BCL  | C2A-C1A | -6.01 | 1.38        | 1.52     |
| 18  | c     | 202 | HEC  | CHA-C1A | 6.00  | 1.50        | 1.38     |
| 11  | A     | 905 | BCL  | C4B-NB  | -6.00 | 1.30        | 1.37     |
| 18  | C     | 301 | HEC  | CHD-C4C | 5.98  | 1.50        | 1.38     |
| 11  | A     | 904 | BCL  | C4B-NB  | -5.98 | 1.30        | 1.37     |
| 10  | a     | 903 | 2GO  | C1D-C2D | -5.96 | 1.33        | 1.45     |
| 12  | A     | 931 | CLA  | O2D-CED | -5.95 | 1.32        | 1.45     |
| 12  | a     | 912 | CLA  | C1B-NB  | -5.94 | 1.30        | 1.37     |
| 18  | c     | 202 | HEC  | C1A-NA  | -5.92 | 1.28        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 17  | A     | 932 | 85N  | O3-C17  | -5.91 | 1.21        | 1.40     |
| 18  | C     | 301 | HEC  | C3C-C4C | -5.89 | 1.35        | 1.46     |
| 10  | a     | 903 | 2GO  | ZN-NC   | 5.87  | 2.22        | 2.03     |
| 10  | A     | 901 | 2GO  | OBB-CAB | -5.87 | 1.09        | 1.23     |
| 18  | C     | 301 | HEC  | C1D-ND  | -5.86 | 1.28        | 1.39     |
| 11  | A     | 905 | BCL  | OBB-CAB | -5.86 | 1.09        | 1.23     |
| 10  | a     | 903 | 2GO  | C1D-ND  | -5.83 | 1.25        | 1.38     |
| 12  | a     | 913 | CLA  | C1D-ND  | 5.80  | 1.45        | 1.37     |
| 12  | a     | 913 | CLA  | C1C-NC  | -5.80 | 1.28        | 1.37     |
| 11  | a     | 909 | BCL  | O1D-CGD | -5.78 | 1.06        | 1.21     |
| 15  | a     | 918 | 85I  | O6-C3   | -5.77 | 1.34        | 1.44     |
| 11  | a     | 909 | BCL  | C4B-NB  | -5.76 | 1.30        | 1.37     |
| 11  | a     | 905 | BCL  | C3C-C4C | -5.69 | 1.44        | 1.51     |
| 18  | C     | 301 | HEC  | O2A-CGA | -5.69 | 1.12        | 1.30     |
| 11  | A     | 903 | BCL  | C1B-NB  | -5.68 | 1.30        | 1.37     |
| 12  | A     | 911 | CLA  | C4B-NB  | -5.67 | 1.30        | 1.37     |
| 11  | a     | 909 | BCL  | C1B-NB  | -5.66 | 1.30        | 1.37     |
| 11  | A     | 906 | BCL  | C1B-NB  | -5.64 | 1.30        | 1.37     |
| 11  | a     | 911 | BCL  | C3C-C4C | -5.61 | 1.44        | 1.51     |
| 11  | A     | 905 | BCL  | C1D-ND  | -5.58 | 1.30        | 1.37     |
| 11  | a     | 907 | BCL  | OBB-CAB | -5.54 | 1.10        | 1.23     |
| 11  | a     | 905 | BCL  | CBB-CAB | -5.49 | 1.39        | 1.50     |
| 11  | a     | 908 | BCL  | C1B-NB  | -5.48 | 1.30        | 1.37     |
| 10  | a     | 903 | 2GO  | C4D-ND  | -5.45 | 1.25        | 1.38     |
| 11  | A     | 909 | BCL  | CHC-C4B | 5.42  | 1.51        | 1.39     |
| 11  | A     | 903 | BCL  | CBB-CAB | -5.41 | 1.39        | 1.50     |
| 11  | A     | 908 | BCL  | C3C-C4C | -5.39 | 1.44        | 1.51     |
| 19  | E     | 101 | 84Q  | C15-C16 | 5.39  | 1.64        | 1.51     |
| 11  | a     | 909 | BCL  | O2D-CED | -5.37 | 1.33        | 1.45     |
| 12  | A     | 912 | CLA  | C1B-NB  | -5.37 | 1.30        | 1.37     |
| 15  | A     | 916 | 85I  | O6-C3   | 5.35  | 1.53        | 1.44     |
| 11  | a     | 904 | BCL  | C4B-NB  | -5.31 | 1.30        | 1.37     |
| 11  | a     | 906 | BCL  | C1B-NB  | -5.30 | 1.30        | 1.37     |
| 11  | A     | 903 | BCL  | C3C-C4C | -5.29 | 1.44        | 1.51     |
| 12  | A     | 911 | CLA  | C1B-NB  | -5.27 | 1.30        | 1.37     |
| 12  | a     | 912 | CLA  | CHC-C1C | 5.23  | 1.49        | 1.38     |
| 11  | a     | 909 | BCL  | C1D-ND  | -5.22 | 1.31        | 1.37     |
| 12  | A     | 910 | CLA  | C4B-NB  | -5.22 | 1.31        | 1.37     |
| 11  | A     | 909 | BCL  | C1D-ND  | -5.21 | 1.31        | 1.37     |
| 11  | A     | 907 | BCL  | C2-C3   | 5.20  | 1.45        | 1.33     |
| 11  | a     | 910 | BCL  | C1D-ND  | -5.20 | 1.31        | 1.37     |
| 11  | A     | 907 | BCL  | OBB-CAB | -5.18 | 1.11        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | A     | 907 | BCL  | C5-C3   | 5.16  | 1.61        | 1.51     |
| 18  | C     | 301 | HEC  | C4B-NB  | -5.15 | 1.29        | 1.39     |
| 18  | C     | 301 | HEC  | C1C-NC  | -5.13 | 1.29        | 1.39     |
| 12  | A     | 911 | CLA  | C9-C8   | 5.11  | 1.68        | 1.52     |
| 11  | A     | 903 | BCL  | O1A-CGA | -5.07 | 1.07        | 1.22     |
| 11  | A     | 908 | BCL  | C1B-NB  | -5.06 | 1.31        | 1.37     |
| 11  | A     | 902 | BCL  | C2A-C1A | -5.06 | 1.40        | 1.52     |
| 11  | a     | 905 | BCL  | O1D-CGD | -5.05 | 1.08        | 1.21     |
| 11  | a     | 907 | BCL  | C4B-NB  | -5.05 | 1.31        | 1.37     |
| 11  | A     | 907 | BCL  | CBB-CAB | -5.04 | 1.40        | 1.50     |
| 12  | a     | 914 | CLA  | C1C-NC  | -5.04 | 1.29        | 1.37     |
| 11  | A     | 909 | BCL  | OBD-CAD | -5.04 | 1.13        | 1.22     |
| 11  | A     | 905 | BCL  | C1B-NB  | -5.02 | 1.31        | 1.37     |
| 11  | A     | 904 | BCL  | CHC-C4B | 5.02  | 1.50        | 1.39     |
| 10  | a     | 903 | 2GO  | C4B-NB  | 5.00  | 1.48        | 1.38     |
| 12  | A     | 911 | CLA  | MG-NC   | 4.98  | 2.18        | 2.06     |
| 11  | a     | 906 | BCL  | CAA-C2A | -4.98 | 1.45        | 1.54     |
| 18  | C     | 301 | HEC  | CBB-CAB | -4.96 | 1.31        | 1.49     |
| 12  | A     | 931 | CLA  | O2D-CGD | 4.93  | 1.45        | 1.33     |
| 11  | A     | 903 | BCL  | C1D-ND  | -4.92 | 1.31        | 1.37     |
| 18  | C     | 301 | HEC  | O2D-CGD | -4.91 | 1.14        | 1.30     |
| 11  | A     | 908 | BCL  | C1D-ND  | -4.89 | 1.31        | 1.37     |
| 12  | A     | 910 | CLA  | C1D-ND  | 4.89  | 1.44        | 1.37     |
| 12  | a     | 912 | CLA  | C1D-ND  | 4.88  | 1.44        | 1.37     |
| 11  | a     | 906 | BCL  | C1D-ND  | -4.87 | 1.31        | 1.37     |
| 10  | a     | 903 | 2GO  | C4C-C3C | 4.85  | 1.53        | 1.45     |
| 12  | A     | 910 | CLA  | C1B-NB  | -4.84 | 1.31        | 1.37     |
| 11  | A     | 909 | BCL  | CHB-C4A | -4.83 | 1.25        | 1.37     |
| 12  | a     | 912 | CLA  | O2D-CED | -4.79 | 1.34        | 1.45     |
| 18  | C     | 301 | HEC  | CBC-CAC | -4.77 | 1.31        | 1.49     |
| 11  | a     | 906 | BCL  | OBBCAB  | -4.77 | 1.12        | 1.23     |
| 11  | A     | 909 | BCL  | CBB-CAB | -4.77 | 1.40        | 1.50     |
| 11  | A     | 906 | BCL  | O1D-CGD | -4.75 | 1.09        | 1.21     |
| 11  | A     | 905 | BCL  | C3C-C4C | -4.71 | 1.45        | 1.51     |
| 12  | A     | 911 | CLA  | C7-C8   | -4.71 | 1.29        | 1.52     |
| 11  | a     | 909 | BCL  | C3C-C4C | -4.70 | 1.45        | 1.51     |
| 11  | a     | 906 | BCL  | C3C-C4C | -4.68 | 1.45        | 1.51     |
| 11  | A     | 902 | BCL  | O2D-CED | -4.67 | 1.34        | 1.45     |
| 11  | A     | 902 | BCL  | C3C-C4C | -4.67 | 1.45        | 1.51     |
| 10  | A     | 901 | 2GO  | CHA-C1A | 4.66  | 1.51        | 1.41     |
| 11  | a     | 907 | BCL  | C2A-C1A | -4.64 | 1.41        | 1.52     |
| 11  | A     | 907 | BCL  | CHC-C1C | -4.64 | 1.26        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | a     | 904 | BCL  | O1A-CGA | -4.63 | 1.08        | 1.22     |
| 11  | A     | 904 | BCL  | O2A-CGA | 4.62  | 1.46        | 1.30     |
| 11  | a     | 905 | BCL  | O2A-CGA | 4.58  | 1.46        | 1.33     |
| 11  | A     | 903 | BCL  | O1D-CGD | -4.56 | 1.09        | 1.21     |
| 11  | a     | 911 | BCL  | O2D-CED | -4.55 | 1.35        | 1.45     |
| 11  | a     | 910 | BCL  | O1D-CGD | -4.55 | 1.09        | 1.21     |
| 12  | A     | 931 | CLA  | O2A-CGA | 4.54  | 1.46        | 1.33     |
| 11  | A     | 902 | BCL  | CHB-C1B | 4.54  | 1.49        | 1.39     |
| 12  | a     | 915 | CLA  | C1C-NC  | -4.54 | 1.30        | 1.37     |
| 18  | C     | 301 | HEC  | CAB-C3B | 4.54  | 1.49        | 1.35     |
| 11  | A     | 906 | BCL  | O1A-CGA | -4.49 | 1.09        | 1.22     |
| 18  | c     | 202 | HEC  | O2D-CGD | -4.48 | 1.16        | 1.30     |
| 11  | A     | 907 | BCL  | O2D-CED | -4.46 | 1.35        | 1.45     |
| 12  | A     | 931 | CLA  | O1A-CGA | -4.46 | 1.09        | 1.22     |
| 11  | a     | 911 | BCL  | OBD-CAD | -4.42 | 1.14        | 1.22     |
| 11  | A     | 909 | BCL  | MG-NA   | 4.40  | 2.16        | 2.06     |
| 18  | C     | 301 | HEC  | C4D-ND  | -4.38 | 1.31        | 1.39     |
| 12  | a     | 914 | CLA  | O1D-CGD | -4.38 | 1.10        | 1.21     |
| 12  | A     | 912 | CLA  | MG-NC   | 4.35  | 2.16        | 2.06     |
| 11  | A     | 907 | BCL  | OBD-CAD | -4.33 | 1.15        | 1.22     |
| 12  | A     | 912 | CLA  | O1D-CGD | -4.32 | 1.10        | 1.21     |
| 12  | A     | 912 | CLA  | C1C-NC  | -4.32 | 1.31        | 1.37     |
| 18  | c     | 202 | HEC  | O1A-CGA | -4.30 | 1.08        | 1.22     |
| 11  | a     | 904 | BCL  | OBB-CAB | -4.30 | 1.13        | 1.23     |
| 12  | a     | 901 | CLA  | O2A-CGA | 4.30  | 1.45        | 1.33     |
| 11  | A     | 905 | BCL  | O2D-CED | -4.29 | 1.35        | 1.45     |
| 11  | a     | 904 | BCL  | O2D-CED | -4.29 | 1.35        | 1.45     |
| 15  | A     | 915 | 85I  | P-O3    | 4.29  | 1.72        | 1.59     |
| 11  | a     | 908 | BCL  | OBB-CAB | -4.29 | 1.13        | 1.23     |
| 11  | A     | 903 | BCL  | C2A-C1A | -4.27 | 1.42        | 1.52     |
| 11  | a     | 904 | BCL  | O2A-CGA | 4.26  | 1.45        | 1.33     |
| 11  | a     | 910 | BCL  | CHC-C4B | 4.20  | 1.48        | 1.39     |
| 12  | a     | 912 | CLA  | O1D-CGD | -4.20 | 1.10        | 1.21     |
| 11  | a     | 909 | BCL  | CBB-CAB | -4.19 | 1.42        | 1.50     |
| 11  | a     | 908 | BCL  | O2D-CED | -4.18 | 1.36        | 1.45     |
| 11  | a     | 911 | BCL  | O2A-C1  | -4.17 | 1.34        | 1.46     |
| 11  | A     | 902 | BCL  | CBB-CAB | -4.17 | 1.42        | 1.50     |
| 10  | a     | 903 | 2GO  | CHA-C1A | 4.15  | 1.50        | 1.41     |
| 12  | a     | 915 | CLA  | C1D-ND  | 4.12  | 1.43        | 1.37     |
| 11  | A     | 905 | BCL  | C3A-C2A | -4.11 | 1.43        | 1.54     |
| 11  | A     | 902 | BCL  | MG-NB   | 4.10  | 2.13        | 2.05     |
| 11  | a     | 910 | BCL  | O1A-CGA | -4.08 | 1.10        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | A     | 902 | BCL  | OBB-CAB | -4.07 | 1.14        | 1.23     |
| 12  | A     | 933 | CLA  | O2A-C1  | -4.07 | 1.35        | 1.46     |
| 11  | A     | 907 | BCL  | CHB-C1B | 4.07  | 1.48        | 1.39     |
| 12  | a     | 901 | CLA  | O2D-CED | -4.06 | 1.36        | 1.45     |
| 11  | a     | 904 | BCL  | O1D-CGD | -4.04 | 1.11        | 1.21     |
| 11  | a     | 910 | BCL  | CBB-CAB | -4.03 | 1.42        | 1.50     |
| 12  | A     | 933 | CLA  | C1C-NC  | -4.03 | 1.31        | 1.37     |
| 15  | a     | 919 | 85I  | C4-C3   | -4.00 | 1.42        | 1.51     |
| 11  | A     | 904 | BCL  | OBB-CAB | -3.99 | 1.14        | 1.23     |
| 11  | A     | 904 | BCL  | CAA-C2A | -3.99 | 1.46        | 1.54     |
| 15  | A     | 915 | 85I  | O4-C5   | -3.98 | 1.21        | 1.33     |
| 11  | a     | 908 | BCL  | O1D-CGD | -3.97 | 1.11        | 1.21     |
| 11  | a     | 905 | BCL  | O2D-CED | -3.97 | 1.36        | 1.45     |
| 11  | a     | 910 | BCL  | O2D-CED | -3.94 | 1.36        | 1.45     |
| 11  | A     | 908 | BCL  | O1D-CGD | -3.93 | 1.11        | 1.21     |
| 11  | A     | 906 | BCL  | OBB-CAB | -3.93 | 1.14        | 1.23     |
| 12  | A     | 912 | CLA  | CHB-C1B | 3.91  | 1.48        | 1.39     |
| 11  | a     | 909 | BCL  | O1A-CGA | -3.90 | 1.10        | 1.22     |
| 18  | c     | 202 | HEC  | C2A-C3A | 3.90  | 1.45        | 1.36     |
| 12  | a     | 914 | CLA  | O2A-CGA | 3.90  | 1.45        | 1.33     |
| 11  | A     | 902 | BCL  | CAA-C2A | -3.89 | 1.47        | 1.54     |
| 15  | A     | 915 | 85I  | P-O     | -3.85 | 1.44        | 1.59     |
| 11  | A     | 904 | BCL  | C2A-C1A | -3.85 | 1.43        | 1.52     |
| 11  | A     | 906 | BCL  | C1B-C2B | -3.84 | 1.34        | 1.43     |
| 11  | a     | 908 | BCL  | CAA-CBA | -3.83 | 1.41        | 1.52     |
| 11  | a     | 905 | BCL  | OBD-CAD | -3.83 | 1.15        | 1.22     |
| 11  | A     | 905 | BCL  | O1D-CGD | -3.83 | 1.11        | 1.21     |
| 11  | a     | 911 | BCL  | O1A-CGA | -3.83 | 1.11        | 1.22     |
| 13  | A     | 913 | LYC  | C14-C12 | -3.81 | 1.27        | 1.35     |
| 12  | A     | 931 | CLA  | OBD-CAD | -3.81 | 1.15        | 1.22     |
| 12  | a     | 915 | CLA  | C3C-C2C | 3.80  | 1.45        | 1.36     |
| 12  | a     | 913 | CLA  | CHC-C1C | 3.80  | 1.46        | 1.38     |
| 18  | C     | 301 | HEC  | C4A-C3A | 3.78  | 1.52        | 1.45     |
| 11  | A     | 908 | BCL  | C3A-C2A | -3.78 | 1.44        | 1.54     |
| 12  | a     | 915 | CLA  | MG-NC   | 3.77  | 2.15        | 2.06     |
| 11  | A     | 909 | BCL  | C2-C3   | 3.77  | 1.41        | 1.33     |
| 11  | a     | 907 | BCL  | CHB-C1B | 3.76  | 1.47        | 1.39     |
| 11  | a     | 911 | BCL  | CHD-C1D | 3.76  | 1.45        | 1.38     |
| 12  | a     | 912 | CLA  | MG-NC   | 3.75  | 2.15        | 2.06     |
| 11  | A     | 907 | BCL  | C6-C5   | 3.75  | 1.65        | 1.52     |
| 11  | A     | 902 | BCL  | O2D-CGD | 3.75  | 1.42        | 1.33     |
| 11  | a     | 910 | BCL  | O2D-CGD | 3.74  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | a     | 901 | CLA  | O1D-CGD | -3.74 | 1.11        | 1.21     |
| 11  | A     | 909 | BCL  | C3A-C2A | -3.73 | 1.44        | 1.54     |
| 11  | A     | 909 | BCL  | CAA-CBA | -3.72 | 1.41        | 1.52     |
| 10  | A     | 901 | 2GO  | C1D-ND  | -3.71 | 1.30        | 1.38     |
| 11  | A     | 903 | BCL  | C3A-C2A | -3.71 | 1.44        | 1.54     |
| 12  | a     | 901 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 12  | a     | 901 | CLA  | CHC-C1C | 3.69  | 1.45        | 1.38     |
| 18  | c     | 202 | HEC  | C1D-ND  | -3.69 | 1.32        | 1.39     |
| 11  | A     | 903 | BCL  | CHB-C1B | 3.67  | 1.47        | 1.39     |
| 12  | a     | 913 | CLA  | CAA-C2A | 3.67  | 1.60        | 1.54     |
| 12  | a     | 901 | CLA  | MG-NC   | 3.67  | 2.15        | 2.06     |
| 18  | C     | 301 | HEC  | C3D-C2D | 3.67  | 1.48        | 1.38     |
| 11  | A     | 909 | BCL  | MG-ND   | -3.65 | 1.98        | 2.05     |
| 11  | A     | 909 | BCL  | CBD-CAD | -3.64 | 1.40        | 1.56     |
| 18  | c     | 202 | HEC  | CAB-C3B | 3.63  | 1.46        | 1.35     |
| 12  | A     | 911 | CLA  | CHB-C4A | -3.63 | 1.28        | 1.37     |
| 11  | A     | 902 | BCL  | O1A-CGA | -3.62 | 1.11        | 1.22     |
| 11  | a     | 906 | BCL  | C2A-C1A | -3.62 | 1.44        | 1.52     |
| 12  | a     | 915 | CLA  | CHB-C4A | -3.62 | 1.28        | 1.37     |
| 12  | a     | 914 | CLA  | MG-NC   | 3.61  | 2.14        | 2.06     |
| 11  | A     | 905 | BCL  | CHC-C4B | 3.61  | 1.47        | 1.39     |
| 11  | A     | 909 | BCL  | O1D-CGD | -3.60 | 1.12        | 1.21     |
| 18  | C     | 301 | HEC  | CAC-C3C | 3.60  | 1.46        | 1.35     |
| 15  | A     | 915 | 85I  | P-O1    | -3.60 | 1.38        | 1.50     |
| 11  | a     | 906 | BCL  | O2A-CGA | 3.59  | 1.42        | 1.30     |
| 10  | A     | 901 | 2GO  | CHA-C4D | -3.59 | 1.30        | 1.40     |
| 12  | a     | 901 | CLA  | C7-C8   | -3.58 | 1.35        | 1.52     |
| 12  | a     | 915 | CLA  | O1A-CGA | -3.56 | 1.11        | 1.22     |
| 10  | a     | 903 | 2GO  | C1C-C2C | 3.56  | 1.51        | 1.44     |
| 12  | a     | 912 | CLA  | O2A-CGA | 3.56  | 1.43        | 1.33     |
| 11  | a     | 907 | BCL  | O2A-CGA | 3.56  | 1.43        | 1.33     |
| 12  | A     | 911 | CLA  | O2D-CED | -3.55 | 1.37        | 1.45     |
| 11  | a     | 907 | BCL  | O2A-C1  | -3.55 | 1.36        | 1.46     |
| 11  | A     | 903 | BCL  | CHC-C4B | 3.54  | 1.47        | 1.39     |
| 12  | A     | 933 | CLA  | CAA-C2A | -3.53 | 1.47        | 1.54     |
| 11  | A     | 909 | BCL  | CBD-CGD | -3.53 | 1.41        | 1.52     |
| 18  | C     | 301 | HEC  | C4A-NA  | -3.53 | 1.33        | 1.39     |
| 11  | A     | 906 | BCL  | CHC-C1C | -3.51 | 1.28        | 1.37     |
| 12  | A     | 933 | CLA  | C1B-NB  | -3.50 | 1.33        | 1.37     |
| 11  | A     | 904 | BCL  | CHB-C1B | 3.47  | 1.47        | 1.39     |
| 12  | a     | 915 | CLA  | O1D-CGD | -3.46 | 1.12        | 1.21     |
| 11  | a     | 907 | BCL  | CAA-C2A | -3.46 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | A     | 911 | CLA  | CHC-C1C | 3.45  | 1.45        | 1.38     |
| 10  | a     | 903 | 2GO  | ZN-NA   | 3.45  | 2.14        | 2.03     |
| 13  | A     | 913 | LYC  | C13-C12 | -3.44 | 1.43        | 1.50     |
| 12  | A     | 911 | CLA  | O2A-C1  | -3.44 | 1.36        | 1.46     |
| 11  | A     | 903 | BCL  | O2A-CGA | 3.43  | 1.43        | 1.33     |
| 12  | A     | 912 | CLA  | O2A-CGA | 3.43  | 1.43        | 1.33     |
| 13  | c     | 201 | LYC  | C13-C12 | -3.43 | 1.43        | 1.50     |
| 11  | a     | 906 | BCL  | MG-NB   | 3.43  | 2.12        | 2.05     |
| 12  | A     | 931 | CLA  | C4D-CHA | 3.42  | 1.50        | 1.38     |
| 12  | A     | 933 | CLA  | O1A-CGA | -3.42 | 1.12        | 1.22     |
| 12  | a     | 901 | CLA  | C1D-C2D | 3.41  | 1.52        | 1.45     |
| 12  | A     | 910 | CLA  | O2A-CGA | 3.41  | 1.43        | 1.33     |
| 18  | c     | 202 | HEC  | C3C-C4C | -3.41 | 1.40        | 1.46     |
| 11  | a     | 905 | BCL  | CAC-C3C | -3.41 | 1.47        | 1.54     |
| 11  | a     | 905 | BCL  | O1A-CGA | -3.40 | 1.12        | 1.22     |
| 12  | A     | 910 | CLA  | C7-C8   | -3.39 | 1.36        | 1.52     |
| 12  | a     | 913 | CLA  | CHC-C4B | 3.36  | 1.47        | 1.39     |
| 12  | a     | 915 | CLA  | CHC-C4B | 3.36  | 1.47        | 1.39     |
| 12  | A     | 911 | CLA  | O1A-CGA | -3.36 | 1.12        | 1.22     |
| 11  | a     | 908 | BCL  | CHC-C4B | 3.36  | 1.46        | 1.39     |
| 10  | a     | 903 | 2GO  | O1D-CGD | -3.36 | 1.14        | 1.21     |
| 11  | A     | 905 | BCL  | CBA-CGA | -3.35 | 1.41        | 1.50     |
| 12  | A     | 931 | CLA  | C10-C8  | -3.34 | 1.36        | 1.52     |
| 11  | a     | 906 | BCL  | CHC-C4B | 3.34  | 1.46        | 1.39     |
| 19  | E     | 101 | 84Q  | C3-C1   | -3.33 | 1.30        | 1.51     |
| 11  | A     | 904 | BCL  | C1B-NB  | -3.33 | 1.33        | 1.37     |
| 11  | a     | 908 | BCL  | CBA-CGA | -3.32 | 1.41        | 1.50     |
| 11  | A     | 907 | BCL  | CMD-C2D | -3.32 | 1.44        | 1.50     |
| 11  | a     | 907 | BCL  | CHD-C1D | 3.32  | 1.44        | 1.38     |
| 18  | c     | 202 | HEC  | CBA-CGA | -3.31 | 1.42        | 1.50     |
| 11  | A     | 902 | BCL  | CBD-CAD | -3.31 | 1.41        | 1.56     |
| 11  | A     | 903 | BCL  | O2D-CGD | 3.30  | 1.41        | 1.33     |
| 11  | a     | 908 | BCL  | C5-C3   | -3.30 | 1.44        | 1.51     |
| 10  | A     | 901 | 2GO  | C3D-C2D | -3.29 | 1.30        | 1.39     |
| 11  | a     | 911 | BCL  | CHC-C1C | -3.27 | 1.29        | 1.37     |
| 12  | A     | 910 | CLA  | C10-C8  | -3.27 | 1.36        | 1.52     |
| 11  | A     | 908 | BCL  | OBb-CAB | -3.26 | 1.15        | 1.23     |
| 12  | a     | 915 | CLA  | O2D-CED | -3.24 | 1.38        | 1.45     |
| 11  | A     | 908 | BCL  | CAA-C2A | -3.24 | 1.48        | 1.54     |
| 11  | A     | 908 | BCL  | CMA-C3A | -3.23 | 1.46        | 1.53     |
| 11  | a     | 904 | BCL  | CHB-C1B | 3.22  | 1.46        | 1.39     |
| 12  | a     | 914 | CLA  | C3C-C2C | 3.21  | 1.43        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | a     | 907 | BCL  | O1D-CGD | -3.21 | 1.13        | 1.21     |
| 19  | E     | 101 | 84Q  | C7-C6   | -3.20 | 1.35        | 1.51     |
| 11  | A     | 907 | BCL  | C2C-C3C | -3.20 | 1.45        | 1.54     |
| 11  | a     | 907 | BCL  | MG-NA   | -3.19 | 1.98        | 2.06     |
| 11  | a     | 907 | BCL  | MG-NB   | 3.19  | 2.12        | 2.05     |
| 11  | A     | 908 | BCL  | MG-NC   | -3.18 | 1.98        | 2.06     |
| 11  | A     | 908 | BCL  | CHB-C4A | -3.18 | 1.29        | 1.37     |
| 12  | a     | 912 | CLA  | CBD-CAD | -3.17 | 1.42        | 1.56     |
| 13  | A     | 913 | LYC  | C10-C11 | -3.17 | 1.26        | 1.34     |
| 12  | a     | 913 | CLA  | O1A-CGA | -3.17 | 1.13        | 1.22     |
| 11  | a     | 909 | BCL  | C3A-C2A | -3.16 | 1.45        | 1.54     |
| 11  | A     | 908 | BCL  | O2A-CGA | 3.16  | 1.42        | 1.33     |
| 18  | c     | 202 | HEC  | CHB-C4A | 3.16  | 1.44        | 1.38     |
| 11  | a     | 907 | BCL  | C1B-NB  | -3.15 | 1.33        | 1.37     |
| 11  | A     | 902 | BCL  | O2A-CGA | 3.15  | 1.42        | 1.33     |
| 11  | a     | 909 | BCL  | CHB-C1B | 3.15  | 1.46        | 1.39     |
| 12  | a     | 913 | CLA  | C10-C8  | 3.15  | 1.68        | 1.52     |
| 11  | A     | 906 | BCL  | CHB-C1B | 3.14  | 1.46        | 1.39     |
| 18  | c     | 202 | HEC  | CBC-CAC | -3.13 | 1.37        | 1.49     |
| 12  | A     | 910 | CLA  | C3A-C2A | -3.13 | 1.46        | 1.54     |
| 11  | a     | 907 | BCL  | C2C-C3C | -3.12 | 1.46        | 1.54     |
| 11  | a     | 910 | BCL  | CHB-C4A | -3.12 | 1.29        | 1.37     |
| 11  | a     | 910 | BCL  | O2A-CGA | 3.11  | 1.42        | 1.33     |
| 11  | a     | 907 | BCL  | CHC-C4B | 3.11  | 1.46        | 1.39     |
| 12  | a     | 901 | CLA  | CHB-C1B | 3.11  | 1.46        | 1.39     |
| 11  | A     | 906 | BCL  | CHB-C4A | -3.11 | 1.29        | 1.37     |
| 11  | A     | 905 | BCL  | CAA-CBA | -3.10 | 1.43        | 1.52     |
| 11  | a     | 908 | BCL  | CHC-C1C | -3.10 | 1.29        | 1.37     |
| 19  | E     | 101 | 84Q  | C9-C8   | -3.09 | 1.36        | 1.51     |
| 11  | a     | 905 | BCL  | CHB-C4A | -3.09 | 1.29        | 1.37     |
| 11  | A     | 903 | BCL  | O2D-CED | -3.08 | 1.38        | 1.45     |
| 11  | a     | 911 | BCL  | C1D-C2D | -3.07 | 1.39        | 1.45     |
| 12  | A     | 931 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 11  | A     | 907 | BCL  | CBD-CAD | -3.06 | 1.43        | 1.56     |
| 11  | a     | 911 | BCL  | C3A-C2A | -3.06 | 1.46        | 1.54     |
| 11  | a     | 910 | BCL  | MG-NA   | 3.06  | 2.13        | 2.06     |
| 12  | A     | 912 | CLA  | CHC-C1C | 3.06  | 1.44        | 1.38     |
| 11  | a     | 906 | BCL  | C3B-C4B | 3.04  | 1.47        | 1.41     |
| 11  | a     | 909 | BCL  | CBD-CAD | -3.04 | 1.43        | 1.56     |
| 12  | A     | 931 | CLA  | CHB-C1B | 3.04  | 1.46        | 1.39     |
| 12  | a     | 901 | CLA  | O2D-CGD | 3.04  | 1.40        | 1.33     |
| 12  | A     | 931 | CLA  | C1D-C2D | -3.04 | 1.39        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | A     | 902 | BCL  | C3A-C2A | -3.02 | 1.46        | 1.54     |
| 11  | a     | 905 | BCL  | C1B-NB  | -3.02 | 1.33        | 1.37     |
| 10  | a     | 903 | 2GO  | CHC-C1C | -3.02 | 1.32        | 1.38     |
| 11  | a     | 909 | BCL  | CHC-C1C | -3.01 | 1.30        | 1.37     |
| 12  | a     | 914 | CLA  | C2A-C1A | -3.01 | 1.45        | 1.52     |
| 12  | a     | 913 | CLA  | O1D-CGD | -3.01 | 1.13        | 1.21     |
| 11  | A     | 902 | BCL  | CHD-C1D | 3.00  | 1.44        | 1.38     |
| 12  | A     | 910 | CLA  | CBD-CAD | -3.00 | 1.43        | 1.56     |
| 11  | a     | 904 | BCL  | CHC-C4B | 2.99  | 1.46        | 1.39     |
| 19  | E     | 101 | 84Q  | C9-C10  | -2.99 | 1.36        | 1.51     |
| 12  | A     | 912 | CLA  | CBD-CAD | -2.99 | 1.43        | 1.56     |
| 11  | A     | 902 | BCL  | O1D-CGD | -2.98 | 1.13        | 1.21     |
| 18  | c     | 202 | HEC  | C4C-NC  | -2.98 | 1.34        | 1.39     |
| 12  | A     | 931 | CLA  | CMA-C3A | -2.98 | 1.46        | 1.53     |
| 11  | a     | 905 | BCL  | C2C-C3C | -2.97 | 1.46        | 1.54     |
| 11  | A     | 909 | BCL  | CHD-C1D | 2.97  | 1.44        | 1.38     |
| 10  | A     | 901 | 2GO  | CBC-CAC | -2.97 | 1.38        | 1.51     |
| 11  | A     | 908 | BCL  | C2C-C3C | -2.96 | 1.46        | 1.54     |
| 12  | a     | 915 | CLA  | CHB-C1B | 2.96  | 1.46        | 1.39     |
| 12  | A     | 911 | CLA  | O1D-CGD | -2.95 | 1.13        | 1.21     |
| 11  | a     | 908 | BCL  | CHB-C1B | 2.95  | 1.46        | 1.39     |
| 11  | a     | 911 | BCL  | CBD-CAD | -2.95 | 1.43        | 1.56     |
| 12  | A     | 933 | CLA  | C3A-C2A | -2.95 | 1.46        | 1.54     |
| 10  | A     | 901 | 2GO  | ZN-NB   | 2.94  | 2.13        | 2.03     |
| 11  | A     | 902 | BCL  | CHC-C1C | -2.94 | 1.30        | 1.37     |
| 12  | a     | 914 | CLA  | C3A-C2A | -2.94 | 1.46        | 1.54     |
| 11  | A     | 906 | BCL  | CHD-C1D | 2.94  | 1.44        | 1.38     |
| 11  | a     | 905 | BCL  | CBD-CAD | -2.94 | 1.43        | 1.56     |
| 11  | a     | 904 | BCL  | C2C-C3C | -2.94 | 1.46        | 1.54     |
| 12  | A     | 910 | CLA  | C3C-C2C | 2.94  | 1.43        | 1.36     |
| 11  | a     | 909 | BCL  | C2C-C3C | -2.93 | 1.46        | 1.54     |
| 12  | A     | 931 | CLA  | CHD-C1D | 2.93  | 1.44        | 1.38     |
| 12  | A     | 910 | CLA  | O1D-CGD | -2.89 | 1.14        | 1.21     |
| 11  | A     | 908 | BCL  | CBD-CAD | -2.89 | 1.43        | 1.56     |
| 12  | a     | 901 | CLA  | CAA-C2A | -2.88 | 1.48        | 1.54     |
| 11  | A     | 904 | BCL  | O2D-CGD | 2.88  | 1.40        | 1.33     |
| 12  | A     | 933 | CLA  | O2D-CED | -2.88 | 1.38        | 1.45     |
| 10  | A     | 901 | 2GO  | CHD-C1D | 2.88  | 1.44        | 1.38     |
| 12  | A     | 931 | CLA  | MG-NB   | 2.88  | 2.11        | 2.05     |
| 13  | A     | 913 | LYC  | C59-C58 | -2.87 | 1.27        | 1.34     |
| 11  | a     | 908 | BCL  | O2D-CGD | 2.86  | 1.40        | 1.33     |
| 12  | a     | 913 | CLA  | MG-NC   | 2.86  | 2.13        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | a     | 905 | BCL  | O2D-CGD | 2.86  | 1.40        | 1.33     |
| 11  | A     | 903 | BCL  | CMD-C2D | -2.85 | 1.44        | 1.50     |
| 11  | A     | 908 | BCL  | O2D-CGD | 2.85  | 1.40        | 1.33     |
| 10  | a     | 903 | 2GO  | CHB-C1B | 2.84  | 1.45        | 1.39     |
| 11  | A     | 907 | BCL  | O2A-C1  | 2.84  | 1.53        | 1.46     |
| 19  | E     | 101 | 84Q  | C6-C5   | -2.84 | 1.37        | 1.51     |
| 11  | A     | 902 | BCL  | C2C-C3C | -2.83 | 1.46        | 1.54     |
| 12  | A     | 912 | CLA  | CHB-C4A | -2.82 | 1.30        | 1.37     |
| 19  | E     | 101 | 84Q  | C8-C7   | -2.81 | 1.37        | 1.51     |
| 11  | a     | 910 | BCL  | CMB-C2B | -2.80 | 1.45        | 1.50     |
| 15  | A     | 915 | 85I  | C33-C32 | -2.80 | 1.37        | 1.51     |
| 11  | A     | 905 | BCL  | CHB-C4A | -2.80 | 1.30        | 1.37     |
| 11  | a     | 911 | BCL  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 12  | a     | 901 | CLA  | CBD-CAD | -2.80 | 1.44        | 1.56     |
| 11  | a     | 907 | BCL  | O1A-CGA | -2.79 | 1.14        | 1.22     |
| 12  | A     | 933 | CLA  | CBD-CAD | -2.79 | 1.44        | 1.56     |
| 12  | A     | 911 | CLA  | CBD-CAD | -2.78 | 1.44        | 1.56     |
| 11  | a     | 904 | BCL  | CBD-CAD | -2.77 | 1.44        | 1.56     |
| 12  | A     | 910 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 11  | A     | 907 | BCL  | C3A-C2A | -2.76 | 1.47        | 1.54     |
| 11  | a     | 908 | BCL  | O1A-CGA | -2.76 | 1.14        | 1.22     |
| 19  | E     | 101 | 84Q  | C5-C4   | -2.75 | 1.38        | 1.51     |
| 12  | a     | 914 | CLA  | CHB-C1B | 2.75  | 1.45        | 1.39     |
| 12  | A     | 912 | CLA  | C1D-C2D | -2.75 | 1.39        | 1.45     |
| 12  | A     | 931 | CLA  | C1C-C2C | -2.75 | 1.38        | 1.44     |
| 18  | c     | 202 | HEC  | CBA-CAA | -2.74 | 1.42        | 1.51     |
| 12  | A     | 911 | CLA  | C10-C8  | -2.74 | 1.39        | 1.52     |
| 11  | A     | 908 | BCL  | MG-NA   | -2.74 | 1.99        | 2.06     |
| 15  | A     | 915 | 85I  | O6-C3   | -2.74 | 1.40        | 1.44     |
| 11  | a     | 907 | BCL  | C3C-C4C | -2.74 | 1.48        | 1.51     |
| 12  | a     | 901 | CLA  | C3C-C2C | 2.74  | 1.42        | 1.36     |
| 12  | A     | 911 | CLA  | CMC-C2C | -2.73 | 1.45        | 1.50     |
| 11  | A     | 903 | BCL  | CBD-CAD | -2.73 | 1.44        | 1.56     |
| 15  | A     | 915 | 85I  | P-O2    | -2.72 | 1.42        | 1.55     |
| 12  | A     | 910 | CLA  | CAA-C2A | -2.71 | 1.49        | 1.54     |
| 15  | A     | 915 | 85I  | O5-C5   | -2.71 | 1.14        | 1.22     |
| 11  | a     | 909 | BCL  | CMD-C2D | -2.71 | 1.45        | 1.50     |
| 11  | A     | 903 | BCL  | CHC-C1C | -2.71 | 1.30        | 1.37     |
| 11  | a     | 907 | BCL  | C1D-C2D | -2.70 | 1.40        | 1.45     |
| 10  | A     | 901 | 2GO  | ZN-ND   | 2.70  | 2.12        | 2.03     |
| 12  | A     | 933 | CLA  | CBA-CGA | -2.70 | 1.42        | 1.50     |
| 18  | C     | 301 | HEC  | O1A-CGA | -2.70 | 1.13        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | a     | 915 | CLA  | O2D-CGD | 2.69  | 1.39        | 1.33     |
| 12  | A     | 912 | CLA  | C2A-C1A | -2.69 | 1.46        | 1.52     |
| 11  | A     | 908 | BCL  | CBD-CGD | -2.69 | 1.44        | 1.52     |
| 11  | a     | 906 | BCL  | O1D-CGD | -2.69 | 1.14        | 1.21     |
| 11  | a     | 909 | BCL  | C5-C3   | -2.69 | 1.45        | 1.51     |
| 18  | C     | 301 | HEC  | C1C-C2C | -2.68 | 1.36        | 1.43     |
| 12  | a     | 912 | CLA  | MG-NB   | 2.68  | 2.11        | 2.05     |
| 18  | C     | 301 | HEC  | CBA-CGA | -2.67 | 1.44        | 1.50     |
| 11  | A     | 907 | BCL  | CHC-C4B | 2.67  | 1.45        | 1.39     |
| 12  | A     | 911 | CLA  | CHD-C1D | 2.67  | 1.43        | 1.38     |
| 12  | a     | 901 | CLA  | C2-C3   | -2.67 | 1.26        | 1.33     |
| 11  | a     | 907 | BCL  | O2D-CED | -2.67 | 1.39        | 1.45     |
| 12  | a     | 914 | CLA  | CBD-CAD | -2.67 | 1.44        | 1.56     |
| 11  | a     | 908 | BCL  | CBD-CAD | -2.66 | 1.44        | 1.56     |
| 12  | A     | 931 | CLA  | MG-NC   | 2.66  | 2.12        | 2.06     |
| 11  | A     | 905 | BCL  | O2A-C1  | -2.65 | 1.39        | 1.46     |
| 12  | A     | 933 | CLA  | CHC-C1C | 2.65  | 1.43        | 1.38     |
| 11  | A     | 907 | BCL  | C2A-C1A | -2.65 | 1.46        | 1.52     |
| 11  | A     | 908 | BCL  | O1A-CGA | -2.64 | 1.14        | 1.22     |
| 11  | a     | 906 | BCL  | CHD-C1D | 2.64  | 1.43        | 1.38     |
| 12  | a     | 914 | CLA  | CHB-C4A | -2.64 | 1.31        | 1.37     |
| 11  | a     | 911 | BCL  | CBB-CAB | -2.62 | 1.45        | 1.50     |
| 11  | a     | 905 | BCL  | CHC-C4B | 2.62  | 1.45        | 1.39     |
| 12  | A     | 910 | CLA  | CHB-C1B | 2.62  | 1.45        | 1.39     |
| 13  | c     | 201 | LYC  | C1-C2   | -2.61 | 1.43        | 1.50     |
| 12  | A     | 912 | CLA  | C3C-C2C | 2.61  | 1.42        | 1.36     |
| 19  | a     | 921 | 84Q  | P-O4    | 2.60  | 1.67        | 1.59     |
| 11  | A     | 905 | BCL  | CBD-CAD | -2.60 | 1.44        | 1.56     |
| 11  | a     | 909 | BCL  | O2D-CGD | 2.60  | 1.39        | 1.33     |
| 12  | A     | 933 | CLA  | CHB-C4A | -2.59 | 1.31        | 1.37     |
| 10  | A     | 901 | 2GO  | C4C-C3C | -2.59 | 1.40        | 1.45     |
| 12  | a     | 914 | CLA  | O1A-CGA | -2.59 | 1.14        | 1.22     |
| 11  | A     | 902 | BCL  | CHB-C4A | -2.59 | 1.31        | 1.37     |
| 12  | A     | 910 | CLA  | CHD-C1D | 2.58  | 1.43        | 1.38     |
| 18  | c     | 202 | HEC  | CMD-C2D | -2.58 | 1.45        | 1.50     |
| 12  | a     | 901 | CLA  | O1A-CGA | -2.58 | 1.14        | 1.22     |
| 11  | A     | 902 | BCL  | CMB-C2B | -2.58 | 1.45        | 1.50     |
| 18  | c     | 202 | HEC  | CAD-C3D | -2.58 | 1.44        | 1.51     |
| 11  | a     | 910 | BCL  | C3A-C2A | -2.58 | 1.47        | 1.54     |
| 12  | a     | 901 | CLA  | C5-C3   | -2.58 | 1.46        | 1.51     |
| 11  | A     | 905 | BCL  | O2A-CGA | 2.58  | 1.40        | 1.33     |
| 11  | A     | 908 | BCL  | CHC-C1C | -2.58 | 1.31        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | a     | 904 | BCL  | CHC-C1C | -2.56 | 1.31        | 1.37     |
| 18  | C     | 301 | HEC  | CHC-C1C | 2.56  | 1.45        | 1.39     |
| 11  | A     | 905 | BCL  | C2C-C3C | -2.56 | 1.47        | 1.54     |
| 12  | A     | 931 | CLA  | MG-NA   | 2.55  | 2.12        | 2.06     |
| 12  | A     | 933 | CLA  | MG-ND   | 2.55  | 2.10        | 2.05     |
| 11  | a     | 908 | BCL  | C3D-C2D | 2.55  | 1.45        | 1.39     |
| 18  | C     | 301 | HEC  | CMB-C2B | -2.55 | 1.45        | 1.50     |
| 13  | c     | 201 | LYC  | C15-C16 | -2.54 | 1.28        | 1.34     |
| 10  | A     | 901 | 2GO  | O1D-CGD | -2.54 | 1.16        | 1.21     |
| 11  | A     | 907 | BCL  | C3C-C4C | -2.54 | 1.48        | 1.51     |
| 18  | C     | 301 | HEC  | CHB-C1B | 2.54  | 1.45        | 1.39     |
| 13  | A     | 913 | LYC  | C11-C12 | -2.53 | 1.40        | 1.46     |
| 12  | A     | 931 | CLA  | C3A-C4A | -2.53 | 1.43        | 1.51     |
| 11  | a     | 911 | BCL  | CBA-CGA | -2.53 | 1.43        | 1.50     |
| 12  | A     | 931 | CLA  | CHC-C1C | 2.53  | 1.43        | 1.38     |
| 18  | C     | 301 | HEC  | C1A-NA  | -2.52 | 1.34        | 1.39     |
| 11  | a     | 904 | BCL  | CBB-CAB | -2.52 | 1.45        | 1.50     |
| 12  | a     | 913 | CLA  | CHB-C1B | 2.52  | 1.45        | 1.39     |
| 12  | a     | 913 | CLA  | CBD-CAD | -2.52 | 1.45        | 1.56     |
| 12  | A     | 910 | CLA  | CBD-CGD | -2.51 | 1.44        | 1.52     |
| 11  | A     | 904 | BCL  | C3A-C2A | -2.51 | 1.47        | 1.54     |
| 11  | A     | 906 | BCL  | C2A-C1A | -2.51 | 1.46        | 1.52     |
| 12  | a     | 912 | CLA  | CHD-C4C | 2.51  | 1.44        | 1.39     |
| 11  | a     | 906 | BCL  | CAA-CBA | -2.51 | 1.45        | 1.52     |
| 11  | a     | 907 | BCL  | CBD-CAD | -2.50 | 1.45        | 1.56     |
| 11  | a     | 910 | BCL  | CHB-C1B | 2.50  | 1.45        | 1.39     |
| 15  | a     | 920 | 85I  | C4-C3   | -2.50 | 1.46        | 1.51     |
| 10  | A     | 901 | 2GO  | C3B-C4B | -2.50 | 1.36        | 1.41     |
| 11  | A     | 904 | BCL  | CMB-C2B | -2.50 | 1.45        | 1.50     |
| 13  | c     | 201 | LYC  | C62-C61 | -2.49 | 1.44        | 1.50     |
| 11  | a     | 904 | BCL  | CAA-CBA | -2.49 | 1.45        | 1.52     |
| 11  | a     | 911 | BCL  | C1B-C2B | -2.49 | 1.37        | 1.43     |
| 11  | a     | 909 | BCL  | C3A-C4A | -2.48 | 1.43        | 1.51     |
| 11  | a     | 911 | BCL  | CHB-C4A | -2.48 | 1.31        | 1.37     |
| 12  | a     | 914 | CLA  | C4D-CHA | 2.47  | 1.46        | 1.38     |
| 11  | a     | 908 | BCL  | MG-ND   | 2.47  | 2.10        | 2.05     |
| 12  | A     | 910 | CLA  | O2D-CED | -2.47 | 1.39        | 1.45     |
| 12  | a     | 913 | CLA  | C5-C3   | -2.47 | 1.46        | 1.51     |
| 17  | g     | 101 | 85N  | O4-C24  | -2.47 | 1.22        | 1.30     |
| 11  | a     | 911 | BCL  | C2C-C3C | -2.46 | 1.47        | 1.54     |
| 12  | A     | 910 | CLA  | O2D-CGD | 2.46  | 1.39        | 1.33     |
| 12  | a     | 901 | CLA  | CMC-C2C | -2.46 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | a     | 901 | CLA  | MG-NB   | 2.45  | 2.10        | 2.05     |
| 10  | a     | 903 | 2GO  | O1A-CGA | -2.45 | 1.15        | 1.22     |
| 11  | A     | 908 | BCL  | C3D-C2D | 2.45  | 1.45        | 1.39     |
| 11  | A     | 904 | BCL  | CBD-CAD | -2.45 | 1.45        | 1.56     |
| 11  | a     | 911 | BCL  | CHB-C1B | 2.45  | 1.44        | 1.39     |
| 15  | a     | 918 | 85I  | C4-C3   | 2.45  | 1.57        | 1.51     |
| 11  | a     | 911 | BCL  | MG-NA   | 2.43  | 2.12        | 2.06     |
| 11  | A     | 908 | BCL  | O2D-CED | -2.42 | 1.39        | 1.45     |
| 11  | a     | 906 | BCL  | C3D-C2D | 2.42  | 1.45        | 1.39     |
| 12  | A     | 910 | CLA  | CMA-C3A | -2.42 | 1.48        | 1.53     |
| 11  | a     | 906 | BCL  | CHB-C1B | 2.42  | 1.44        | 1.39     |
| 12  | A     | 911 | CLA  | CHB-C1B | 2.42  | 1.44        | 1.39     |
| 18  | C     | 301 | HEC  | CHC-C4B | 2.42  | 1.43        | 1.38     |
| 11  | a     | 907 | BCL  | CHB-C4A | -2.42 | 1.31        | 1.37     |
| 11  | a     | 908 | BCL  | C4-C3   | -2.41 | 1.44        | 1.50     |
| 11  | a     | 909 | BCL  | C2C-C1C | -2.41 | 1.44        | 1.51     |
| 11  | a     | 910 | BCL  | MG-NB   | 2.41  | 2.10        | 2.05     |
| 12  | A     | 933 | CLA  | C2A-C1A | -2.41 | 1.46        | 1.52     |
| 11  | a     | 906 | BCL  | CBD-CAD | -2.41 | 1.45        | 1.56     |
| 12  | a     | 913 | CLA  | C3A-C2A | -2.41 | 1.48        | 1.54     |
| 11  | A     | 907 | BCL  | O1A-CGA | -2.40 | 1.15        | 1.22     |
| 13  | A     | 913 | LYC  | C52-C51 | -2.40 | 1.46        | 1.50     |
| 11  | A     | 909 | BCL  | CHB-C1B | 2.40  | 1.44        | 1.39     |
| 11  | A     | 905 | BCL  | CBB-CAB | -2.40 | 1.45        | 1.50     |
| 11  | A     | 906 | BCL  | MG-ND   | 2.40  | 2.10        | 2.05     |
| 11  | A     | 904 | BCL  | CMA-C3A | -2.40 | 1.48        | 1.53     |
| 12  | a     | 913 | CLA  | C2A-C1A | -2.39 | 1.46        | 1.52     |
| 12  | A     | 931 | CLA  | CBD-CGD | 2.39  | 1.59        | 1.52     |
| 11  | a     | 905 | BCL  | C3D-C2D | 2.38  | 1.45        | 1.39     |
| 12  | A     | 910 | CLA  | CMB-C2B | -2.38 | 1.45        | 1.50     |
| 10  | a     | 903 | 2GO  | C1A-C2A | 2.38  | 1.50        | 1.45     |
| 11  | A     | 908 | BCL  | CAC-C3C | -2.37 | 1.49        | 1.54     |
| 12  | A     | 931 | CLA  | C4C-C3C | -2.37 | 1.41        | 1.45     |
| 12  | A     | 931 | CLA  | O2A-C1  | -2.37 | 1.39        | 1.46     |
| 11  | a     | 906 | BCL  | C3A-C4A | -2.36 | 1.44        | 1.51     |
| 12  | A     | 910 | CLA  | C2A-C1A | -2.36 | 1.46        | 1.52     |
| 11  | a     | 911 | BCL  | O1D-CGD | -2.36 | 1.15        | 1.21     |
| 11  | A     | 904 | BCL  | CAA-CBA | -2.36 | 1.45        | 1.52     |
| 11  | a     | 909 | BCL  | C4-C3   | -2.35 | 1.45        | 1.50     |
| 10  | A     | 901 | 2GO  | C1B-C2B | -2.35 | 1.37        | 1.43     |
| 12  | a     | 913 | CLA  | O2A-C1  | -2.35 | 1.39        | 1.46     |
| 11  | a     | 910 | BCL  | CBD-CAD | -2.35 | 1.46        | 1.56     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | a     | 914 | CLA  | C3D-C2D | 2.34  | 1.45        | 1.39     |
| 12  | a     | 914 | CLA  | C4C-C3C | -2.34 | 1.41        | 1.45     |
| 11  | a     | 904 | BCL  | CMA-C3A | -2.34 | 1.48        | 1.53     |
| 11  | A     | 908 | BCL  | C3A-C4A | -2.34 | 1.44        | 1.51     |
| 12  | a     | 915 | CLA  | C3B-C4B | -2.34 | 1.36        | 1.42     |
| 11  | a     | 904 | BCL  | C2A-C1A | -2.34 | 1.47        | 1.52     |
| 11  | A     | 907 | BCL  | CHD-C1D | 2.33  | 1.42        | 1.38     |
| 11  | a     | 906 | BCL  | CBD-CGD | -2.33 | 1.45        | 1.52     |
| 19  | E     | 101 | 84Q  | O-C14   | -2.33 | 1.15        | 1.22     |
| 12  | a     | 914 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 12  | a     | 913 | CLA  | CHB-C4A | -2.32 | 1.31        | 1.37     |
| 12  | A     | 911 | CLA  | O2A-CGA | 2.31  | 1.40        | 1.33     |
| 12  | a     | 913 | CLA  | O2A-CGA | 2.31  | 1.40        | 1.33     |
| 18  | C     | 301 | HEC  | CHD-C1D | 2.31  | 1.44        | 1.39     |
| 11  | A     | 909 | BCL  | O2D-CED | 2.30  | 1.50        | 1.45     |
| 13  | A     | 913 | LYC  | C5-C4   | -2.29 | 1.43        | 1.50     |
| 15  | A     | 915 | 85I  | O7-C20  | -2.28 | 1.15        | 1.22     |
| 11  | A     | 907 | BCL  | CHB-C4A | -2.28 | 1.32        | 1.37     |
| 12  | a     | 915 | CLA  | C3A-C2A | -2.28 | 1.48        | 1.54     |
| 12  | a     | 915 | CLA  | O2A-CGA | 2.28  | 1.40        | 1.33     |
| 10  | A     | 901 | 2GO  | CHB-C4A | -2.28 | 1.33        | 1.38     |
| 11  | A     | 909 | BCL  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 11  | A     | 909 | BCL  | C3B-C4B | 2.27  | 1.45        | 1.41     |
| 12  | a     | 912 | CLA  | CHC-C4B | 2.27  | 1.44        | 1.39     |
| 11  | a     | 907 | BCL  | CAA-CBA | -2.26 | 1.46        | 1.52     |
| 11  | a     | 905 | BCL  | C3A-C2A | -2.26 | 1.48        | 1.54     |
| 11  | a     | 911 | BCL  | C2A-C1A | -2.26 | 1.47        | 1.52     |
| 11  | a     | 909 | BCL  | CMA-C3A | -2.25 | 1.48        | 1.53     |
| 13  | A     | 913 | LYC  | C55-C56 | -2.25 | 1.30        | 1.35     |
| 11  | a     | 907 | BCL  | CBA-CGA | -2.25 | 1.44        | 1.50     |
| 12  | A     | 911 | CLA  | CHC-C4B | 2.25  | 1.44        | 1.39     |
| 11  | a     | 906 | BCL  | C3A-C2A | -2.24 | 1.48        | 1.54     |
| 11  | a     | 907 | BCL  | C3A-C4A | -2.24 | 1.44        | 1.51     |
| 13  | A     | 913 | LYC  | C18-C17 | -2.24 | 1.46        | 1.50     |
| 10  | A     | 901 | 2GO  | C3B-C2B | -2.23 | 1.34        | 1.42     |
| 12  | a     | 914 | CLA  | CBD-CGD | -2.23 | 1.45        | 1.52     |
| 11  | A     | 904 | BCL  | C4D-CHA | 2.23  | 1.46        | 1.38     |
| 10  | A     | 901 | 2GO  | C1C-NC  | -2.22 | 1.34        | 1.38     |
| 11  | a     | 909 | BCL  | CHC-C4B | 2.22  | 1.44        | 1.39     |
| 11  | A     | 909 | BCL  | C9-C8   | -2.22 | 1.45        | 1.52     |
| 11  | A     | 903 | BCL  | CAA-CBA | -2.21 | 1.46        | 1.52     |
| 12  | A     | 933 | CLA  | C2-C3   | -2.21 | 1.28        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | A     | 906 | BCL  | O2A-C1  | -2.21 | 1.40        | 1.46     |
| 11  | A     | 908 | BCL  | CMC-C2C | -2.21 | 1.48        | 1.53     |
| 13  | c     | 201 | LYC  | C21-C20 | -2.20 | 1.30        | 1.36     |
| 11  | A     | 909 | BCL  | C2A-C1A | -2.20 | 1.47        | 1.52     |
| 11  | a     | 908 | BCL  | O2A-CGA | 2.20  | 1.39        | 1.33     |
| 13  | c     | 201 | LYC  | C14-C12 | -2.20 | 1.30        | 1.35     |
| 11  | A     | 908 | BCL  | CHD-C4C | 2.20  | 1.45        | 1.39     |
| 11  | A     | 904 | BCL  | C1D-ND  | -2.19 | 1.35        | 1.37     |
| 12  | a     | 912 | CLA  | C3D-C2D | 2.19  | 1.45        | 1.39     |
| 12  | a     | 915 | CLA  | MG-NB   | 2.19  | 2.10        | 2.05     |
| 11  | A     | 908 | BCL  | CHD-C1D | 2.19  | 1.42        | 1.38     |
| 13  | c     | 201 | LYC  | C18-C17 | -2.19 | 1.46        | 1.50     |
| 10  | a     | 903 | 2GO  | C3B-C2B | -2.19 | 1.35        | 1.42     |
| 11  | a     | 904 | BCL  | MG-NB   | 2.18  | 2.10        | 2.05     |
| 11  | a     | 909 | BCL  | C2-C3   | -2.18 | 1.28        | 1.33     |
| 11  | A     | 909 | BCL  | CBA-CGA | -2.18 | 1.44        | 1.50     |
| 11  | A     | 903 | BCL  | C2C-C3C | -2.17 | 1.48        | 1.54     |
| 12  | a     | 912 | CLA  | C2A-C1A | -2.17 | 1.47        | 1.52     |
| 12  | A     | 933 | CLA  | C3D-C2D | 2.16  | 1.44        | 1.39     |
| 12  | a     | 913 | CLA  | C3C-C2C | 2.15  | 1.41        | 1.36     |
| 11  | A     | 909 | BCL  | C2C-C3C | -2.15 | 1.48        | 1.54     |
| 11  | a     | 911 | BCL  | CAC-C3C | -2.15 | 1.49        | 1.54     |
| 12  | A     | 933 | CLA  | MG-NC   | 2.14  | 2.11        | 2.06     |
| 12  | A     | 933 | CLA  | MG-NB   | 2.14  | 2.10        | 2.05     |
| 11  | a     | 911 | BCL  | C3B-C4B | 2.14  | 1.45        | 1.41     |
| 12  | a     | 912 | CLA  | C4C-C3C | -2.14 | 1.41        | 1.45     |
| 11  | A     | 904 | BCL  | CHD-C1D | 2.14  | 1.42        | 1.38     |
| 11  | A     | 907 | BCL  | C1-C2   | 2.13  | 1.55        | 1.49     |
| 12  | A     | 912 | CLA  | CHD-C1D | 2.13  | 1.42        | 1.38     |
| 11  | a     | 909 | BCL  | CHB-C4A | -2.12 | 1.32        | 1.37     |
| 11  | A     | 906 | BCL  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 12  | a     | 901 | CLA  | O2A-C1  | -2.12 | 1.40        | 1.46     |
| 11  | A     | 903 | BCL  | CHB-C4A | -2.12 | 1.32        | 1.37     |
| 12  | a     | 914 | CLA  | O2D-CED | -2.11 | 1.40        | 1.45     |
| 11  | A     | 907 | BCL  | C7-C8   | 2.11  | 1.63        | 1.52     |
| 11  | a     | 909 | BCL  | CHD-C1D | 2.11  | 1.42        | 1.38     |
| 19  | E     | 101 | 84Q  | C-C1    | -2.11 | 1.40        | 1.51     |
| 12  | A     | 911 | CLA  | CHD-C4C | 2.10  | 1.44        | 1.39     |
| 11  | a     | 907 | BCL  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 11  | a     | 910 | BCL  | C4D-CHA | 2.09  | 1.45        | 1.38     |
| 11  | A     | 902 | BCL  | OBD-CAD | -2.09 | 1.18        | 1.22     |
| 11  | a     | 907 | BCL  | CBB-CAB | -2.09 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 12  | a     | 915 | CLA  | CBD-CAD | -2.09 | 1.47        | 1.56     |
| 13  | c     | 201 | LYC  | C63-C64 | -2.09 | 1.46        | 1.53     |
| 11  | a     | 904 | BCL  | CAC-C3C | -2.08 | 1.50        | 1.54     |
| 13  | c     | 201 | LYC  | C19-C17 | -2.08 | 1.31        | 1.35     |
| 11  | a     | 910 | BCL  | CHD-C4C | 2.08  | 1.45        | 1.39     |
| 11  | A     | 906 | BCL  | CHC-C4B | 2.08  | 1.44        | 1.39     |
| 11  | A     | 908 | BCL  | C5-C3   | -2.08 | 1.47        | 1.51     |
| 11  | a     | 908 | BCL  | C3C-C4C | -2.08 | 1.49        | 1.51     |
| 12  | a     | 914 | CLA  | CHD-C1D | 2.08  | 1.42        | 1.38     |
| 11  | A     | 907 | BCL  | C6-C7   | 2.08  | 1.60        | 1.52     |
| 11  | A     | 904 | BCL  | CHC-C1C | -2.07 | 1.32        | 1.37     |
| 18  | C     | 301 | HEC  | C4D-C3D | 2.07  | 1.48        | 1.44     |
| 11  | A     | 909 | BCL  | O2A-CGA | 2.07  | 1.39        | 1.33     |
| 10  | a     | 903 | 2GO  | ZN-ND   | 2.07  | 2.10        | 2.03     |
| 11  | A     | 908 | BCL  | CHC-C4B | 2.06  | 1.44        | 1.39     |
| 11  | A     | 904 | BCL  | C3D-C2D | 2.06  | 1.44        | 1.39     |
| 11  | A     | 905 | BCL  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 11  | A     | 904 | BCL  | CBA-CGA | -2.06 | 1.45        | 1.50     |
| 11  | a     | 911 | BCL  | CHD-C4C | 2.05  | 1.44        | 1.39     |
| 15  | A     | 915 | 85I  | C28-C27 | 2.05  | 1.62        | 1.51     |
| 11  | a     | 908 | BCL  | CMC-C2C | -2.05 | 1.48        | 1.53     |
| 12  | a     | 912 | CLA  | O1A-CGA | -2.05 | 1.16        | 1.22     |
| 12  | A     | 910 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 12  | a     | 915 | CLA  | CHD-C1D | 2.05  | 1.42        | 1.38     |
| 11  | A     | 904 | BCL  | CHB-C4A | -2.05 | 1.32        | 1.37     |
| 11  | A     | 905 | BCL  | C3B-C4B | 2.04  | 1.45        | 1.41     |
| 11  | a     | 905 | BCL  | CHC-C1C | -2.04 | 1.32        | 1.37     |
| 18  | C     | 301 | HEC  | C2A-C3A | 2.04  | 1.41        | 1.36     |
| 12  | A     | 911 | CLA  | C2A-C1A | -2.03 | 1.47        | 1.52     |
| 11  | A     | 908 | BCL  | CBB-CAB | -2.03 | 1.46        | 1.50     |
| 11  | A     | 907 | BCL  | C3A-C4A | -2.03 | 1.45        | 1.51     |
| 12  | A     | 912 | CLA  | C3A-C2A | -2.02 | 1.49        | 1.54     |
| 12  | A     | 933 | CLA  | CHC-C4B | 2.02  | 1.43        | 1.39     |
| 11  | a     | 908 | BCL  | C3B-C4B | 2.01  | 1.45        | 1.41     |
| 12  | A     | 931 | CLA  | CBD-CAD | -2.00 | 1.47        | 1.56     |

All (1088) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A     | 909 | BCL  | O2D-CGD-CBD | 21.23 | 148.34      | 111.23   |
| 11  | A     | 906 | BCL  | O2D-CGD-CBD | 18.55 | 143.66      | 111.23   |
| 11  | a     | 908 | BCL  | C4A-NA-C1A  | 18.53 | 115.13      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 12  | A     | 931 | CLA  | O2D-CGD-CBD | 18.40  | 143.39      | 111.23   |
| 11  | a     | 907 | BCL  | C4A-NA-C1A  | 16.33  | 114.13      | 106.68   |
| 12  | a     | 913 | CLA  | C1D-ND-C4D  | -15.86 | 95.18       | 106.31   |
| 11  | a     | 909 | BCL  | O2D-CGD-CBD | 15.58  | 138.47      | 111.23   |
| 11  | A     | 906 | BCL  | O2D-CGD-O1D | -15.57 | 93.54       | 123.85   |
| 11  | A     | 905 | BCL  | O2D-CGD-CBD | 15.05  | 137.54      | 111.23   |
| 13  | c     | 201 | LYC  | C21-C50-C51 | 15.00  | 148.32      | 127.28   |
| 11  | A     | 907 | BCL  | O2D-CGD-CBD | 14.77  | 137.06      | 111.23   |
| 11  | A     | 903 | BCL  | O2D-CGD-CBD | 14.59  | 136.73      | 111.23   |
| 11  | A     | 907 | BCL  | C4A-NA-C1A  | 14.39  | 113.25      | 106.68   |
| 12  | a     | 913 | CLA  | O2D-CGD-CBD | 14.37  | 136.34      | 111.23   |
| 11  | a     | 910 | BCL  | O2D-CGD-CBD | 14.19  | 136.04      | 111.23   |
| 11  | a     | 904 | BCL  | O2D-CGD-CBD | 14.05  | 135.79      | 111.23   |
| 11  | a     | 905 | BCL  | O2D-CGD-CBD | 13.97  | 135.66      | 111.23   |
| 12  | A     | 912 | CLA  | C2C-C1C-NC  | 13.41  | 124.07      | 109.98   |
| 11  | a     | 908 | BCL  | O2D-CGD-CBD | 13.20  | 134.31      | 111.23   |
| 12  | a     | 913 | CLA  | O2D-CGD-O1D | -13.19 | 98.18       | 123.85   |
| 13  | c     | 201 | LYC  | C53-C51-C50 | 13.17  | 139.72      | 119.01   |
| 11  | a     | 910 | BCL  | C1C-NC-C4C  | 13.06  | 112.64      | 106.68   |
| 15  | A     | 917 | 85I  | O4-C4-C3    | 12.72  | 142.19      | 109.54   |
| 11  | A     | 902 | BCL  | O2D-CGD-CBD | 12.67  | 133.38      | 111.23   |
| 11  | A     | 903 | BCL  | O2D-CGD-O1D | -12.47 | 99.57       | 123.85   |
| 10  | A     | 901 | 2GO  | CMA-C3A-C4A | -12.29 | 105.83      | 125.03   |
| 10  | a     | 903 | 2GO  | CMA-C3A-C4A | -12.12 | 106.10      | 125.03   |
| 13  | c     | 201 | LYC  | C15-C14-C12 | 12.04  | 144.16      | 127.28   |
| 11  | a     | 907 | BCL  | O2D-CGD-CBD | 12.02  | 132.25      | 111.23   |
| 12  | A     | 931 | CLA  | O2D-CGD-O1D | -11.97 | 100.55      | 123.85   |
| 12  | a     | 914 | CLA  | C3B-C4B-NB  | 11.83  | 121.09      | 110.53   |
| 15  | A     | 916 | 85I  | O4-C4-C3    | 11.67  | 139.49      | 109.54   |
| 12  | A     | 911 | CLA  | C1D-ND-C4D  | -11.66 | 98.13       | 106.31   |
| 11  | A     | 909 | BCL  | O2A-CGA-CBA | 11.17  | 145.89      | 111.83   |
| 11  | a     | 908 | BCL  | CBA-CAA-C2A | -11.11 | 80.73       | 113.79   |
| 18  | C     | 301 | HEC  | CBB-CAB-C3B | -11.04 | 105.38      | 127.43   |
| 10  | A     | 901 | 2GO  | C4A-C3A-C2A | -10.97 | 95.44       | 106.98   |
| 11  | a     | 910 | BCL  | O2A-CGA-CBA | 10.93  | 145.16      | 111.83   |
| 12  | A     | 933 | CLA  | O2D-CGD-CBD | 10.90  | 130.29      | 111.23   |
| 11  | a     | 909 | BCL  | O2D-CGD-O1D | -10.89 | 102.65      | 123.85   |
| 15  | A     | 917 | 85I  | P-O3-C3     | 10.78  | 161.93      | 120.93   |
| 11  | a     | 907 | BCL  | C1C-NC-C4C  | -10.72 | 101.79      | 106.68   |
| 12  | a     | 901 | CLA  | O2D-CGD-CBD | 10.61  | 129.78      | 111.23   |
| 12  | A     | 933 | CLA  | O2D-CGD-O1D | -10.60 | 103.22      | 123.85   |
| 11  | a     | 905 | BCL  | O2D-CGD-O1D | -10.56 | 103.29      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 11  | A     | 909 | BCL  | O1D-CGD-CBD | -10.53 | 103.75      | 124.52   |
| 13  | c     | 201 | LYC  | C20-C19-C17 | 10.52  | 142.03      | 127.28   |
| 12  | a     | 915 | CLA  | O2D-CGD-CBD | 10.50  | 129.59      | 111.23   |
| 13  | c     | 201 | LYC  | C21-C20-C19 | 10.47  | 144.94      | 123.52   |
| 11  | A     | 907 | BCL  | C6-C5-C3    | 10.31  | 138.58      | 113.47   |
| 11  | A     | 908 | BCL  | O2D-CGD-CBD | 10.27  | 129.19      | 111.23   |
| 11  | A     | 907 | BCL  | O2D-CGD-O1D | -10.26 | 103.87      | 123.85   |
| 12  | a     | 914 | CLA  | O2D-CGD-CBD | 10.25  | 129.14      | 111.23   |
| 15  | a     | 920 | 85I  | O4-C4-C3    | 10.19  | 135.69      | 109.54   |
| 11  | A     | 906 | BCL  | C2D-C1D-ND  | 9.86   | 119.89      | 110.13   |
| 11  | a     | 910 | BCL  | O2A-CGA-O1A | -9.82  | 99.07       | 123.63   |
| 11  | a     | 908 | BCL  | O2D-CGD-O1D | -9.79  | 104.80      | 123.85   |
| 11  | a     | 909 | BCL  | C4A-NA-C1A  | 9.78   | 111.14      | 106.68   |
| 12  | A     | 931 | CLA  | CED-O2D-CGD | 9.65   | 137.80      | 115.92   |
| 11  | A     | 907 | BCL  | O2A-CGA-CBA | 9.61   | 141.15      | 111.83   |
| 11  | A     | 906 | BCL  | C4A-NA-C1A  | 9.59   | 111.06      | 106.68   |
| 12  | A     | 931 | CLA  | C3B-C2B-C1B | -9.55  | 95.92       | 107.17   |
| 15  | a     | 918 | 85I  | O4-C4-C3    | 9.53   | 134.01      | 109.54   |
| 12  | A     | 931 | CLA  | C1D-ND-C4D  | 9.46   | 112.95      | 106.31   |
| 11  | a     | 908 | BCL  | C1-C2-C3    | 9.42   | 141.63      | 126.20   |
| 11  | A     | 905 | BCL  | O2D-CGD-O1D | -9.39  | 105.57      | 123.85   |
| 11  | a     | 904 | BCL  | C4A-NA-C1A  | 9.38   | 110.96      | 106.68   |
| 11  | a     | 904 | BCL  | O2D-CGD-O1D | -9.32  | 105.70      | 123.85   |
| 11  | a     | 906 | BCL  | CMD-C2D-C1D | 9.32   | 141.14      | 124.73   |
| 11  | a     | 909 | BCL  | C1-C2-C3    | 9.28   | 141.40      | 126.20   |
| 17  | A     | 932 | 85N  | C18-O3-C17  | 9.26   | 133.48      | 113.83   |
| 11  | a     | 910 | BCL  | C1-O2A-CGA  | 9.19   | 138.90      | 116.65   |
| 12  | A     | 910 | CLA  | O2D-CGD-CBD | 9.13   | 127.19      | 111.23   |
| 11  | A     | 902 | BCL  | C1-O2A-CGA  | 9.12   | 138.74      | 116.65   |
| 11  | A     | 906 | BCL  | C3D-C2D-C1D | -9.06  | 93.47       | 105.83   |
| 11  | A     | 906 | BCL  | CHD-C1D-ND  | -9.05  | 112.06      | 124.80   |
| 11  | A     | 903 | BCL  | O2A-CGA-CBA | 9.03   | 139.35      | 111.83   |
| 12  | a     | 912 | CLA  | O2D-CGD-O1D | -9.01  | 106.30      | 123.85   |
| 11  | a     | 911 | BCL  | C3D-C2D-C1D | -8.94  | 93.64       | 105.83   |
| 10  | A     | 901 | 2GO  | C1A-NA-C4A  | 8.85   | 120.05      | 106.80   |
| 11  | A     | 907 | BCL  | C3D-C2D-C1D | -8.80  | 93.82       | 105.83   |
| 11  | a     | 911 | BCL  | C2D-C1D-ND  | 8.78   | 118.82      | 110.13   |
| 11  | A     | 906 | BCL  | C1D-ND-C4D  | -8.73  | 100.19      | 106.31   |
| 15  | A     | 915 | 85I  | P-O3-C3     | 8.69   | 154.00      | 120.93   |
| 18  | c     | 202 | HEC  | CBB-CAB-C3B | -8.67  | 110.11      | 127.43   |
| 12  | A     | 933 | CLA  | C3B-C2B-C1B | -8.63  | 97.00       | 107.17   |
| 12  | A     | 933 | CLA  | C4-C3-C5    | 8.61   | 126.27      | 116.13   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A     | 903 | BCL  | CMD-C2D-C1D | 8.54  | 139.77      | 124.73   |
| 11  | A     | 907 | BCL  | C7-C6-C5    | 8.53  | 136.00      | 113.26   |
| 12  | A     | 912 | CLA  | C3C-C4C-NC  | 8.51  | 121.33      | 110.43   |
| 12  | a     | 901 | CLA  | C1D-ND-C4D  | -8.51 | 100.34      | 106.31   |
| 10  | A     | 901 | 2GO  | CAC-C3C-C2C | -8.50 | 111.94      | 127.56   |
| 12  | a     | 901 | CLA  | O2A-CGA-CBA | 8.48  | 137.70      | 111.83   |
| 11  | a     | 905 | BCL  | O2A-CGA-CBA | 8.45  | 137.61      | 111.83   |
| 15  | A     | 915 | 85I  | O6-C3-C4    | -8.41 | 75.44       | 107.08   |
| 11  | A     | 909 | BCL  | O2D-CGD-O1D | -8.32 | 107.65      | 123.85   |
| 11  | a     | 911 | BCL  | C1-C2-C3    | 8.28  | 139.77      | 126.20   |
| 11  | A     | 905 | BCL  | CMD-C2D-C1D | 8.23  | 139.22      | 124.73   |
| 12  | A     | 933 | CLA  | CED-O2D-CGD | 8.23  | 134.59      | 115.92   |
| 11  | a     | 911 | BCL  | C1-O2A-CGA  | 8.21  | 136.52      | 116.65   |
| 11  | a     | 910 | BCL  | O2D-CGD-O1D | -8.21 | 107.87      | 123.85   |
| 12  | A     | 910 | CLA  | C2C-C1C-NC  | 8.20  | 118.60      | 109.98   |
| 12  | A     | 912 | CLA  | C3B-C2B-C1B | -8.19 | 97.52       | 107.17   |
| 11  | A     | 908 | BCL  | C2B-C1B-NB  | 8.19  | 118.81      | 110.33   |
| 15  | A     | 915 | 85I  | O4-C4-C3    | 8.13  | 130.42      | 109.54   |
| 11  | A     | 905 | BCL  | C3D-C2D-C1D | -8.13 | 94.73       | 105.83   |
| 10  | a     | 903 | 2GO  | C4C-C3C-C2C | -8.08 | 95.13       | 106.89   |
| 11  | A     | 904 | BCL  | C1C-NC-C4C  | -8.06 | 103.00      | 106.68   |
| 15  | a     | 919 | 85I  | O3-C3-C4    | 8.06  | 137.40      | 107.08   |
| 11  | A     | 907 | BCL  | C1C-NC-C4C  | -8.06 | 103.00      | 106.68   |
| 12  | A     | 911 | CLA  | C3C-C4C-NC  | 8.05  | 120.74      | 110.43   |
| 12  | A     | 910 | CLA  | CMD-C2D-C1D | 8.03  | 138.88      | 124.73   |
| 11  | A     | 907 | BCL  | CMD-C2D-C1D | 7.98  | 138.78      | 124.73   |
| 11  | a     | 909 | BCL  | CMD-C2D-C1D | 7.97  | 138.76      | 124.73   |
| 12  | A     | 931 | CLA  | C2D-C1D-ND  | -7.96 | 102.25      | 110.13   |
| 12  | A     | 933 | CLA  | CMB-C2B-C1B | 7.96  | 137.53      | 125.42   |
| 11  | A     | 909 | BCL  | O2A-C1-C2   | 7.95  | 138.71      | 108.11   |
| 11  | A     | 907 | BCL  | C1-O2A-CGA  | 7.95  | 135.90      | 116.65   |
| 15  | A     | 916 | 85I  | P-O3-C3     | 7.92  | 151.08      | 120.93   |
| 12  | a     | 901 | CLA  | C3C-C4C-NC  | 7.92  | 120.57      | 110.43   |
| 12  | a     | 915 | CLA  | O2D-CGD-O1D | -7.87 | 108.53      | 123.85   |
| 12  | a     | 913 | CLA  | CMD-C2D-C1D | 7.86  | 138.57      | 124.73   |
| 12  | a     | 914 | CLA  | O2D-CGD-O1D | -7.85 | 108.58      | 123.85   |
| 11  | a     | 908 | BCL  | OBb-CAB-CBB | -7.83 | 102.22      | 119.77   |
| 12  | A     | 931 | CLA  | CMC-C2C-C1C | 7.83  | 137.26      | 125.03   |
| 11  | A     | 904 | BCL  | CMD-C2D-C1D | 7.82  | 138.50      | 124.73   |
| 11  | a     | 909 | BCL  | O2A-CGA-O1A | -7.81 | 104.08      | 123.63   |
| 13  | c     | 201 | LYC  | C13-C12-C14 | -7.77 | 110.23      | 122.82   |
| 12  | A     | 911 | CLA  | C2C-C1C-NC  | 7.77  | 118.14      | 109.98   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | A     | 931 | CLA  | C4A-NA-C1A  | 7.73  | 110.21      | 106.68   |
| 13  | A     | 913 | LYC  | C10-C9-C7   | -7.73 | 116.82      | 127.69   |
| 12  | a     | 901 | CLA  | C6-C7-C8    | 7.73  | 141.65      | 115.97   |
| 11  | a     | 910 | BCL  | C1-C2-C3    | -7.67 | 113.63      | 126.20   |
| 11  | a     | 910 | BCL  | C4A-NA-C1A  | -7.66 | 103.19      | 106.68   |
| 11  | a     | 905 | BCL  | CMD-C2D-C1D | 7.62  | 138.16      | 124.73   |
| 12  | A     | 933 | CLA  | C4A-NA-C1A  | 7.62  | 110.15      | 106.68   |
| 15  | a     | 920 | 85I  | O6-C3-C4    | 7.60  | 135.66      | 107.08   |
| 15  | a     | 919 | 85I  | P-O3-C3     | 7.60  | 149.84      | 120.93   |
| 13  | c     | 201 | LYC  | C16-C17-C19 | 7.60  | 130.96      | 119.01   |
| 11  | a     | 907 | BCL  | C1-C2-C3    | -7.59 | 113.76      | 126.20   |
| 12  | A     | 911 | CLA  | C4A-NA-C1A  | 7.56  | 110.13      | 106.68   |
| 11  | a     | 908 | BCL  | C3A-C2A-C1A | 7.52  | 112.60      | 101.34   |
| 13  | c     | 201 | LYC  | C15-C16-C17 | 7.50  | 146.92      | 126.36   |
| 12  | a     | 912 | CLA  | C2B-C1B-NB  | 7.49  | 118.09      | 110.33   |
| 12  | A     | 931 | CLA  | C1-O2A-CGA  | 7.46  | 134.72      | 116.65   |
| 12  | a     | 912 | CLA  | C1D-ND-C4D  | -7.42 | 101.10      | 106.31   |
| 11  | A     | 905 | BCL  | C4A-NA-C1A  | 7.40  | 110.06      | 106.68   |
| 11  | a     | 911 | BCL  | O2A-CGA-CBA | 7.37  | 134.30      | 111.83   |
| 11  | A     | 907 | BCL  | C1-C2-C3    | 7.37  | 138.27      | 126.20   |
| 11  | A     | 903 | BCL  | C1-O2A-CGA  | 7.36  | 134.47      | 116.65   |
| 11  | a     | 905 | BCL  | C3D-C2D-C1D | -7.36 | 95.79       | 105.83   |
| 12  | A     | 933 | CLA  | C2B-C1B-NB  | 7.29  | 117.89      | 110.33   |
| 12  | A     | 910 | CLA  | C1D-ND-C4D  | -7.29 | 101.20      | 106.31   |
| 11  | A     | 909 | BCL  | C4A-NA-C1A  | -7.27 | 103.36      | 106.68   |
| 12  | a     | 912 | CLA  | O2D-CGD-CBD | 7.27  | 123.93      | 111.23   |
| 11  | A     | 905 | BCL  | CBA-CAA-C2A | -7.19 | 92.40       | 113.79   |
| 11  | A     | 907 | BCL  | CED-O2D-CGD | 7.19  | 132.22      | 115.92   |
| 12  | A     | 912 | CLA  | C1D-ND-C4D  | -7.17 | 101.28      | 106.31   |
| 12  | A     | 912 | CLA  | C1C-C2C-C3C | -7.16 | 99.45       | 106.98   |
| 11  | a     | 908 | BCL  | C3D-C2D-C1D | -7.15 | 96.07       | 105.83   |
| 12  | A     | 912 | CLA  | O2D-CGD-O1D | -7.15 | 109.94      | 123.85   |
| 12  | a     | 901 | CLA  | C11-C10-C8  | -7.09 | 92.41       | 115.97   |
| 12  | a     | 912 | CLA  | CMD-C2D-C1D | 7.07  | 137.18      | 124.73   |
| 10  | A     | 901 | 2GO  | C1C-NC-C4C  | 7.01  | 115.78      | 106.47   |
| 11  | A     | 909 | BCL  | C3D-C2D-C1D | -7.00 | 96.28       | 105.83   |
| 12  | A     | 911 | CLA  | CMD-C2D-C1D | 6.99  | 137.04      | 124.73   |
| 11  | a     | 906 | BCL  | C3D-C2D-C1D | -6.99 | 96.30       | 105.83   |
| 12  | a     | 913 | CLA  | C11-C10-C8  | -6.98 | 92.78       | 115.97   |
| 11  | a     | 906 | BCL  | C2B-C1B-NB  | 6.97  | 117.55      | 110.33   |
| 11  | a     | 904 | BCL  | O2A-CGA-CBA | 6.97  | 133.07      | 111.83   |
| 18  | c     | 202 | HEC  | O2A-CGA-O1A | -6.95 | 105.45      | 123.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | E     | 101 | 84Q  | O1-C15-C16  | 6.95  | 127.38      | 109.54   |
| 13  | c     | 201 | LYC  | C18-C17-C16 | -6.95 | 107.48      | 118.09   |
| 11  | a     | 905 | BCL  | C2B-C1B-NB  | 6.94  | 117.52      | 110.33   |
| 12  | A     | 911 | CLA  | CHD-C4C-C3C | -6.87 | 114.76      | 124.77   |
| 11  | A     | 903 | BCL  | O1A-CGA-CBA | -6.84 | 97.03       | 123.78   |
| 12  | a     | 913 | CLA  | C3D-C2D-C1D | -6.84 | 96.50       | 105.83   |
| 11  | A     | 905 | BCL  | C2B-C1B-NB  | 6.84  | 117.42      | 110.33   |
| 12  | a     | 901 | CLA  | CMD-C2D-C1D | 6.83  | 136.76      | 124.73   |
| 11  | A     | 902 | BCL  | O2D-CGD-O1D | -6.80 | 110.61      | 123.85   |
| 10  | a     | 903 | 2GO  | CHA-CBD-CAD | -6.78 | 100.71      | 107.06   |
| 12  | a     | 912 | CLA  | C3B-C4B-NB  | 6.75  | 116.56      | 110.53   |
| 11  | A     | 905 | BCL  | C3A-C2A-C1A | 6.75  | 111.44      | 101.34   |
| 11  | a     | 911 | BCL  | CED-O2D-CGD | 6.74  | 131.20      | 115.92   |
| 12  | A     | 931 | CLA  | CHD-C4C-C3C | -6.74 | 114.95      | 124.77   |
| 12  | a     | 913 | CLA  | C3B-C2B-C1B | -6.73 | 99.24       | 107.17   |
| 12  | a     | 914 | CLA  | C2B-C1B-NB  | 6.66  | 117.23      | 110.33   |
| 12  | A     | 912 | CLA  | O2D-CGD-CBD | 6.66  | 122.87      | 111.23   |
| 11  | a     | 908 | BCL  | CMD-C2D-C1D | 6.65  | 136.45      | 124.73   |
| 12  | A     | 933 | CLA  | C3B-C4B-NB  | 6.65  | 116.47      | 110.53   |
| 13  | c     | 201 | LYC  | C52-C51-C50 | -6.63 | 112.08      | 122.82   |
| 11  | A     | 904 | BCL  | C3D-C2D-C1D | -6.62 | 96.79       | 105.83   |
| 11  | a     | 908 | BCL  | OBB-CAB-C3B | 6.56  | 132.02      | 120.43   |
| 12  | a     | 901 | CLA  | C2C-C1C-NC  | 6.56  | 116.87      | 109.98   |
| 12  | a     | 912 | CLA  | C3B-C2B-C1B | -6.55 | 99.45       | 107.17   |
| 12  | A     | 911 | CLA  | C3D-C2D-C1D | -6.54 | 96.91       | 105.83   |
| 11  | A     | 902 | BCL  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 10  | a     | 903 | 2GO  | C1A-NA-C4A  | 6.52  | 116.56      | 106.80   |
| 11  | A     | 909 | BCL  | C2B-C1B-NB  | 6.50  | 117.07      | 110.33   |
| 11  | a     | 907 | BCL  | O2D-CGD-O1D | -6.49 | 111.21      | 123.85   |
| 10  | a     | 903 | 2GO  | CAC-C3C-C4C | -6.48 | 116.36      | 124.79   |
| 12  | a     | 912 | CLA  | O2A-CGA-CBA | 6.48  | 131.59      | 111.83   |
| 12  | a     | 914 | CLA  | CHD-C4C-C3C | -6.48 | 115.33      | 124.77   |
| 11  | a     | 911 | BCL  | CMD-C2D-C1D | 6.48  | 136.13      | 124.73   |
| 13  | c     | 201 | LYC  | C52-C51-C53 | -6.47 | 108.20      | 118.09   |
| 12  | A     | 912 | CLA  | CAC-C3C-C4C | 6.47  | 133.21      | 124.79   |
| 11  | a     | 904 | BCL  | CED-O2D-CGD | 6.43  | 130.50      | 115.92   |
| 11  | A     | 905 | BCL  | CAA-C2A-C3A | -6.42 | 95.66       | 113.00   |
| 12  | a     | 915 | CLA  | C4-C3-C5    | 6.40  | 123.67      | 116.13   |
| 10  | a     | 903 | 2GO  | C1A-C2A-C3A | -6.39 | 98.20       | 106.63   |
| 11  | a     | 907 | BCL  | CBA-CAA-C2A | -6.38 | 94.82       | 113.79   |
| 11  | a     | 910 | BCL  | O2A-C1-C2   | 6.37  | 132.62      | 108.11   |
| 11  | a     | 905 | BCL  | C4A-NA-C1A  | 6.36  | 109.58      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A     | 905 | BCL  | C1D-ND-C4D  | -6.36 | 101.85      | 106.31   |
| 11  | A     | 905 | BCL  | C2D-C1D-ND  | 6.31  | 116.37      | 110.13   |
| 13  | c     | 201 | LYC  | C20-C21-C50 | -6.31 | 110.61      | 123.52   |
| 12  | A     | 912 | CLA  | CMA-C3A-C4A | 6.31  | 128.73      | 111.77   |
| 11  | a     | 911 | BCL  | O2D-CGD-CBD | 6.30  | 122.25      | 111.23   |
| 11  | a     | 905 | BCL  | CHD-C1D-ND  | -6.30 | 115.93      | 124.80   |
| 12  | a     | 915 | CLA  | CMB-C2B-C1B | 6.29  | 134.99      | 125.42   |
| 12  | a     | 915 | CLA  | C4A-NA-C1A  | -6.28 | 103.81      | 106.68   |
| 12  | a     | 901 | CLA  | C2B-C1B-NB  | 6.25  | 116.80      | 110.33   |
| 11  | A     | 903 | BCL  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 12  | A     | 933 | CLA  | C3D-C2D-C1D | -6.24 | 97.31       | 105.83   |
| 12  | a     | 915 | CLA  | CMD-C2D-C1D | 6.23  | 135.70      | 124.73   |
| 12  | A     | 910 | CLA  | O2D-CGD-O1D | -6.23 | 111.73      | 123.85   |
| 11  | a     | 909 | BCL  | C1-O2A-CGA  | 6.23  | 131.72      | 116.65   |
| 11  | a     | 905 | BCL  | C4-C3-C2    | -6.22 | 107.65      | 123.63   |
| 11  | A     | 907 | BCL  | O1A-CGA-CBA | -6.21 | 99.48       | 123.78   |
| 13  | c     | 201 | LYC  | C11-C12-C14 | 6.20  | 128.77      | 119.01   |
| 12  | a     | 913 | CLA  | CAC-C3C-C4C | 6.20  | 132.86      | 124.79   |
| 11  | A     | 909 | BCL  | C4-C3-C5    | -6.20 | 104.47      | 115.23   |
| 11  | a     | 909 | BCL  | CHD-C1D-ND  | -6.20 | 116.08      | 124.80   |
| 11  | A     | 907 | BCL  | C2D-C1D-ND  | 6.20  | 116.26      | 110.13   |
| 11  | A     | 905 | BCL  | CHD-C1D-ND  | -6.14 | 116.16      | 124.80   |
| 12  | a     | 914 | CLA  | C3C-C4C-NC  | 6.13  | 118.29      | 110.43   |
| 11  | a     | 911 | BCL  | C1C-NC-C4C  | 6.13  | 109.48      | 106.68   |
| 11  | a     | 905 | BCL  | CMB-C2B-C1B | 6.13  | 134.75      | 125.42   |
| 10  | A     | 901 | 2GO  | CMC-C2C-C1C | -6.13 | 115.46      | 125.03   |
| 11  | A     | 906 | BCL  | OBB-CAB-C3B | 6.13  | 131.27      | 120.43   |
| 12  | a     | 901 | CLA  | CHD-C4C-C3C | -6.12 | 115.85      | 124.77   |
| 12  | A     | 911 | CLA  | C4C-C3C-C2C | -6.11 | 98.00       | 106.89   |
| 11  | a     | 910 | BCL  | CMD-C2D-C1D | 6.09  | 135.44      | 124.73   |
| 11  | a     | 904 | BCL  | CMD-C2D-C1D | 6.06  | 135.40      | 124.73   |
| 12  | a     | 914 | CLA  | C4B-C3B-C2B | -6.05 | 99.78       | 107.30   |
| 11  | A     | 903 | BCL  | CBB-CAB-C3B | 6.04  | 133.15      | 120.40   |
| 12  | a     | 912 | CLA  | CMB-C2B-C1B | 6.04  | 134.61      | 125.42   |
| 11  | A     | 902 | BCL  | C2B-C1B-NB  | 6.01  | 116.56      | 110.33   |
| 12  | a     | 901 | CLA  | O2D-CGD-O1D | -5.99 | 112.19      | 123.85   |
| 11  | A     | 904 | BCL  | CMB-C2B-C1B | 5.98  | 134.52      | 125.42   |
| 12  | A     | 911 | CLA  | C3B-C2B-C1B | -5.98 | 100.12      | 107.17   |
| 11  | a     | 907 | BCL  | C16-C15-C13 | -5.97 | 96.12       | 115.97   |
| 11  | a     | 904 | BCL  | CHD-C1D-ND  | -5.97 | 116.40      | 124.80   |
| 12  | A     | 931 | CLA  | O2A-CGA-CBA | 5.97  | 130.04      | 111.83   |
| 11  | A     | 902 | BCL  | CMD-C2D-C1D | 5.96  | 135.23      | 124.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | A     | 901 | 2GO  | C4D-ND-C1D  | 5.94  | 116.86      | 106.68   |
| 11  | a     | 907 | BCL  | CMD-C2D-C1D | 5.94  | 135.19      | 124.73   |
| 10  | A     | 901 | 2GO  | C2B-C1B-NB  | -5.91 | 101.61      | 109.02   |
| 11  | A     | 906 | BCL  | O2A-CGA-O1A | -5.90 | 108.86      | 123.63   |
| 10  | a     | 903 | 2GO  | CMC-C2C-C1C | -5.90 | 115.82      | 125.03   |
| 11  | A     | 909 | BCL  | C1C-NC-C4C  | 5.89  | 109.36      | 106.68   |
| 11  | a     | 908 | BCL  | C2A-C3A-C4A | -5.88 | 92.37       | 101.87   |
| 11  | a     | 909 | BCL  | C4-C3-C2    | -5.88 | 108.53      | 123.63   |
| 11  | A     | 907 | BCL  | C4-C3-C2    | -5.87 | 108.55      | 123.63   |
| 11  | a     | 904 | BCL  | C3C-C4C-CHD | -5.85 | 111.06      | 123.39   |
| 11  | A     | 909 | BCL  | CMD-C2D-C1D | 5.84  | 135.02      | 124.73   |
| 10  | a     | 903 | 2GO  | C16-C15-C13 | 5.84  | 135.38      | 115.97   |
| 12  | a     | 915 | CLA  | O2A-CGA-O1A | -5.84 | 109.02      | 123.63   |
| 11  | A     | 906 | BCL  | CED-O2D-CGD | 5.83  | 129.14      | 115.92   |
| 10  | A     | 901 | 2GO  | CAC-C3C-C4C | -5.83 | 117.20      | 124.79   |
| 13  | A     | 913 | LYC  | C59-C60-C61 | 5.82  | 135.88      | 127.69   |
| 11  | a     | 904 | BCL  | C1-C2-C3    | -5.80 | 116.69      | 126.20   |
| 11  | A     | 909 | BCL  | O2A-CGA-O1A | -5.80 | 109.12      | 123.63   |
| 18  | c     | 202 | HEC  | CBC-CAC-C3C | -5.80 | 115.85      | 127.43   |
| 11  | a     | 906 | BCL  | CAC-C3C-C4C | -5.78 | 99.76       | 112.58   |
| 15  | a     | 920 | 85I  | P-O3-C3     | -5.78 | 98.96       | 120.93   |
| 11  | a     | 910 | BCL  | CED-O2D-CGD | 5.77  | 129.01      | 115.92   |
| 18  | C     | 301 | HEC  | C4C-NC-C1C  | 5.73  | 115.17      | 105.82   |
| 12  | a     | 912 | CLA  | CED-O2D-CGD | 5.71  | 128.86      | 115.92   |
| 12  | a     | 912 | CLA  | C2C-C1C-NC  | 5.70  | 115.96      | 109.98   |
| 11  | A     | 903 | BCL  | O2A-C1-C2   | 5.69  | 130.02      | 108.11   |
| 19  | E     | 101 | 84Q  | P-O4-C16    | 5.69  | 142.59      | 120.93   |
| 11  | a     | 905 | BCL  | CED-O2D-CGD | 5.69  | 128.83      | 115.92   |
| 12  | a     | 915 | CLA  | C3D-C2D-C1D | -5.65 | 98.12       | 105.83   |
| 11  | a     | 905 | BCL  | C1-C2-C3    | 5.64  | 135.43      | 126.20   |
| 12  | A     | 931 | CLA  | C2C-C1C-NC  | 5.64  | 115.90      | 109.98   |
| 10  | A     | 901 | 2GO  | C2D-C1D-ND  | -5.64 | 101.77      | 110.35   |
| 11  | A     | 902 | BCL  | C3C-C4C-CHD | -5.62 | 111.54      | 123.39   |
| 11  | a     | 909 | BCL  | C3D-C2D-C1D | -5.61 | 98.17       | 105.83   |
| 18  | C     | 301 | HEC  | C1D-C2D-C3D | -5.60 | 100.41      | 106.82   |
| 11  | A     | 909 | BCL  | C9-C8-C10   | -5.58 | 91.39       | 111.27   |
| 11  | a     | 911 | BCL  | O2A-C1-C2   | 5.57  | 129.53      | 108.11   |
| 11  | A     | 906 | BCL  | C1-O2A-CGA  | 5.55  | 130.10      | 116.65   |
| 12  | a     | 901 | CLA  | C4C-C3C-C2C | -5.55 | 98.81       | 106.89   |
| 12  | A     | 912 | CLA  | C4A-NA-C1A  | 5.51  | 109.19      | 106.68   |
| 12  | a     | 901 | CLA  | C3B-C2B-C1B | -5.51 | 100.68      | 107.17   |
| 12  | a     | 914 | CLA  | CED-O2D-CGD | 5.49  | 128.38      | 115.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | a     | 915 | CLA  | C3B-C4B-NB  | 5.49  | 115.43      | 110.53   |
| 12  | a     | 915 | CLA  | C3C-C4C-NC  | 5.49  | 117.46      | 110.43   |
| 13  | A     | 913 | LYC  | C18-C17-C19 | -5.48 | 113.94      | 122.82   |
| 11  | a     | 906 | BCL  | C1C-NC-C4C  | -5.48 | 104.18      | 106.68   |
| 11  | A     | 905 | BCL  | CAA-C2A-C1A | -5.46 | 94.09       | 111.97   |
| 11  | A     | 904 | BCL  | C4A-NA-C1A  | 5.46  | 109.17      | 106.68   |
| 11  | A     | 905 | BCL  | C1C-NC-C4C  | 5.45  | 109.17      | 106.68   |
| 11  | A     | 903 | BCL  | CHD-C1D-ND  | -5.44 | 117.14      | 124.80   |
| 10  | A     | 901 | 2GO  | C1B-NB-C4B  | 5.43  | 114.60      | 106.52   |
| 10  | A     | 901 | 2GO  | C1-O2A-CGA  | 5.43  | 129.78      | 116.65   |
| 12  | A     | 910 | CLA  | C1C-C2C-C3C | -5.41 | 101.29      | 106.98   |
| 11  | a     | 909 | BCL  | O2A-C1-C2   | -5.40 | 87.33       | 108.11   |
| 12  | A     | 911 | CLA  | O2D-CGD-O1D | -5.39 | 113.35      | 123.85   |
| 13  | c     | 201 | LYC  | C1-C2-C4    | -5.39 | 106.48      | 122.66   |
| 12  | A     | 931 | CLA  | C2B-C1B-NB  | 5.39  | 115.91      | 110.33   |
| 12  | a     | 915 | CLA  | CMC-C2C-C1C | 5.39  | 133.45      | 125.03   |
| 18  | c     | 202 | HEC  | O2A-CGA-CBA | 5.38  | 131.00      | 114.00   |
| 12  | A     | 911 | CLA  | O2A-CGA-CBA | 5.37  | 128.21      | 111.83   |
| 13  | c     | 201 | LYC  | C14-C15-C16 | -5.36 | 107.67      | 123.20   |
| 11  | a     | 906 | BCL  | C3C-C4C-CHD | -5.35 | 112.10      | 123.39   |
| 11  | a     | 908 | BCL  | CAA-C2A-C1A | -5.34 | 94.47       | 111.97   |
| 12  | a     | 915 | CLA  | O2A-CGA-CBA | 5.34  | 128.12      | 111.83   |
| 11  | a     | 907 | BCL  | C2B-C1B-NB  | 5.33  | 115.85      | 110.33   |
| 11  | a     | 909 | BCL  | CED-O2D-CGD | 5.29  | 127.92      | 115.92   |
| 18  | C     | 301 | HEC  | C4A-C3A-C2A | -5.29 | 99.12       | 106.97   |
| 11  | A     | 904 | BCL  | C3C-C4C-CHD | -5.29 | 112.25      | 123.39   |
| 11  | a     | 909 | BCL  | O2A-CGA-CBA | 5.28  | 127.93      | 111.83   |
| 11  | a     | 908 | BCL  | CHD-C1D-ND  | -5.27 | 117.38      | 124.80   |
| 11  | a     | 911 | BCL  | C2B-C1B-NB  | 5.27  | 115.79      | 110.33   |
| 11  | a     | 904 | BCL  | C3D-C2D-C1D | -5.27 | 98.64       | 105.83   |
| 11  | A     | 908 | BCL  | CAA-C2A-C3A | -5.26 | 98.80       | 113.00   |
| 12  | a     | 901 | CLA  | C3D-C4D-ND  | 5.25  | 118.53      | 109.99   |
| 11  | a     | 908 | BCL  | CED-O2D-CGD | 5.25  | 127.83      | 115.92   |
| 12  | a     | 914 | CLA  | CBA-CAA-C2A | -5.24 | 98.19       | 113.79   |
| 11  | A     | 902 | BCL  | O2A-CGA-CBA | 5.22  | 127.75      | 111.83   |
| 11  | a     | 906 | BCL  | CHD-C1D-ND  | -5.20 | 117.48      | 124.80   |
| 11  | A     | 903 | BCL  | C3C-C4C-CHD | -5.19 | 112.46      | 123.39   |
| 12  | A     | 912 | CLA  | C2B-C1B-NB  | 5.18  | 115.69      | 110.33   |
| 11  | a     | 908 | BCL  | C2B-C1B-NB  | 5.17  | 115.69      | 110.33   |
| 11  | A     | 903 | BCL  | CBA-CAA-C2A | 5.17  | 129.18      | 113.79   |
| 11  | A     | 908 | BCL  | C3D-C2D-C1D | -5.16 | 98.78       | 105.83   |
| 11  | a     | 908 | BCL  | C5-C3-C2    | 5.16  | 132.75      | 121.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | a     | 907 | BCL  | C1D-ND-C4D  | 5.16  | 109.93      | 106.31   |
| 12  | a     | 901 | CLA  | CMB-C2B-C1B | 5.16  | 133.27      | 125.42   |
| 18  | C     | 301 | HEC  | CHD-C4C-C3C | 5.14  | 133.88      | 125.21   |
| 11  | a     | 904 | BCL  | C1-O2A-CGA  | 5.14  | 129.09      | 116.65   |
| 13  | c     | 201 | LYC  | C3-C2-C4    | 5.14  | 138.07      | 122.66   |
| 13  | A     | 913 | LYC  | C13-C12-C11 | 5.14  | 125.93      | 118.09   |
| 11  | a     | 906 | BCL  | O2D-CGD-O1D | -5.14 | 113.85      | 123.85   |
| 11  | A     | 905 | BCL  | CMA-C3A-C4A | 5.13  | 125.56      | 111.77   |
| 10  | A     | 901 | 2GO  | C2A-C1A-NA  | -5.12 | 105.19      | 109.15   |
| 11  | a     | 905 | BCL  | C3C-C4C-CHD | -5.12 | 112.59      | 123.39   |
| 13  | A     | 913 | LYC  | C57-C56-C55 | 5.08  | 131.04      | 122.82   |
| 11  | A     | 906 | BCL  | CMD-C2D-C1D | 5.08  | 133.67      | 124.73   |
| 11  | a     | 906 | BCL  | C4A-NA-C1A  | 5.07  | 108.99      | 106.68   |
| 12  | a     | 912 | CLA  | C3C-C4C-NC  | 5.06  | 116.91      | 110.43   |
| 12  | A     | 911 | CLA  | CAC-C3C-C4C | 5.04  | 131.34      | 124.79   |
| 12  | A     | 910 | CLA  | C3C-C4C-NC  | 5.03  | 116.88      | 110.43   |
| 12  | A     | 931 | CLA  | CHD-C4C-NC  | 5.03  | 132.03      | 124.23   |
| 17  | A     | 932 | 85N  | O3-C17-O6   | 5.02  | 124.04      | 110.65   |
| 12  | a     | 913 | CLA  | O2A-CGA-CBA | 5.01  | 127.12      | 111.83   |
| 11  | a     | 911 | BCL  | C4A-NA-C1A  | 5.01  | 108.96      | 106.68   |
| 12  | A     | 933 | CLA  | C1-O2A-CGA  | 5.01  | 128.77      | 116.65   |
| 13  | c     | 201 | LYC  | C5-C4-C2    | 5.00  | 144.33      | 127.64   |
| 12  | A     | 933 | CLA  | C2C-C1C-NC  | 5.00  | 115.23      | 109.98   |
| 12  | A     | 910 | CLA  | C2B-C1B-NB  | 5.00  | 115.51      | 110.33   |
| 11  | a     | 908 | BCL  | CAA-C2A-C3A | -4.99 | 99.51       | 113.00   |
| 11  | A     | 908 | BCL  | C1-C2-C3    | -4.99 | 118.02      | 126.20   |
| 13  | c     | 201 | LYC  | C10-C9-C7   | 4.99  | 134.70      | 127.69   |
| 11  | a     | 911 | BCL  | OBB-CAB-C3B | -4.98 | 111.63      | 120.43   |
| 12  | a     | 913 | CLA  | C1-O2A-CGA  | 4.98  | 128.70      | 116.65   |
| 12  | A     | 910 | CLA  | C3B-C2B-C1B | -4.96 | 101.32      | 107.17   |
| 12  | A     | 910 | CLA  | C6-C7-C8    | 4.96  | 132.44      | 115.97   |
| 10  | a     | 903 | 2GO  | CAA-C2A-C3A | -4.95 | 118.60      | 127.87   |
| 11  | A     | 904 | BCL  | CBC-CAC-C3C | 4.95  | 123.91      | 113.41   |
| 11  | A     | 903 | BCL  | C3D-C2D-C1D | -4.94 | 99.09       | 105.83   |
| 11  | a     | 907 | BCL  | O2A-CGA-CBA | 4.94  | 126.89      | 111.83   |
| 12  | a     | 914 | CLA  | C2C-C1C-NC  | 4.93  | 115.16      | 109.98   |
| 11  | A     | 902 | BCL  | CBC-CAC-C3C | 4.92  | 123.86      | 113.41   |
| 12  | A     | 931 | CLA  | C1C-C2C-C3C | -4.91 | 101.81      | 106.98   |
| 11  | A     | 904 | BCL  | O2D-CGD-CBD | 4.90  | 119.79      | 111.23   |
| 13  | c     | 201 | LYC  | C10-C11-C12 | 4.89  | 139.77      | 126.36   |
| 11  | A     | 902 | BCL  | CED-O2D-CGD | 4.89  | 127.00      | 115.92   |
| 12  | a     | 912 | CLA  | CHB-C1B-NB  | -4.88 | 116.72      | 124.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A     | 909 | BCL  | C1-O2A-CGA  | 4.87  | 128.45      | 116.65   |
| 19  | a     | 921 | 84Q  | O1-C15-C16  | 4.86  | 122.03      | 109.54   |
| 12  | a     | 913 | CLA  | C3D-C4D-ND  | 4.86  | 117.89      | 109.99   |
| 12  | a     | 915 | CLA  | CAC-C3C-C4C | 4.85  | 131.10      | 124.79   |
| 12  | a     | 913 | CLA  | CHD-C4C-C3C | -4.85 | 117.70      | 124.77   |
| 12  | A     | 933 | CLA  | CAC-C3C-C4C | 4.85  | 131.10      | 124.79   |
| 11  | A     | 908 | BCL  | CHD-C1D-ND  | -4.83 | 118.01      | 124.80   |
| 18  | C     | 301 | HEC  | CAD-C3D-C4D | 4.82  | 134.35      | 124.94   |
| 11  | A     | 909 | BCL  | O1A-CGA-CBA | -4.82 | 104.93      | 123.78   |
| 12  | a     | 901 | CLA  | C3D-C2D-C1D | -4.81 | 99.27       | 105.83   |
| 11  | A     | 905 | BCL  | C3C-C4C-CHD | -4.80 | 113.28      | 123.39   |
| 12  | a     | 914 | CLA  | C4C-C3C-C2C | -4.79 | 99.91       | 106.89   |
| 11  | A     | 904 | BCL  | CED-O2D-CGD | 4.79  | 126.78      | 115.92   |
| 10  | A     | 901 | 2GO  | CHC-C1C-NC  | 4.77  | 130.90      | 124.75   |
| 11  | A     | 909 | BCL  | OBB-CAB-C3B | -4.77 | 111.99      | 120.43   |
| 15  | a     | 918 | 85I  | P-O3-C3     | 4.77  | 139.07      | 120.93   |
| 12  | A     | 910 | CLA  | C4A-NA-C1A  | -4.77 | 104.50      | 106.68   |
| 10  | a     | 903 | 2GO  | C2B-C1B-NB  | -4.76 | 103.05      | 109.02   |
| 12  | A     | 931 | CLA  | C4D-C3D-CAD | -4.75 | 102.94      | 108.11   |
| 19  | E     | 101 | 84Q  | O4-C16-C15  | 4.74  | 124.93      | 107.08   |
| 10  | a     | 903 | 2GO  | C3A-C4A-NA  | -4.73 | 102.95      | 109.06   |
| 12  | A     | 912 | CLA  | CHD-C4C-C3C | -4.73 | 117.87      | 124.77   |
| 12  | A     | 910 | CLA  | C3D-C2D-C1D | -4.73 | 99.38       | 105.83   |
| 11  | A     | 908 | BCL  | O2A-CGA-CBA | 4.73  | 126.25      | 111.83   |
| 11  | a     | 904 | BCL  | C1D-ND-C4D  | -4.72 | 103.00      | 106.31   |
| 12  | A     | 933 | CLA  | CMC-C2C-C1C | 4.71  | 132.39      | 125.03   |
| 12  | A     | 931 | CLA  | O1D-CGD-CBD | -4.70 | 115.24      | 124.52   |
| 11  | a     | 910 | BCL  | CMB-C2B-C1B | 4.69  | 132.57      | 125.42   |
| 18  | C     | 301 | HEC  | C2A-C1A-NA  | 4.69  | 114.85      | 110.32   |
| 11  | A     | 908 | BCL  | O1D-CGD-CBD | -4.68 | 115.28      | 124.52   |
| 11  | A     | 908 | BCL  | CMD-C2D-C1D | 4.68  | 132.97      | 124.73   |
| 11  | A     | 903 | BCL  | OBB-CAB-CBB | -4.68 | 109.29      | 119.77   |
| 18  | c     | 202 | HEC  | CHA-C1A-NA  | -4.68 | 119.36      | 124.45   |
| 11  | a     | 910 | BCL  | C5-C3-C2    | 4.67  | 131.64      | 121.17   |
| 12  | a     | 915 | CLA  | C3B-C2B-C1B | -4.67 | 101.67      | 107.17   |
| 11  | a     | 905 | BCL  | C5-C3-C2    | 4.66  | 131.64      | 121.17   |
| 12  | a     | 913 | CLA  | C3C-C4C-NC  | 4.65  | 116.39      | 110.43   |
| 12  | A     | 912 | CLA  | CMD-C2D-C1D | 4.65  | 132.92      | 124.73   |
| 12  | A     | 910 | CLA  | C11-C10-C8  | 4.65  | 131.42      | 115.97   |
| 11  | a     | 911 | BCL  | CHD-C1D-ND  | -4.64 | 118.27      | 124.80   |
| 15  | A     | 915 | 85I  | O3-P-O1     | 4.63  | 124.61      | 109.81   |
| 11  | a     | 909 | BCL  | C5-C3-C2    | 4.63  | 131.55      | 121.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | a     | 907 | BCL  | CED-O2D-CGD | 4.63  | 126.41      | 115.92   |
| 18  | c     | 202 | HEC  | O2D-CGD-O1D | -4.63 | 111.44      | 123.33   |
| 12  | A     | 933 | CLA  | CHB-C1B-NB  | -4.62 | 117.11      | 124.05   |
| 12  | a     | 912 | CLA  | O2A-CGA-O1A | -4.62 | 112.07      | 123.63   |
| 18  | C     | 301 | HEC  | CHA-C1A-NA  | -4.62 | 119.42      | 124.45   |
| 11  | A     | 902 | BCL  | CAA-CBA-CGA | -4.62 | 100.09      | 113.21   |
| 19  | a     | 921 | 84Q  | O4-C16-C15  | 4.61  | 124.42      | 107.08   |
| 12  | A     | 912 | CLA  | CED-O2D-CGD | 4.60  | 126.35      | 115.92   |
| 11  | a     | 905 | BCL  | OBB-CAB-CBB | -4.59 | 109.48      | 119.77   |
| 12  | a     | 914 | CLA  | O2A-CGA-CBA | 4.59  | 129.48      | 112.14   |
| 12  | A     | 933 | CLA  | O2A-CGA-O1A | -4.59 | 112.16      | 123.63   |
| 18  | c     | 202 | HEC  | C1D-C2D-C3D | -4.58 | 101.57      | 106.82   |
| 11  | A     | 903 | BCL  | C1-C2-C3    | 4.58  | 133.70      | 126.20   |
| 12  | A     | 911 | CLA  | O2A-CGA-O1A | -4.57 | 112.20      | 123.63   |
| 18  | c     | 202 | HEC  | C4D-ND-C1D  | 4.55  | 113.24      | 105.82   |
| 12  | a     | 912 | CLA  | C1C-C2C-C3C | -4.55 | 102.20      | 106.98   |
| 11  | a     | 909 | BCL  | C2B-C1B-NB  | 4.54  | 115.04      | 110.33   |
| 11  | a     | 905 | BCL  | O1A-CGA-CBA | -4.54 | 106.03      | 123.78   |
| 12  | A     | 912 | CLA  | C3D-C4D-ND  | 4.52  | 117.33      | 109.99   |
| 11  | A     | 905 | BCL  | CED-O2D-CGD | 4.52  | 126.16      | 115.92   |
| 12  | a     | 912 | CLA  | C3D-C4D-ND  | 4.49  | 117.28      | 109.99   |
| 10  | a     | 903 | 2GO  | C4A-C3A-C2A | -4.48 | 102.27      | 106.98   |
| 11  | A     | 907 | BCL  | C4-C3-C5    | 4.47  | 122.98      | 115.23   |
| 12  | A     | 931 | CLA  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 18  | C     | 301 | HEC  | O2A-CGA-O1A | -4.46 | 111.87      | 123.33   |
| 11  | A     | 907 | BCL  | CHD-C1D-ND  | -4.45 | 118.53      | 124.80   |
| 13  | A     | 913 | LYC  | C8-C7-C6    | 4.45  | 122.95      | 115.23   |
| 12  | a     | 915 | CLA  | CED-O2D-CGD | 4.44  | 125.98      | 115.92   |
| 12  | A     | 933 | CLA  | C1C-C2C-C3C | -4.43 | 102.32      | 106.98   |
| 11  | a     | 906 | BCL  | CAA-C2A-C1A | -4.43 | 97.46       | 111.97   |
| 13  | c     | 201 | LYC  | C9-C10-C11  | 4.43  | 136.03      | 123.20   |
| 12  | a     | 913 | CLA  | C2A-C1A-CHA | -4.43 | 116.18      | 123.87   |
| 12  | A     | 910 | CLA  | C3B-C4B-NB  | 4.39  | 114.44      | 110.53   |
| 12  | a     | 914 | CLA  | C3B-C2B-C1B | -4.38 | 102.00      | 107.17   |
| 12  | a     | 913 | CLA  | C4C-C3C-C2C | -4.37 | 100.53      | 106.89   |
| 11  | A     | 909 | BCL  | CAA-C2A-C1A | 4.37  | 126.31      | 111.97   |
| 10  | A     | 901 | 2GO  | C1A-C2A-C3A | -4.37 | 100.86      | 106.63   |
| 11  | A     | 902 | BCL  | O1D-CGD-CBD | -4.37 | 115.90      | 124.52   |
| 10  | A     | 901 | 2GO  | CMC-C2C-C3C | -4.37 | 114.34      | 126.15   |
| 10  | a     | 903 | 2GO  | CHB-C4A-NA  | 4.35  | 130.35      | 124.75   |
| 12  | A     | 911 | CLA  | O2D-CGD-CBD | 4.33  | 118.80      | 111.23   |
| 10  | A     | 901 | 2GO  | CHB-C4A-NA  | 4.33  | 130.32      | 124.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A     | 902 | BCL  | CHD-C1D-ND  | -4.33 | 118.72      | 124.80   |
| 12  | A     | 911 | CLA  | C10-C8-C7   | 4.31  | 133.92      | 112.07   |
| 11  | A     | 908 | BCL  | O2D-CGD-O1D | -4.31 | 115.46      | 123.85   |
| 12  | A     | 931 | CLA  | C4D-CHA-C1A | -4.31 | 116.11      | 121.24   |
| 12  | A     | 910 | CLA  | CHD-C4C-C3C | -4.31 | 118.49      | 124.77   |
| 11  | a     | 904 | BCL  | O1A-CGA-CBA | -4.28 | 107.02      | 123.78   |
| 12  | A     | 931 | CLA  | C3D-C4D-ND  | -4.28 | 103.03      | 109.99   |
| 11  | a     | 910 | BCL  | O1D-CGD-CBD | -4.28 | 116.09      | 124.52   |
| 11  | a     | 910 | BCL  | C2A-C1A-CHA | -4.27 | 116.45      | 123.87   |
| 12  | A     | 911 | CLA  | CHC-C1C-NC  | -4.27 | 117.88      | 124.31   |
| 12  | a     | 915 | CLA  | C4C-C3C-C2C | -4.26 | 100.69      | 106.89   |
| 12  | A     | 912 | CLA  | C4C-C3C-C2C | -4.26 | 100.69      | 106.89   |
| 10  | a     | 903 | 2GO  | C4D-ND-C1D  | 4.24  | 113.95      | 106.68   |
| 11  | A     | 905 | BCL  | C1-O2A-CGA  | 4.24  | 126.91      | 116.65   |
| 11  | A     | 906 | BCL  | C1-C2-C3    | -4.23 | 119.26      | 126.20   |
| 11  | a     | 906 | BCL  | OBb-CAB-CBB | -4.23 | 110.30      | 119.77   |
| 11  | a     | 909 | BCL  | C6-C5-C3    | -4.23 | 103.17      | 113.47   |
| 12  | A     | 910 | CLA  | O2A-CGA-CBA | 4.22  | 124.70      | 111.83   |
| 12  | a     | 901 | CLA  | C9-C8-C7    | 4.20  | 126.26      | 111.27   |
| 12  | A     | 912 | CLA  | CMB-C2B-C1B | 4.20  | 131.82      | 125.42   |
| 11  | A     | 908 | BCL  | C3C-C4C-CHD | -4.19 | 114.56      | 123.39   |
| 11  | a     | 910 | BCL  | C4D-C3D-CAD | 4.19  | 112.65      | 108.11   |
| 11  | a     | 907 | BCL  | O1D-CGD-CBD | -4.18 | 116.28      | 124.52   |
| 12  | a     | 901 | CLA  | O2A-CGA-O1A | -4.16 | 113.23      | 123.63   |
| 13  | c     | 201 | LYC  | C57-C56-C58 | 4.15  | 124.43      | 118.09   |
| 11  | a     | 908 | BCL  | C2D-C1D-ND  | 4.15  | 114.23      | 110.13   |
| 11  | A     | 906 | BCL  | O2A-CGA-CBA | 4.14  | 124.45      | 111.83   |
| 11  | A     | 903 | BCL  | CED-O2D-CGD | 4.14  | 125.30      | 115.92   |
| 13  | c     | 201 | LYC  | C59-C60-C61 | 4.13  | 133.50      | 127.69   |
| 18  | C     | 301 | HEC  | C2D-C1D-ND  | 4.13  | 116.77      | 110.14   |
| 12  | a     | 912 | CLA  | C1-C2-C3    | -4.13 | 119.43      | 126.20   |
| 11  | a     | 910 | BCL  | OBb-CAB-CBB | -4.13 | 110.53      | 119.77   |
| 11  | A     | 909 | BCL  | CHC-C4B-NB  | -4.12 | 117.87      | 124.05   |
| 12  | a     | 913 | CLA  | CED-O2D-CGD | 4.10  | 125.21      | 115.92   |
| 12  | a     | 914 | CLA  | CMC-C2C-C1C | 4.10  | 131.43      | 125.03   |
| 11  | a     | 911 | BCL  | O2D-CGD-O1D | -4.08 | 115.90      | 123.85   |
| 12  | a     | 901 | CLA  | CHD-C1D-ND  | -4.08 | 119.06      | 124.80   |
| 10  | A     | 901 | 2GO  | CAA-C2A-C3A | -4.07 | 120.25      | 127.87   |
| 13  | c     | 201 | LYC  | C57-C56-C55 | -4.07 | 116.23      | 122.82   |
| 11  | a     | 907 | BCL  | C3C-C4C-CHD | -4.06 | 114.83      | 123.39   |
| 15  | A     | 916 | 85I  | O2-P-O      | -4.06 | 89.16       | 107.57   |
| 11  | a     | 907 | BCL  | C1-O2A-CGA  | 4.06  | 126.48      | 116.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | a     | 904 | BCL  | CMC-C2C-C1C | 4.06  | 122.68      | 111.77   |
| 11  | a     | 907 | BCL  | CMC-C2C-C1C | 4.06  | 122.68      | 111.77   |
| 11  | A     | 905 | BCL  | O1D-CGD-CBD | -4.06 | 116.52      | 124.52   |
| 12  | a     | 912 | CLA  | C4-C3-C2    | -4.05 | 113.21      | 123.63   |
| 12  | A     | 931 | CLA  | C4-C3-C5    | 4.05  | 122.26      | 115.23   |
| 12  | A     | 912 | CLA  | CAA-CBA-CGA | 4.04  | 124.67      | 113.21   |
| 12  | a     | 912 | CLA  | C6-C7-C8    | -4.02 | 102.59      | 115.97   |
| 12  | a     | 913 | CLA  | C4-C3-C5    | 4.02  | 122.21      | 115.23   |
| 11  | a     | 906 | BCL  | CED-O2D-CGD | 4.01  | 125.01      | 115.92   |
| 12  | A     | 912 | CLA  | CHC-C1C-C2C | -4.00 | 115.58      | 126.95   |
| 11  | A     | 902 | BCL  | C9-C8-C10   | -4.00 | 97.01       | 111.27   |
| 12  | A     | 912 | CLA  | CMC-C2C-C1C | 4.00  | 131.28      | 125.03   |
| 11  | A     | 908 | BCL  | CAA-CBA-CGA | -3.98 | 101.90      | 113.21   |
| 12  | a     | 913 | CLA  | CMC-C2C-C1C | 3.98  | 131.26      | 125.03   |
| 12  | a     | 912 | CLA  | CAC-C3C-C4C | 3.98  | 129.97      | 124.79   |
| 12  | a     | 915 | CLA  | CHB-C4A-NA  | 3.98  | 130.14      | 124.40   |
| 12  | a     | 913 | CLA  | C2D-C1D-ND  | 3.96  | 114.05      | 110.13   |
| 11  | a     | 907 | BCL  | CBB-CAB-C3B | 3.96  | 128.75      | 120.40   |
| 11  | A     | 903 | BCL  | C2B-C1B-NB  | 3.96  | 114.43      | 110.33   |
| 12  | a     | 912 | CLA  | C12-C11-C10 | -3.95 | 95.56       | 113.28   |
| 11  | A     | 904 | BCL  | CHD-C1D-ND  | -3.95 | 119.24      | 124.80   |
| 10  | A     | 901 | 2GO  | CBB-CAB-C3B | 3.95  | 128.73      | 120.40   |
| 12  | a     | 914 | CLA  | CAC-C3C-C4C | 3.95  | 129.93      | 124.79   |
| 11  | a     | 908 | BCL  | C3C-C4C-CHD | -3.94 | 115.08      | 123.39   |
| 11  | a     | 911 | BCL  | C1D-ND-C4D  | -3.94 | 103.55      | 106.31   |
| 11  | A     | 907 | BCL  | OBB-CAB-C3B | 3.92  | 127.37      | 120.43   |
| 12  | A     | 931 | CLA  | CMB-C2B-C1B | 3.92  | 131.39      | 125.42   |
| 18  | C     | 301 | HEC  | CBC-CAC-C3C | -3.92 | 119.61      | 127.43   |
| 11  | a     | 906 | BCL  | CMB-C2B-C1B | 3.92  | 131.38      | 125.42   |
| 12  | A     | 911 | CLA  | C6-C7-C8    | 3.91  | 128.97      | 115.97   |
| 19  | E     | 101 | 84Q  | O2-C16-C15  | -3.91 | 92.36       | 107.08   |
| 12  | a     | 915 | CLA  | C1-O2A-CGA  | 3.91  | 126.12      | 116.65   |
| 17  | A     | 932 | 85N  | O3-C17-C16  | 3.91  | 122.01      | 107.06   |
| 12  | A     | 933 | CLA  | C1-C2-C3    | -3.89 | 119.82      | 126.20   |
| 11  | A     | 902 | BCL  | CMB-C2B-C1B | 3.89  | 131.34      | 125.42   |
| 18  | c     | 202 | HEC  | CMC-C2C-C3C | 3.89  | 135.69      | 126.55   |
| 12  | a     | 913 | CLA  | C4D-CHA-C1A | -3.88 | 116.61      | 121.24   |
| 12  | a     | 901 | CLA  | C1C-C2C-C3C | -3.88 | 102.90      | 106.98   |
| 11  | a     | 907 | BCL  | C4-C3-C5    | 3.87  | 121.94      | 115.23   |
| 11  | A     | 907 | BCL  | C3C-C4C-CHD | -3.87 | 115.24      | 123.39   |
| 11  | a     | 904 | BCL  | C3D-C4D-ND  | 3.87  | 116.27      | 109.99   |
| 12  | A     | 911 | CLA  | C1-O2A-CGA  | 3.86  | 126.00      | 116.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | a     | 908 | BCL  | C16-C17-C18 | -3.86 | 98.71       | 115.94   |
| 18  | C     | 301 | HEC  | C1D-CHD-C4C | 3.85  | 136.53      | 124.66   |
| 11  | A     | 904 | BCL  | O1A-CGA-CBA | -3.85 | 110.89      | 123.09   |
| 18  | C     | 301 | HEC  | O2A-CGA-CBA | 3.84  | 126.14      | 114.00   |
| 12  | A     | 933 | CLA  | O2A-C1-C2   | -3.84 | 93.34       | 108.11   |
| 11  | A     | 907 | BCL  | CAA-CBA-CGA | 3.83  | 124.09      | 113.21   |
| 11  | A     | 902 | BCL  | C14-C13-C12 | 3.83  | 124.92      | 111.27   |
| 11  | a     | 910 | BCL  | CAA-C2A-C1A | 3.82  | 124.48      | 111.97   |
| 11  | A     | 902 | BCL  | CMA-C3A-C2A | -3.81 | 99.23       | 113.98   |
| 12  | a     | 914 | CLA  | CHD-C1D-ND  | -3.80 | 119.45      | 124.80   |
| 11  | A     | 903 | BCL  | C6-C5-C3    | 3.80  | 122.73      | 113.47   |
| 12  | a     | 901 | CLA  | O1A-CGA-CBA | -3.80 | 108.91      | 123.78   |
| 18  | c     | 202 | HEC  | CAA-C2A-C1A | 3.80  | 132.58      | 124.85   |
| 18  | c     | 202 | HEC  | C4D-CHA-C1A | 3.78  | 136.33      | 124.66   |
| 11  | A     | 904 | BCL  | O2A-CGA-CBA | 3.78  | 125.95      | 114.00   |
| 11  | a     | 911 | BCL  | O1A-CGA-CBA | -3.78 | 109.01      | 123.78   |
| 11  | a     | 907 | BCL  | CHC-C4B-NB  | -3.78 | 118.38      | 124.05   |
| 12  | a     | 913 | CLA  | CMB-C2B-C1B | 3.76  | 131.15      | 125.42   |
| 12  | a     | 912 | CLA  | C3D-C2D-C1D | -3.76 | 100.70      | 105.83   |
| 12  | A     | 933 | CLA  | C1D-ND-C4D  | -3.75 | 103.68      | 106.31   |
| 12  | A     | 910 | CLA  | C4D-CHA-C1A | -3.75 | 116.77      | 121.24   |
| 11  | A     | 908 | BCL  | CAC-C3C-C4C | -3.75 | 104.26      | 112.58   |
| 12  | a     | 914 | CLA  | C3D-C4D-ND  | 3.75  | 116.08      | 109.99   |
| 12  | a     | 913 | CLA  | O2A-CGA-O1A | -3.74 | 114.27      | 123.63   |
| 11  | A     | 907 | BCL  | C9-C8-C10   | -3.74 | 97.94       | 111.27   |
| 13  | A     | 913 | LYC  | C13-C12-C14 | -3.73 | 116.77      | 122.82   |
| 12  | a     | 914 | CLA  | C1D-ND-C4D  | -3.72 | 103.70      | 106.31   |
| 11  | A     | 909 | BCL  | C4D-C3D-CAD | 3.72  | 112.14      | 108.11   |
| 12  | a     | 913 | CLA  | C9-C8-C7    | 3.71  | 124.50      | 111.27   |
| 10  | A     | 901 | 2GO  | C2C-C1C-NC  | -3.70 | 104.28      | 109.06   |
| 12  | A     | 910 | CLA  | C1-O2A-CGA  | 3.70  | 125.61      | 116.65   |
| 11  | a     | 906 | BCL  | CAA-CBA-CGA | -3.70 | 102.63      | 112.49   |
| 11  | A     | 902 | BCL  | C2A-C1A-CHA | -3.70 | 117.45      | 123.87   |
| 11  | a     | 905 | BCL  | CBC-CAC-C3C | -3.69 | 105.58      | 113.41   |
| 18  | C     | 301 | HEC  | C3A-C4A-NA  | 3.68  | 116.45      | 109.64   |
| 11  | a     | 907 | BCL  | CHB-C1B-NB  | -3.68 | 118.53      | 124.05   |
| 11  | A     | 902 | BCL  | C3D-C2D-C1D | -3.68 | 100.81      | 105.83   |
| 12  | A     | 911 | CLA  | CED-O2D-CGD | 3.67  | 124.24      | 115.92   |
| 11  | a     | 907 | BCL  | C3D-C2D-C1D | -3.67 | 100.82      | 105.83   |
| 11  | a     | 907 | BCL  | CHB-C4A-NA  | 3.67  | 129.70      | 124.40   |
| 12  | A     | 910 | CLA  | CGD-CBD-CAD | -3.66 | 98.99       | 110.85   |
| 11  | A     | 902 | BCL  | C11-C12-C13 | 3.66  | 128.12      | 115.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | a     | 918 | 85I  | O3-C3-C4    | 3.66  | 120.84      | 107.08   |
| 11  | a     | 909 | BCL  | C3C-C4C-CHD | -3.65 | 115.70      | 123.39   |
| 12  | A     | 911 | CLA  | C2A-C1A-CHA | -3.64 | 117.55      | 123.87   |
| 12  | a     | 912 | CLA  | C4D-C3D-CAD | -3.63 | 104.17      | 108.11   |
| 11  | a     | 904 | BCL  | CHC-C4B-NB  | -3.62 | 118.62      | 124.05   |
| 12  | A     | 933 | CLA  | C6-C5-C3    | -3.61 | 96.56       | 113.70   |
| 12  | A     | 910 | CLA  | CHD-C1D-ND  | -3.60 | 119.73      | 124.80   |
| 11  | A     | 903 | BCL  | C3A-C2A-C1A | 3.60  | 106.73      | 101.34   |
| 11  | a     | 904 | BCL  | C2B-C1B-NB  | 3.60  | 114.06      | 110.33   |
| 12  | A     | 911 | CLA  | CHC-C4B-NB  | 3.60  | 129.45      | 124.05   |
| 12  | a     | 912 | CLA  | CHD-C4C-C3C | -3.60 | 119.53      | 124.77   |
| 11  | A     | 907 | BCL  | C9-C8-C7    | 3.58  | 124.03      | 111.27   |
| 11  | A     | 902 | BCL  | C3A-C2A-C1A | 3.57  | 106.69      | 101.34   |
| 11  | a     | 907 | BCL  | CHD-C1D-ND  | -3.56 | 119.79      | 124.80   |
| 11  | a     | 911 | BCL  | C3C-C4C-CHD | -3.56 | 115.88      | 123.39   |
| 11  | a     | 905 | BCL  | CHB-C1B-NB  | -3.54 | 118.73      | 124.05   |
| 11  | a     | 906 | BCL  | OBD-CAD-C3D | -3.53 | 120.16      | 128.42   |
| 12  | A     | 933 | CLA  | CHB-C4A-NA  | 3.53  | 129.49      | 124.40   |
| 10  | a     | 903 | 2GO  | O2D-CGD-CBD | 3.53  | 118.16      | 111.82   |
| 11  | a     | 906 | BCL  | CHC-C4B-NB  | -3.52 | 118.78      | 124.05   |
| 12  | a     | 901 | CLA  | CED-O2D-CGD | 3.51  | 123.88      | 115.92   |
| 12  | a     | 912 | CLA  | C9-C8-C10   | -3.51 | 98.76       | 111.27   |
| 18  | c     | 202 | HEC  | C4A-NA-C1A  | 3.51  | 111.54      | 105.82   |
| 12  | A     | 912 | CLA  | C2A-C1A-CHA | -3.50 | 117.80      | 123.87   |
| 11  | A     | 908 | BCL  | C2D-C1D-ND  | 3.50  | 113.59      | 110.13   |
| 11  | A     | 903 | BCL  | C1D-ND-C4D  | -3.50 | 103.86      | 106.31   |
| 11  | A     | 903 | BCL  | C6-C7-C8    | 3.50  | 127.58      | 115.97   |
| 11  | A     | 902 | BCL  | C1-C2-C3    | -3.48 | 120.49      | 126.20   |
| 11  | a     | 905 | BCL  | CHB-C4A-NA  | 3.48  | 129.43      | 124.40   |
| 18  | C     | 301 | HEC  | CAA-C2A-C3A | -3.48 | 121.35      | 127.87   |
| 13  | A     | 913 | LYC  | C64-C65-C66 | -3.47 | 116.07      | 127.64   |
| 11  | A     | 905 | BCL  | C3D-C4D-ND  | 3.47  | 115.62      | 109.99   |
| 18  | c     | 202 | HEC  | C2C-C1C-NC  | 3.46  | 115.69      | 110.14   |
| 12  | A     | 912 | CLA  | O2A-CGA-O1A | -3.46 | 112.88      | 123.20   |
| 11  | A     | 907 | BCL  | C2B-C1B-NB  | 3.45  | 113.91      | 110.33   |
| 11  | A     | 909 | BCL  | CED-O2D-CGD | 3.45  | 123.74      | 115.92   |
| 10  | A     | 901 | 2GO  | OBB-CAB-CBB | -3.44 | 112.07      | 119.77   |
| 12  | A     | 910 | CLA  | CHC-C1C-C2C | -3.43 | 117.19      | 126.95   |
| 18  | C     | 301 | HEC  | CMC-C2C-C1C | 3.42  | 130.63      | 125.42   |
| 11  | a     | 906 | BCL  | O2D-CGD-CBD | 3.42  | 117.22      | 111.23   |
| 11  | a     | 904 | BCL  | O1D-CGD-CBD | -3.42 | 117.77      | 124.52   |
| 12  | A     | 933 | CLA  | CBA-CAA-C2A | -3.42 | 103.62      | 113.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | a     | 907 | BCL  | OBB-CAB-C3B | -3.42 | 114.39      | 120.43   |
| 11  | A     | 905 | BCL  | C2A-C3A-C4A | -3.42 | 96.35       | 101.87   |
| 18  | c     | 202 | HEC  | O2D-CGD-CBD | 3.41  | 124.76      | 114.00   |
| 12  | a     | 912 | CLA  | C4-C3-C5    | 3.40  | 121.13      | 115.23   |
| 12  | A     | 931 | CLA  | CHA-C4D-ND  | 3.40  | 139.56      | 132.55   |
| 12  | a     | 901 | CLA  | O1D-CGD-CBD | -3.39 | 117.82      | 124.52   |
| 12  | a     | 901 | CLA  | CAC-C3C-C2C | 3.39  | 133.79      | 127.56   |
| 12  | a     | 912 | CLA  | CHC-C1C-NC  | -3.39 | 119.21      | 124.31   |
| 18  | c     | 202 | HEC  | C3D-C4D-ND  | -3.38 | 106.40      | 110.15   |
| 18  | C     | 301 | HEC  | CHD-C1D-ND  | -3.38 | 117.74      | 123.86   |
| 12  | A     | 931 | CLA  | O1A-CGA-CBA | -3.37 | 110.59      | 123.78   |
| 12  | A     | 910 | CLA  | C2A-C1A-CHA | -3.36 | 118.04      | 123.87   |
| 11  | A     | 909 | BCL  | CMA-C3A-C4A | 3.36  | 120.80      | 111.77   |
| 11  | A     | 902 | BCL  | CAC-C3C-C4C | -3.36 | 105.13      | 112.58   |
| 11  | a     | 908 | BCL  | C9-C8-C10   | -3.36 | 99.31       | 111.27   |
| 12  | a     | 913 | CLA  | CHD-C1D-ND  | -3.35 | 120.09      | 124.80   |
| 12  | A     | 931 | CLA  | C3B-C4B-NB  | 3.34  | 113.51      | 110.53   |
| 12  | a     | 901 | CLA  | C4-C3-C5    | 3.34  | 121.03      | 115.23   |
| 11  | A     | 909 | BCL  | CHB-C1B-C2B | -3.34 | 117.73      | 127.43   |
| 11  | A     | 909 | BCL  | CHA-C1A-NA  | -3.33 | 118.85      | 126.39   |
| 12  | A     | 912 | CLA  | C1-O2A-CGA  | 3.33  | 126.73      | 116.07   |
| 12  | A     | 912 | CLA  | C1D-CHD-C4C | -3.33 | 118.95      | 126.02   |
| 11  | a     | 907 | BCL  | C7-C6-C5    | -3.33 | 104.40      | 113.26   |
| 13  | A     | 913 | LYC  | C20-C21-C50 | 3.32  | 130.31      | 123.52   |
| 11  | A     | 909 | BCL  | CHD-C1D-ND  | -3.32 | 120.13      | 124.80   |
| 12  | a     | 901 | CLA  | CHC-C4B-NB  | -3.31 | 119.08      | 124.05   |
| 18  | c     | 202 | HEC  | C1A-C2A-C3A | -3.30 | 102.76      | 107.11   |
| 11  | a     | 910 | BCL  | C16-C15-C13 | 3.30  | 126.93      | 115.97   |
| 12  | a     | 912 | CLA  | C4A-NA-C1A  | -3.30 | 105.17      | 106.68   |
| 11  | a     | 909 | BCL  | OBB-CAB-C3B | 3.30  | 126.26      | 120.43   |
| 11  | a     | 907 | BCL  | C6-C7-C8    | -3.29 | 105.02      | 115.97   |
| 11  | A     | 905 | BCL  | O2A-CGA-CBA | 3.29  | 121.87      | 111.83   |
| 11  | a     | 909 | BCL  | C1C-NC-C4C  | -3.29 | 105.18      | 106.68   |
| 11  | A     | 905 | BCL  | CHC-C4B-NB  | -3.29 | 119.12      | 124.05   |
| 12  | a     | 915 | CLA  | CMA-C3A-C4A | 3.28  | 120.59      | 111.77   |
| 11  | a     | 909 | BCL  | O1D-CGD-CBD | -3.28 | 118.05      | 124.52   |
| 10  | a     | 903 | 2GO  | CHD-C1D-C2D | 3.28  | 132.31      | 125.49   |
| 11  | a     | 909 | BCL  | C2D-C1D-ND  | 3.28  | 113.37      | 110.13   |
| 11  | A     | 909 | BCL  | C10-C8-C7   | 3.28  | 128.67      | 112.07   |
| 11  | a     | 905 | BCL  | C4D-CHA-C1A | 3.27  | 125.14      | 121.24   |
| 12  | a     | 912 | CLA  | CAA-CBA-CGA | -3.27 | 103.94      | 113.21   |
| 12  | a     | 914 | CLA  | CHB-C4A-NA  | 3.26  | 129.11      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | a     | 915 | CLA  | C2A-C1A-CHA | -3.26 | 118.21      | 123.87   |
| 18  | C     | 301 | HEC  | CAA-C2A-C1A | 3.25  | 131.45      | 124.85   |
| 12  | A     | 933 | CLA  | C3C-C4C-NC  | 3.24  | 114.58      | 110.43   |
| 11  | A     | 902 | BCL  | C4-C3-C2    | -3.23 | 115.32      | 123.63   |
| 11  | A     | 907 | BCL  | C5-C3-C2    | 3.23  | 128.43      | 121.17   |
| 11  | a     | 910 | BCL  | C3D-C2D-C1D | -3.21 | 101.45      | 105.83   |
| 13  | A     | 913 | LYC  | C58-C56-C55 | -3.20 | 113.98      | 119.01   |
| 12  | a     | 915 | CLA  | C4D-CHA-C1A | -3.20 | 117.43      | 121.24   |
| 12  | A     | 911 | CLA  | CMB-C2B-C1B | 3.19  | 130.28      | 125.42   |
| 13  | A     | 913 | LYC  | C16-C17-C19 | 3.19  | 124.03      | 119.01   |
| 11  | A     | 909 | BCL  | C3C-C4C-CHD | -3.19 | 116.67      | 123.39   |
| 10  | A     | 901 | 2GO  | C3D-C4D-ND  | -3.19 | 104.57      | 110.51   |
| 11  | A     | 905 | BCL  | CMB-C2B-C1B | 3.19  | 130.27      | 125.42   |
| 12  | a     | 912 | CLA  | C4C-C3C-C2C | -3.18 | 102.26      | 106.89   |
| 11  | a     | 905 | BCL  | OBB-CAB-C3B | 3.18  | 126.06      | 120.43   |
| 11  | A     | 905 | BCL  | C16-C15-C13 | -3.18 | 105.40      | 115.97   |
| 10  | A     | 901 | 2GO  | CHA-C1A-C2A | 3.17  | 132.93      | 128.14   |
| 12  | A     | 931 | CLA  | C6-C7-C8    | 3.17  | 126.49      | 115.97   |
| 12  | a     | 914 | CLA  | CMD-C2D-C1D | 3.16  | 130.29      | 124.73   |
| 12  | A     | 911 | CLA  | C3B-C4B-NB  | -3.16 | 107.71      | 110.53   |
| 12  | A     | 933 | CLA  | CMD-C2D-C1D | 3.15  | 130.27      | 124.73   |
| 12  | A     | 931 | CLA  | C1D-CHD-C4C | -3.14 | 119.34      | 126.02   |
| 12  | A     | 931 | CLA  | CHD-C1D-C2D | 3.13  | 132.01      | 125.49   |
| 18  | C     | 301 | HEC  | C4B-NB-C1B  | 3.13  | 110.93      | 105.82   |
| 11  | A     | 906 | BCL  | CMC-C2C-C1C | 3.13  | 120.19      | 111.77   |
| 12  | A     | 910 | CLA  | CMB-C2B-C1B | 3.13  | 130.19      | 125.42   |
| 11  | a     | 910 | BCL  | C4D-CHA-C1A | -3.12 | 117.52      | 121.24   |
| 11  | A     | 904 | BCL  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |
| 11  | A     | 908 | BCL  | OBB-CAB-C3B | -3.11 | 114.94      | 120.43   |
| 10  | A     | 901 | 2GO  | CHD-C1D-C2D | 3.10  | 131.94      | 125.49   |
| 11  | a     | 911 | BCL  | CBB-CAB-C3B | 3.10  | 126.95      | 120.40   |
| 19  | E     | 101 | 84Q  | O4-P-O6     | 3.10  | 119.70      | 109.81   |
| 10  | a     | 903 | 2GO  | C3C-C4C-NC  | 3.09  | 115.94      | 110.16   |
| 13  | c     | 201 | LYC  | C8-C7-C9    | -3.09 | 109.15      | 122.50   |
| 12  | A     | 931 | CLA  | C4B-C3B-C2B | 3.09  | 111.14      | 107.30   |
| 12  | A     | 931 | CLA  | C11-C10-C8  | 3.09  | 126.23      | 115.97   |
| 18  | C     | 301 | HEC  | O2D-CGD-O1D | -3.09 | 115.39      | 123.33   |
| 18  | C     | 301 | HEC  | CMB-C2B-C1B | 3.08  | 130.11      | 125.42   |
| 12  | a     | 912 | CLA  | C17-C16-C15 | -3.08 | 99.47       | 113.28   |
| 13  | A     | 913 | LYC  | C59-C58-C56 | -3.08 | 117.93      | 126.36   |
| 12  | a     | 915 | CLA  | CHC-C1C-NC  | -3.07 | 119.68      | 124.31   |
| 11  | a     | 908 | BCL  | OBD-CAD-C3D | -3.07 | 121.23      | 128.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | a     | 901 | CLA  | C7-C6-C5    | -3.07 | 105.07      | 113.26   |
| 11  | a     | 905 | BCL  | C4-C3-C5    | 3.07  | 120.55      | 115.23   |
| 10  | a     | 903 | 2GO  | C2D-C1D-ND  | -3.06 | 105.69      | 110.35   |
| 15  | A     | 915 | 85I  | O2-P-O      | -3.06 | 93.69       | 107.57   |
| 12  | a     | 915 | CLA  | C1C-C2C-C3C | -3.06 | 103.76      | 106.98   |
| 10  | a     | 903 | 2GO  | OBB-CAB-CBB | -3.06 | 112.92      | 119.77   |
| 11  | A     | 908 | BCL  | CMB-C2B-C1B | 3.06  | 130.07      | 125.42   |
| 12  | a     | 901 | CLA  | C6-C5-C3    | 3.06  | 120.91      | 113.47   |
| 13  | A     | 913 | LYC  | C1-C2-C4    | -3.05 | 113.49      | 122.66   |
| 18  | c     | 202 | HEC  | CHA-C1A-C2A | 3.05  | 129.68      | 124.86   |
| 12  | a     | 913 | CLA  | CAA-CBA-CGA | 3.05  | 121.86      | 113.21   |
| 11  | A     | 904 | BCL  | CMA-C3A-C2A | -3.05 | 102.21      | 113.98   |
| 11  | A     | 902 | BCL  | O1A-CGA-CBA | -3.04 | 111.88      | 123.78   |
| 11  | A     | 908 | BCL  | C3B-C2B-C1B | -3.04 | 96.68       | 106.40   |
| 11  | A     | 907 | BCL  | O2A-C1-C2   | 3.04  | 119.80      | 108.11   |
| 11  | A     | 907 | BCL  | O1D-CGD-CBD | -3.03 | 118.53      | 124.52   |
| 11  | A     | 903 | BCL  | C3D-C4D-ND  | 3.03  | 114.92      | 109.99   |
| 10  | a     | 903 | 2GO  | CHA-CBD-CGD | -3.03 | 115.51      | 125.24   |
| 11  | a     | 910 | BCL  | C3D-C4D-ND  | 3.03  | 114.90      | 109.99   |
| 11  | a     | 910 | BCL  | C11-C12-C13 | 3.02  | 126.00      | 115.97   |
| 11  | A     | 906 | BCL  | C3D-C4D-ND  | 3.02  | 114.89      | 109.99   |
| 11  | a     | 904 | BCL  | C3B-C4B-NB  | 3.01  | 113.74      | 109.76   |
| 13  | c     | 201 | LYC  | C54-C55-C56 | 3.01  | 131.50      | 127.28   |
| 18  | C     | 301 | HEC  | C1C-CHC-C4B | 3.00  | 133.92      | 124.66   |
| 11  | a     | 908 | BCL  | CHC-C4B-NB  | -2.99 | 119.56      | 124.05   |
| 11  | a     | 906 | BCL  | C3B-C4B-NB  | 2.99  | 113.70      | 109.76   |
| 11  | a     | 904 | BCL  | CMC-C2C-C3C | -2.99 | 102.44      | 113.98   |
| 12  | a     | 914 | CLA  | C3D-C2D-C1D | -2.98 | 101.76      | 105.83   |
| 12  | a     | 913 | CLA  | C4A-NA-C1A  | -2.97 | 105.32      | 106.68   |
| 12  | A     | 910 | CLA  | CMA-C3A-C4A | -2.97 | 103.80      | 111.77   |
| 12  | A     | 933 | CLA  | CHD-C1D-ND  | -2.96 | 120.63      | 124.80   |
| 12  | A     | 931 | CLA  | CHC-C4B-NB  | 2.96  | 128.50      | 124.05   |
| 12  | a     | 901 | CLA  | C14-C13-C15 | -2.96 | 100.71      | 111.27   |
| 12  | a     | 915 | CLA  | C2B-C1B-NB  | 2.96  | 113.40      | 110.33   |
| 11  | a     | 905 | BCL  | CHD-C1D-C2D | 2.96  | 131.64      | 125.49   |
| 11  | a     | 909 | BCL  | CHC-C1C-NC  | 2.95  | 128.66      | 124.40   |
| 10  | A     | 901 | 2GO  | C4C-C3C-C2C | -2.94 | 102.61      | 106.89   |
| 11  | a     | 905 | BCL  | C3B-C2B-C1B | -2.93 | 97.04       | 106.40   |
| 11  | a     | 905 | BCL  | C11-C12-C13 | 2.93  | 125.70      | 115.97   |
| 12  | A     | 912 | CLA  | CAA-C2A-C1A | 2.92  | 121.55      | 111.97   |
| 11  | A     | 903 | BCL  | CMD-C2D-C3D | -2.92 | 121.00      | 127.69   |
| 11  | a     | 905 | BCL  | CMA-C3A-C4A | 2.91  | 119.60      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | A     | 933 | CLA  | C3D-C4D-ND  | 2.91  | 114.72      | 109.99   |
| 11  | a     | 905 | BCL  | O2A-CGA-O1A | -2.91 | 116.35      | 123.63   |
| 11  | A     | 905 | BCL  | CAB-C3B-C2B | -2.91 | 121.70      | 127.74   |
| 11  | A     | 909 | BCL  | CBB-CAB-C3B | 2.91  | 126.53      | 120.40   |
| 11  | a     | 904 | BCL  | CHB-C1B-NB  | -2.90 | 119.69      | 124.05   |
| 11  | a     | 908 | BCL  | C3D-C4D-ND  | 2.90  | 114.70      | 109.99   |
| 10  | A     | 901 | 2GO  | CHA-CBD-CAD | -2.90 | 104.35      | 107.06   |
| 11  | A     | 903 | BCL  | CMB-C2B-C1B | 2.90  | 129.83      | 125.42   |
| 18  | c     | 202 | HEC  | CMD-C2D-C1D | 2.89  | 129.83      | 125.42   |
| 12  | a     | 901 | CLA  | C1-C2-C3    | -2.88 | 121.48      | 126.20   |
| 11  | a     | 907 | BCL  | O1A-CGA-CBA | -2.88 | 112.53      | 123.78   |
| 12  | a     | 915 | CLA  | C2D-C1D-ND  | -2.87 | 107.28      | 110.13   |
| 15  | a     | 919 | 85I  | O4-C4-C3    | 2.87  | 116.91      | 109.54   |
| 12  | a     | 915 | CLA  | C4B-C3B-C2B | -2.87 | 103.74      | 107.30   |
| 11  | a     | 911 | BCL  | C6-C5-C3    | 2.87  | 120.45      | 113.47   |
| 11  | a     | 911 | BCL  | C3A-C2A-C1A | 2.86  | 105.62      | 101.34   |
| 11  | A     | 905 | BCL  | O2A-C1-C2   | 2.86  | 119.10      | 108.11   |
| 12  | a     | 914 | CLA  | CHC-C4B-NB  | -2.86 | 119.76      | 124.05   |
| 11  | A     | 902 | BCL  | O2A-C1-C2   | 2.85  | 119.07      | 108.11   |
| 10  | a     | 903 | 2GO  | C1D-CHD-C4C | 2.85  | 132.07      | 126.02   |
| 12  | A     | 933 | CLA  | C4D-C3D-CAD | -2.84 | 105.02      | 108.11   |
| 12  | a     | 914 | CLA  | CHB-C1B-NB  | -2.84 | 119.79      | 124.05   |
| 12  | A     | 910 | CLA  | C10-C8-C7   | 2.84  | 126.47      | 112.07   |
| 12  | a     | 901 | CLA  | CAA-C2A-C3A | -2.84 | 105.32      | 113.00   |
| 12  | A     | 912 | CLA  | CHC-C1C-NC  | -2.84 | 120.04      | 124.31   |
| 12  | a     | 915 | CLA  | CHD-C4C-C3C | -2.83 | 120.64      | 124.77   |
| 11  | A     | 903 | BCL  | CMC-C2C-C1C | 2.83  | 119.39      | 111.77   |
| 12  | a     | 915 | CLA  | C4D-C3D-CAD | -2.83 | 105.03      | 108.11   |
| 12  | A     | 910 | CLA  | CMA-C3A-C2A | -2.83 | 103.05      | 113.98   |
| 10  | a     | 903 | 2GO  | O1D-CGD-CBD | -2.82 | 119.49      | 124.60   |
| 10  | a     | 903 | 2GO  | CMC-C2C-C3C | -2.82 | 118.53      | 126.15   |
| 12  | A     | 911 | CLA  | CHD-C1D-ND  | -2.81 | 120.84      | 124.80   |
| 11  | a     | 911 | BCL  | CMA-C3A-C4A | 2.81  | 119.33      | 111.77   |
| 18  | c     | 202 | HEC  | CHC-C4B-C3B | -2.81 | 120.47      | 125.21   |
| 12  | a     | 914 | CLA  | CMA-C3A-C2A | -2.81 | 103.12      | 113.98   |
| 18  | c     | 202 | HEC  | CHA-C4D-C3D | 2.80  | 131.44      | 125.30   |
| 12  | a     | 912 | CLA  | C2A-C1A-CHA | -2.80 | 119.00      | 123.87   |
| 12  | a     | 912 | CLA  | CMC-C2C-C1C | 2.80  | 129.41      | 125.03   |
| 11  | a     | 911 | BCL  | O2A-CGA-O1A | -2.79 | 116.64      | 123.63   |
| 11  | a     | 910 | BCL  | C3A-C2A-C1A | -2.79 | 97.16       | 101.34   |
| 12  | a     | 912 | CLA  | C9-C8-C7    | 2.79  | 121.22      | 111.27   |
| 12  | a     | 915 | CLA  | CBC-CAC-C3C | -2.79 | 104.86      | 112.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | a     | 913 | CLA  | CHA-C4D-ND  | -2.79 | 126.80      | 132.55   |
| 11  | A     | 903 | BCL  | CBC-CAC-C3C | 2.78  | 119.32      | 113.41   |
| 13  | A     | 913 | LYC  | C5-C4-C2    | 2.78  | 136.92      | 127.64   |
| 11  | a     | 904 | BCL  | C2D-C1D-ND  | 2.78  | 112.88      | 110.13   |
| 19  | E     | 101 | 84Q  | O7-P-O6     | -2.78 | 97.92       | 108.94   |
| 11  | A     | 908 | BCL  | OBB-CAB-CBB | 2.77  | 125.98      | 119.77   |
| 11  | A     | 908 | BCL  | CED-O2D-CGD | 2.77  | 122.20      | 115.92   |
| 10  | A     | 901 | 2GO  | CAA-C2A-C1A | -2.77 | 120.55      | 128.30   |
| 11  | A     | 906 | BCL  | OBB-CAB-CBB | -2.77 | 113.57      | 119.77   |
| 11  | A     | 908 | BCL  | CMA-C3A-C2A | -2.77 | 103.29      | 113.98   |
| 10  | a     | 903 | 2GO  | CBB-CAB-C3B | 2.77  | 126.23      | 120.40   |
| 11  | A     | 909 | BCL  | CMB-C2B-C1B | 2.76  | 129.62      | 125.42   |
| 11  | a     | 905 | BCL  | CMC-C2C-C1C | 2.76  | 119.18      | 111.77   |
| 18  | c     | 202 | HEC  | C1D-CHD-C4C | 2.76  | 133.16      | 124.66   |
| 10  | A     | 901 | 2GO  | C1-C2-C3    | 2.75  | 130.71      | 126.20   |
| 18  | c     | 202 | HEC  | CHC-C4B-NB  | 2.75  | 127.45      | 124.45   |
| 12  | a     | 914 | CLA  | C1D-CHD-C4C | -2.75 | 120.18      | 126.02   |
| 12  | a     | 912 | CLA  | CHD-C1D-ND  | -2.74 | 120.94      | 124.80   |
| 12  | A     | 910 | CLA  | C6-C5-C3    | -2.74 | 106.79      | 113.47   |
| 11  | a     | 911 | BCL  | CAA-C2A-C1A | 2.74  | 120.96      | 111.97   |
| 12  | A     | 911 | CLA  | C3D-C4D-ND  | 2.73  | 114.42      | 109.99   |
| 11  | a     | 909 | BCL  | CMA-C3A-C4A | 2.72  | 119.09      | 111.77   |
| 12  | A     | 911 | CLA  | C1-C2-C3    | -2.72 | 121.74      | 126.20   |
| 12  | A     | 931 | CLA  | CMD-C2D-C1D | 2.72  | 129.52      | 124.73   |
| 11  | a     | 911 | BCL  | C4D-CHA-C1A | -2.72 | 118.00      | 121.24   |
| 12  | a     | 912 | CLA  | C4B-C3B-C2B | -2.72 | 103.92      | 107.30   |
| 11  | A     | 906 | BCL  | CBC-CAC-C3C | 2.72  | 119.17      | 113.41   |
| 11  | A     | 907 | BCL  | C6-C7-C8    | 2.72  | 124.99      | 115.97   |
| 18  | C     | 301 | HEC  | C1B-CHB-C4A | 2.71  | 133.04      | 124.66   |
| 11  | A     | 904 | BCL  | C4D-CHA-C1A | -2.71 | 118.01      | 121.24   |
| 18  | C     | 301 | HEC  | C4D-CHA-C1A | 2.71  | 133.01      | 124.66   |
| 11  | A     | 903 | BCL  | CAA-C2A-C3A | 2.71  | 120.31      | 113.00   |
| 18  | C     | 301 | HEC  | CMA-C3A-C4A | 2.70  | 129.49      | 124.73   |
| 11  | a     | 908 | BCL  | C4-C3-C2    | -2.70 | 116.69      | 123.63   |
| 11  | a     | 910 | BCL  | C4-C3-C2    | -2.70 | 116.69      | 123.63   |
| 12  | a     | 914 | CLA  | CHD-C1D-C2D | 2.70  | 131.10      | 125.49   |
| 11  | A     | 907 | BCL  | CHB-C1B-NB  | -2.70 | 120.00      | 124.05   |
| 11  | a     | 908 | BCL  | C4-C3-C5    | -2.70 | 110.55      | 115.23   |
| 10  | A     | 901 | 2GO  | C3A-C4A-NA  | -2.69 | 105.58      | 109.06   |
| 11  | A     | 902 | BCL  | CHD-C1D-C2D | 2.68  | 131.07      | 125.49   |
| 11  | A     | 908 | BCL  | C3D-C4D-ND  | 2.68  | 114.35      | 109.99   |
| 18  | C     | 301 | HEC  | CMD-C2D-C3D | 2.68  | 131.31      | 125.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 12  | A     | 933 | CLA  | CHA-C4D-ND  | -2.68 | 127.03      | 132.55   |
| 12  | A     | 911 | CLA  | C6-C5-C3    | 2.67  | 119.98      | 113.47   |
| 11  | A     | 909 | BCL  | C15-C13-C12 | 2.67  | 125.60      | 112.07   |
| 11  | A     | 907 | BCL  | C15-C13-C14 | -2.67 | 98.63       | 110.53   |
| 11  | a     | 905 | BCL  | OBD-CAD-C3D | -2.66 | 122.20      | 128.42   |
| 11  | A     | 909 | BCL  | C5-C3-C2    | 2.66  | 127.14      | 121.17   |
| 18  | c     | 202 | HEC  | CMB-C2B-C3B | 2.66  | 132.80      | 126.55   |
| 18  | C     | 301 | HEC  | CHB-C4A-C3A | -2.65 | 119.98      | 125.49   |
| 11  | a     | 905 | BCL  | O2A-C1-C2   | 2.65  | 118.30      | 108.11   |
| 10  | A     | 901 | 2GO  | CHA-CBD-CGD | -2.64 | 116.76      | 125.24   |
| 12  | A     | 931 | CLA  | CHB-C4A-NA  | 2.63  | 128.19      | 124.40   |
| 12  | a     | 915 | CLA  | OBD-CAD-C3D | -2.63 | 122.27      | 128.42   |
| 12  | A     | 910 | CLA  | CMD-C2D-C3D | -2.62 | 121.67      | 127.69   |
| 12  | a     | 913 | CLA  | C2B-C1B-NB  | 2.62  | 113.05      | 110.33   |
| 11  | A     | 905 | BCL  | C14-C13-C12 | 2.62  | 120.62      | 111.27   |
| 11  | a     | 909 | BCL  | CHC-C4B-NB  | -2.62 | 120.12      | 124.05   |
| 11  | A     | 905 | BCL  | CHB-C1B-C2B | -2.62 | 119.83      | 127.43   |
| 11  | a     | 908 | BCL  | O2A-CGA-O1A | 2.62  | 130.17      | 123.63   |
| 11  | A     | 903 | BCL  | C1C-NC-C4C  | -2.61 | 105.49      | 106.68   |
| 11  | a     | 906 | BCL  | C2D-C1D-ND  | 2.61  | 112.71      | 110.13   |
| 12  | a     | 912 | CLA  | O1D-CGD-CBD | 2.61  | 129.66      | 124.52   |
| 11  | A     | 902 | BCL  | C4-C3-C5    | 2.61  | 119.75      | 115.23   |
| 11  | A     | 908 | BCL  | CHB-C4A-NA  | 2.60  | 128.16      | 124.40   |
| 12  | a     | 912 | CLA  | CMD-C2D-C3D | -2.60 | 121.74      | 127.69   |
| 11  | A     | 904 | BCL  | OBD-CAD-C3D | -2.60 | 122.35      | 128.42   |
| 18  | c     | 202 | HEC  | C4A-C3A-C2A | -2.60 | 103.12      | 106.97   |
| 11  | a     | 906 | BCL  | CBC-CAC-C3C | 2.59  | 118.91      | 113.41   |
| 12  | A     | 931 | CLA  | C16-C15-C13 | -2.59 | 107.37      | 115.97   |
| 11  | a     | 905 | BCL  | C1D-ND-C4D  | 2.58  | 108.12      | 106.31   |
| 10  | A     | 901 | 2GO  | CHB-C1B-NB  | 2.58  | 128.71      | 124.24   |
| 11  | a     | 909 | BCL  | CBB-CAB-C3B | -2.58 | 114.96      | 120.40   |
| 11  | a     | 906 | BCL  | CHB-C1B-NB  | -2.58 | 120.18      | 124.05   |
| 11  | A     | 909 | BCL  | CAC-C3C-C4C | -2.58 | 106.86      | 112.58   |
| 12  | A     | 931 | CLA  | C11-C12-C13 | -2.58 | 107.39      | 115.97   |
| 11  | A     | 902 | BCL  | C9-C8-C7    | -2.58 | 102.09      | 111.27   |
| 11  | A     | 908 | BCL  | C7-C6-C5    | -2.57 | 106.40      | 113.26   |
| 11  | A     | 907 | BCL  | C2C-C3C-C4C | -2.57 | 97.49       | 101.34   |
| 11  | a     | 904 | BCL  | C6-C5-C3    | 2.57  | 119.73      | 113.47   |
| 13  | A     | 913 | LYC  | C18-C17-C16 | 2.57  | 122.01      | 118.09   |
| 10  | a     | 903 | 2GO  | C15-C13-C12 | -2.57 | 99.06       | 112.07   |
| 11  | A     | 903 | BCL  | C2A-C1A-CHA | -2.56 | 119.42      | 123.87   |
| 11  | a     | 908 | BCL  | CAB-C3B-C2B | -2.56 | 122.43      | 127.74   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | a     | 910 | BCL  | C3C-C4C-CHD | -2.56 | 118.00      | 123.39   |
| 12  | A     | 910 | CLA  | C4C-C3C-C2C | -2.56 | 103.17      | 106.89   |
| 12  | A     | 912 | CLA  | C3A-C2A-C1A | -2.55 | 97.52       | 101.34   |
| 11  | a     | 911 | BCL  | CAB-C3B-C2B | -2.55 | 122.45      | 127.74   |
| 11  | a     | 910 | BCL  | CBA-CAA-C2A | 2.55  | 121.37      | 113.79   |
| 18  | C     | 301 | HEC  | CAD-C3D-C2D | -2.55 | 121.36      | 127.07   |
| 12  | a     | 913 | CLA  | C9-C8-C10   | -2.54 | 102.21      | 111.27   |
| 11  | A     | 907 | BCL  | C1D-ND-C4D  | -2.54 | 104.53      | 106.31   |
| 11  | a     | 908 | BCL  | CBB-CAB-C3B | 2.53  | 125.74      | 120.40   |
| 11  | A     | 908 | BCL  | CHB-C1B-NB  | -2.52 | 120.26      | 124.05   |
| 11  | A     | 909 | BCL  | C3B-C2B-C1B | -2.52 | 98.34       | 106.40   |
| 12  | a     | 915 | CLA  | CAA-CBA-CGA | 2.52  | 120.36      | 113.21   |
| 11  | A     | 908 | BCL  | C1-O2A-CGA  | 2.52  | 122.75      | 116.65   |
| 15  | A     | 915 | 85I  | O-P-O1      | -2.51 | 98.97       | 108.94   |
| 11  | a     | 904 | BCL  | CHD-C1D-C2D | 2.51  | 130.72      | 125.49   |
| 11  | A     | 906 | BCL  | CBA-CAA-C2A | 2.51  | 121.26      | 113.79   |
| 11  | A     | 906 | BCL  | C4D-CHA-C1A | 2.51  | 124.24      | 121.24   |
| 13  | A     | 913 | LYC  | C55-C54-C53 | -2.51 | 115.93      | 123.20   |
| 11  | A     | 904 | BCL  | CAA-C2A-C1A | -2.51 | 103.76      | 111.97   |
| 12  | A     | 912 | CLA  | CHD-C4C-NC  | -2.51 | 120.34      | 124.23   |
| 11  | A     | 903 | BCL  | C2D-C1D-ND  | 2.51  | 112.61      | 110.13   |
| 12  | A     | 931 | CLA  | OBD-CAD-C3D | -2.50 | 122.57      | 128.42   |
| 11  | A     | 906 | BCL  | CBB-CAB-C3B | -2.50 | 115.13      | 120.40   |
| 18  | C     | 301 | HEC  | CMC-C2C-C3C | 2.50  | 132.43      | 126.55   |
| 11  | a     | 906 | BCL  | CBB-CAB-C3B | 2.50  | 125.67      | 120.40   |
| 12  | A     | 910 | CLA  | C4B-C3B-C2B | -2.50 | 104.20      | 107.30   |
| 11  | a     | 910 | BCL  | CBB-CAB-C3B | 2.49  | 125.65      | 120.40   |
| 13  | c     | 201 | LYC  | C5-C6-C7    | 2.49  | 121.43      | 113.19   |
| 12  | a     | 914 | CLA  | CMB-C2B-C3B | 2.49  | 132.40      | 126.55   |
| 10  | a     | 903 | 2GO  | C1B-NB-C4B  | 2.48  | 110.20      | 106.52   |
| 11  | a     | 909 | BCL  | C4-C3-C5    | 2.47  | 119.51      | 115.23   |
| 11  | a     | 905 | BCL  | C6-C5-C3    | 2.46  | 119.47      | 113.47   |
| 12  | a     | 914 | CLA  | O2A-CGA-O1A | -2.46 | 115.85      | 123.20   |
| 11  | A     | 906 | BCL  | C3C-C4C-CHD | -2.46 | 118.21      | 123.39   |
| 11  | a     | 911 | BCL  | C4-C3-C2    | 2.46  | 129.94      | 123.63   |
| 12  | a     | 913 | CLA  | CHC-C1C-NC  | -2.46 | 120.61      | 124.31   |
| 11  | A     | 902 | BCL  | CHB-C1B-NB  | -2.46 | 120.36      | 124.05   |
| 11  | a     | 906 | BCL  | CMD-C2D-C3D | -2.45 | 122.08      | 127.69   |
| 11  | A     | 905 | BCL  | C3B-C2B-C1B | -2.44 | 98.60       | 106.40   |
| 13  | A     | 913 | LYC  | C20-C19-C17 | -2.44 | 123.86      | 127.28   |
| 12  | A     | 931 | CLA  | C9-C8-C10   | 2.44  | 119.96      | 111.27   |
| 11  | a     | 909 | BCL  | CHD-C1D-C2D | 2.43  | 130.55      | 125.49   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | E     | 101 | 84Q  | C19-C18-C17 | 2.43  | 122.61      | 113.69   |
| 11  | a     | 910 | BCL  | C1D-CHD-C4C | -2.43 | 120.76      | 126.62   |
| 12  | A     | 911 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 12  | a     | 913 | CLA  | CMA-C3A-C4A | 2.43  | 118.30      | 111.77   |
| 11  | A     | 908 | BCL  | O1A-CGA-CBA | -2.42 | 114.33      | 123.78   |
| 15  | A     | 917 | 85I  | O3-C3-C4    | 2.41  | 116.16      | 107.08   |
| 18  | c     | 202 | HEC  | CBA-CAA-C2A | -2.41 | 105.86      | 112.53   |
| 12  | a     | 913 | CLA  | C2C-C1C-NC  | 2.41  | 112.52      | 109.98   |
| 11  | a     | 909 | BCL  | C1D-ND-C4D  | -2.41 | 104.62      | 106.31   |
| 11  | a     | 910 | BCL  | CAA-CBA-CGA | 2.40  | 120.02      | 113.21   |
| 11  | A     | 908 | BCL  | CMB-C2B-C3B | 2.40  | 133.22      | 125.67   |
| 11  | A     | 907 | BCL  | C11-C12-C13 | 2.39  | 126.62      | 115.94   |
| 11  | A     | 904 | BCL  | C2A-C1A-CHA | -2.39 | 119.72      | 123.87   |
| 12  | A     | 910 | CLA  | CMC-C2C-C3C | 2.39  | 132.61      | 126.15   |
| 11  | A     | 909 | BCL  | CBA-CAA-C2A | 2.39  | 120.89      | 113.79   |
| 11  | a     | 908 | BCL  | C16-C15-C13 | -2.38 | 108.04      | 115.97   |
| 11  | A     | 907 | BCL  | C11-C10-C8  | 2.38  | 123.86      | 115.97   |
| 11  | A     | 907 | BCL  | OBB-CAB-CBB | -2.37 | 114.45      | 119.77   |
| 12  | A     | 911 | CLA  | C2D-C1D-ND  | 2.37  | 112.47      | 110.13   |
| 13  | c     | 201 | LYC  | C59-C58-C56 | -2.37 | 119.86      | 126.36   |
| 12  | a     | 912 | CLA  | C7-C6-C5    | 2.37  | 119.58      | 113.26   |
| 11  | A     | 907 | BCL  | C4D-C3D-CAD | -2.37 | 105.53      | 108.11   |
| 11  | a     | 907 | BCL  | CHD-C1D-C2D | 2.37  | 130.41      | 125.49   |
| 11  | a     | 911 | BCL  | C16-C15-C13 | 2.36  | 123.82      | 115.97   |
| 11  | A     | 903 | BCL  | CHB-C1B-C2B | -2.36 | 120.57      | 127.43   |
| 12  | a     | 901 | CLA  | CBA-CAA-C2A | 2.36  | 120.80      | 113.79   |
| 12  | A     | 910 | CLA  | CHB-C1B-NB  | -2.35 | 120.52      | 124.05   |
| 10  | a     | 903 | 2GO  | C3D-C4D-ND  | -2.35 | 106.13      | 110.51   |
| 11  | A     | 906 | BCL  | C4-C3-C5    | 2.34  | 118.88      | 116.13   |
| 12  | a     | 914 | CLA  | O1A-CGA-CBA | -2.34 | 114.64      | 123.78   |
| 15  | A     | 915 | 85I  | O6-C20-C21  | 2.33  | 116.53      | 111.48   |
| 11  | a     | 910 | BCL  | CMC-C2C-C1C | 2.33  | 118.04      | 111.77   |
| 11  | a     | 908 | BCL  | CHB-C1B-C2B | -2.33 | 120.66      | 127.43   |
| 15  | A     | 916 | 85I  | O2-P-O3     | 2.32  | 116.14      | 106.70   |
| 12  | a     | 912 | CLA  | C6-C5-C3    | 2.32  | 119.11      | 113.47   |
| 11  | A     | 902 | BCL  | C1D-CHD-C4C | -2.31 | 121.04      | 126.62   |
| 19  | E     | 101 | 84Q  | O5-P-O4     | -2.31 | 97.31       | 106.70   |
| 11  | A     | 905 | BCL  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 11  | a     | 908 | BCL  | C1-O2A-CGA  | -2.29 | 111.09      | 116.65   |
| 12  | A     | 910 | CLA  | C1D-CHD-C4C | -2.29 | 121.15      | 126.02   |
| 11  | a     | 911 | BCL  | C4-C3-C5    | -2.29 | 111.25      | 115.23   |
| 12  | A     | 911 | CLA  | CMA-C3A-C4A | 2.29  | 117.93      | 111.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | a     | 903 | 2GO  | CAC-C3C-C2C | -2.29 | 123.35      | 127.56   |
| 12  | a     | 915 | CLA  | C2C-C1C-NC  | 2.29  | 112.39      | 109.98   |
| 17  | G     | 101 | 85N  | O3-C17-O6   | 2.29  | 116.76      | 110.65   |
| 11  | A     | 903 | BCL  | CHD-C1D-C2D | 2.29  | 130.24      | 125.49   |
| 12  | A     | 912 | CLA  | O2A-CGA-CBA | 2.28  | 120.77      | 112.14   |
| 11  | A     | 905 | BCL  | C9-C8-C10   | -2.28 | 103.14      | 111.27   |
| 12  | A     | 933 | CLA  | O2A-CGA-CBA | 2.28  | 118.79      | 111.83   |
| 12  | A     | 931 | CLA  | CAA-C2A-C3A | 2.28  | 119.16      | 113.00   |
| 15  | A     | 916 | 85I  | C7-C6-C5    | -2.28 | 105.34      | 113.69   |
| 12  | A     | 911 | CLA  | C2B-C1B-NB  | 2.28  | 112.69      | 110.33   |
| 11  | a     | 906 | BCL  | CMC-C2C-C1C | 2.27  | 117.89      | 111.77   |
| 12  | A     | 931 | CLA  | CHB-C1B-NB  | -2.27 | 120.64      | 124.05   |
| 17  | G     | 101 | 85N  | O2-C16-C17  | -2.27 | 103.72      | 109.54   |
| 12  | a     | 913 | CLA  | CBC-CAC-C3C | 2.26  | 118.56      | 112.42   |
| 11  | a     | 911 | BCL  | CMB-C2B-C3B | 2.26  | 132.81      | 125.67   |
| 11  | a     | 908 | BCL  | C11-C10-C8  | -2.26 | 108.44      | 115.97   |
| 11  | a     | 905 | BCL  | C2D-C1D-ND  | 2.26  | 112.36      | 110.13   |
| 11  | a     | 906 | BCL  | O2A-CGA-CBA | 2.26  | 121.14      | 114.00   |
| 12  | A     | 931 | CLA  | CMB-C2B-C3B | 2.25  | 131.85      | 126.55   |
| 11  | A     | 909 | BCL  | C11-C12-C13 | 2.25  | 123.45      | 115.97   |
| 11  | a     | 908 | BCL  | CMB-C2B-C3B | 2.25  | 132.77      | 125.67   |
| 12  | a     | 913 | CLA  | C4-C3-C2    | -2.25 | 117.85      | 123.63   |
| 12  | a     | 915 | CLA  | CBA-CAA-C2A | -2.24 | 107.12      | 113.79   |
| 11  | A     | 908 | BCL  | CHB-C1B-C2B | -2.24 | 120.92      | 127.43   |
| 12  | a     | 914 | CLA  | C1C-C2C-C3C | -2.24 | 104.62      | 106.98   |
| 12  | a     | 901 | CLA  | CMD-C2D-C3D | -2.23 | 122.57      | 127.69   |
| 11  | A     | 904 | BCL  | CAC-C3C-C4C | -2.23 | 107.63      | 112.58   |
| 11  | a     | 905 | BCL  | CHC-C4B-NB  | -2.22 | 120.71      | 124.05   |
| 11  | A     | 907 | BCL  | C4D-CHA-C1A | 2.22  | 123.89      | 121.24   |
| 12  | a     | 915 | CLA  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 11  | a     | 910 | BCL  | O1A-CGA-CBA | -2.22 | 115.11      | 123.78   |
| 18  | C     | 301 | HEC  | C4A-NA-C1A  | -2.22 | 102.21      | 105.82   |
| 11  | A     | 905 | BCL  | O1A-CGA-CBA | -2.21 | 115.12      | 123.78   |
| 11  | A     | 908 | BCL  | C1D-ND-C4D  | -2.21 | 104.76      | 106.31   |
| 11  | a     | 909 | BCL  | C9-C8-C7    | 2.20  | 119.13      | 111.27   |
| 15  | a     | 918 | 85I  | O6-C3-C4    | 2.20  | 115.36      | 107.08   |
| 11  | A     | 902 | BCL  | CHC-C4B-NB  | -2.20 | 120.75      | 124.05   |
| 11  | A     | 906 | BCL  | CMB-C2B-C1B | 2.20  | 128.77      | 125.42   |
| 11  | A     | 908 | BCL  | C4D-C3D-CAD | -2.20 | 105.72      | 108.11   |
| 11  | A     | 907 | BCL  | CMA-C3A-C4A | 2.20  | 117.68      | 111.77   |
| 11  | a     | 910 | BCL  | C20-C18-C17 | 2.19  | 124.52      | 111.55   |
| 12  | A     | 912 | CLA  | CHB-C1B-C2B | -2.19 | 121.07      | 127.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 10  | a     | 903 | 2GO  | C1C-C2C-C3C | -2.19 | 104.68      | 106.98   |
| 10  | a     | 903 | 2GO  | C3B-C2B-C1B | 2.19  | 113.39      | 106.40   |
| 12  | a     | 914 | CLA  | C4D-CHA-C1A | 2.18  | 123.85      | 121.24   |
| 11  | A     | 907 | BCL  | CBA-CAA-C2A | 2.18  | 120.28      | 113.79   |
| 12  | a     | 915 | CLA  | C4-C3-C2    | -2.18 | 118.03      | 123.63   |
| 11  | a     | 908 | BCL  | CHA-C1A-NA  | 2.18  | 131.32      | 126.39   |
| 12  | A     | 931 | CLA  | CHC-C4B-C3B | -2.17 | 117.96      | 127.37   |
| 11  | a     | 905 | BCL  | C4D-C3D-CAD | -2.16 | 105.76      | 108.11   |
| 11  | a     | 911 | BCL  | C15-C13-C12 | -2.15 | 101.15      | 112.07   |
| 12  | A     | 933 | CLA  | C4C-C3C-C2C | -2.15 | 103.76      | 106.89   |
| 11  | A     | 902 | BCL  | C6-C5-C3    | 2.15  | 118.71      | 113.47   |
| 12  | A     | 933 | CLA  | CHD-C4C-C3C | -2.14 | 121.66      | 124.77   |
| 11  | A     | 906 | BCL  | CAC-C3C-C4C | 2.13  | 117.31      | 112.58   |
| 11  | a     | 909 | BCL  | C3D-C4D-ND  | 2.13  | 113.45      | 109.99   |
| 17  | A     | 932 | 85N  | O5-C24-C19  | -2.13 | 117.20      | 122.86   |
| 11  | A     | 905 | BCL  | CMC-C2C-C3C | -2.13 | 105.76      | 113.98   |
| 11  | a     | 904 | BCL  | C4-C3-C2    | -2.12 | 118.17      | 123.63   |
| 11  | a     | 910 | BCL  | CMD-C2D-C3D | -2.12 | 122.82      | 127.69   |
| 11  | a     | 910 | BCL  | C14-C13-C15 | 2.12  | 118.84      | 111.27   |
| 15  | A     | 916 | 85I  | O3-C3-C4    | 2.12  | 115.07      | 107.08   |
| 11  | A     | 903 | BCL  | C3B-C2B-C1B | -2.12 | 99.62       | 106.40   |
| 11  | a     | 908 | BCL  | C1D-CHD-C4C | -2.12 | 121.51      | 126.62   |
| 10  | a     | 903 | 2GO  | CHD-C1D-ND  | -2.12 | 121.32      | 124.82   |
| 11  | a     | 904 | BCL  | C1D-CHD-C4C | -2.11 | 121.52      | 126.62   |
| 13  | A     | 913 | LYC  | C15-C14-C12 | -2.11 | 124.32      | 127.28   |
| 12  | a     | 915 | CLA  | C4B-CHC-C1C | 2.11  | 131.20      | 126.25   |
| 12  | a     | 912 | CLA  | C4B-CHC-C1C | 2.10  | 131.19      | 126.25   |
| 12  | a     | 913 | CLA  | C2A-C3A-C4A | -2.10 | 98.48       | 101.87   |
| 13  | A     | 913 | LYC  | C57-C56-C58 | -2.10 | 114.89      | 118.09   |
| 12  | A     | 911 | CLA  | C15-C13-C12 | 2.10  | 122.69      | 112.07   |
| 11  | a     | 910 | BCL  | C4-C3-C5    | -2.09 | 111.59      | 115.23   |
| 18  | c     | 202 | HEC  | C2B-C1B-NB  | 2.09  | 113.50      | 110.14   |
| 12  | A     | 910 | CLA  | CBA-CAA-C2A | 2.09  | 120.01      | 113.79   |
| 11  | a     | 911 | BCL  | OBD-CAD-C3D | -2.09 | 123.54      | 128.42   |
| 11  | a     | 909 | BCL  | CMD-C2D-C3D | -2.09 | 122.90      | 127.69   |
| 12  | a     | 901 | CLA  | CHC-C1C-NC  | -2.08 | 121.17      | 124.31   |
| 11  | A     | 907 | BCL  | CMB-C2B-C1B | 2.08  | 128.59      | 125.42   |
| 11  | A     | 903 | BCL  | CMA-C3A-C2A | -2.08 | 105.93      | 113.98   |
| 11  | a     | 904 | BCL  | CBC-CAC-C3C | 2.08  | 117.82      | 113.41   |
| 11  | a     | 906 | BCL  | O1D-CGD-CBD | 2.08  | 128.61      | 124.52   |
| 11  | A     | 903 | BCL  | C12-C11-C10 | -2.07 | 103.99      | 113.28   |
| 11  | a     | 907 | BCL  | CAB-C3B-C2B | -2.07 | 123.44      | 127.74   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A     | 909 | BCL  | C12-C11-C10 | 2.07  | 122.56      | 113.28   |
| 11  | a     | 905 | BCL  | C7-C6-C5    | 2.06  | 118.77      | 113.26   |
| 12  | a     | 914 | CLA  | CHC-C1C-NC  | -2.06 | 121.20      | 124.31   |
| 11  | A     | 908 | BCL  | O2A-C1-C2   | 2.06  | 116.04      | 108.11   |
| 10  | a     | 903 | 2GO  | CAA-C2A-C1A | -2.06 | 122.53      | 128.30   |
| 11  | A     | 906 | BCL  | CMD-C2D-C3D | 2.06  | 132.41      | 127.69   |
| 12  | A     | 931 | CLA  | CMC-C2C-C3C | -2.06 | 120.58      | 126.15   |
| 12  | A     | 933 | CLA  | C2A-C1A-CHA | -2.06 | 120.30      | 123.87   |
| 12  | A     | 910 | CLA  | C3D-C4D-ND  | 2.05  | 113.33      | 109.99   |
| 11  | A     | 905 | BCL  | C12-C11-C10 | 2.05  | 122.47      | 113.28   |
| 11  | A     | 904 | BCL  | C2B-C1B-NB  | 2.05  | 112.45      | 110.33   |
| 12  | A     | 912 | CLA  | CBC-CAC-C3C | -2.03 | 106.91      | 112.42   |
| 11  | a     | 908 | BCL  | O1D-CGD-CBD | -2.03 | 120.51      | 124.52   |
| 11  | a     | 907 | BCL  | C3B-C2B-C1B | -2.03 | 99.92       | 106.40   |
| 11  | A     | 905 | BCL  | OBB-CAB-C3B | -2.03 | 116.85      | 120.43   |
| 12  | a     | 913 | CLA  | C1C-C2C-C3C | -2.02 | 104.85      | 106.98   |
| 12  | a     | 915 | CLA  | CHB-C1B-NB  | -2.02 | 121.01      | 124.05   |
| 15  | A     | 915 | 85I  | C33-C32-C31 | 2.02  | 123.53      | 111.55   |
| 12  | a     | 915 | CLA  | C6-C5-C3    | -2.02 | 104.11      | 113.70   |
| 15  | A     | 915 | 85I  | C34-C32-C31 | 2.02  | 123.52      | 111.55   |
| 12  | A     | 931 | CLA  | C3C-C4C-NC  | 2.02  | 113.02      | 110.43   |
| 12  | a     | 901 | CLA  | CHB-C1B-C2B | -2.02 | 121.56      | 127.43   |
| 11  | A     | 904 | BCL  | C2C-C3C-C4C | -2.02 | 98.32       | 101.34   |
| 12  | a     | 913 | CLA  | C6-C5-C3    | 2.02  | 118.38      | 113.47   |
| 11  | A     | 908 | BCL  | C14-C13-C12 | -2.02 | 104.09      | 111.27   |
| 11  | a     | 909 | BCL  | C9-C8-C10   | -2.01 | 104.10      | 111.27   |
| 11  | a     | 908 | BCL  | C3B-C2B-C1B | -2.01 | 99.98       | 106.40   |
| 11  | A     | 907 | BCL  | CAC-C3C-C4C | -2.01 | 108.13      | 112.58   |
| 11  | A     | 902 | BCL  | CBB-CAB-C3B | -2.01 | 116.17      | 120.40   |
| 12  | A     | 910 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 11  | A     | 909 | BCL  | C2D-C1D-ND  | 2.01  | 112.11      | 110.13   |
| 11  | a     | 906 | BCL  | CHD-C1D-C2D | 2.00  | 129.66      | 125.49   |
| 15  | A     | 916 | 85I  | O6-C20-C21  | 2.00  | 115.81      | 111.48   |
| 12  | A     | 911 | CLA  | CHA-C4D-ND  | -2.00 | 128.42      | 132.55   |
| 11  | a     | 911 | BCL  | C7-C6-C5    | -2.00 | 107.93      | 113.26   |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 12  | A     | 910 | CLA  | C8   |
| 12  | A     | 911 | CLA  | C8   |
| 15  | A     | 916 | 85I  | C3   |

All (640) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | a     | 903 | 2GO  | C1A-C2A-CAA-CBA |
| 11  | A     | 902 | BCL  | C3A-C2A-CAA-CBA |
| 11  | A     | 902 | BCL  | C11-C12-C13-C14 |
| 11  | A     | 903 | BCL  | C1A-C2A-CAA-CBA |
| 11  | A     | 904 | BCL  | C1A-C2A-CAA-CBA |
| 11  | A     | 905 | BCL  | C1A-C2A-CAA-CBA |
| 11  | A     | 905 | BCL  | CBA-CGA-O2A-C1  |
| 11  | A     | 905 | BCL  | O1A-CGA-O2A-C1  |
| 11  | A     | 905 | BCL  | CBD-CGD-O2D-CED |
| 11  | A     | 905 | BCL  | C2-C3-C5-C6     |
| 11  | A     | 905 | BCL  | C4-C3-C5-C6     |
| 11  | A     | 906 | BCL  | CBD-CGD-O2D-CED |
| 11  | A     | 906 | BCL  | O1D-CGD-O2D-CED |
| 11  | A     | 907 | BCL  | C2C-C3C-CAC-CBC |
| 11  | A     | 907 | BCL  | C4C-C3C-CAC-CBC |
| 11  | A     | 907 | BCL  | CBD-CGD-O2D-CED |
| 11  | a     | 904 | BCL  | C4C-C3C-CAC-CBC |
| 11  | a     | 904 | BCL  | CHA-CBD-CGD-O2D |
| 11  | a     | 904 | BCL  | CBD-CGD-O2D-CED |
| 11  | a     | 905 | BCL  | C1A-C2A-CAA-CBA |
| 11  | a     | 905 | BCL  | C3A-C2A-CAA-CBA |
| 11  | a     | 905 | BCL  | CHA-CBD-CGD-O1D |
| 11  | a     | 905 | BCL  | CHA-CBD-CGD-O2D |
| 11  | a     | 906 | BCL  | C1A-C2A-CAA-CBA |
| 11  | a     | 908 | BCL  | C1A-C2A-CAA-CBA |
| 11  | a     | 908 | BCL  | CBD-CGD-O2D-CED |
| 11  | a     | 911 | BCL  | C1A-C2A-CAA-CBA |
| 11  | a     | 911 | BCL  | C3A-C2A-CAA-CBA |
| 12  | A     | 933 | CLA  | CHA-CBD-CGD-O1D |
| 12  | A     | 933 | CLA  | CHA-CBD-CGD-O2D |
| 12  | a     | 912 | CLA  | CBD-CGD-O2D-CED |
| 12  | a     | 913 | CLA  | CBD-CGD-O2D-CED |
| 12  | a     | 913 | CLA  | C6-C7-C8-C9     |
| 12  | a     | 915 | CLA  | CHA-CBD-CGD-O1D |
| 12  | a     | 915 | CLA  | CHA-CBD-CGD-O2D |
| 12  | a     | 915 | CLA  | C2-C3-C5-C6     |
| 12  | a     | 915 | CLA  | C4-C3-C5-C6     |
| 13  | c     | 201 | LYC  | C57-C56-C58-C59 |
| 15  | A     | 915 | 85I  | C4-C3-O3-P      |
| 15  | A     | 915 | 85I  | O7-C20-O6-C3    |
| 15  | A     | 915 | 85I  | C21-C20-O6-C3   |
| 15  | A     | 916 | 85I  | N-C1-C2-O       |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 15  | A     | 916 | 85I  | O6-C3-C4-O4    |
| 15  | A     | 916 | 85I  | C4-C3-O3-P     |
| 15  | A     | 916 | 85I  | C4-C3-O6-C20   |
| 15  | A     | 916 | 85I  | O3-C3-O6-C20   |
| 15  | A     | 916 | 85I  | O7-C20-O6-C3   |
| 15  | A     | 917 | 85I  | C4-C3-O6-C20   |
| 15  | A     | 917 | 85I  | C2-O-P-O2      |
| 15  | A     | 917 | 85I  | C2-O-P-O3      |
| 15  | A     | 917 | 85I  | C3-O3-P-O      |
| 15  | A     | 917 | 85I  | O7-C20-O6-C3   |
| 15  | a     | 918 | 85I  | C2-C1-N-C      |
| 15  | a     | 918 | 85I  | O3-C3-C4-O4    |
| 15  | a     | 918 | 85I  | O6-C3-C4-O4    |
| 15  | a     | 918 | 85I  | C4-C3-O6-C20   |
| 15  | a     | 918 | 85I  | O7-C20-O6-C3   |
| 15  | a     | 919 | 85I  | O6-C3-C4-O4    |
| 15  | a     | 919 | 85I  | C4-C3-O3-P     |
| 15  | a     | 919 | 85I  | O3-C3-O6-C20   |
| 15  | a     | 919 | 85I  | C6-C5-O4-C4    |
| 15  | a     | 919 | 85I  | C2-O-P-O1      |
| 15  | a     | 919 | 85I  | C2-O-P-O3      |
| 15  | a     | 920 | 85I  | C2-C1-N-C      |
| 15  | a     | 920 | 85I  | O3-C3-C4-O4    |
| 15  | a     | 920 | 85I  | O6-C3-C4-O4    |
| 15  | a     | 920 | 85I  | C4-C3-O6-C20   |
| 15  | a     | 920 | 85I  | C2-O-P-O1      |
| 15  | a     | 920 | 85I  | C2-O-P-O2      |
| 15  | a     | 920 | 85I  | C2-O-P-O3      |
| 15  | a     | 920 | 85I  | O7-C20-O6-C3   |
| 17  | A     | 932 | 85N  | O3-C17-O6-C25  |
| 17  | A     | 932 | 85N  | O2-C16-C17-O6  |
| 17  | A     | 932 | 85N  | C16-C17-O3-C18 |
| 17  | A     | 932 | 85N  | C20-C19-C24-O4 |
| 17  | A     | 932 | 85N  | C20-C19-C24-O5 |
| 17  | G     | 101 | 85N  | C19-C20-N1-C21 |
| 17  | G     | 101 | 85N  | C19-C20-N1-C22 |
| 17  | G     | 101 | 85N  | C19-C20-N1-C23 |
| 17  | G     | 101 | 85N  | O3-C18-C19-C20 |
| 17  | G     | 101 | 85N  | O3-C18-C19-C24 |
| 17  | G     | 101 | 85N  | C20-C19-C24-O4 |
| 17  | G     | 101 | 85N  | C20-C19-C24-O5 |
| 17  | a     | 902 | 85N  | O7-C25-O6-C17  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | a     | 902 | 85N  | C26-C25-O6-C17  |
| 17  | a     | 902 | 85N  | O2-C16-C17-O3   |
| 17  | g     | 101 | 85N  | C16-C17-O6-C25  |
| 17  | g     | 101 | 85N  | O7-C25-O6-C17   |
| 17  | g     | 101 | 85N  | O2-C16-C17-O6   |
| 18  | C     | 301 | HEC  | C2B-C3B-CAB-CBB |
| 18  | C     | 301 | HEC  | C4B-C3B-CAB-CBB |
| 18  | C     | 301 | HEC  | C2C-C3C-CAC-CBC |
| 18  | C     | 301 | HEC  | C4C-C3C-CAC-CBC |
| 18  | c     | 202 | HEC  | C2B-C3B-CAB-CBB |
| 18  | c     | 202 | HEC  | C4B-C3B-CAB-CBB |
| 18  | c     | 202 | HEC  | C2C-C3C-CAC-CBC |
| 18  | c     | 202 | HEC  | C4C-C3C-CAC-CBC |
| 19  | E     | 101 | 84Q  | O3-C17-O2-C16   |
| 19  | E     | 101 | 84Q  | C16-O4-P-O7     |
| 19  | E     | 101 | 84Q  | O7-C32-C33-N    |
| 19  | E     | 101 | 84Q  | O1-C15-C16-O2   |
| 19  | E     | 101 | 84Q  | O1-C15-C16-O4   |
| 19  | a     | 921 | 84Q  | O4-C16-O2-C17   |
| 19  | a     | 921 | 84Q  | O3-C17-O2-C16   |
| 19  | a     | 921 | 84Q  | C32-O7-P-O6     |
| 19  | a     | 921 | 84Q  | C32-O7-P-O5     |
| 19  | a     | 921 | 84Q  | C32-O7-P-O4     |
| 19  | a     | 921 | 84Q  | C16-O4-P-O7     |
| 19  | a     | 921 | 84Q  | C15-C16-O4-P    |
| 19  | a     | 921 | 84Q  | O1-C15-C16-O4   |
| 11  | a     | 904 | BCL  | O1D-CGD-O2D-CED |
| 11  | A     | 902 | BCL  | O1D-CGD-O2D-CED |
| 11  | A     | 905 | BCL  | O1D-CGD-O2D-CED |
| 11  | a     | 909 | BCL  | O1D-CGD-O2D-CED |
| 11  | A     | 902 | BCL  | CBD-CGD-O2D-CED |
| 11  | A     | 903 | BCL  | CBD-CGD-O2D-CED |
| 11  | a     | 905 | BCL  | CBD-CGD-O2D-CED |
| 11  | a     | 909 | BCL  | CBD-CGD-O2D-CED |
| 11  | A     | 907 | BCL  | O1A-CGA-O2A-C1  |
| 11  | a     | 907 | BCL  | O1A-CGA-O2A-C1  |
| 11  | a     | 911 | BCL  | O1A-CGA-O2A-C1  |
| 15  | a     | 919 | 85I  | O5-C5-O4-C4     |
| 12  | A     | 911 | CLA  | C3-C5-C6-C7     |
| 12  | a     | 913 | CLA  | C3-C5-C6-C7     |
| 11  | A     | 903 | BCL  | O1D-CGD-O2D-CED |
| 11  | A     | 907 | BCL  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | a     | 913 | CLA  | O1D-CGD-O2D-CED |
| 11  | A     | 907 | BCL  | CBA-CGA-O2A-C1  |
| 11  | a     | 907 | BCL  | CBA-CGA-O2A-C1  |
| 11  | a     | 908 | BCL  | O1A-CGA-O2A-C1  |
| 10  | a     | 903 | 2GO  | C4C-C3C-CAC-CBC |
| 11  | a     | 908 | BCL  | O1D-CGD-O2D-CED |
| 12  | A     | 910 | CLA  | CBD-CGD-O2D-CED |
| 12  | A     | 910 | CLA  | C3-C5-C6-C7     |
| 11  | a     | 908 | BCL  | CBA-CGA-O2A-C1  |
| 11  | a     | 911 | BCL  | CBA-CGA-O2A-C1  |
| 11  | A     | 903 | BCL  | C4-C3-C5-C6     |
| 11  | A     | 907 | BCL  | C4-C3-C5-C6     |
| 11  | a     | 908 | BCL  | C4-C3-C5-C6     |
| 12  | A     | 910 | CLA  | C4-C3-C5-C6     |
| 13  | c     | 201 | LYC  | C5-C6-C7-C8     |
| 11  | A     | 903 | BCL  | C2-C3-C5-C6     |
| 11  | A     | 907 | BCL  | C2-C3-C5-C6     |
| 11  | a     | 908 | BCL  | C2-C3-C5-C6     |
| 12  | A     | 910 | CLA  | C2-C3-C5-C6     |
| 13  | c     | 201 | LYC  | C5-C6-C7-C9     |
| 11  | A     | 903 | BCL  | C2A-CAA-CBA-CGA |
| 11  | a     | 907 | BCL  | C2A-CAA-CBA-CGA |
| 11  | a     | 910 | BCL  | C2A-CAA-CBA-CGA |
| 11  | a     | 909 | BCL  | C3-C5-C6-C7     |
| 17  | g     | 101 | 85N  | C14-C15-O2-C16  |
| 15  | A     | 917 | 85I  | O5-C5-O4-C4     |
| 17  | G     | 101 | 85N  | O1-C15-O2-C16   |
| 10  | A     | 901 | 2GO  | C1A-C2A-CAA-CBA |
| 11  | a     | 905 | BCL  | O1D-CGD-O2D-CED |
| 12  | a     | 912 | CLA  | O1D-CGD-O2D-CED |
| 12  | a     | 901 | CLA  | CBD-CGD-O2D-CED |
| 10  | A     | 901 | 2GO  | C4C-C3C-CAC-CBC |
| 17  | G     | 101 | 85N  | C14-C15-O2-C16  |
| 12  | A     | 910 | CLA  | O1D-CGD-O2D-CED |
| 15  | a     | 918 | 85I  | C21-C20-O6-C3   |
| 12  | A     | 911 | CLA  | CBD-CGD-O2D-CED |
| 12  | a     | 914 | CLA  | CBA-CGA-O2A-C1  |
| 15  | A     | 917 | 85I  | C6-C5-O4-C4     |
| 17  | g     | 101 | 85N  | O1-C15-O2-C16   |
| 13  | c     | 201 | LYC  | C4-C5-C6-C7     |
| 17  | a     | 902 | 85N  | C11-C10-C9-C8   |
| 11  | A     | 909 | BCL  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | a     | 914 | CLA  | CBD-CGD-O2D-CED |
| 12  | a     | 915 | CLA  | CBD-CGD-O2D-CED |
| 15  | A     | 917 | 85I  | C7-C8-C9-C10    |
| 15  | A     | 917 | 85I  | C10-C11-C12-C13 |
| 15  | A     | 915 | 85I  | C12-C13-C14-C15 |
| 11  | A     | 902 | BCL  | CBA-CGA-O2A-C1  |
| 19  | E     | 101 | 84Q  | C13-C14-O1-C15  |
| 19  | a     | 921 | 84Q  | C13-C14-O1-C15  |
| 11  | A     | 902 | BCL  | C4-C3-C5-C6     |
| 11  | A     | 902 | BCL  | C2-C3-C5-C6     |
| 11  | A     | 903 | BCL  | C11-C10-C8-C9   |
| 11  | A     | 903 | BCL  | C14-C13-C15-C16 |
| 11  | A     | 907 | BCL  | C11-C10-C8-C9   |
| 11  | A     | 908 | BCL  | C11-C10-C8-C9   |
| 11  | a     | 908 | BCL  | C14-C13-C15-C16 |
| 11  | a     | 910 | BCL  | C14-C13-C15-C16 |
| 12  | A     | 911 | CLA  | C6-C7-C8-C9     |
| 12  | A     | 931 | CLA  | C6-C7-C8-C9     |
| 12  | a     | 901 | CLA  | C6-C7-C8-C9     |
| 15  | A     | 917 | 85I  | C25-C26-C27-C28 |
| 12  | a     | 914 | CLA  | O1A-CGA-O2A-C1  |
| 19  | E     | 101 | 84Q  | O-C14-O1-C15    |
| 19  | a     | 921 | 84Q  | O-C14-O1-C15    |
| 13  | c     | 201 | LYC  | C15-C16-C17-C19 |
| 13  | c     | 201 | LYC  | C55-C56-C58-C59 |
| 12  | a     | 912 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 921 | 84Q  | C11-C12-C13-C14 |
| 11  | A     | 909 | BCL  | C2-C1-O2A-CGA   |
| 12  | A     | 910 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 921 | 84Q  | C1-C3-C4-C5     |
| 11  | a     | 907 | BCL  | C11-C12-C13-C15 |
| 19  | E     | 101 | 84Q  | C18-C17-O2-C16  |
| 17  | a     | 902 | 85N  | C25-C26-C27-C28 |
| 15  | A     | 915 | 85I  | O5-C5-O4-C4     |
| 12  | a     | 901 | CLA  | C15-C16-C17-C18 |
| 11  | A     | 905 | BCL  | C2A-CAA-CBA-CGA |
| 11  | a     | 908 | BCL  | C5-C6-C7-C8     |
| 15  | a     | 919 | 85I  | C14-C15-C16-C17 |
| 11  | A     | 909 | BCL  | C3-C5-C6-C7     |
| 11  | a     | 905 | BCL  | C15-C16-C17-C18 |
| 11  | a     | 907 | BCL  | C5-C6-C7-C8     |
| 11  | a     | 909 | BCL  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | A     | 910 | CLA  | C8-C10-C11-C12  |
| 11  | a     | 909 | BCL  | C10-C11-C12-C13 |
| 17  | A     | 932 | 85N  | C34-C35-C36-C37 |
| 15  | A     | 917 | 85I  | C29-C30-C31-C32 |
| 15  | a     | 920 | 85I  | C29-C30-C31-C32 |
| 12  | A     | 911 | CLA  | C15-C16-C17-C18 |
| 15  | A     | 915 | 85I  | C6-C5-O4-C4     |
| 12  | A     | 910 | CLA  | C5-C6-C7-C8     |
| 12  | a     | 901 | CLA  | C2A-CAA-CBA-CGA |
| 12  | A     | 931 | CLA  | O1D-CGD-O2D-CED |
| 11  | A     | 902 | BCL  | C13-C15-C16-C17 |
| 11  | a     | 907 | BCL  | C10-C11-C12-C13 |
| 11  | a     | 909 | BCL  | C5-C6-C7-C8     |
| 12  | a     | 901 | CLA  | C5-C6-C7-C8     |
| 12  | a     | 912 | CLA  | C8-C10-C11-C12  |
| 10  | a     | 903 | 2GO  | C15-C16-C17-C18 |
| 12  | A     | 931 | CLA  | C8-C10-C11-C12  |
| 12  | a     | 901 | CLA  | C13-C15-C16-C17 |
| 12  | A     | 931 | CLA  | C13-C15-C16-C17 |
| 15  | a     | 920 | 85I  | C14-C15-C16-C17 |
| 13  | A     | 913 | LYC  | C4-C5-C6-C7     |
| 15  | a     | 919 | 85I  | C15-C16-C17-C19 |
| 10  | a     | 903 | 2GO  | C13-C15-C16-C17 |
| 13  | c     | 201 | LYC  | C15-C16-C17-C18 |
| 11  | A     | 902 | BCL  | O1A-CGA-O2A-C1  |
| 11  | A     | 905 | BCL  | C10-C11-C12-C13 |
| 12  | A     | 931 | CLA  | C15-C16-C17-C18 |
| 13  | c     | 201 | LYC  | C17-C19-C20-C21 |
| 12  | A     | 931 | CLA  | C16-C17-C18-C20 |
| 17  | a     | 902 | 85N  | C1-C2-C4-C5     |
| 11  | a     | 908 | BCL  | C3-C5-C6-C7     |
| 11  | a     | 905 | BCL  | C13-C15-C16-C17 |
| 11  | a     | 909 | BCL  | CBA-CGA-O2A-C1  |
| 11  | A     | 903 | BCL  | C16-C17-C18-C20 |
| 12  | A     | 931 | CLA  | C16-C17-C18-C19 |
| 15  | A     | 917 | 85I  | C30-C31-C32-C34 |
| 17  | g     | 101 | 85N  | C27-C28-C29-C30 |
| 19  | E     | 101 | 84Q  | C7-C8-C9-C10    |
| 19  | a     | 921 | 84Q  | C9-C10-C11-C12  |
| 15  | A     | 917 | 85I  | C11-C10-C9-C8   |
| 15  | a     | 919 | 85I  | C12-C13-C14-C15 |
| 17  | A     | 932 | 85N  | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | A     | 916 | 85I  | C25-C26-C27-C28 |
| 15  | a     | 920 | 85I  | C9-C10-C11-C12  |
| 19  | a     | 921 | 84Q  | C4-C5-C6-C7     |
| 15  | A     | 915 | 85I  | C22-C23-C24-C25 |
| 15  | a     | 919 | 85I  | C21-C22-C23-C24 |
| 15  | a     | 920 | 85I  | C11-C12-C13-C14 |
| 15  | a     | 920 | 85I  | C20-C21-C22-C23 |
| 19  | E     | 101 | 84Q  | C17-C18-C19-C20 |
| 17  | A     | 932 | 85N  | C27-C28-C29-C30 |
| 11  | a     | 910 | BCL  | C16-C17-C18-C19 |
| 19  | E     | 101 | 84Q  | C-C1-C3-C4      |
| 19  | E     | 101 | 84Q  | C2-C1-C3-C4     |
| 12  | A     | 911 | CLA  | O1D-CGD-O2D-CED |
| 11  | A     | 908 | BCL  | C2A-CAA-CBA-CGA |
| 15  | a     | 919 | 85I  | C6-C7-C8-C9     |
| 15  | a     | 919 | 85I  | C9-C10-C11-C12  |
| 12  | a     | 913 | CLA  | C15-C16-C17-C18 |
| 11  | A     | 909 | BCL  | C11-C10-C8-C7   |
| 12  | A     | 911 | CLA  | C11-C12-C13-C15 |
| 11  | a     | 910 | BCL  | C10-C11-C12-C13 |
| 17  | a     | 902 | 85N  | C26-C27-C28-C29 |
| 19  | a     | 921 | 84Q  | C19-C20-C21-C22 |
| 11  | A     | 904 | BCL  | C3A-C2A-CAA-CBA |
| 11  | A     | 905 | BCL  | C3A-C2A-CAA-CBA |
| 11  | A     | 909 | BCL  | C3A-C2A-CAA-CBA |
| 11  | a     | 906 | BCL  | C3A-C2A-CAA-CBA |
| 11  | a     | 908 | BCL  | C3A-C2A-CAA-CBA |
| 12  | A     | 931 | CLA  | C4-C3-C5-C6     |
| 12  | a     | 901 | CLA  | C3A-C2A-CAA-CBA |
| 12  | A     | 931 | CLA  | C5-C6-C7-C8     |
| 11  | a     | 910 | BCL  | C16-C17-C18-C20 |
| 15  | A     | 916 | 85I  | C30-C31-C32-C33 |
| 15  | A     | 917 | 85I  | C15-C16-C17-C19 |
| 15  | a     | 919 | 85I  | C22-C23-C24-C25 |
| 15  | A     | 916 | 85I  | C22-C23-C24-C25 |
| 15  | A     | 916 | 85I  | C27-C28-C29-C30 |
| 15  | a     | 918 | 85I  | C21-C22-C23-C24 |
| 15  | A     | 915 | 85I  | C10-C11-C12-C13 |
| 15  | a     | 918 | 85I  | C26-C27-C28-C29 |
| 15  | a     | 919 | 85I  | C11-C10-C9-C8   |
| 17  | G     | 101 | 85N  | C10-C11-C12-C13 |
| 15  | A     | 916 | 85I  | C21-C20-O6-C3   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | a     | 902 | 85N  | C11-C12-C13-C14 |
| 15  | a     | 919 | 85I  | C10-C11-C12-C13 |
| 17  | g     | 101 | 85N  | C5-C6-C7-C8     |
| 11  | A     | 903 | BCL  | C16-C17-C18-C19 |
| 15  | A     | 917 | 85I  | C30-C31-C32-C33 |
| 15  | a     | 919 | 85I  | C30-C31-C32-C34 |
| 15  | A     | 917 | 85I  | C20-C21-C22-C23 |
| 12  | a     | 915 | CLA  | C2B-C3B-CAB-CBB |
| 15  | A     | 916 | 85I  | C24-C25-C26-C27 |
| 15  | A     | 917 | 85I  | C12-C13-C14-C15 |
| 15  | A     | 915 | 85I  | C26-C27-C28-C29 |
| 12  | A     | 931 | CLA  | C2A-CAA-CBA-CGA |
| 17  | a     | 902 | 85N  | C12-C13-C14-C15 |
| 17  | a     | 902 | 85N  | C7-C8-C9-C10    |
| 19  | a     | 921 | 84Q  | C3-C4-C5-C6     |
| 15  | A     | 917 | 85I  | C26-C27-C28-C29 |
| 15  | A     | 916 | 85I  | C20-C21-C22-C23 |
| 17  | G     | 101 | 85N  | C26-C27-C28-C29 |
| 17  | a     | 902 | 85N  | C5-C6-C7-C8     |
| 15  | A     | 916 | 85I  | C7-C8-C9-C10    |
| 15  | a     | 920 | 85I  | C21-C20-O6-C3   |
| 17  | g     | 101 | 85N  | C26-C25-O6-C17  |
| 12  | a     | 901 | CLA  | O1D-CGD-O2D-CED |
| 15  | a     | 918 | 85I  | C22-C23-C24-C25 |
| 15  | a     | 920 | 85I  | C7-C8-C9-C10    |
| 19  | E     | 101 | 84Q  | C10-C11-C12-C13 |
| 15  | a     | 919 | 85I  | C25-C26-C27-C28 |
| 15  | a     | 919 | 85I  | C13-C14-C15-C16 |
| 11  | a     | 904 | BCL  | CBA-CGA-O2A-C1  |
| 17  | G     | 101 | 85N  | C1-C2-C4-C5     |
| 17  | a     | 902 | 85N  | C17-C16-O2-C15  |
| 15  | A     | 916 | 85I  | C5-C6-C7-C8     |
| 15  | A     | 916 | 85I  | C12-C13-C14-C15 |
| 12  | a     | 901 | CLA  | C8-C10-C11-C12  |
| 15  | a     | 920 | 85I  | C25-C26-C27-C28 |
| 15  | a     | 919 | 85I  | C30-C31-C32-C33 |
| 15  | a     | 920 | 85I  | C30-C31-C32-C33 |
| 17  | g     | 101 | 85N  | C11-C12-C13-C14 |
| 11  | a     | 908 | BCL  | C13-C15-C16-C17 |
| 19  | E     | 101 | 84Q  | C19-C20-C21-C22 |
| 17  | a     | 902 | 85N  | C3-C2-C4-C5     |
| 15  | a     | 918 | 85I  | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | A     | 917 | 85I  | C21-C22-C23-C24 |
| 15  | a     | 919 | 85I  | C7-C8-C9-C10    |
| 17  | a     | 902 | 85N  | C10-C11-C12-C13 |
| 15  | a     | 919 | 85I  | C11-C12-C13-C14 |
| 15  | A     | 916 | 85I  | C11-C10-C9-C8   |
| 15  | A     | 916 | 85I  | C13-C14-C15-C16 |
| 19  | E     | 101 | 84Q  | C20-C21-C22-C23 |
| 17  | a     | 902 | 85N  | C28-C29-C30-C31 |
| 15  | A     | 917 | 85I  | C22-C23-C24-C25 |
| 17  | g     | 101 | 85N  | C26-C27-C28-C29 |
| 10  | a     | 903 | 2GO  | C2C-C3C-CAC-CBC |
| 19  | a     | 921 | 84Q  | C6-C7-C8-C9     |
| 19  | E     | 101 | 84Q  | C16-C15-O1-C14  |
| 11  | a     | 904 | BCL  | C2A-CAA-CBA-CGA |
| 12  | a     | 901 | CLA  | CBA-CGA-O2A-C1  |
| 15  | A     | 915 | 85I  | C7-C8-C9-C10    |
| 19  | a     | 921 | 84Q  | C25-C26-C27-C28 |
| 11  | A     | 905 | BCL  | C5-C6-C7-C8     |
| 15  | A     | 917 | 85I  | C15-C16-C17-C18 |
| 11  | a     | 909 | BCL  | O1A-CGA-O2A-C1  |
| 11  | A     | 908 | BCL  | C3-C5-C6-C7     |
| 11  | A     | 902 | BCL  | C1A-C2A-CAA-CBA |
| 11  | A     | 908 | BCL  | C1A-C2A-CAA-CBA |
| 11  | A     | 909 | BCL  | C1A-C2A-CAA-CBA |
| 11  | a     | 910 | BCL  | C1A-C2A-CAA-CBA |
| 11  | A     | 903 | BCL  | C10-C11-C12-C13 |
| 11  | A     | 908 | BCL  | C8-C10-C11-C12  |
| 15  | A     | 917 | 85I  | C28-C29-C30-C31 |
| 19  | E     | 101 | 84Q  | C11-C12-C13-C14 |
| 11  | a     | 910 | BCL  | C12-C13-C15-C16 |
| 12  | a     | 901 | CLA  | C6-C7-C8-C10    |
| 12  | a     | 913 | CLA  | C11-C10-C8-C7   |
| 15  | a     | 920 | 85I  | C26-C27-C28-C29 |
| 15  | a     | 918 | 85I  | C30-C31-C32-C34 |
| 19  | a     | 921 | 84Q  | C18-C17-O2-C16  |
| 11  | a     | 904 | BCL  | C2C-C3C-CAC-CBC |
| 12  | A     | 912 | CLA  | CBD-CGD-O2D-CED |
| 15  | a     | 918 | 85I  | C5-C6-C7-C8     |
| 17  | a     | 902 | 85N  | C18-C19-C24-O4  |
| 17  | a     | 902 | 85N  | C30-C31-C32-C33 |
| 11  | A     | 909 | BCL  | C15-C16-C17-C18 |
| 11  | A     | 905 | BCL  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | A     | 917 | 85I  | C5-C6-C7-C8     |
| 12  | a     | 913 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 921 | 84Q  | C5-C6-C7-C8     |
| 17  | G     | 101 | 85N  | C7-C8-C9-C10    |
| 11  | A     | 909 | BCL  | C8-C10-C11-C12  |
| 12  | a     | 912 | CLA  | C13-C15-C16-C17 |
| 12  | a     | 914 | CLA  | O1D-CGD-O2D-CED |
| 11  | a     | 905 | BCL  | CBA-CGA-O2A-C1  |
| 15  | a     | 919 | 85I  | C23-C24-C25-C26 |
| 15  | a     | 920 | 85I  | C21-C22-C23-C24 |
| 17  | a     | 902 | 85N  | C29-C30-C31-C32 |
| 19  | E     | 101 | 84Q  | C3-C4-C5-C6     |
| 15  | A     | 916 | 85I  | C14-C15-C16-C17 |
| 19  | a     | 921 | 84Q  | C23-C24-C25-C26 |
| 11  | A     | 902 | BCL  | C2B-C3B-CAB-CBB |
| 17  | A     | 932 | 85N  | C29-C30-C31-C32 |
| 15  | A     | 916 | 85I  | C6-C7-C8-C9     |
| 13  | c     | 201 | LYC  | C58-C59-C60-C61 |
| 12  | A     | 933 | CLA  | O1D-CGD-O2D-CED |
| 12  | a     | 912 | CLA  | CBA-CGA-O2A-C1  |
| 15  | A     | 917 | 85I  | C6-C7-C8-C9     |
| 19  | a     | 921 | 84Q  | C10-C11-C12-C13 |
| 12  | A     | 912 | CLA  | O1D-CGD-O2D-CED |
| 11  | a     | 908 | BCL  | C15-C16-C17-C18 |
| 15  | a     | 919 | 85I  | C28-C29-C30-C31 |
| 17  | G     | 101 | 85N  | C11-C12-C13-C14 |
| 19  | E     | 101 | 84Q  | C22-C23-C24-C25 |
| 12  | a     | 913 | CLA  | C16-C17-C18-C20 |
| 11  | A     | 903 | BCL  | C6-C7-C8-C9     |
| 11  | a     | 905 | BCL  | C11-C12-C13-C14 |
| 11  | a     | 908 | BCL  | C6-C7-C8-C9     |
| 12  | a     | 912 | CLA  | C6-C7-C8-C9     |
| 12  | A     | 933 | CLA  | C4B-C3B-CAB-CBB |
| 12  | a     | 915 | CLA  | C4B-C3B-CAB-CBB |
| 15  | A     | 915 | 85I  | C25-C26-C27-C28 |
| 11  | A     | 902 | BCL  | C11-C12-C13-C15 |
| 11  | A     | 902 | BCL  | C12-C13-C15-C16 |
| 11  | A     | 903 | BCL  | C6-C7-C8-C10    |
| 11  | A     | 905 | BCL  | C11-C10-C8-C7   |
| 11  | A     | 908 | BCL  | C12-C13-C15-C16 |
| 11  | a     | 908 | BCL  | C6-C7-C8-C10    |
| 11  | a     | 908 | BCL  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | A     | 910 | CLA  | C11-C10-C8-C7   |
| 12  | A     | 911 | CLA  | C11-C10-C8-C7   |
| 12  | a     | 901 | CLA  | C11-C10-C8-C7   |
| 11  | a     | 905 | BCL  | C10-C11-C12-C13 |
| 11  | a     | 905 | BCL  | O1A-CGA-O2A-C1  |
| 11  | A     | 903 | BCL  | C3A-C2A-CAA-CBA |
| 11  | A     | 908 | BCL  | C3A-C2A-CAA-CBA |
| 12  | a     | 915 | CLA  | O1D-CGD-O2D-CED |
| 15  | a     | 919 | 85I  | C15-C16-C17-C18 |
| 17  | a     | 902 | 85N  | O2-C16-C17-O6   |
| 17  | g     | 101 | 85N  | O2-C16-C17-O3   |
| 19  | a     | 921 | 84Q  | O1-C15-C16-O2   |
| 15  | A     | 916 | 85I  | C30-C31-C32-C34 |
| 15  | a     | 918 | 85I  | C30-C31-C32-C33 |
| 17  | G     | 101 | 85N  | C3-C2-C4-C5     |
| 11  | a     | 908 | BCL  | C10-C11-C12-C13 |
| 17  | G     | 101 | 85N  | C6-C7-C8-C9     |
| 11  | a     | 904 | BCL  | C8-C10-C11-C12  |
| 17  | a     | 902 | 85N  | C2-C4-C5-C6     |
| 10  | a     | 903 | 2GO  | C3A-C2A-CAA-CBA |
| 17  | A     | 932 | 85N  | C28-C29-C30-C31 |
| 15  | A     | 915 | 85I  | C30-C31-C32-C33 |
| 11  | a     | 909 | BCL  | C1-C2-C3-C5     |
| 15  | a     | 919 | 85I  | O7-C20-O6-C3    |
| 19  | E     | 101 | 84Q  | C6-C7-C8-C9     |
| 11  | A     | 908 | BCL  | C14-C13-C15-C16 |
| 15  | A     | 917 | 85I  | C21-C20-O6-C3   |
| 11  | a     | 905 | BCL  | C3-C5-C6-C7     |
| 10  | A     | 901 | 2GO  | C10-C11-C12-C13 |
| 19  | E     | 101 | 84Q  | C1-C3-C4-C5     |
| 15  | a     | 918 | 85I  | C11-C12-C13-C14 |
| 15  | a     | 918 | 85I  | C12-C13-C14-C15 |
| 12  | a     | 912 | CLA  | C3-C5-C6-C7     |
| 15  | a     | 919 | 85I  | N-C1-C2-O       |
| 15  | a     | 920 | 85I  | C30-C31-C32-C34 |
| 19  | a     | 921 | 84Q  | C2-C1-C3-C4     |
| 12  | A     | 911 | CLA  | C10-C11-C12-C13 |
| 11  | A     | 903 | BCL  | C11-C10-C8-C7   |
| 11  | a     | 905 | BCL  | C11-C12-C13-C15 |
| 11  | A     | 902 | BCL  | C2A-CAA-CBA-CGA |
| 17  | A     | 932 | 85N  | C1-C2-C4-C5     |
| 15  | A     | 915 | 85I  | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | a     | 904 | BCL  | O1A-CGA-O2A-C1  |
| 12  | a     | 901 | CLA  | O1A-CGA-O2A-C1  |
| 15  | A     | 915 | 85I  | C21-C22-C23-C24 |
| 15  | a     | 920 | 85I  | C27-C28-C29-C30 |
| 15  | a     | 919 | 85I  | C29-C30-C31-C32 |
| 17  | A     | 932 | 85N  | C25-C26-C27-C28 |
| 11  | a     | 909 | BCL  | C16-C17-C18-C19 |
| 12  | A     | 911 | CLA  | C16-C17-C18-C19 |
| 11  | A     | 903 | BCL  | C5-C6-C7-C8     |
| 15  | a     | 920 | 85I  | C1-C2-O-P       |
| 19  | a     | 921 | 84Q  | C33-C32-O7-P    |
| 15  | A     | 916 | 85I  | C23-C24-C25-C26 |
| 15  | a     | 920 | 85I  | C13-C14-C15-C16 |
| 17  | a     | 902 | 85N  | C33-C34-C35-C36 |
| 12  | A     | 910 | CLA  | C10-C11-C12-C13 |
| 12  | A     | 911 | CLA  | C5-C6-C7-C8     |
| 19  | E     | 101 | 84Q  | C24-C25-C26-C27 |
| 19  | E     | 101 | 84Q  | C27-C28-C29-C31 |
| 11  | a     | 905 | BCL  | C5-C6-C7-C8     |
| 15  | A     | 916 | 85I  | C10-C11-C12-C13 |
| 19  | a     | 921 | 84Q  | C-C1-C3-C4      |
| 11  | A     | 905 | BCL  | C12-C13-C15-C16 |
| 11  | A     | 907 | BCL  | C6-C7-C8-C10    |
| 11  | A     | 907 | BCL  | C11-C10-C8-C7   |
| 11  | A     | 908 | BCL  | C11-C10-C8-C7   |
| 11  | a     | 907 | BCL  | C11-C10-C8-C7   |
| 11  | a     | 910 | BCL  | C11-C12-C13-C15 |
| 15  | a     | 918 | 85I  | C27-C28-C29-C30 |
| 17  | a     | 902 | 85N  | C18-C19-C24-O5  |
| 11  | A     | 902 | BCL  | C14-C13-C15-C16 |
| 12  | A     | 911 | CLA  | C11-C12-C13-C14 |
| 12  | A     | 931 | CLA  | C11-C12-C13-C14 |
| 12  | a     | 913 | CLA  | C11-C10-C8-C9   |
| 15  | a     | 918 | 85I  | C7-C8-C9-C10    |
| 11  | A     | 906 | BCL  | CAD-CBD-CGD-O2D |
| 11  | a     | 908 | BCL  | CAD-CBD-CGD-O2D |
| 17  | A     | 932 | 85N  | C19-C18-O3-C17  |
| 15  | a     | 918 | 85I  | C23-C24-C25-C26 |
| 17  | g     | 101 | 85N  | C1-C2-C4-C5     |
| 12  | a     | 912 | CLA  | O1A-CGA-O2A-C1  |
| 11  | a     | 908 | BCL  | CAD-CBD-CGD-O1D |
| 15  | A     | 915 | 85I  | C2-O-P-O1       |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | a     | 919 | 85I  | C2-O-P-O2       |
| 15  | a     | 919 | 85I  | C3-O3-P-O       |
| 19  | E     | 101 | 84Q  | C32-O7-P-O4     |
| 12  | A     | 933 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 921 | 84Q  | C7-C8-C9-C10    |
| 11  | A     | 907 | BCL  | C8-C10-C11-C12  |
| 11  | A     | 906 | BCL  | O1A-CGA-O2A-C1  |
| 13  | c     | 201 | LYC  | C9-C10-C11-C12  |
| 11  | a     | 904 | BCL  | C10-C11-C12-C13 |
| 15  | a     | 920 | 85I  | C6-C7-C8-C9     |
| 10  | a     | 903 | 2GO  | C14-C13-C15-C16 |
| 11  | a     | 910 | BCL  | C11-C12-C13-C14 |
| 12  | a     | 901 | CLA  | C11-C12-C13-C14 |
| 10  | a     | 903 | 2GO  | C11-C12-C13-C15 |
| 15  | a     | 919 | 85I  | C20-C21-C22-C23 |
| 11  | A     | 908 | BCL  | C16-C17-C18-C19 |
| 11  | a     | 909 | BCL  | CAA-CBA-CGA-O2A |
| 17  | A     | 932 | 85N  | C3-C2-C4-C5     |
| 15  | a     | 919 | 85I  | C21-C20-O6-C3   |
| 12  | a     | 901 | CLA  | C16-C17-C18-C20 |
| 17  | g     | 101 | 85N  | C7-C8-C9-C10    |
| 11  | A     | 902 | BCL  | CAA-CBA-CGA-O2A |
| 12  | a     | 912 | CLA  | C4-C3-C5-C6     |
| 17  | G     | 101 | 85N  | C25-C26-C27-C28 |
| 10  | a     | 903 | 2GO  | C8-C10-C11-C12  |
| 15  | a     | 920 | 85I  | C22-C23-C24-C25 |
| 15  | a     | 920 | 85I  | C10-C11-C12-C13 |
| 12  | A     | 931 | CLA  | C11-C12-C13-C15 |
| 15  | A     | 916 | 85I  | C26-C27-C28-C29 |
| 15  | a     | 919 | 85I  | C24-C25-C26-C27 |
| 13  | c     | 201 | LYC  | C52-C51-C53-C54 |
| 12  | A     | 910 | CLA  | C16-C17-C18-C20 |
| 15  | a     | 918 | 85I  | C9-C10-C11-C12  |
| 15  | A     | 915 | 85I  | O3-C3-C4-O4     |
| 11  | a     | 907 | BCL  | C11-C12-C13-C14 |
| 12  | a     | 901 | CLA  | C14-C13-C15-C16 |
| 15  | A     | 915 | 85I  | C6-C7-C8-C9     |
| 18  | c     | 202 | HEC  | CAD-CBD-CGD-O2D |
| 18  | C     | 301 | HEC  | CAD-CBD-CGD-O2D |
| 12  | a     | 901 | CLA  | C1A-C2A-CAA-CBA |
| 13  | c     | 201 | LYC  | C21-C50-C51-C53 |
| 15  | a     | 920 | 85I  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | a     | 901 | CLA  | C2B-C3B-CAB-CBB |
| 11  | A     | 904 | BCL  | CAA-CBA-CGA-O2A |
| 12  | a     | 912 | CLA  | C2-C3-C5-C6     |
| 11  | a     | 906 | BCL  | CAA-CBA-CGA-O1A |
| 11  | A     | 903 | BCL  | C12-C13-C15-C16 |
| 12  | A     | 931 | CLA  | C6-C7-C8-C10    |
| 12  | a     | 901 | CLA  | C12-C13-C15-C16 |
| 17  | g     | 101 | 85N  | C3-C2-C4-C5     |
| 11  | a     | 909 | BCL  | C13-C15-C16-C17 |
| 19  | E     | 101 | 84Q  | C23-C24-C25-C26 |
| 15  | A     | 916 | 85I  | C15-C16-C17-C19 |
| 11  | A     | 905 | BCL  | C2-C1-O2A-CGA   |
| 11  | a     | 908 | BCL  | C2A-CAA-CBA-CGA |
| 11  | A     | 904 | BCL  | CAA-CBA-CGA-O1A |
| 18  | C     | 301 | HEC  | CAD-CBD-CGD-O1D |
| 12  | A     | 931 | CLA  | C2-C3-C5-C6     |
| 11  | a     | 906 | BCL  | CAA-CBA-CGA-O2A |
| 19  | a     | 921 | 84Q  | C27-C28-C29-C30 |
| 11  | a     | 904 | BCL  | CAA-CBA-CGA-O2A |
| 13  | c     | 201 | LYC  | C13-C12-C14-C15 |
| 13  | c     | 201 | LYC  | C21-C50-C51-C52 |
| 15  | A     | 917 | 85I  | N-C1-C2-O       |
| 15  | A     | 917 | 85I  | C23-C24-C25-C26 |
| 11  | A     | 909 | BCL  | C6-C7-C8-C10    |
| 12  | A     | 910 | CLA  | C6-C7-C8-C10    |
| 15  | a     | 918 | 85I  | C28-C29-C30-C31 |
| 17  | g     | 101 | 85N  | C11-C10-C9-C8   |
| 11  | A     | 908 | BCL  | C6-C7-C8-C9     |
| 11  | A     | 909 | BCL  | C11-C10-C8-C9   |
| 15  | A     | 917 | 85I  | C3-O3-P-O1      |
| 15  | a     | 919 | 85I  | C3-O3-P-O1      |
| 19  | E     | 101 | 84Q  | C16-O4-P-O5     |
| 10  | A     | 901 | 2GO  | C16-C17-C18-C20 |
| 13  | c     | 201 | LYC  | C11-C12-C14-C15 |
| 12  | A     | 931 | CLA  | CBD-CGD-O2D-CED |
| 11  | A     | 909 | BCL  | O1D-CGD-O2D-CED |
| 11  | A     | 902 | BCL  | C8-C10-C11-C12  |
| 11  | A     | 907 | BCL  | C11-C12-C13-C14 |
| 15  | a     | 918 | 85I  | C24-C25-C26-C27 |
| 15  | a     | 920 | 85I  | C11-C10-C9-C8   |
| 18  | c     | 202 | HEC  | CAD-CBD-CGD-O1D |
| 12  | a     | 901 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | A     | 902 | BCL  | C4B-C3B-CAB-CBB |
| 11  | A     | 907 | BCL  | C6-C7-C8-C9     |
| 11  | a     | 907 | BCL  | C11-C10-C8-C9   |
| 12  | a     | 901 | CLA  | C11-C10-C8-C9   |
| 12  | a     | 901 | CLA  | C16-C17-C18-C19 |
| 15  | a     | 919 | 85I  | C26-C27-C28-C29 |
| 11  | A     | 903 | BCL  | CAA-CBA-CGA-O2A |
| 11  | a     | 904 | BCL  | C2-C1-O2A-CGA   |
| 11  | a     | 911 | BCL  | C2-C1-O2A-CGA   |
| 15  | A     | 915 | 85I  | C5-C6-C7-C8     |
| 19  | a     | 921 | 84Q  | C27-C28-C29-C31 |
| 12  | A     | 931 | CLA  | C3-C5-C6-C7     |
| 11  | a     | 907 | BCL  | C13-C15-C16-C17 |
| 11  | A     | 909 | BCL  | C11-C12-C13-C14 |
| 17  | A     | 932 | 85N  | C4-C5-C6-C7     |
| 19  | a     | 921 | 84Q  | C22-C23-C24-C25 |
| 15  | a     | 919 | 85I  | O4-C5-C6-C7     |
| 17  | a     | 902 | 85N  | C13-C14-C15-O2  |
| 18  | C     | 301 | HEC  | CAA-CBA-CGA-O2A |
| 11  | a     | 910 | BCL  | CAA-CBA-CGA-O2A |
| 15  | A     | 916 | 85I  | O4-C5-C6-C7     |
| 19  | a     | 921 | 84Q  | C11-C10-C9-C8   |
| 11  | A     | 908 | BCL  | C6-C7-C8-C10    |
| 11  | a     | 905 | BCL  | C6-C7-C8-C10    |
| 12  | A     | 931 | CLA  | C11-C10-C8-C7   |
| 12  | a     | 912 | CLA  | C11-C10-C8-C7   |
| 12  | a     | 913 | CLA  | C6-C7-C8-C10    |
| 17  | A     | 932 | 85N  | C2-C4-C5-C6     |
| 10  | a     | 903 | 2GO  | CAD-CBD-CGD-O1D |
| 12  | A     | 910 | CLA  | C2A-CAA-CBA-CGA |
| 12  | a     | 901 | CLA  | CAA-CBA-CGA-O1A |
| 10  | a     | 903 | 2GO  | CAD-CBD-CGD-O2D |
| 17  | g     | 101 | 85N  | C2-C4-C5-C6     |
| 17  | g     | 101 | 85N  | C13-C14-C15-O2  |
| 17  | G     | 101 | 85N  | C13-C14-C15-O2  |
| 15  | a     | 919 | 85I  | O5-C5-C6-C7     |
| 18  | c     | 202 | HEC  | CAA-CBA-CGA-O2A |
| 15  | a     | 920 | 85I  | O4-C5-C6-C7     |
| 11  | a     | 910 | BCL  | CAA-CBA-CGA-O1A |
| 17  | g     | 101 | 85N  | C13-C14-C15-O1  |
| 15  | A     | 917 | 85I  | C14-C15-C16-C17 |
| 11  | A     | 907 | BCL  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | A     | 903 | BCL  | CAA-CBA-CGA-O1A |
| 11  | A     | 903 | BCL  | O1A-CGA-O2A-C1  |
| 17  | A     | 932 | 85N  | C7-C8-C9-C10    |
| 12  | a     | 901 | CLA  | C2-C1-O2A-CGA   |
| 17  | a     | 902 | 85N  | C13-C14-C15-O1  |
| 17  | A     | 932 | 85N  | C18-C19-C20-N1  |
| 11  | A     | 908 | BCL  | CAA-CBA-CGA-O2A |
| 17  | A     | 932 | 85N  | O6-C25-C26-C27  |
| 17  | A     | 932 | 85N  | O7-C25-C26-C27  |
| 15  | A     | 916 | 85I  | O5-C5-C6-C7     |

There are no ring outliers.

44 monomers are involved in 203 short contacts:

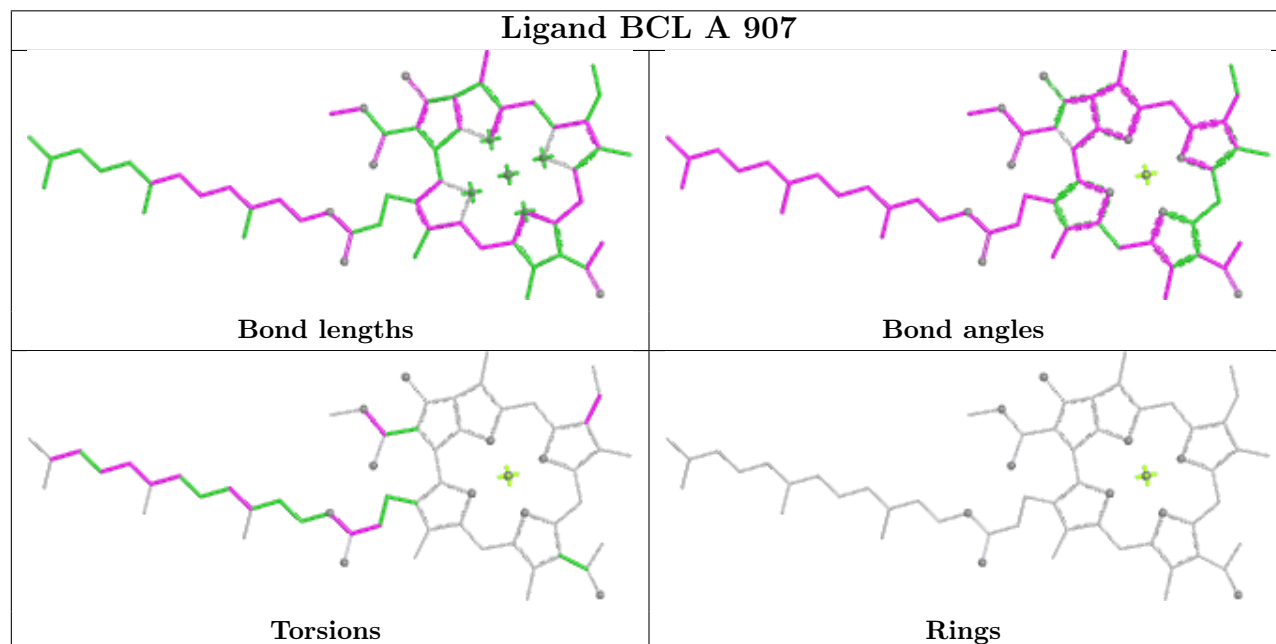
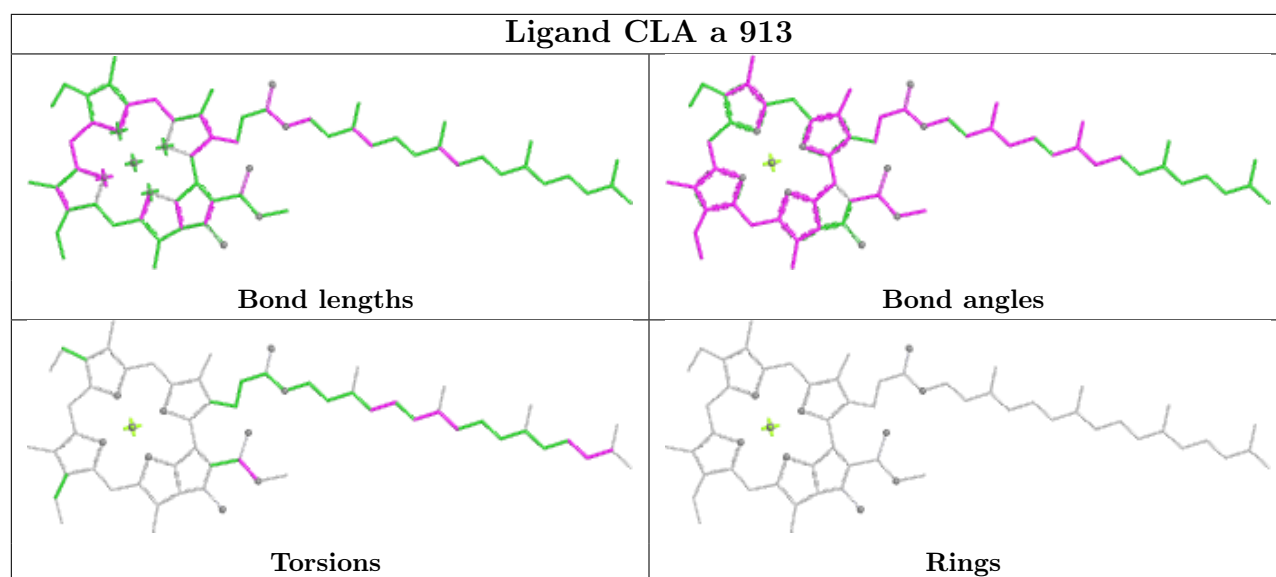
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | a     | 913 | CLA  | 6       | 0            |
| 11  | A     | 907 | BCL  | 4       | 0            |
| 11  | A     | 903 | BCL  | 6       | 0            |
| 15  | A     | 915 | 85I  | 2       | 0            |
| 11  | a     | 905 | BCL  | 7       | 0            |
| 11  | a     | 911 | BCL  | 4       | 0            |
| 12  | a     | 914 | CLA  | 2       | 0            |
| 17  | g     | 101 | 85N  | 1       | 0            |
| 20  | a     | 917 | SF4  | 5       | 0            |
| 11  | A     | 906 | BCL  | 6       | 0            |
| 12  | a     | 915 | CLA  | 2       | 0            |
| 18  | c     | 202 | HEC  | 5       | 0            |
| 11  | A     | 904 | BCL  | 2       | 0            |
| 15  | A     | 916 | 85I  | 1       | 0            |
| 20  | B     | 201 | SF4  | 10      | 0            |
| 11  | a     | 907 | BCL  | 4       | 0            |
| 17  | a     | 902 | 85N  | 3       | 0            |
| 12  | A     | 910 | CLA  | 12      | 0            |
| 12  | A     | 911 | CLA  | 8       | 0            |
| 15  | A     | 917 | 85I  | 3       | 0            |
| 10  | a     | 903 | 2GO  | 1       | 0            |
| 10  | A     | 901 | 2GO  | 3       | 0            |
| 11  | a     | 904 | BCL  | 8       | 0            |
| 13  | A     | 913 | LYC  | 7       | 0            |
| 11  | a     | 906 | BCL  | 1       | 0            |
| 11  | A     | 902 | BCL  | 8       | 0            |
| 11  | A     | 909 | BCL  | 2       | 0            |

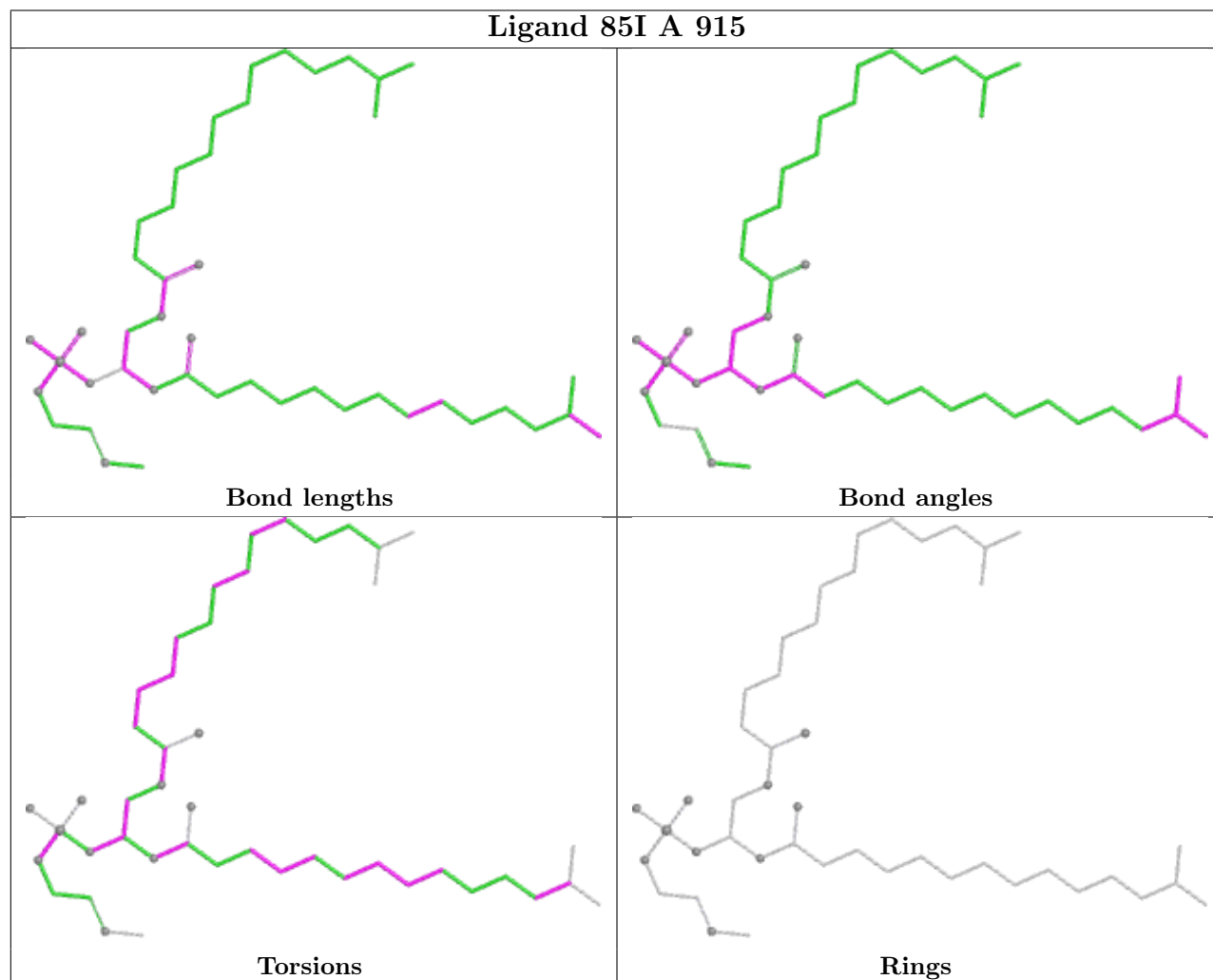
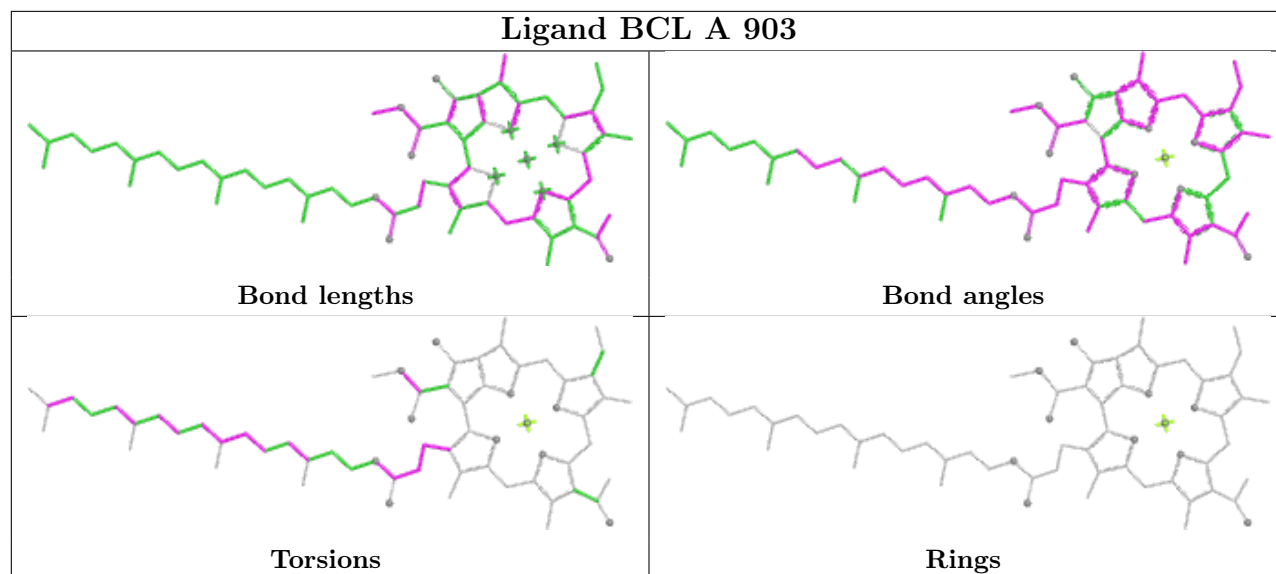
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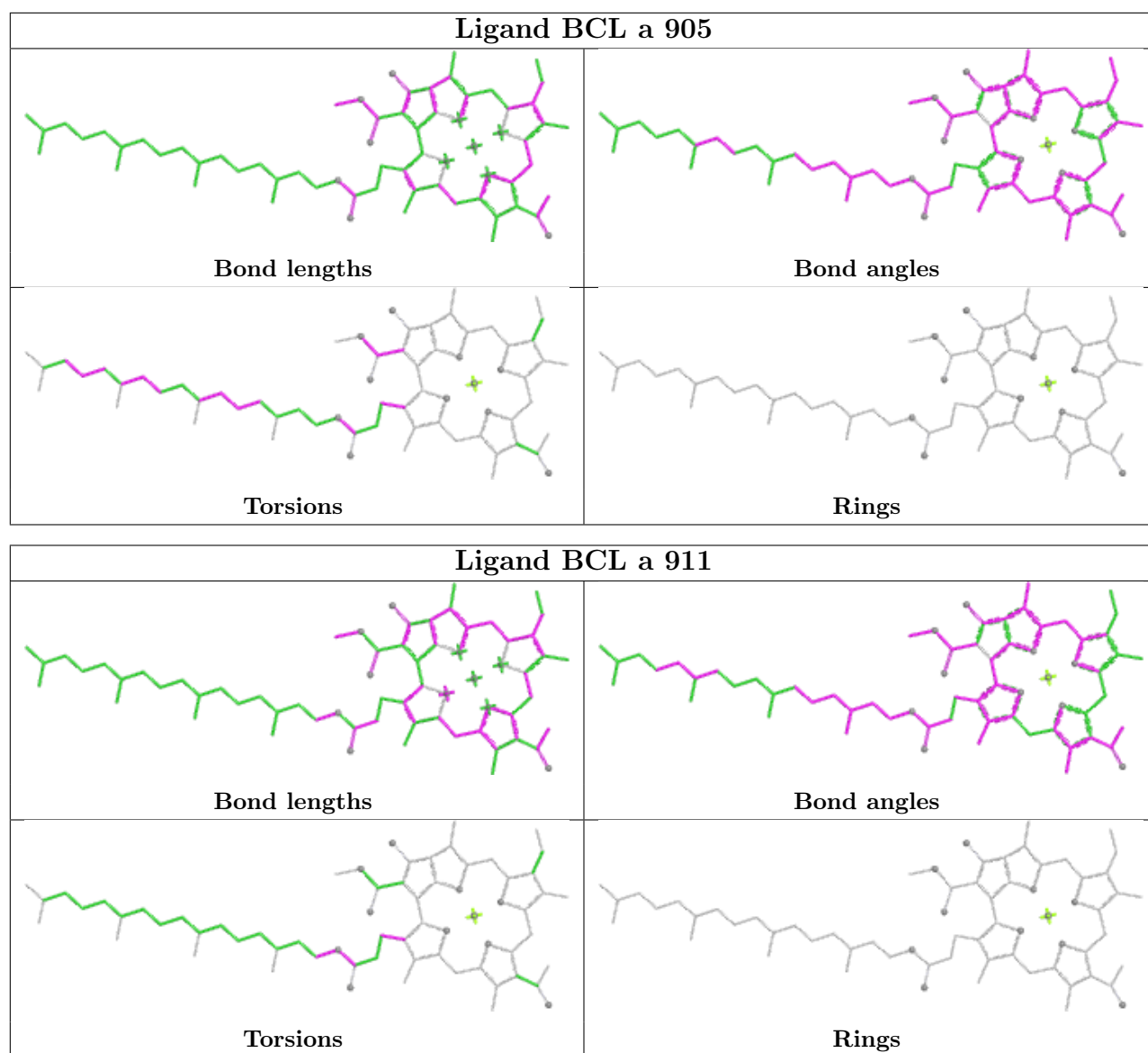
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 15  | a     | 919 | 85I  | 1       | 0            |
| 11  | a     | 908 | BCL  | 9       | 0            |
| 11  | A     | 908 | BCL  | 8       | 0            |
| 17  | G     | 101 | 85N  | 7       | 0            |
| 11  | A     | 905 | BCL  | 8       | 0            |
| 12  | A     | 912 | CLA  | 1       | 0            |
| 12  | A     | 931 | CLA  | 7       | 0            |
| 15  | a     | 920 | 85I  | 4       | 0            |
| 12  | a     | 901 | CLA  | 3       | 0            |
| 18  | C     | 301 | HEC  | 9       | 0            |
| 12  | a     | 912 | CLA  | 3       | 0            |
| 11  | a     | 910 | BCL  | 5       | 0            |
| 12  | A     | 933 | CLA  | 2       | 0            |
| 17  | A     | 932 | 85N  | 8       | 0            |
| 20  | B     | 202 | SF4  | 3       | 0            |
| 11  | a     | 909 | BCL  | 6       | 0            |
| 13  | c     | 201 | LYC  | 5       | 0            |

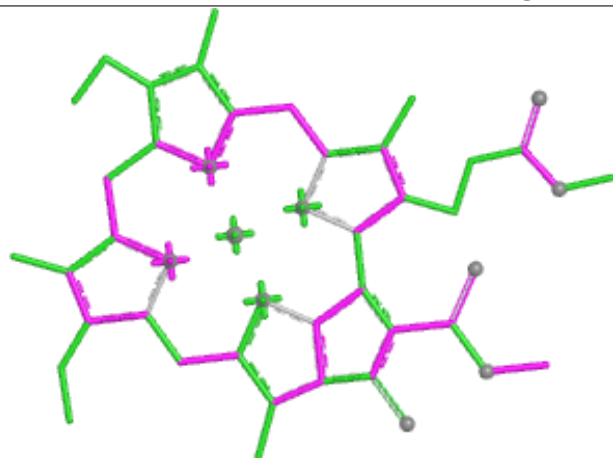
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



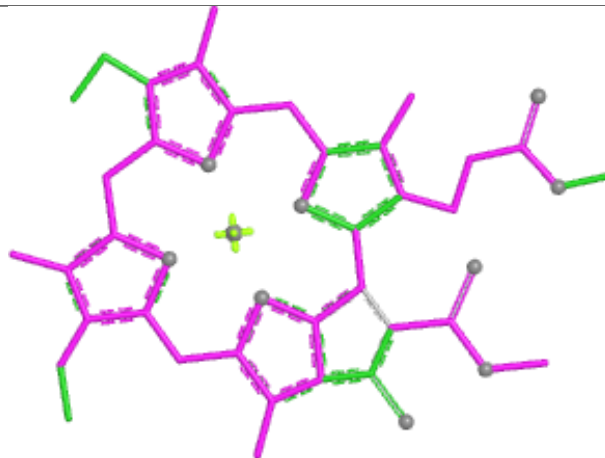




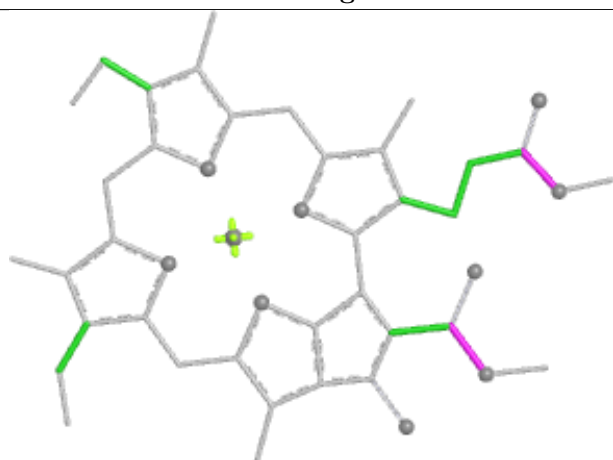
## Ligand CLA a 914



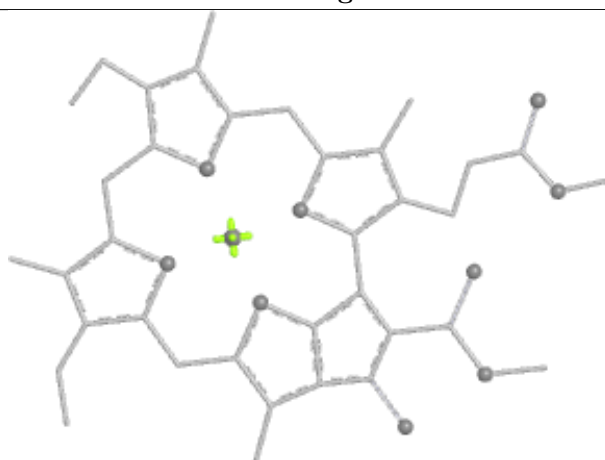
Bond lengths



Bond angles

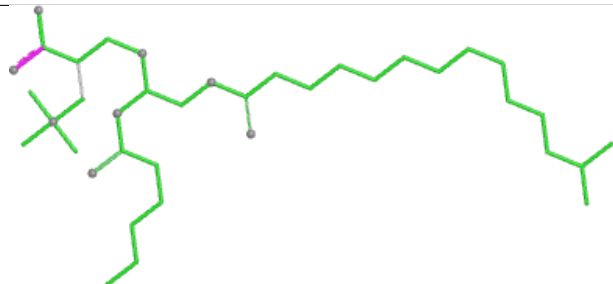


Torsions

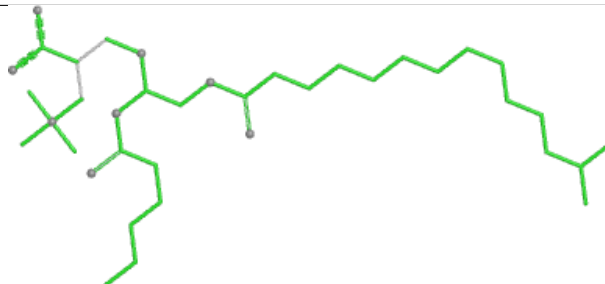


Rings

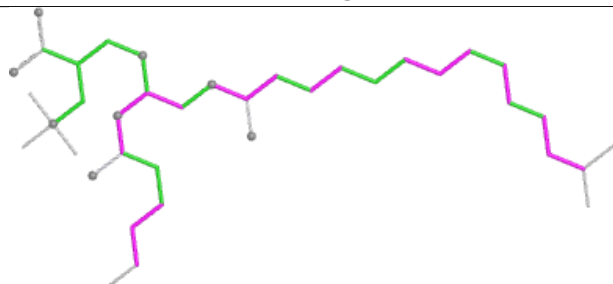
## Ligand 85N g 101



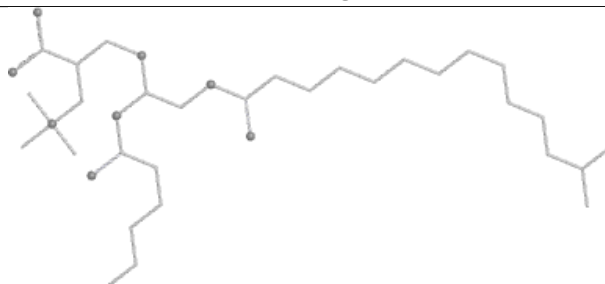
Bond lengths



Bond angles

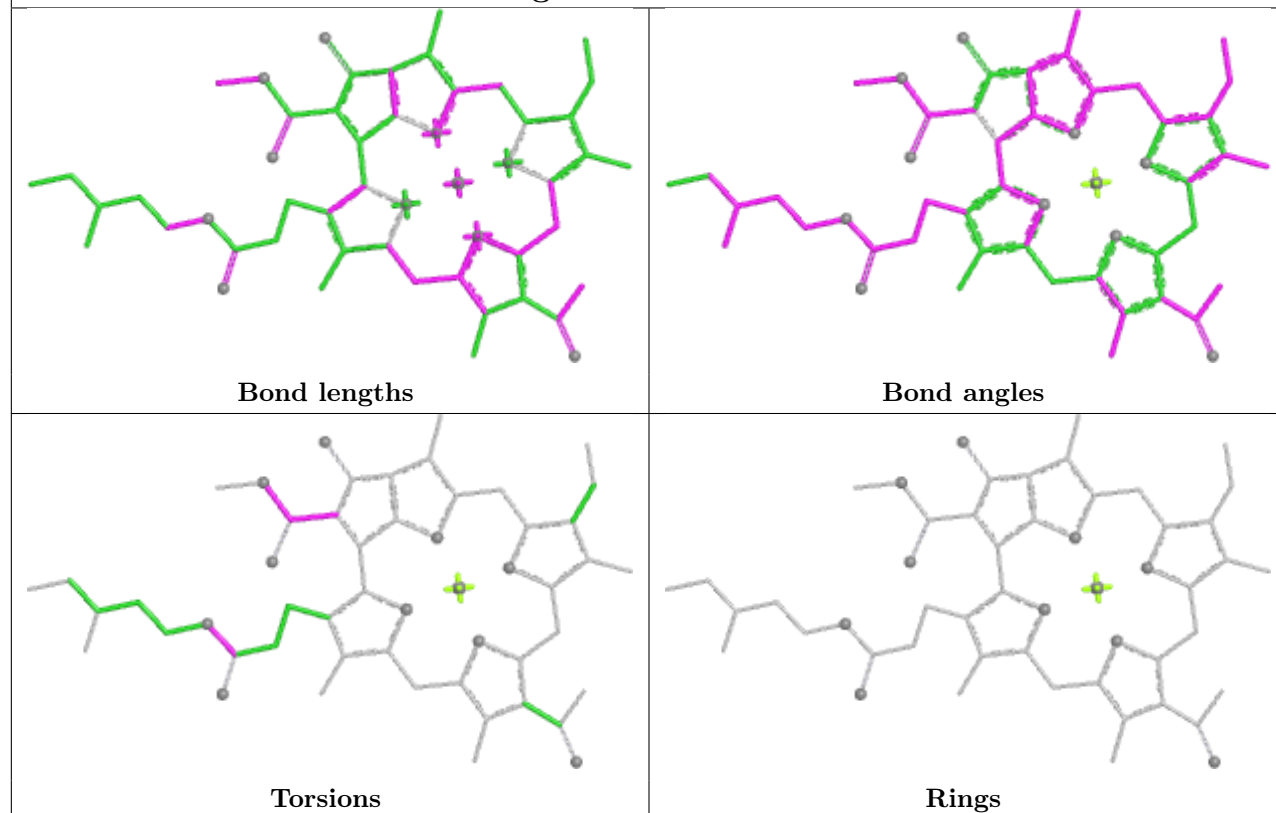


Torsions

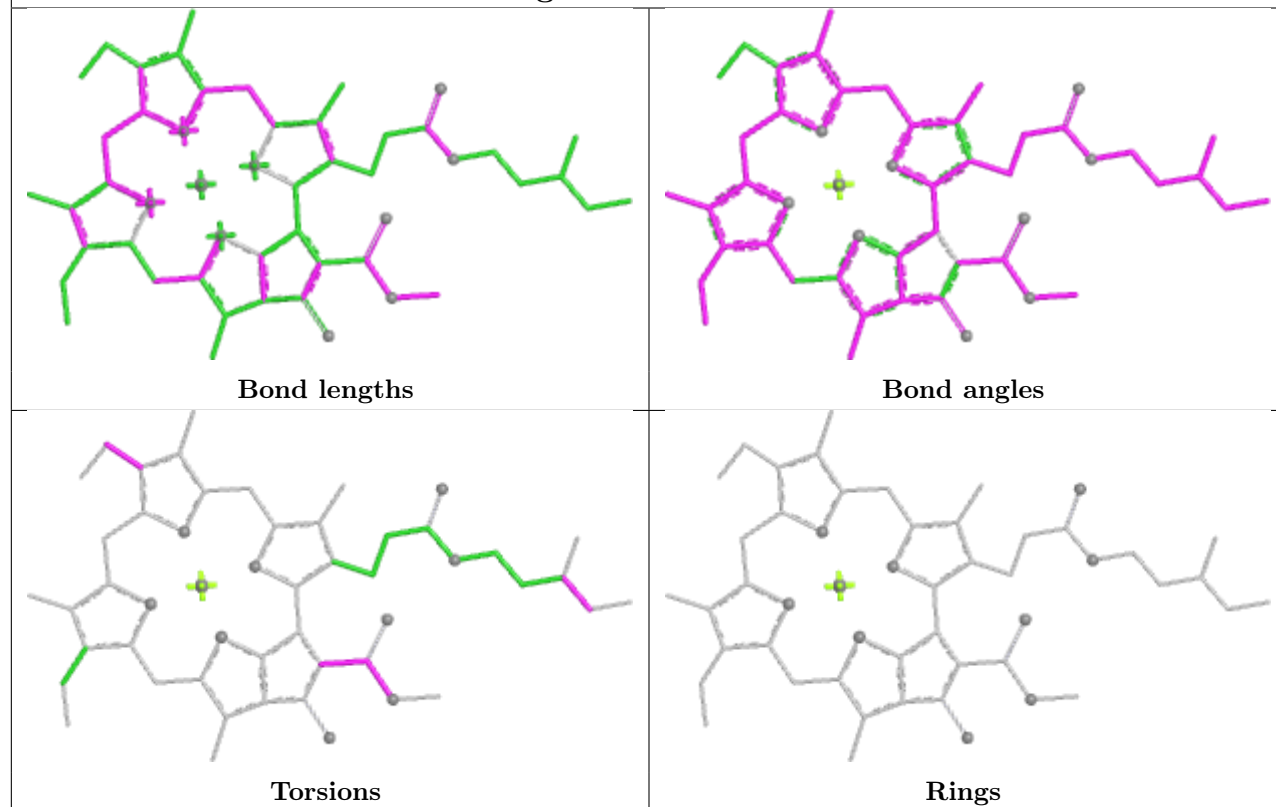


Rings

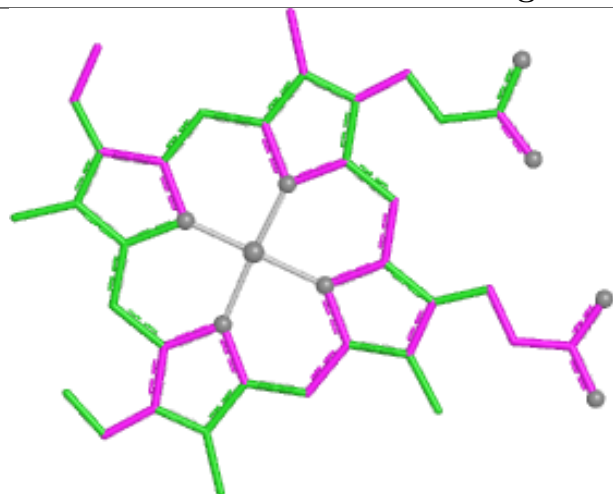
## Ligand BCL A 906



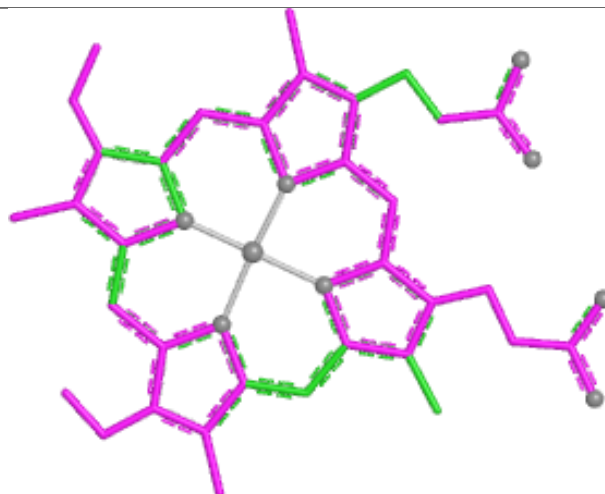
## Ligand CLA a 915



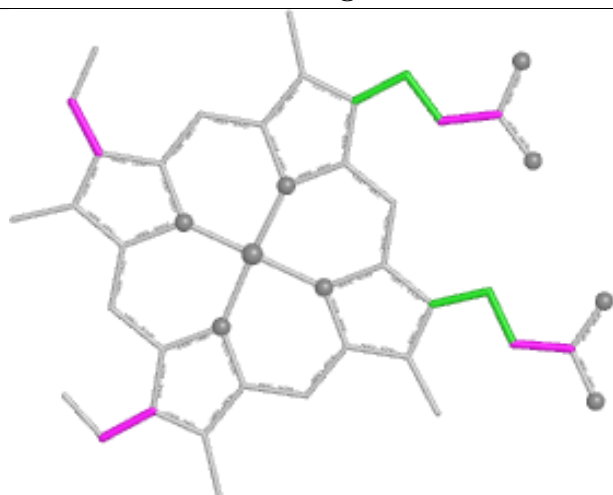
## Ligand HEC c 202



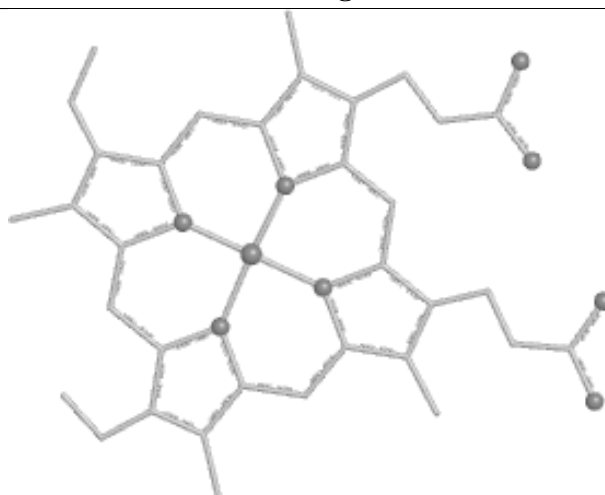
Bond lengths



Bond angles

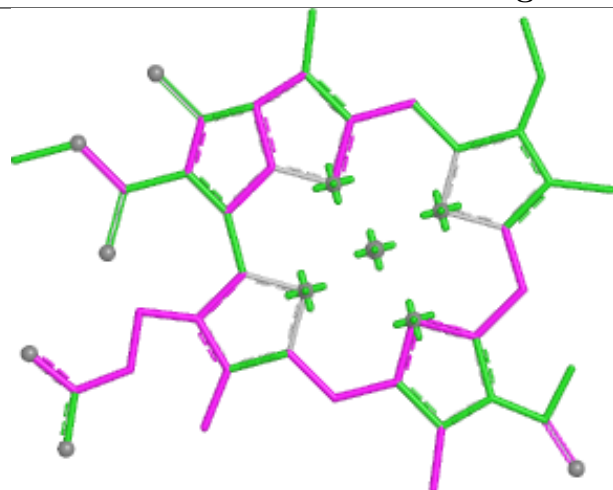


Torsions

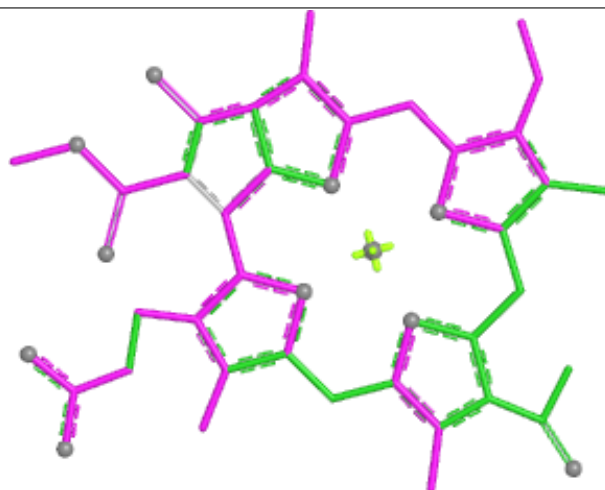


Rings

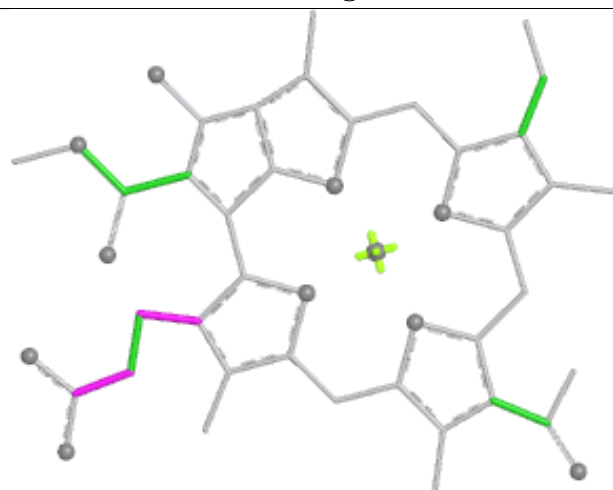
## Ligand BCL A 904



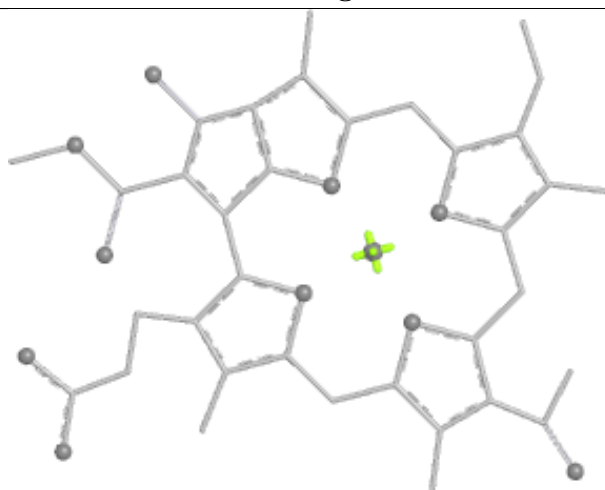
Bond lengths



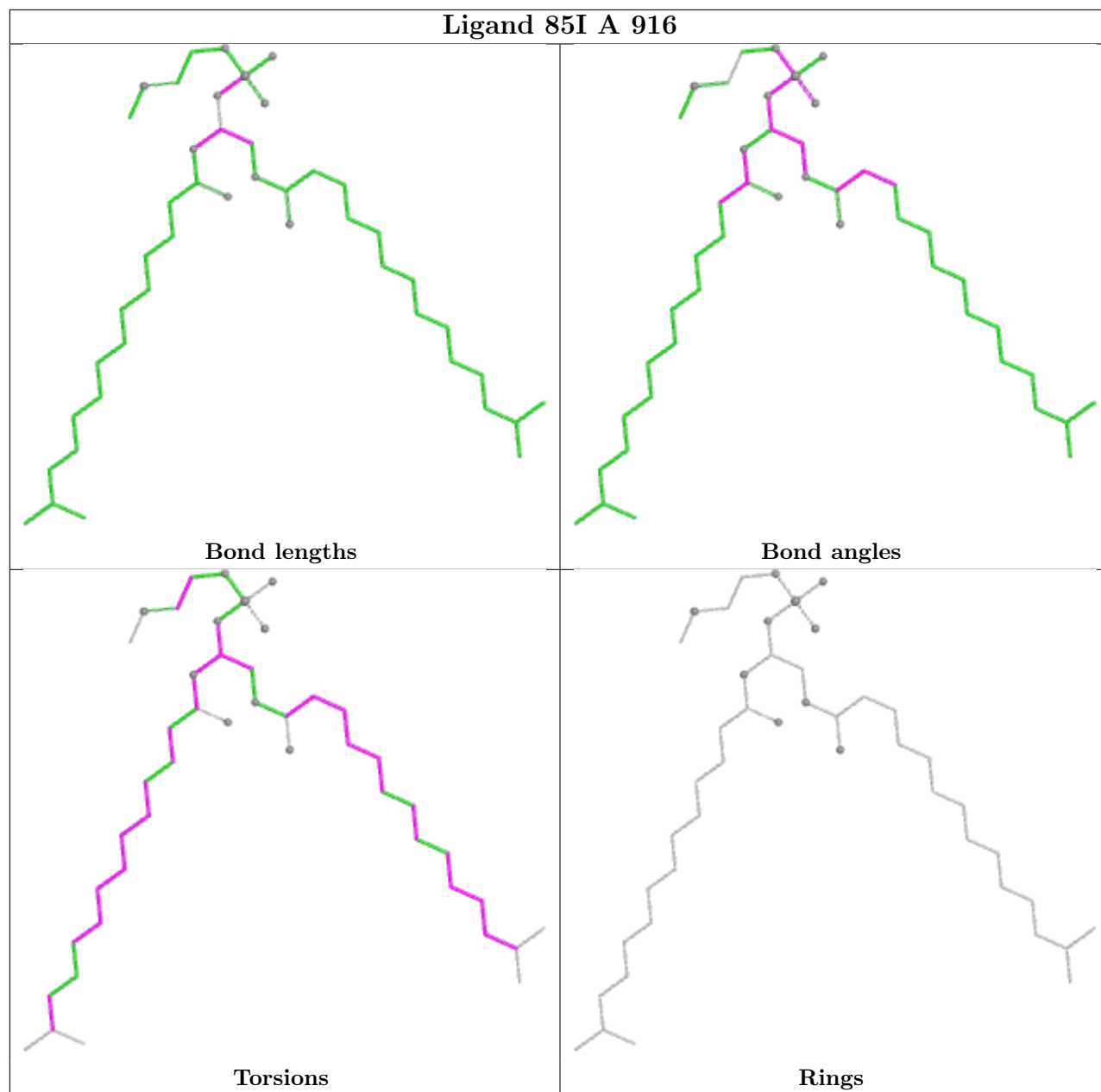
Bond angles



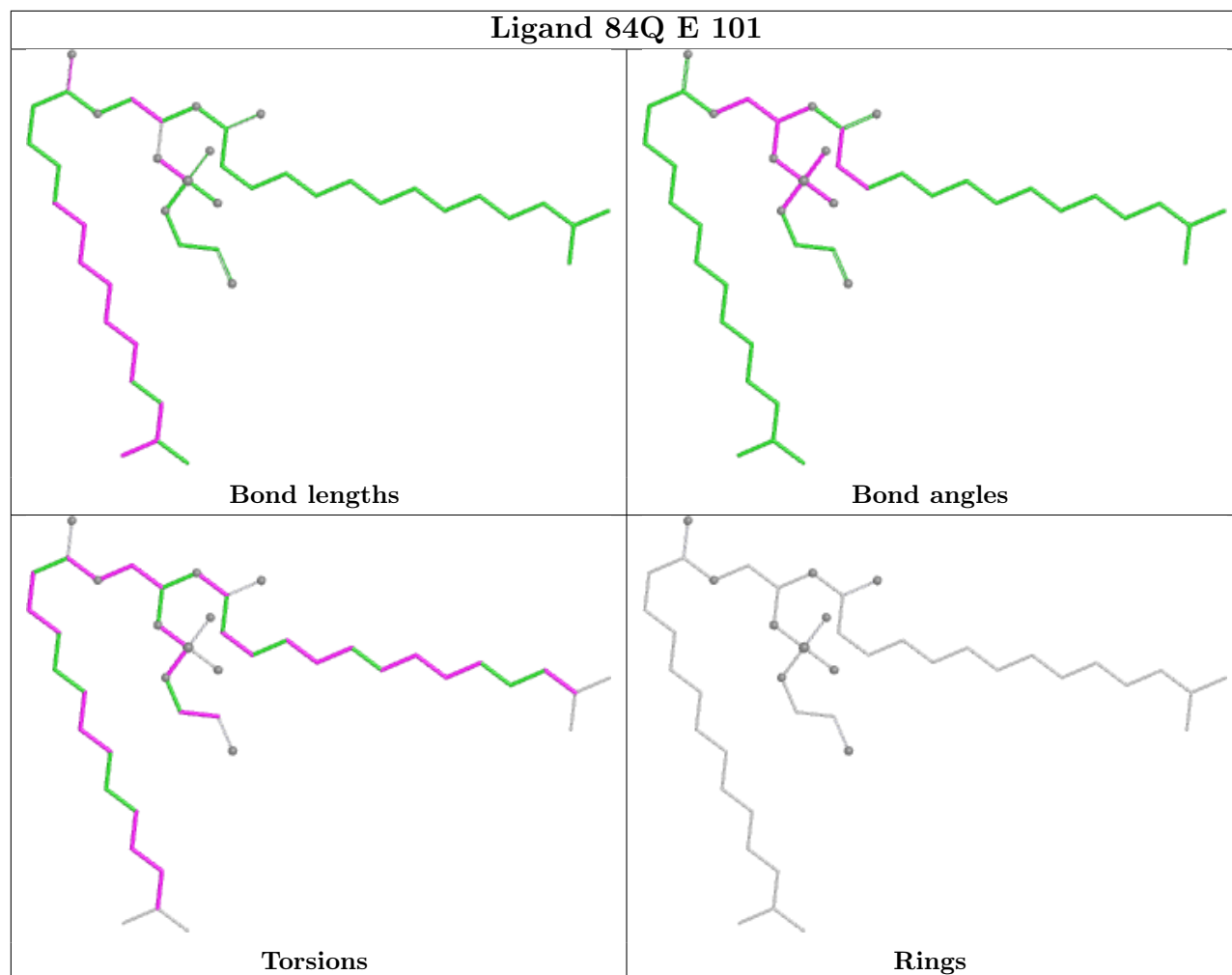
Torsions



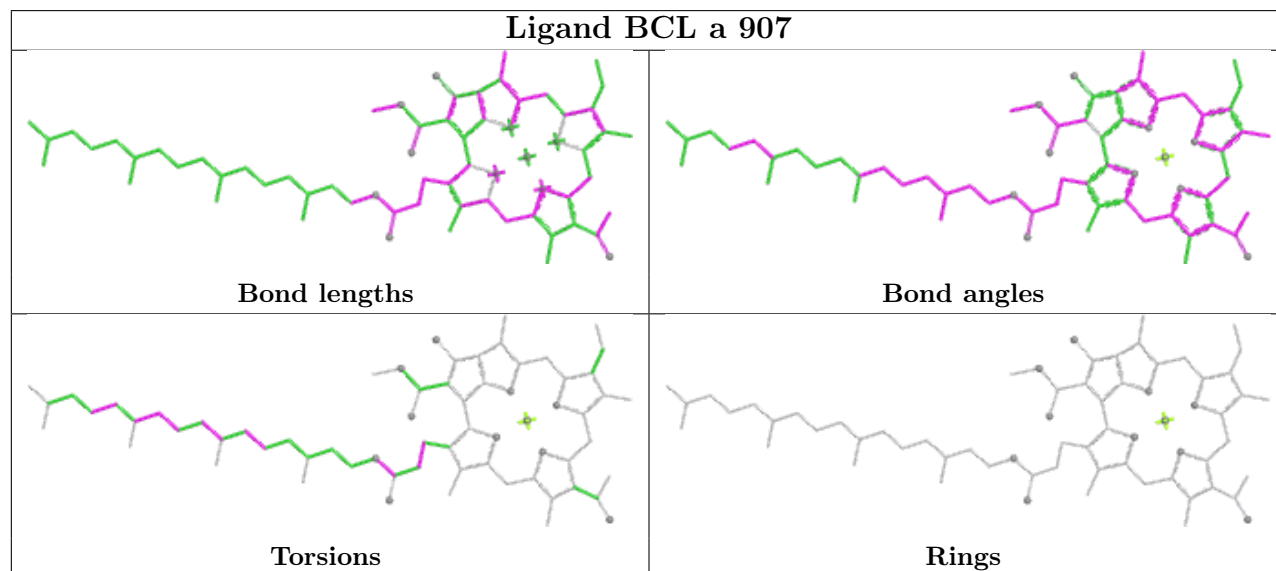
Rings

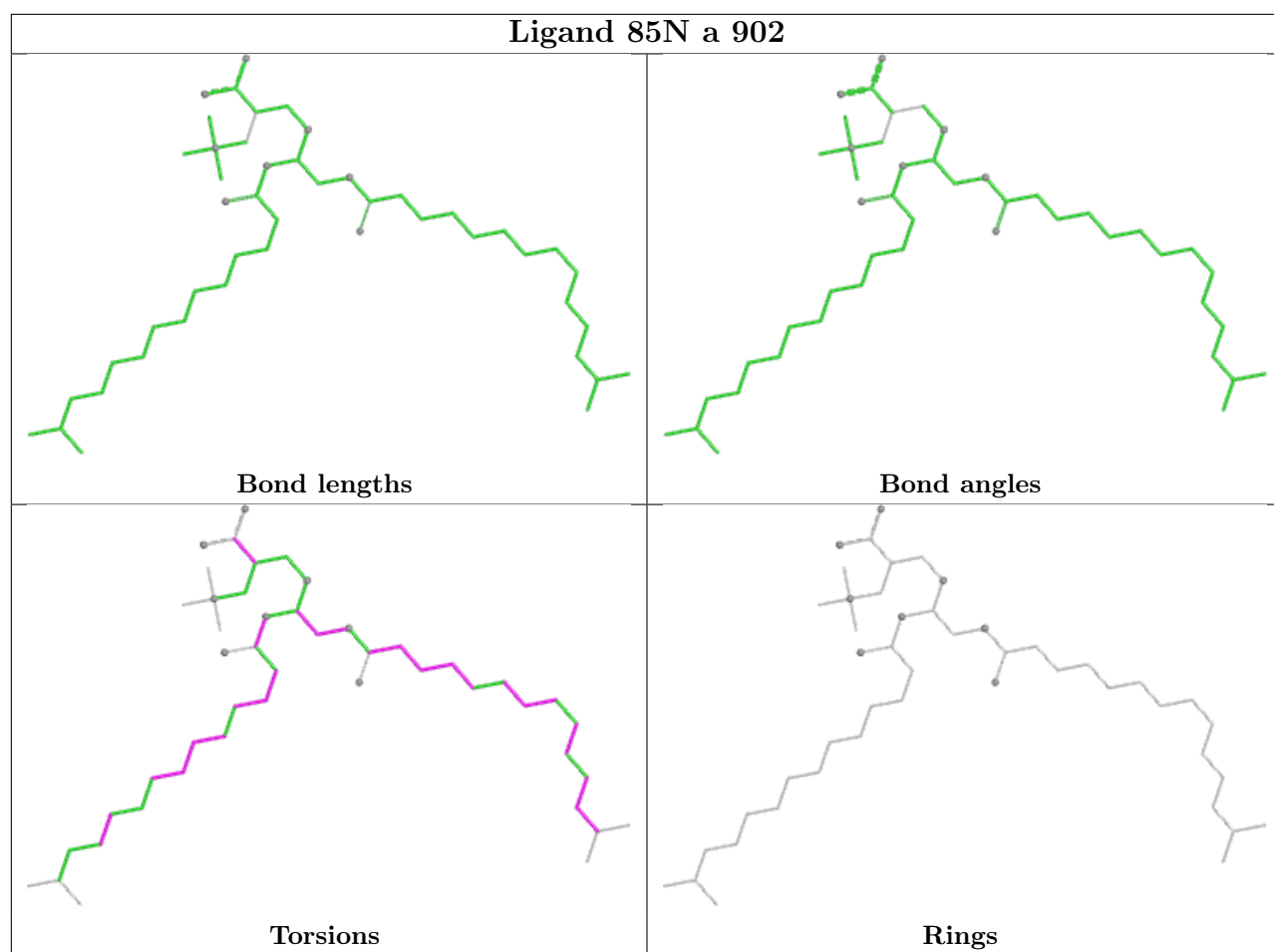


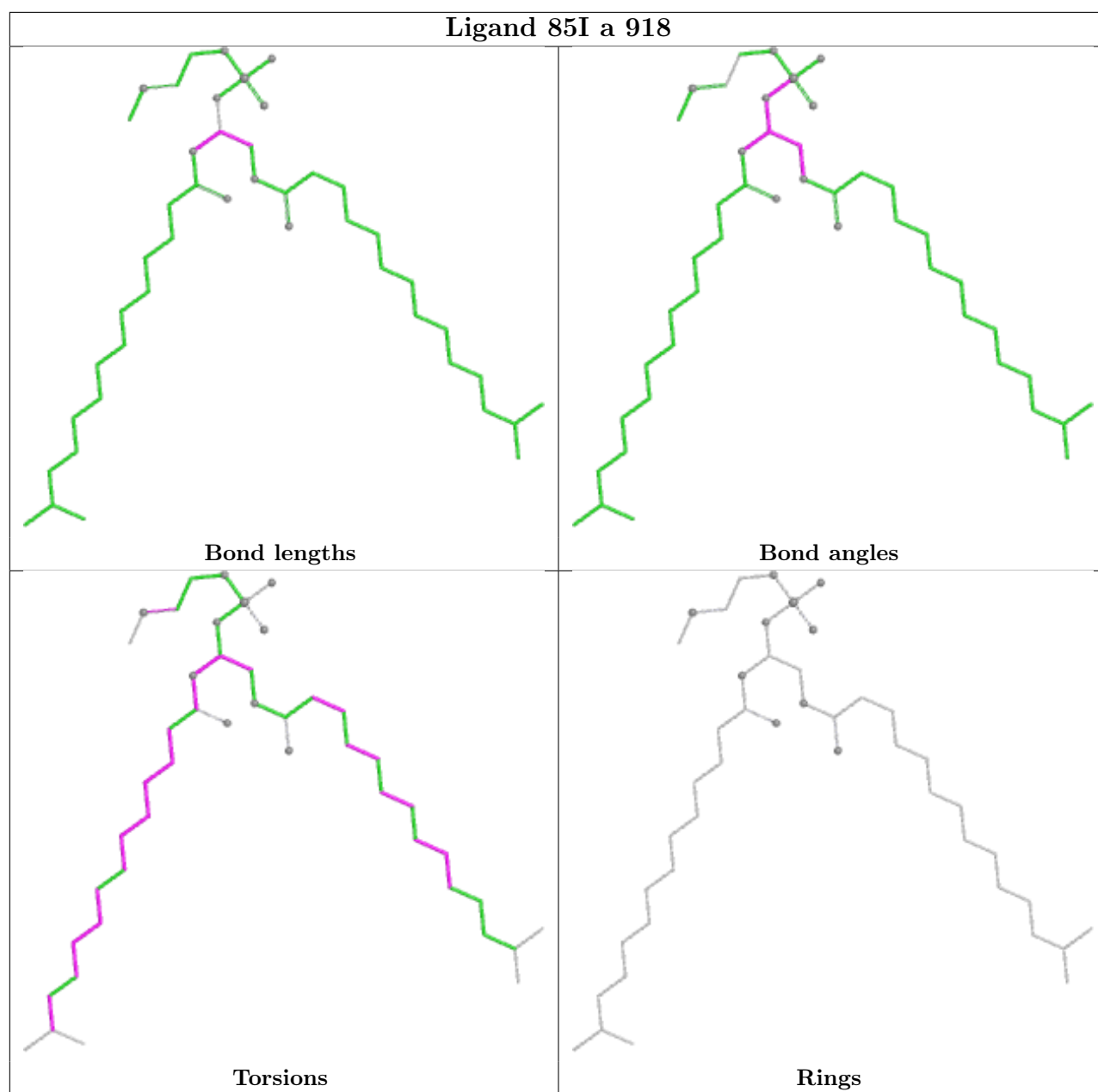
## Ligand 84Q E 101

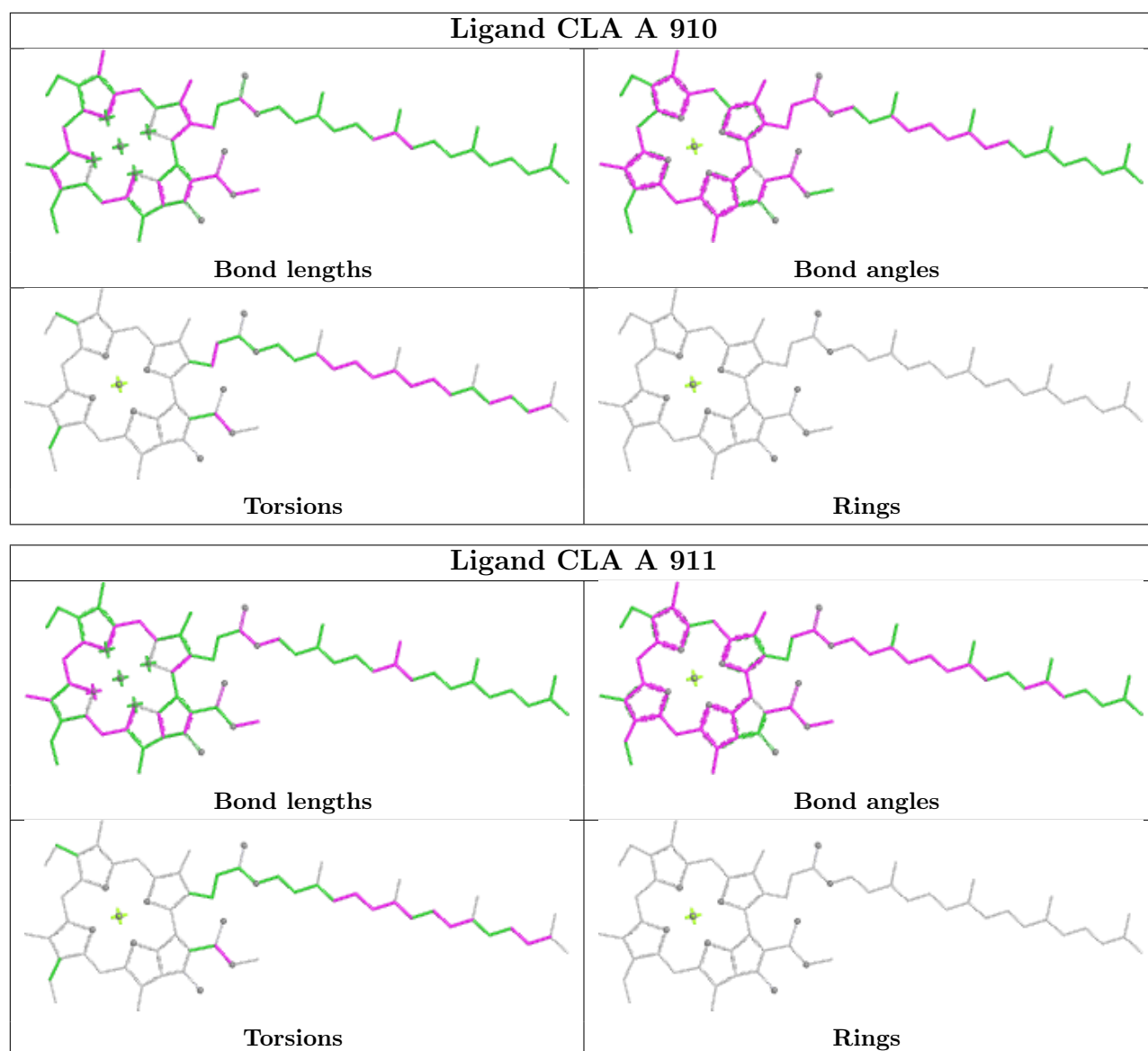


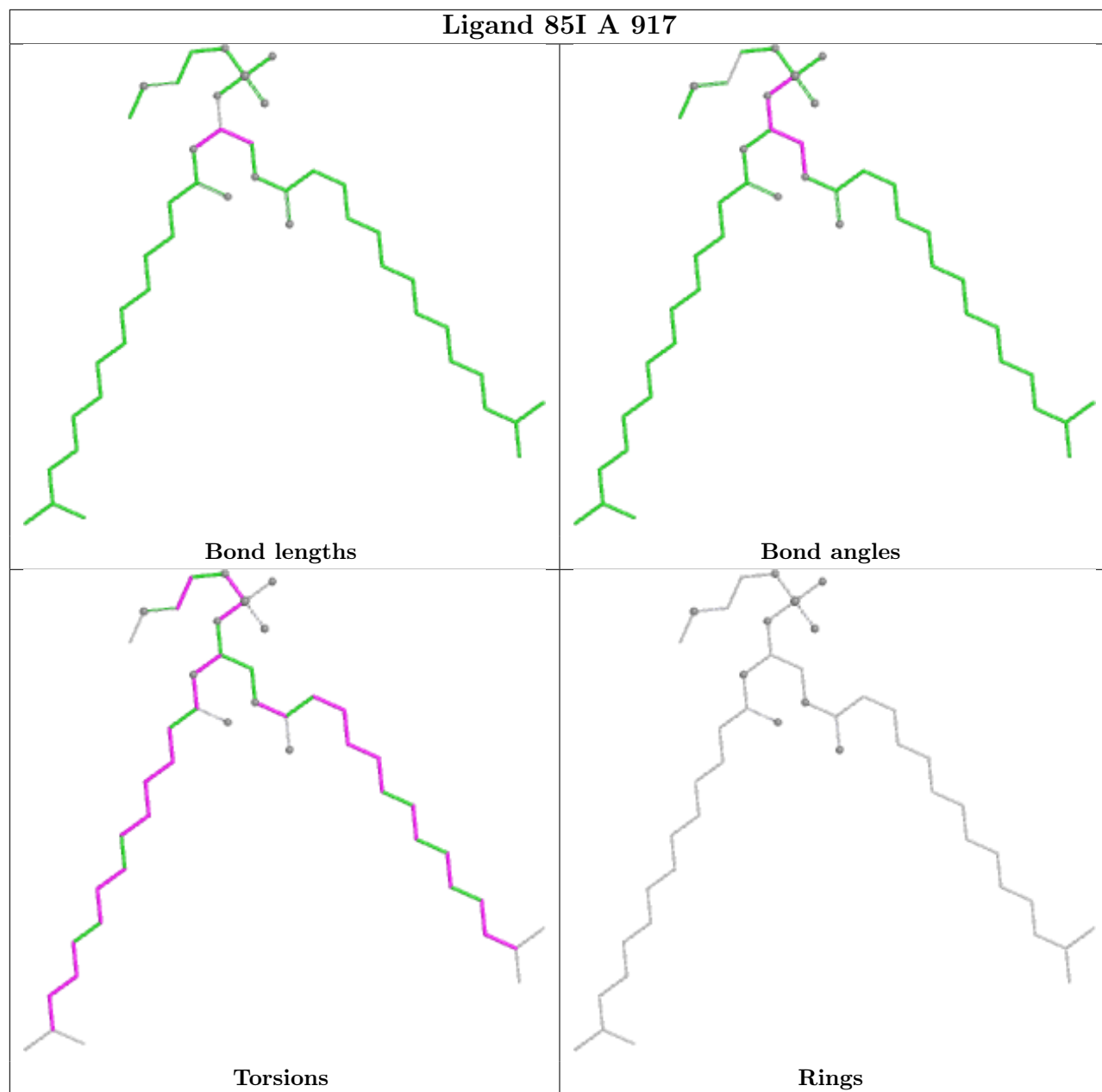
## Ligand BCL a 907



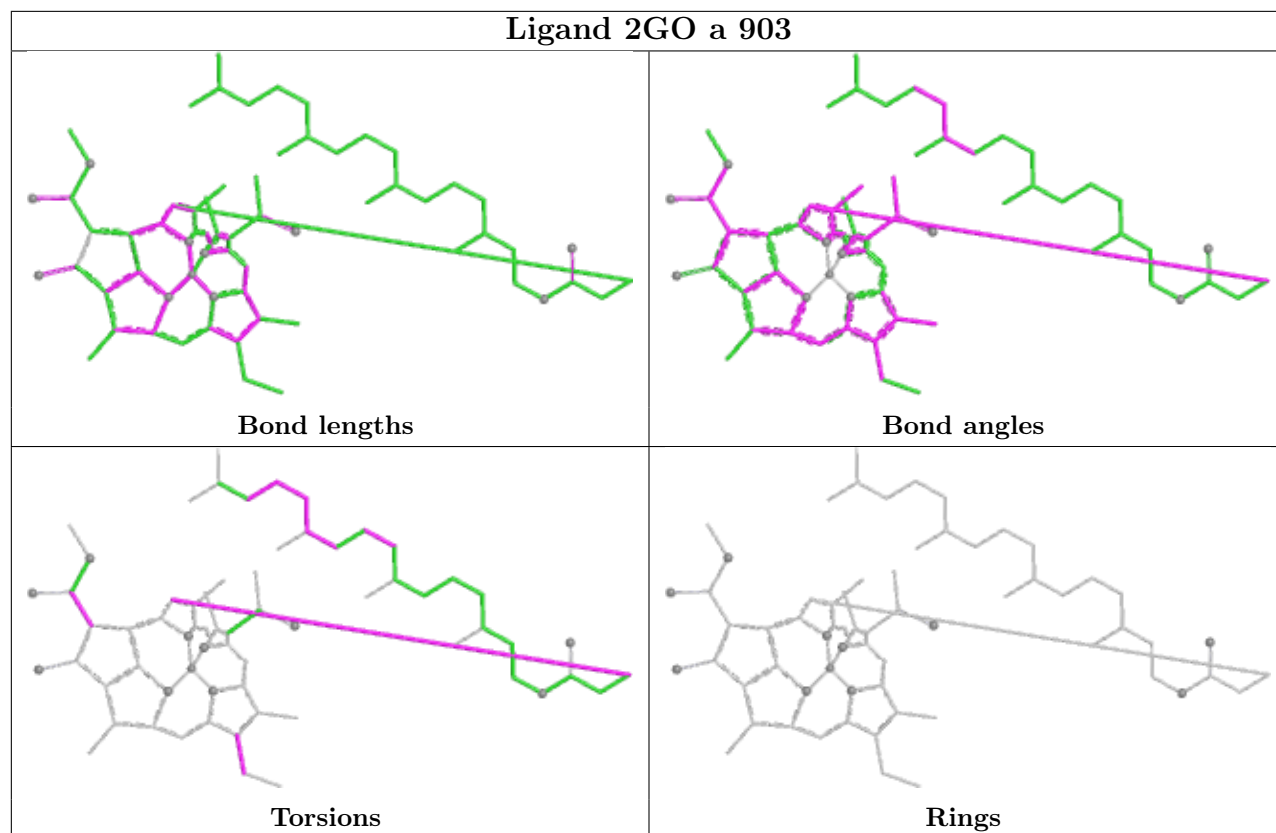




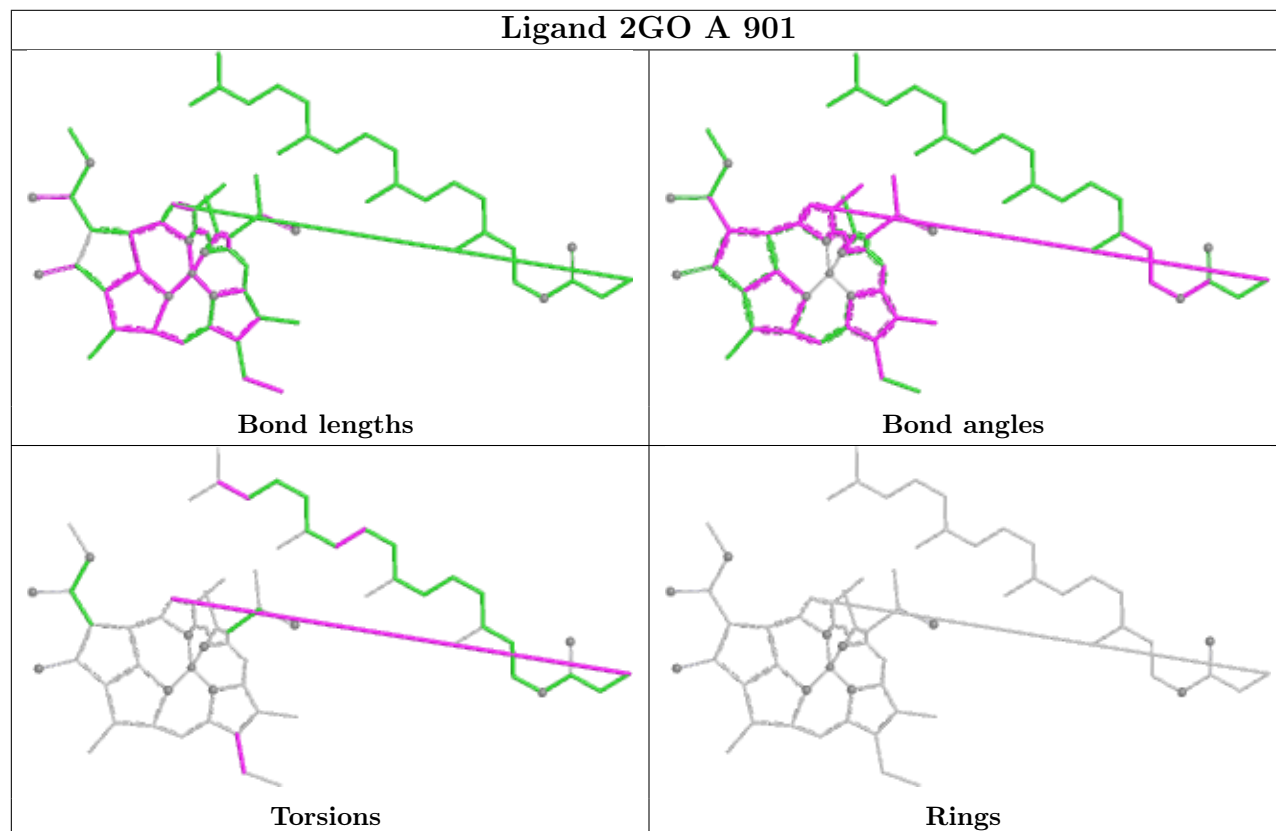


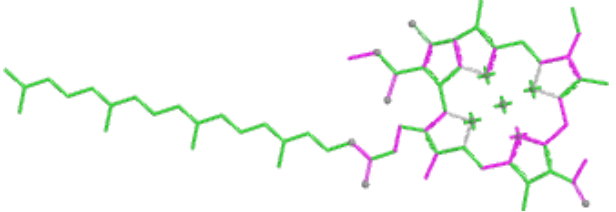
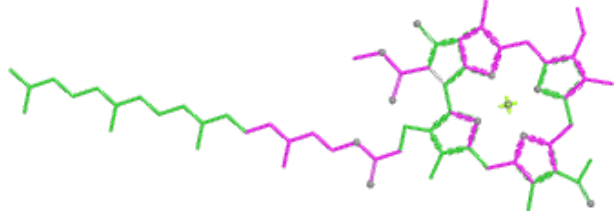
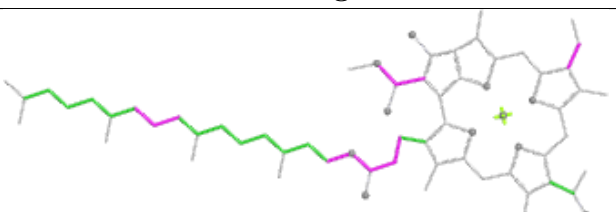
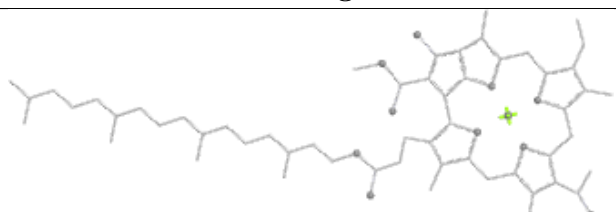
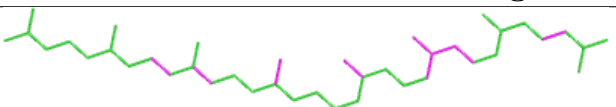
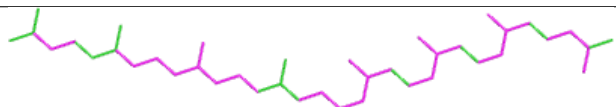
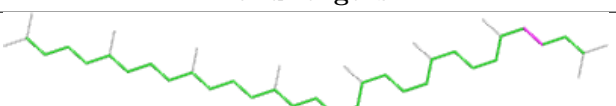
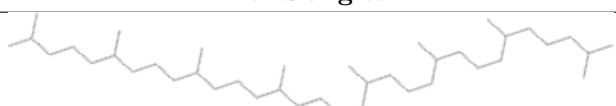


## Ligand 2GO a 903

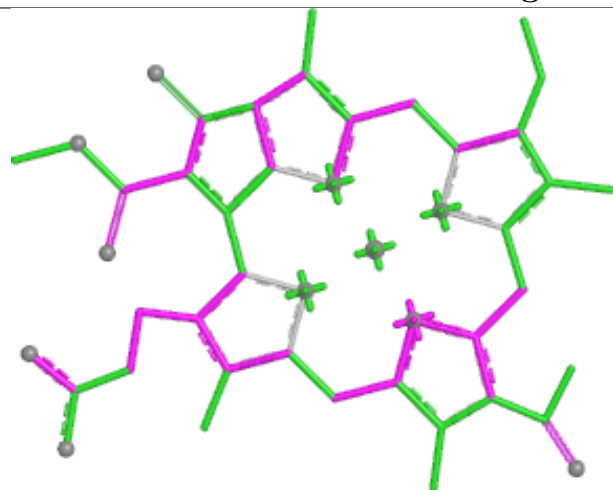


## Ligand 2GO A 901

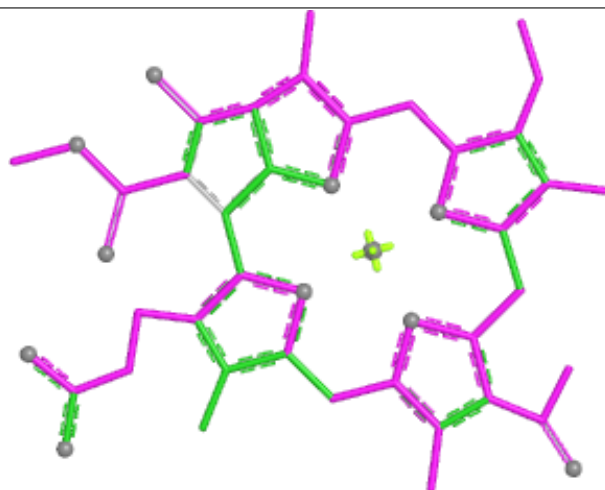


| Ligand BCL a 904                                                                                      |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand LYC A 913                                                                                      |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>    |  <p>Rings</p>      |

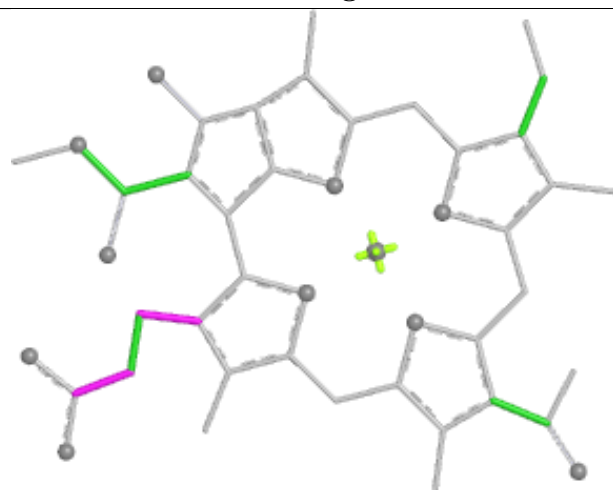
## Ligand BCL a 906



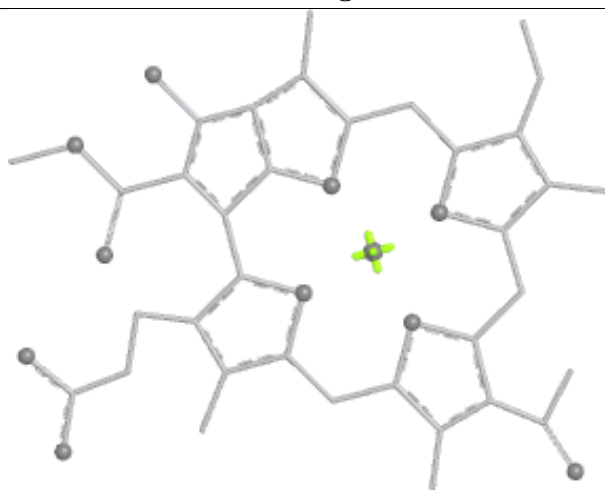
Bond lengths



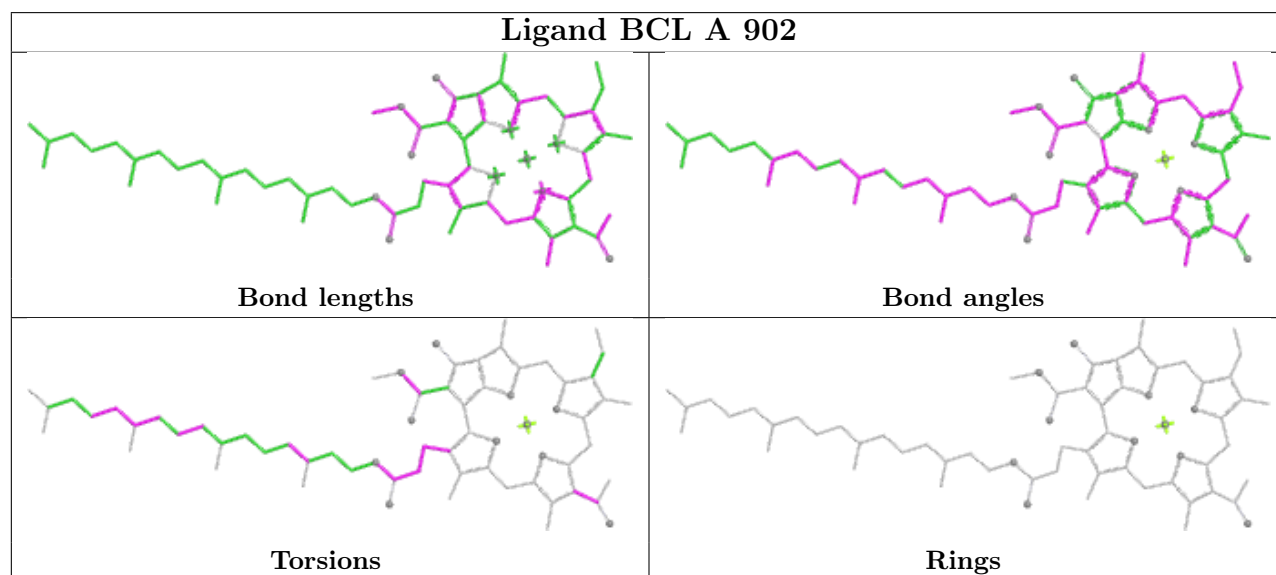
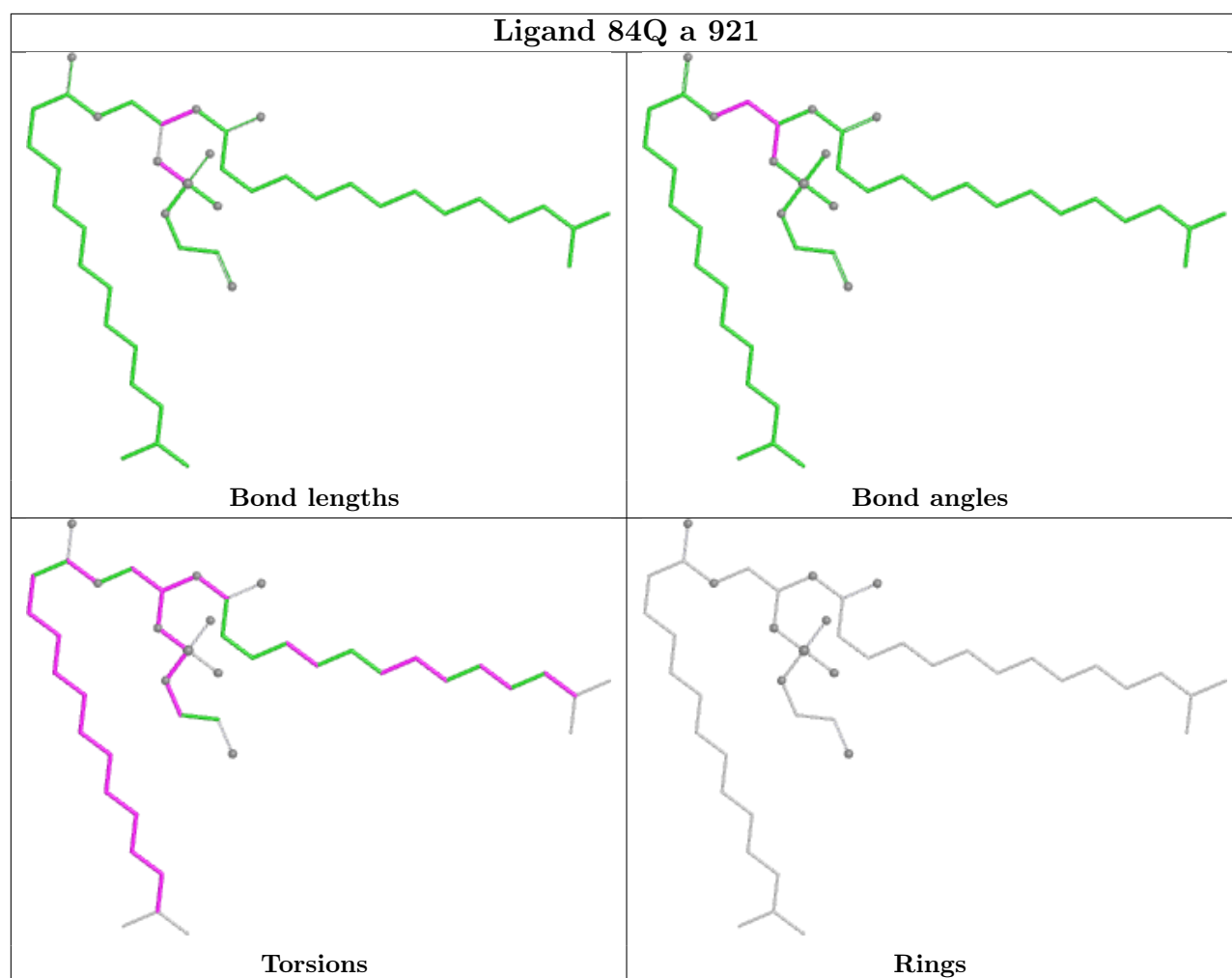
Bond angles

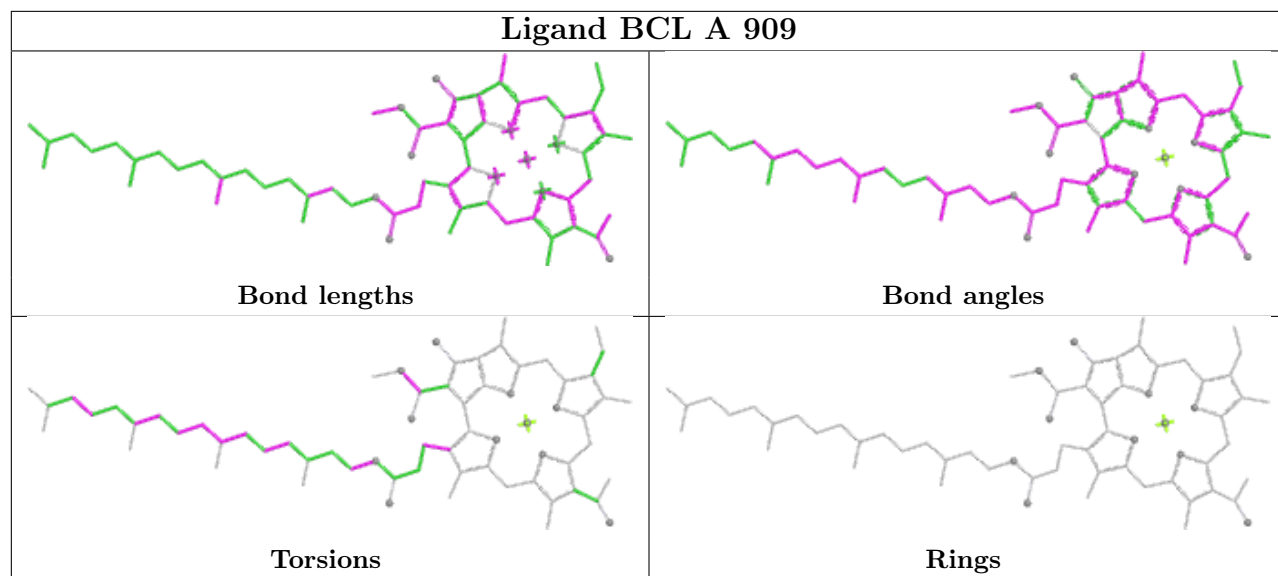


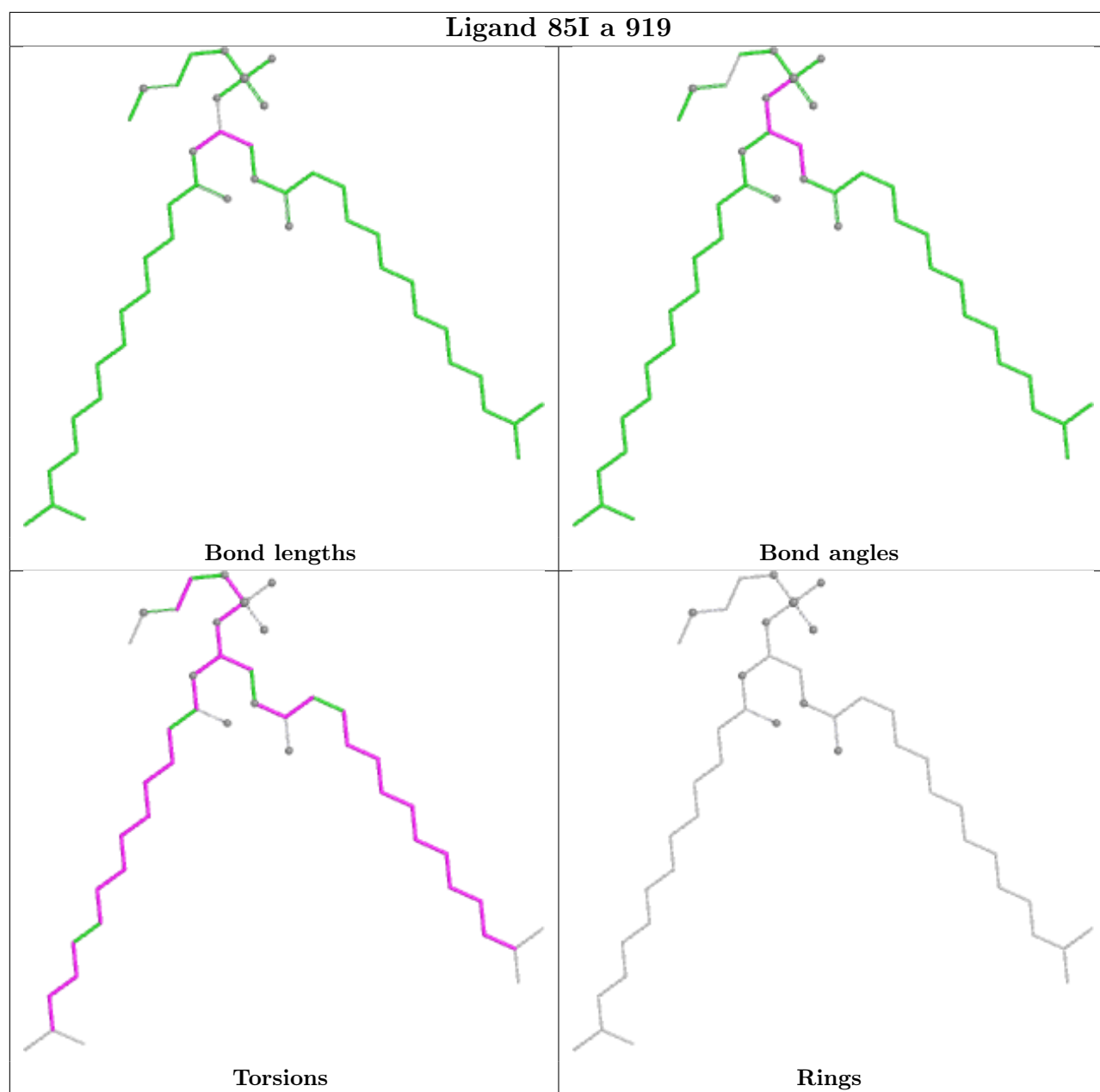
Torsions

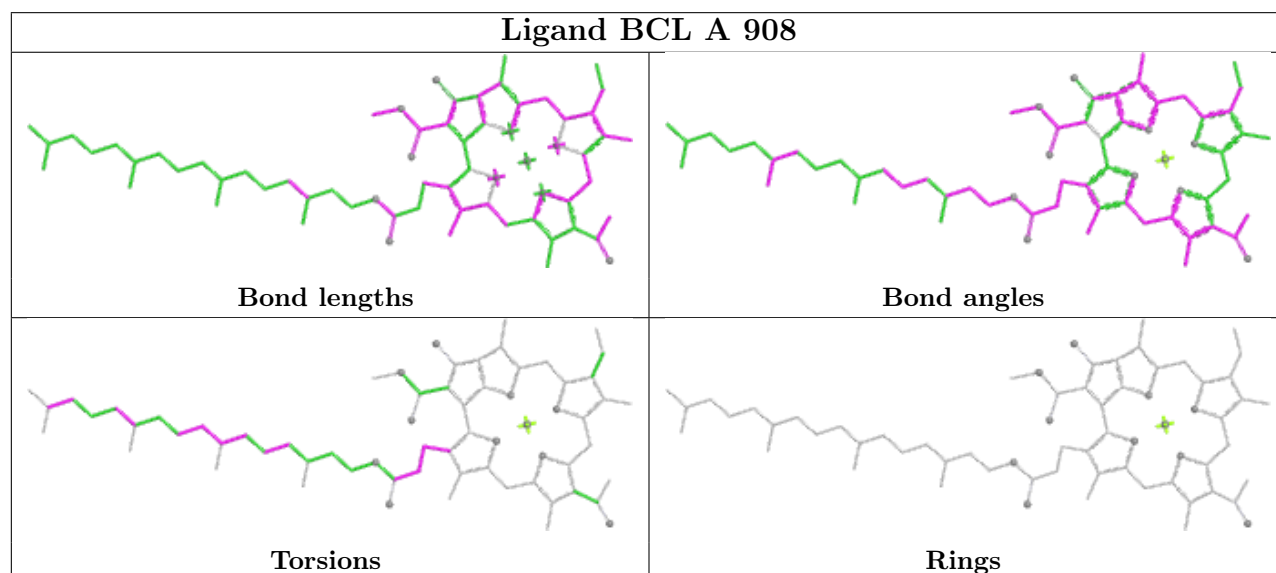
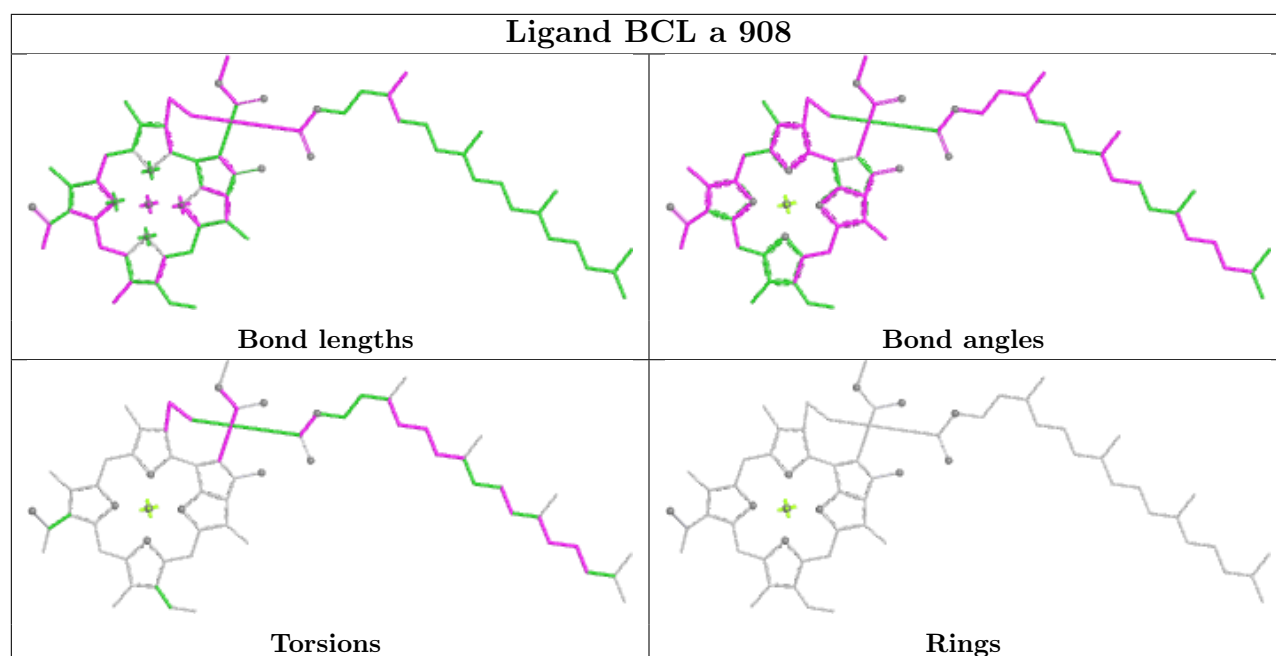


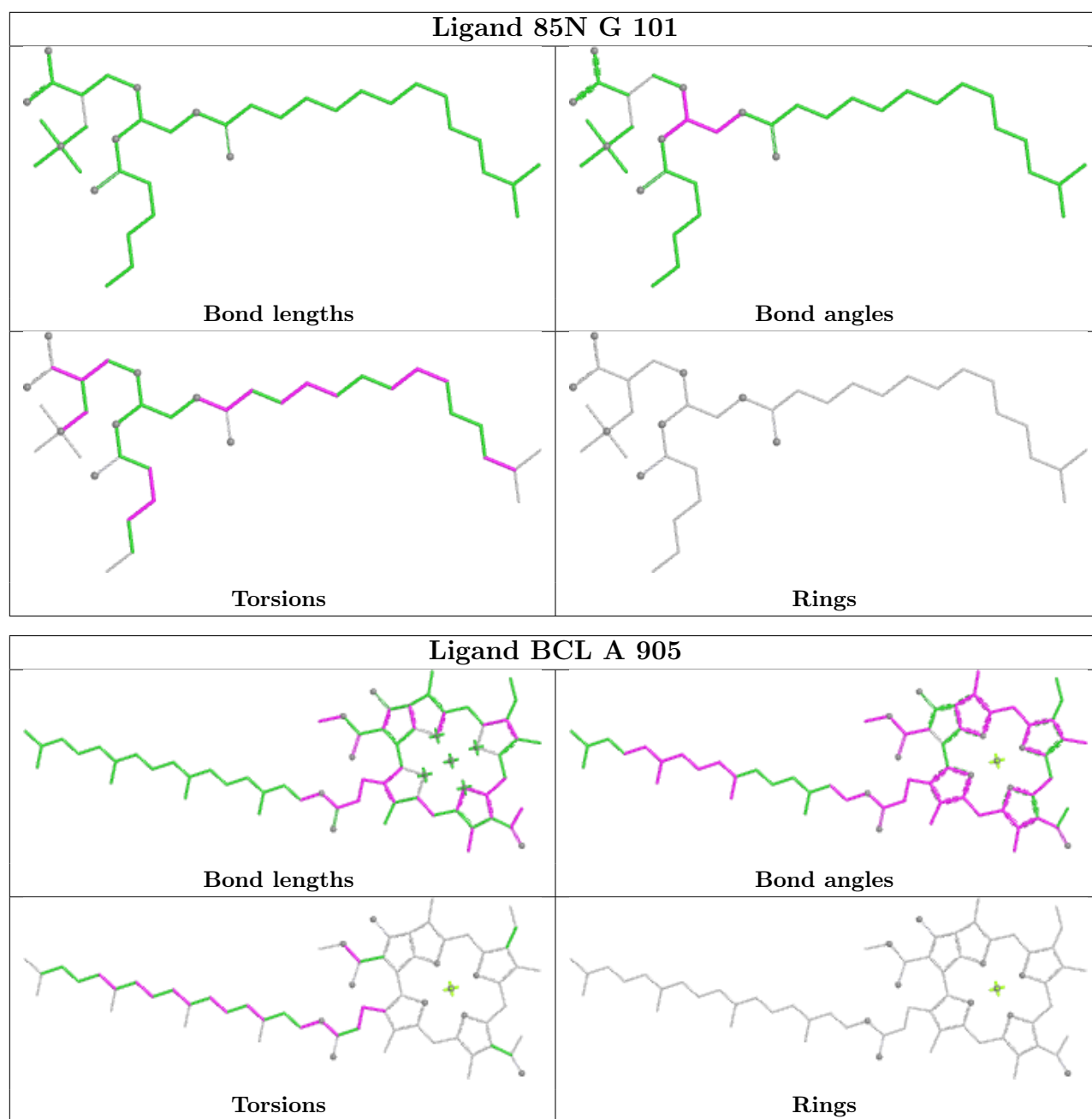
Rings



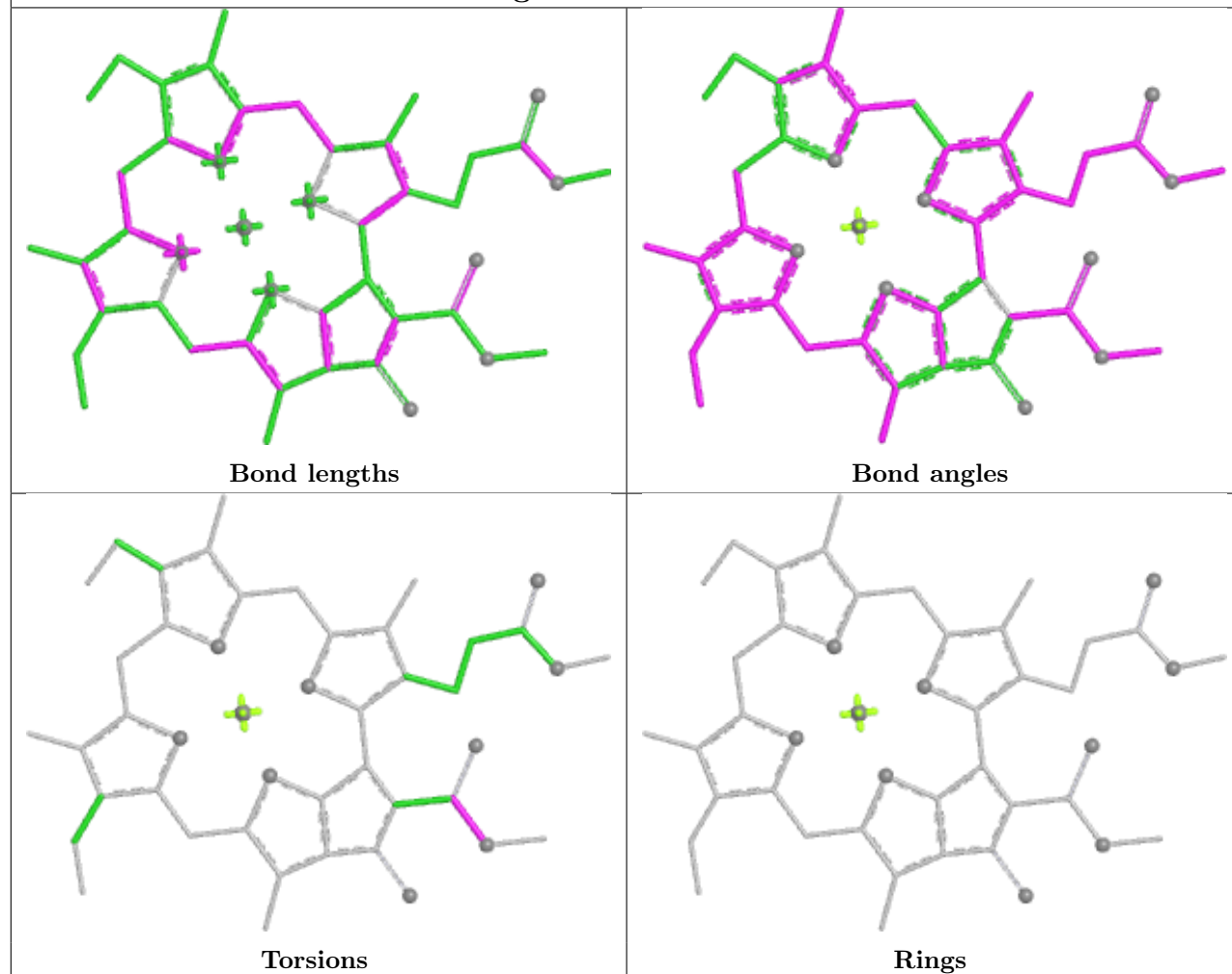




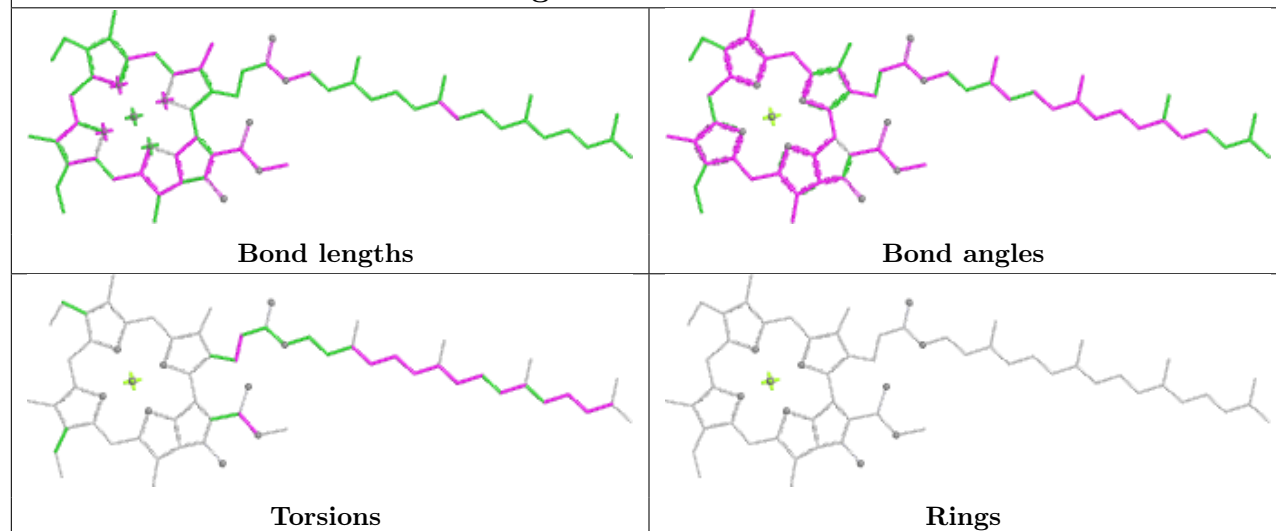


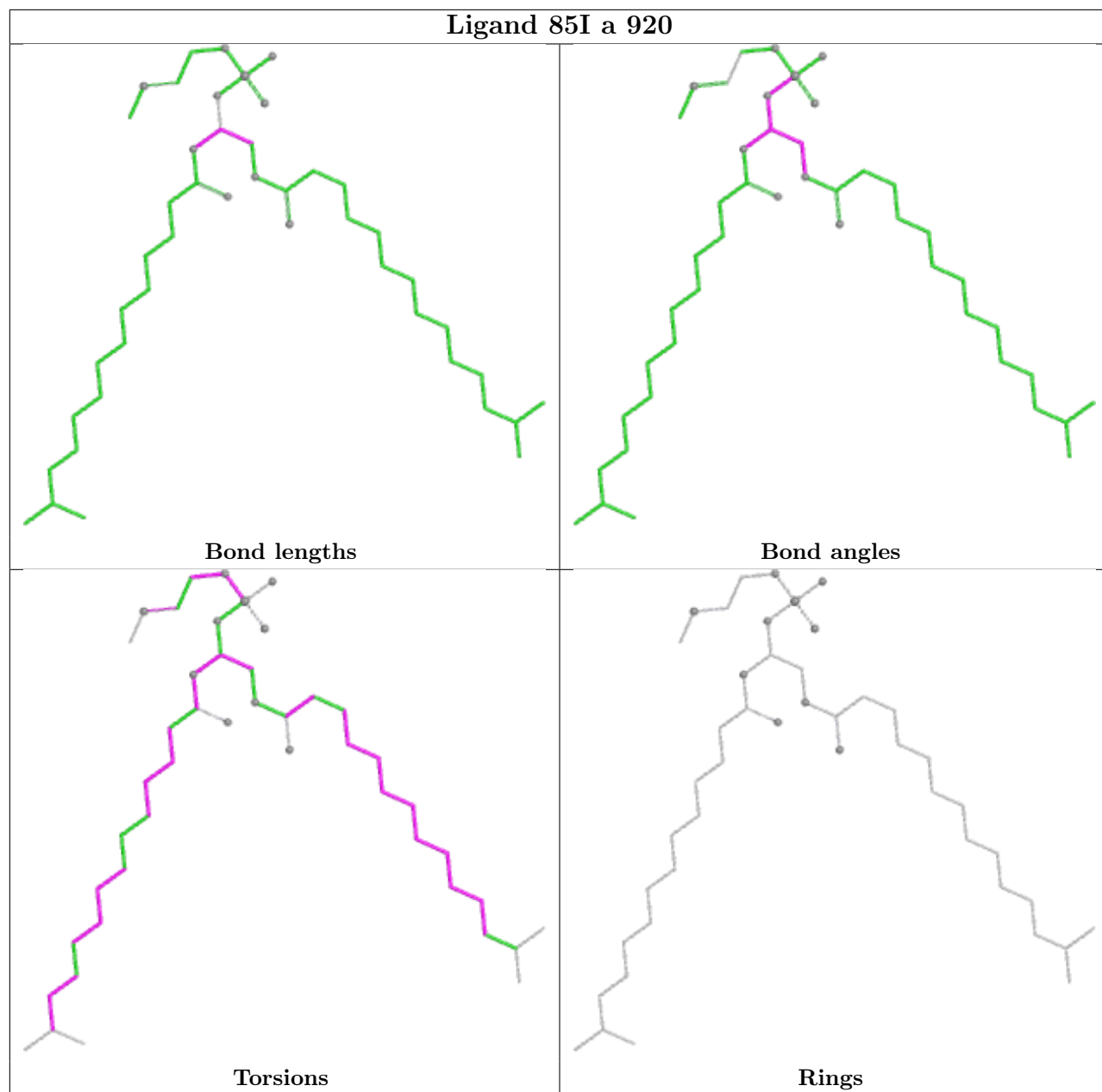


## Ligand CLA A 912

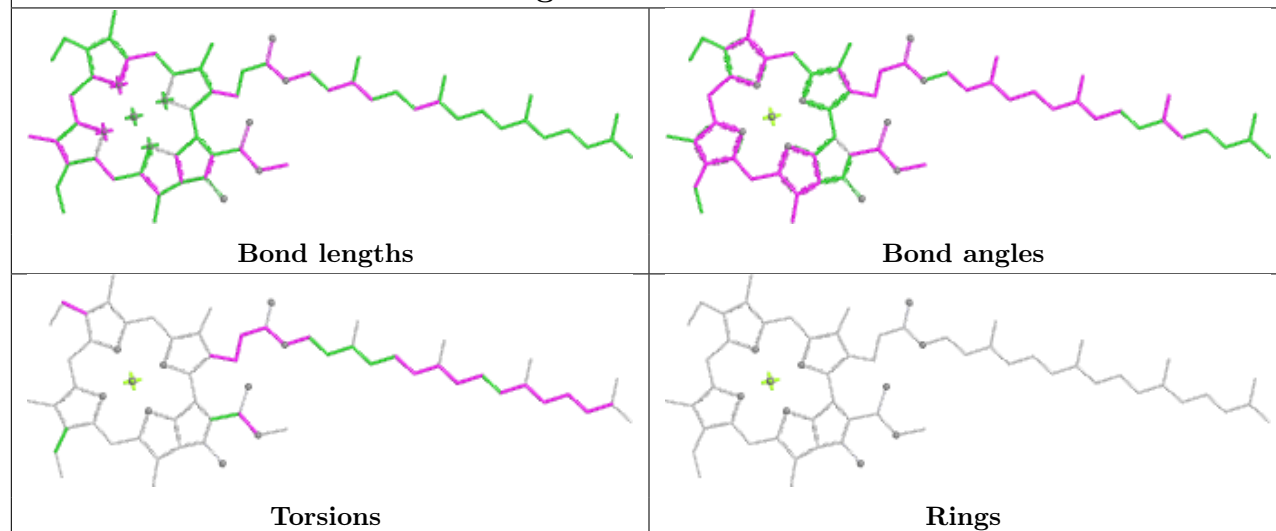


## Ligand CLA A 931

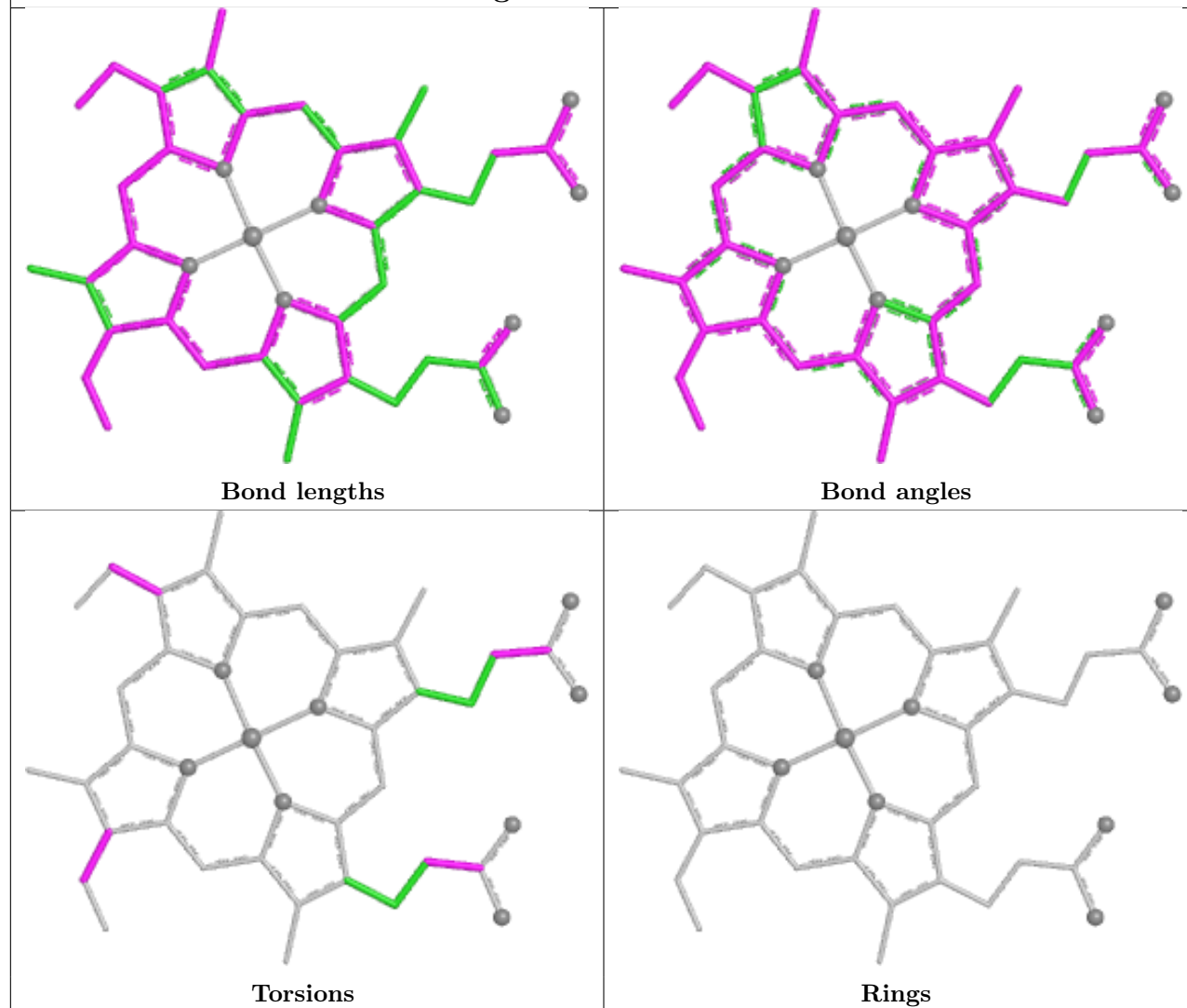


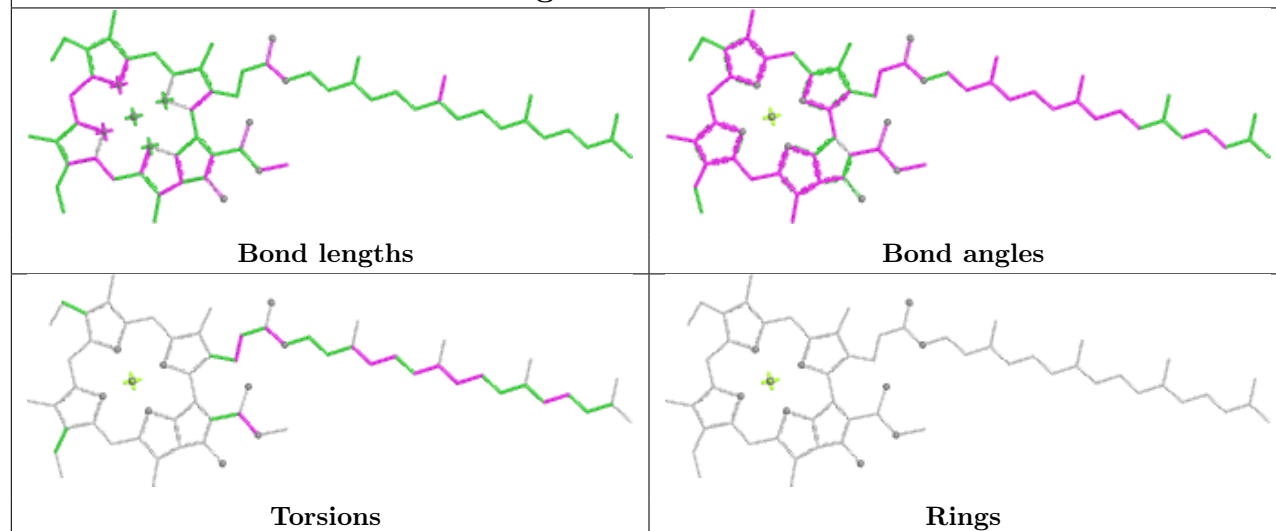
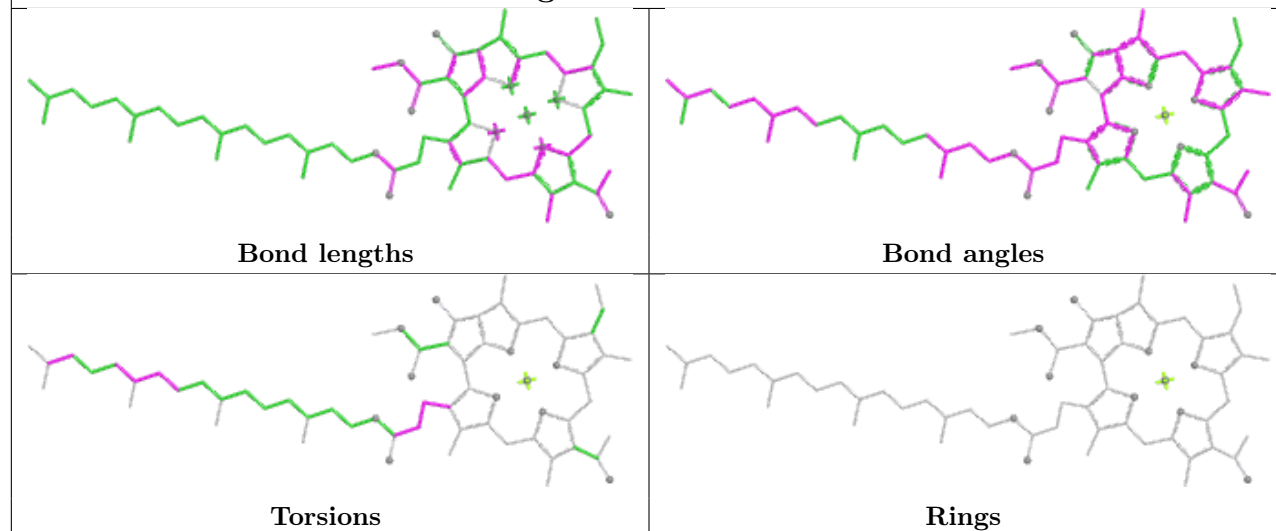


## Ligand CLA a 901

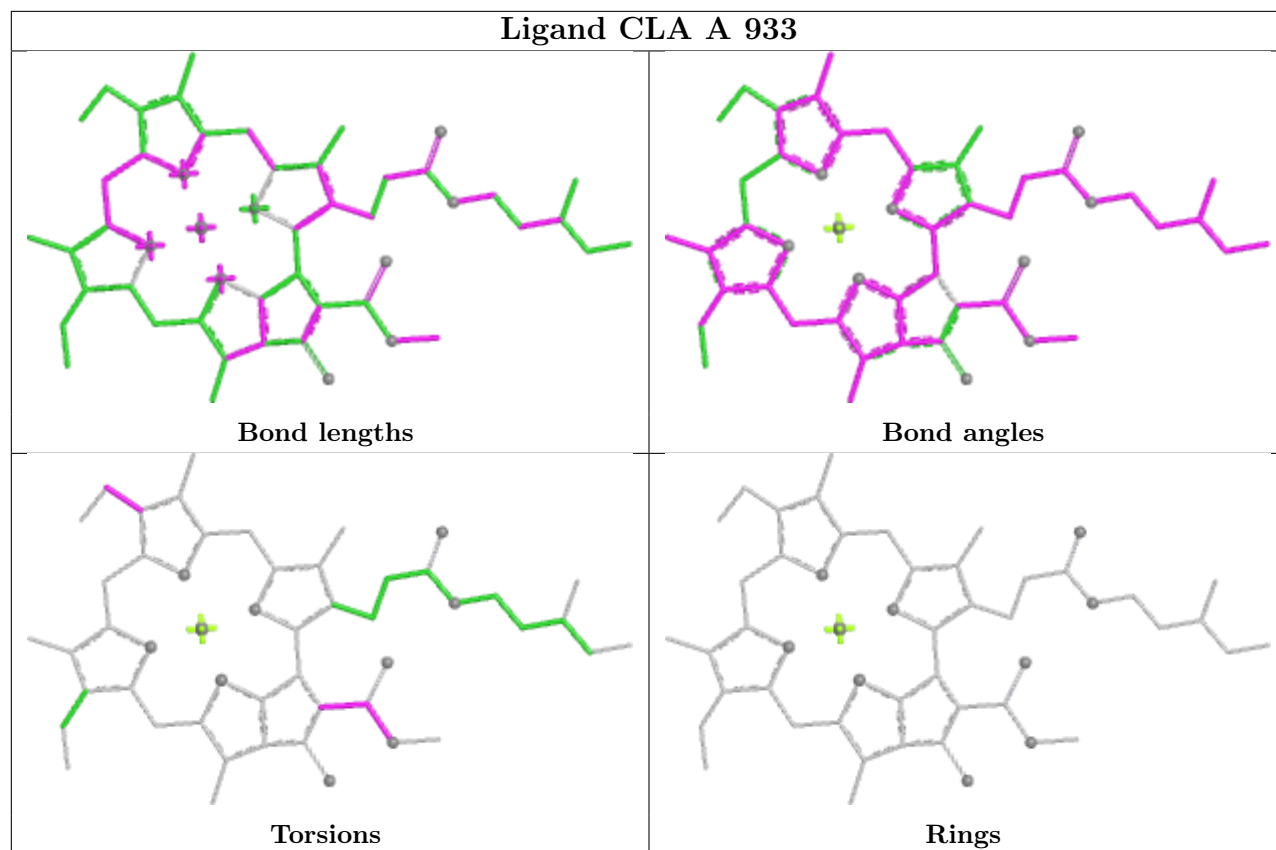


## Ligand HEC C 301

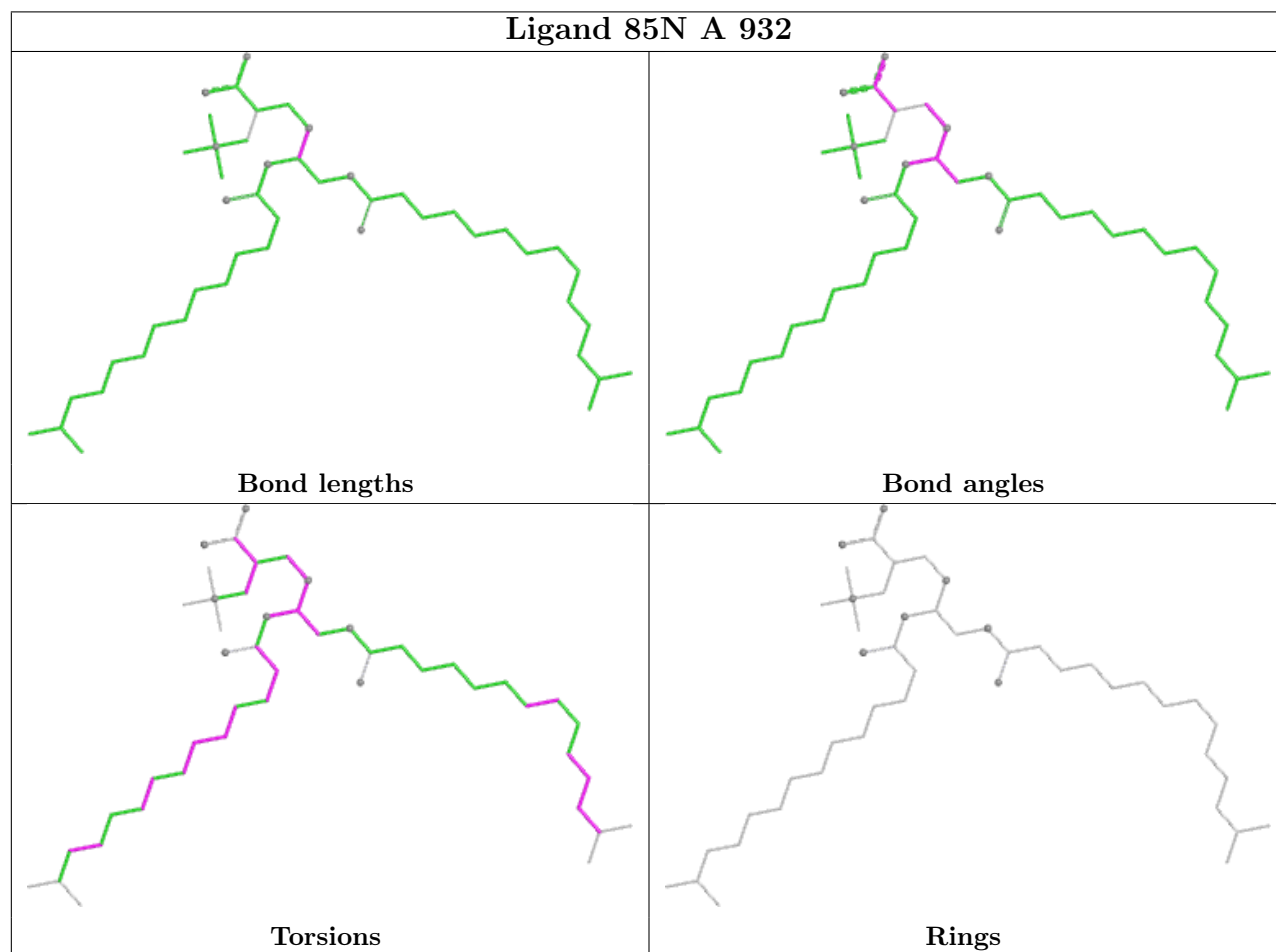


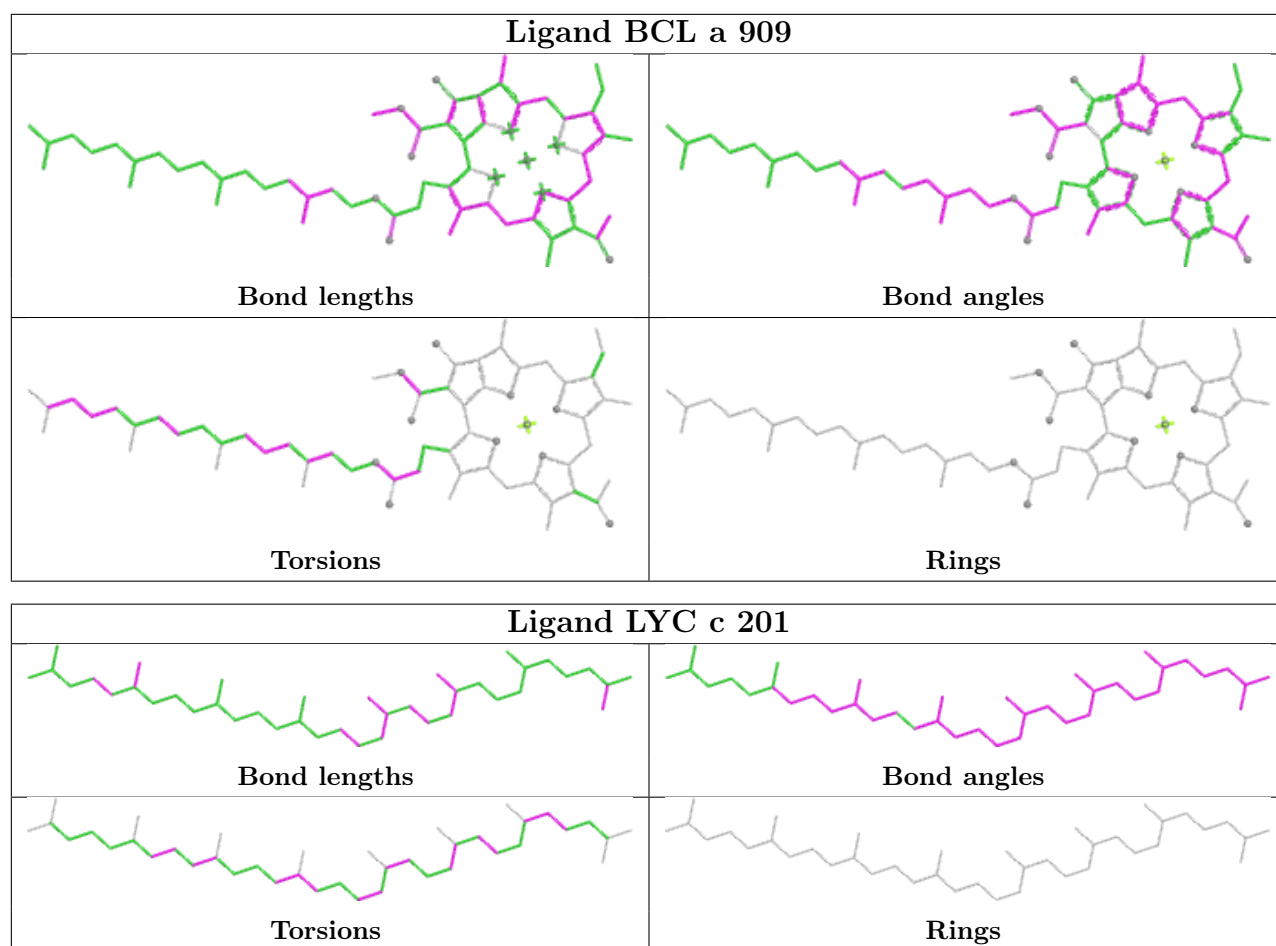
**Ligand CLA a 912****Ligand BCL a 910**

## Ligand CLA A 933



## Ligand 85N A 932





## 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.

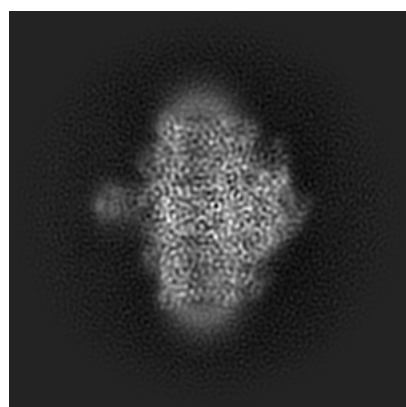
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32228. These allow visual inspection of the internal detail of the map and identification of artifacts.

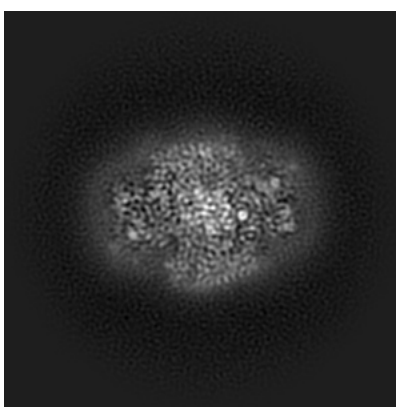
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

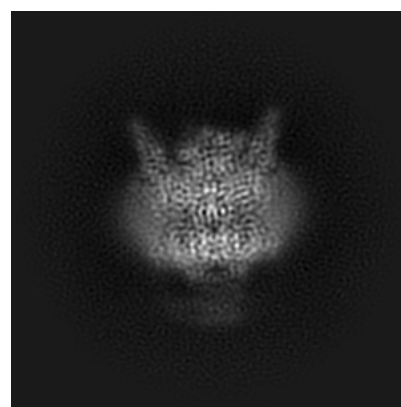
#### 6.1.1 Primary map



X



Y

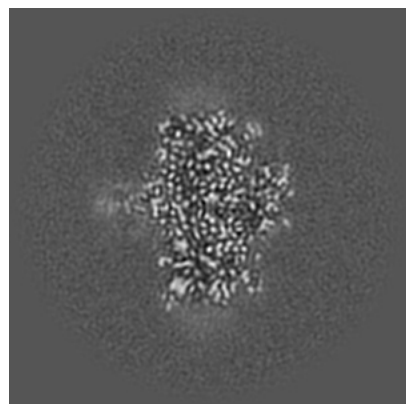


Z

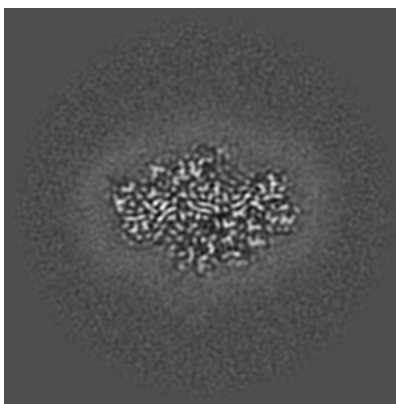
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

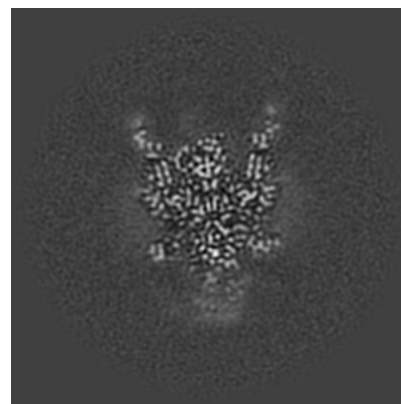
#### 6.2.1 Primary map



X Index: 110



Y Index: 110

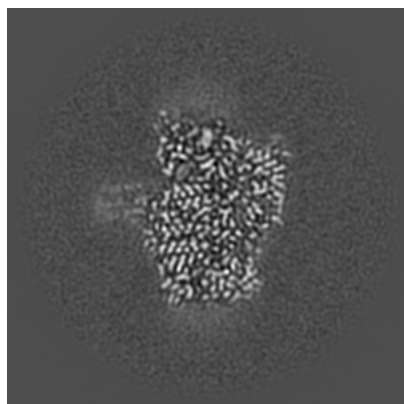


Z Index: 110

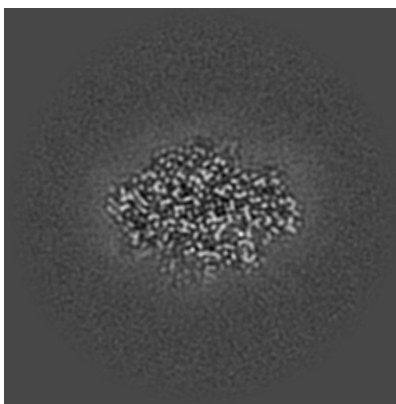
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

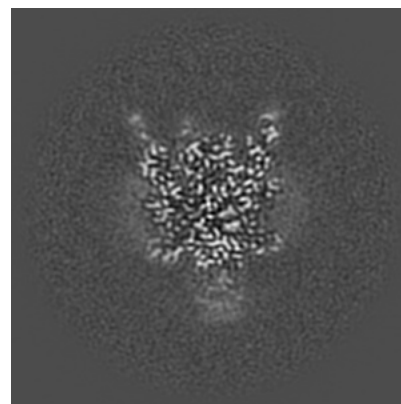
### 6.3.1 Primary map



X Index: 116



Y Index: 118

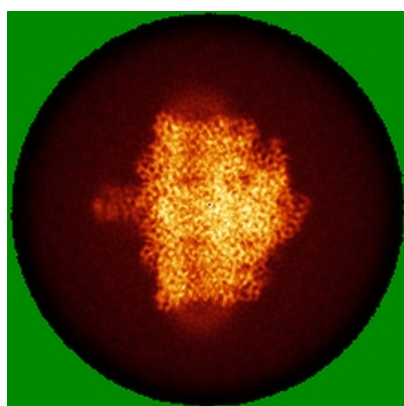


Z Index: 107

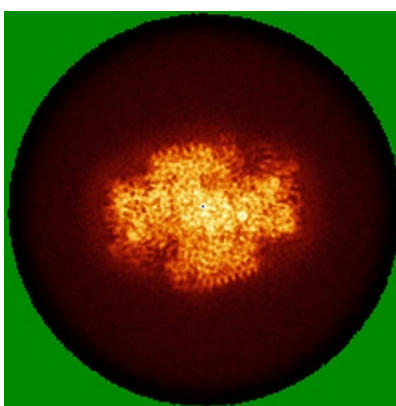
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

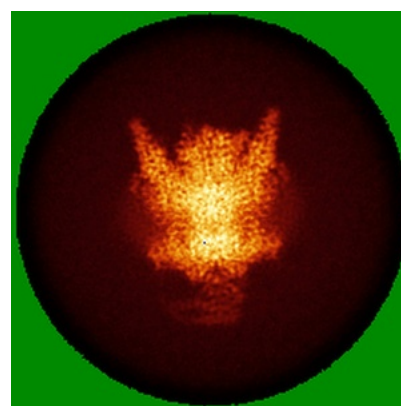
### 6.4.1 Primary map



X



Y

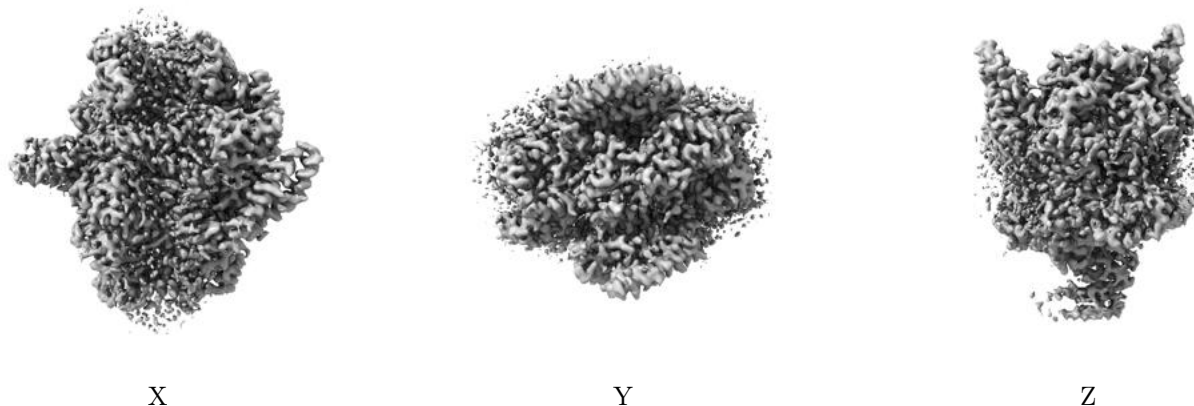


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

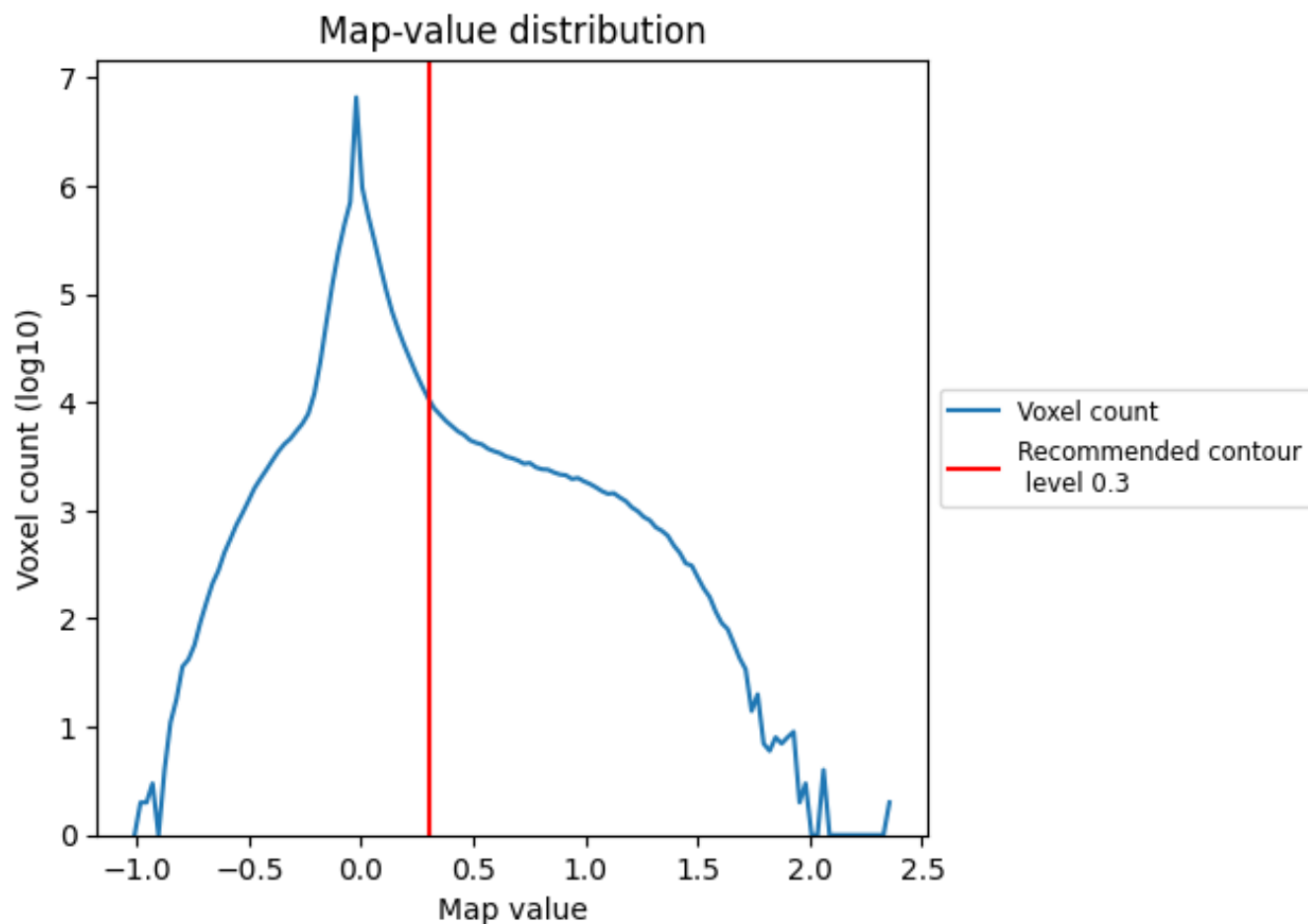
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

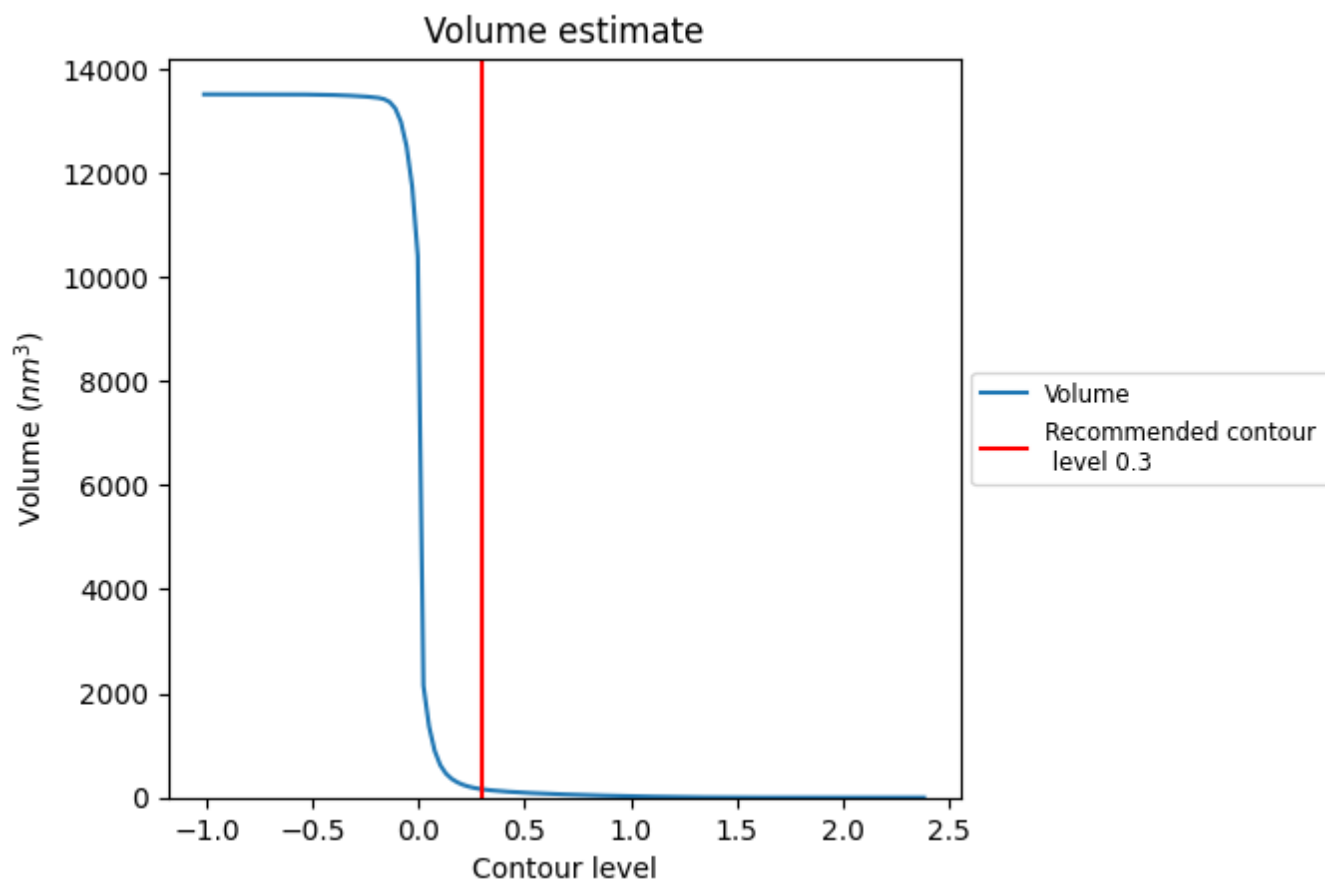
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

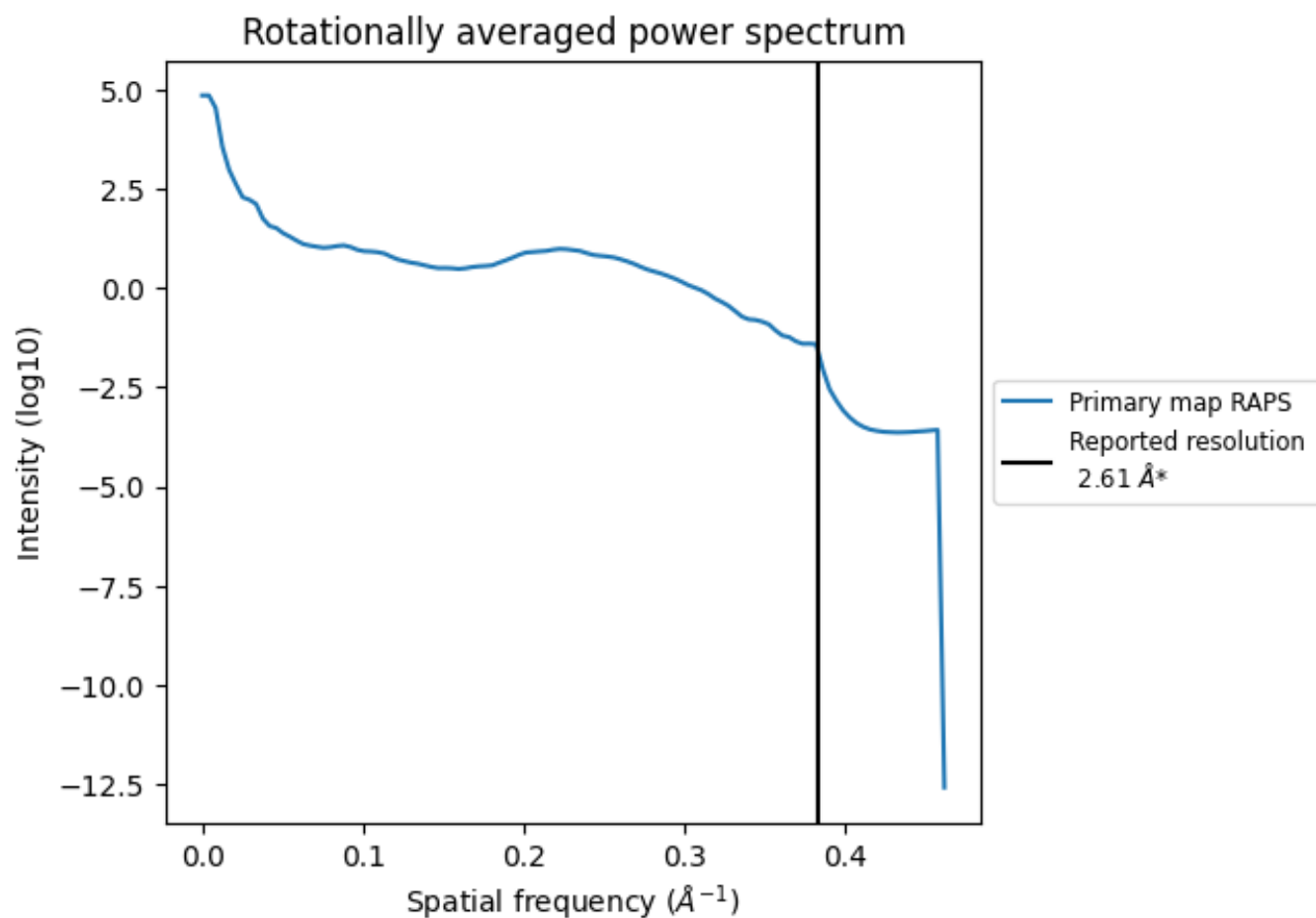
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160  $\text{nm}^3$ ; this corresponds to an approximate mass of 144 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.383 Å<sup>-1</sup>

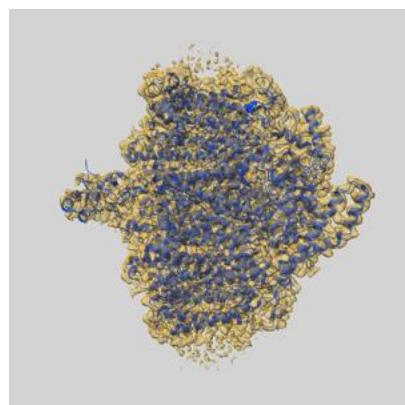
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

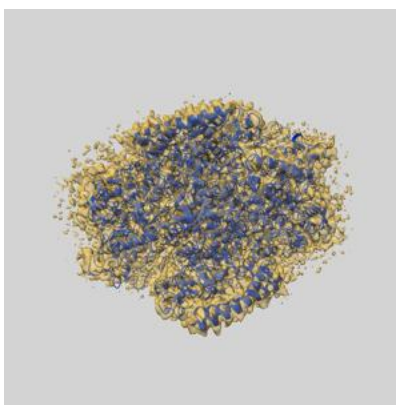
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32228 and PDB model 7VZG. Per-residue inclusion information can be found in section 3 on page 14.

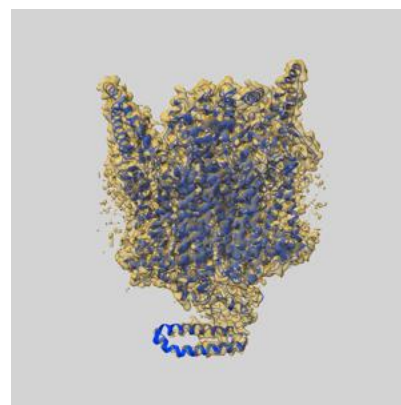
### 9.1 Map-model overlay [i](#)



X



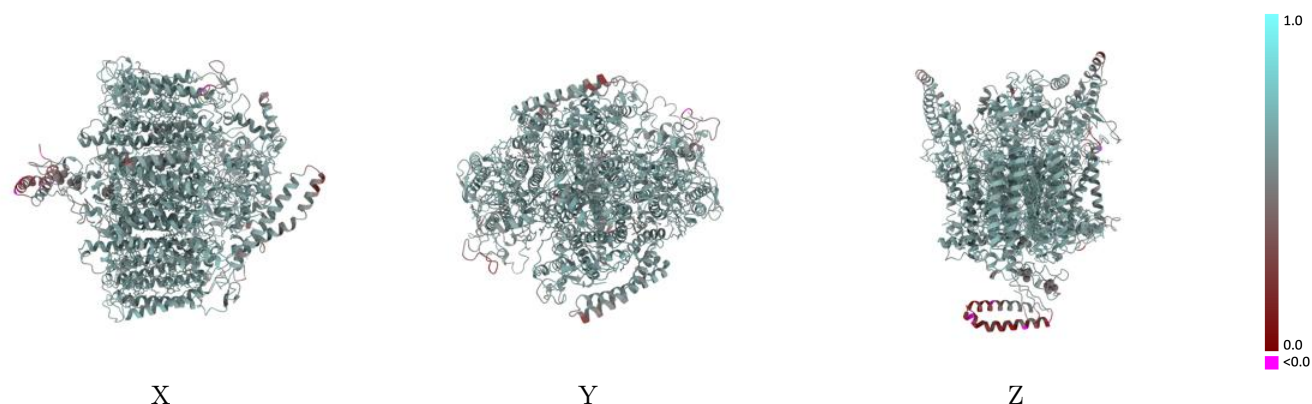
Y



Z

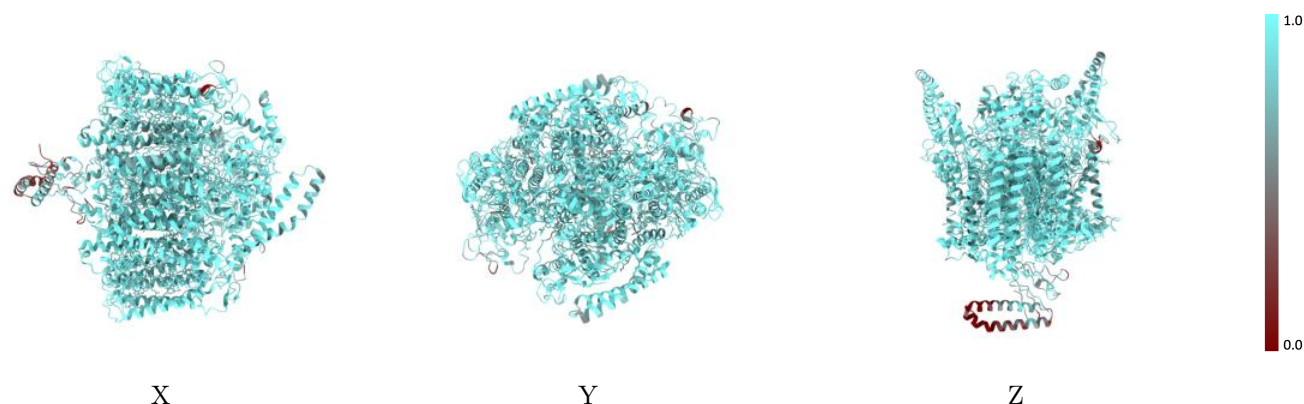
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



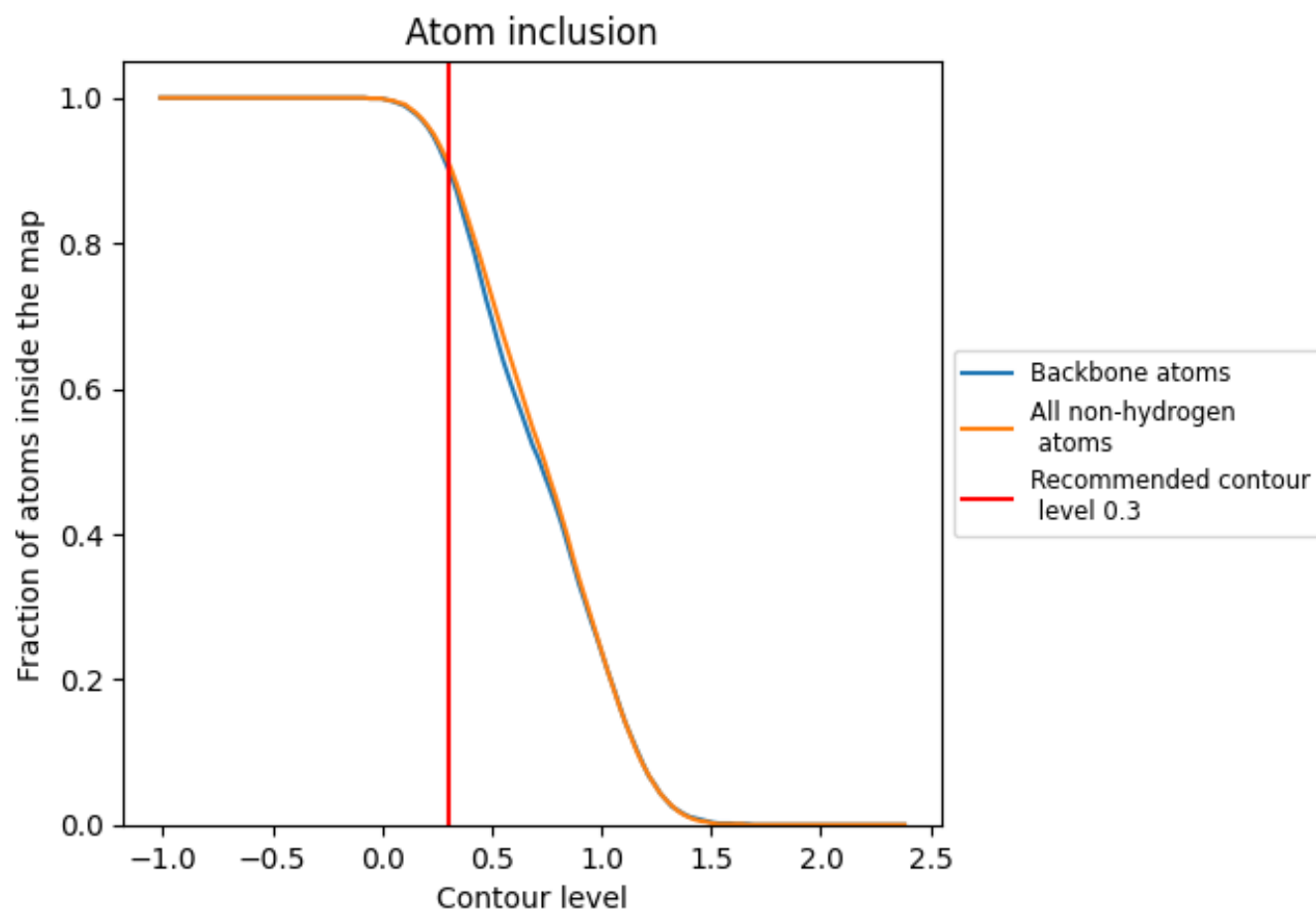
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.9120 | <div></div> 0.5780 |
| A     | <div></div> 0.9440 | <div></div> 0.5910 |
| B     | <div></div> 0.6700 | <div></div> 0.5210 |
| C     | <div></div> 0.9320 | <div></div> 0.5780 |
| D     | <div></div> 0.3570 | <div></div> 0.2470 |
| E     | <div></div> 0.9080 | <div></div> 0.5740 |
| F     | <div></div> 0.9330 | <div></div> 0.5960 |
| G     | <div></div> 0.7090 | <div></div> 0.5340 |
| H     | <div></div> 0.8420 | <div></div> 0.5600 |
| a     | <div></div> 0.9440 | <div></div> 0.5910 |
| c     | <div></div> 0.9260 | <div></div> 0.5760 |
| e     | <div></div> 0.8900 | <div></div> 0.5780 |
| f     | <div></div> 0.9440 | <div></div> 0.5880 |
| g     | <div></div> 0.8310 | <div></div> 0.5940 |
| h     | <div></div> 0.8530 | <div></div> 0.5780 |

