



## Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:27 PM JST

PDB ID : 9KQP  
EMDB ID : EMD-62511  
Title : PSI-LHCI supercomplex binding with 10 Lhcas from *C. subellipsoidea*  
Authors : Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.  
Deposited on : 2024-11-26  
Resolution : 1.92 Å (reported)  
Based on initial model : 6zzx

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.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

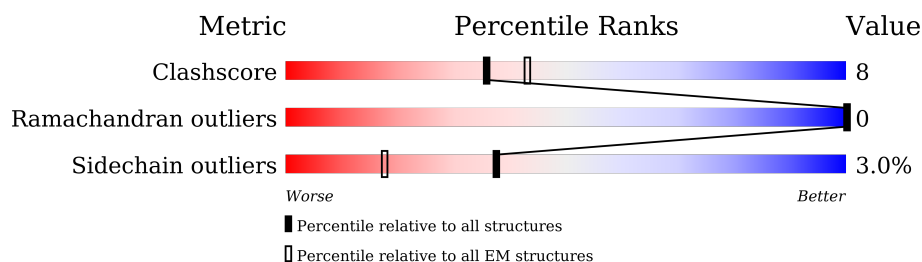
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.92 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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     | 751    | <br>89%      9%      •            |
| 2   | B     | 734    | <br>92%      8%                   |
| 3   | C     | 81     | <br>95%      • •                  |
| 4   | D     | 192    | <br>67%      7%      26%          |
| 5   | E     | 71     | <br>83%      •      15%           |
| 6   | F     | 245    | <br>62%      5%      33%          |
| 7   | G     | 138    | <br>67%      7%      •      25%   |
| 8   | H     | 133    | <br>7%      57%      11%      32% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9   | I     | 36     |                  |
| 10  | J     | 41     |                  |
| 11  | K     | 131    |                  |
| 12  | M     | 31     |                  |
| 13  | a     | 229    |                  |
| 13  | b     | 229    |                  |
| 14  | 3     | 246    |                  |
| 15  | 7     | 259    |                  |
| 16  | 8     | 255    |                  |
| 17  | 9     | 230    |                  |
| 18  | L     | 210    |                  |
| 19  | O     | 142    |                  |
| 20  | 2     | 273    |                  |
| 21  | 4     | 246    |                  |
| 22  | 5     | 274    |                  |
| 23  | 6     | 272    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 29  | UNL  | 3     | 306 | -         | -        | X       | -                |
| 30  | CL0  | A     | 813 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 305 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 313 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 2     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 2     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 317 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 319 | X         | -        | -       | -                |
| 31  | CLA  | 3     | 320 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 306 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 319 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 320 | X         | -        | -       | -                |
| 31  | CLA  | 4     | 321 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 5     | 323 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 6     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 309 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | 7     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 7     | 322 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 307 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 308 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 309 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 310 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 8     | 321 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 311 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 312 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 313 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 314 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 315 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 316 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 318 | X         | -        | -       | -                |
| 31  | CLA  | 9     | 321 | X         | -        | -       | -                |
| 31  | CLA  | A     | 814 | X         | -        | -       | -                |
| 31  | CLA  | A     | 816 | X         | -        | -       | -                |
| 31  | CLA  | A     | 817 | X         | -        | -       | -                |
| 31  | CLA  | A     | 818 | X         | -        | -       | -                |
| 31  | CLA  | A     | 819 | X         | -        | -       | -                |
| 31  | CLA  | A     | 821 | X         | -        | -       | -                |
| 31  | CLA  | A     | 824 | X         | -        | -       | -                |
| 31  | CLA  | A     | 826 | X         | -        | -       | -                |
| 31  | CLA  | A     | 834 | X         | -        | -       | -                |
| 31  | CLA  | A     | 838 | X         | -        | -       | -                |
| 31  | CLA  | A     | 841 | X         | -        | -       | -                |
| 31  | CLA  | A     | 849 | X         | -        | -       | -                |
| 31  | CLA  | A     | 850 | X         | -        | -       | -                |
| 31  | CLA  | A     | 851 | X         | -        | -       | -                |
| 31  | CLA  | A     | 854 | X         | -        | -       | -                |
| 31  | CLA  | A     | 856 | X         | -        | -       | -                |
| 31  | CLA  | A     | 857 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | B     | 811 | X         | -        | -       | -                |
| 31  | CLA  | B     | 812 | X         | -        | -       | -                |
| 31  | CLA  | B     | 814 | X         | -        | -       | -                |
| 31  | CLA  | B     | 815 | X         | -        | -       | -                |
| 31  | CLA  | B     | 817 | X         | -        | -       | -                |
| 31  | CLA  | B     | 818 | X         | -        | -       | -                |
| 31  | CLA  | B     | 819 | X         | -        | -       | -                |
| 31  | CLA  | B     | 822 | X         | -        | -       | -                |
| 31  | CLA  | B     | 823 | X         | -        | -       | -                |
| 31  | CLA  | B     | 827 | X         | -        | -       | -                |
| 31  | CLA  | B     | 828 | X         | -        | -       | -                |
| 31  | CLA  | B     | 832 | X         | -        | -       | -                |
| 31  | CLA  | B     | 833 | X         | -        | -       | -                |
| 31  | CLA  | B     | 834 | X         | -        | -       | -                |
| 31  | CLA  | B     | 835 | X         | -        | -       | -                |
| 31  | CLA  | B     | 840 | X         | -        | -       | -                |
| 31  | CLA  | B     | 842 | X         | -        | -       | -                |
| 31  | CLA  | B     | 843 | X         | -        | -       | -                |
| 31  | CLA  | B     | 844 | X         | -        | -       | -                |
| 31  | CLA  | B     | 848 | X         | -        | -       | -                |
| 31  | CLA  | B     | 849 | X         | -        | -       | -                |
| 31  | CLA  | F     | 301 | X         | -        | -       | -                |
| 31  | CLA  | F     | 305 | X         | -        | -       | -                |
| 31  | CLA  | F     | 306 | X         | -        | -       | -                |
| 31  | CLA  | G     | 204 | X         | -        | -       | -                |
| 31  | CLA  | G     | 205 | X         | -        | -       | -                |
| 31  | CLA  | G     | 206 | X         | -        | -       | -                |
| 31  | CLA  | H     | 901 | X         | -        | -       | -                |
| 31  | CLA  | H     | 902 | X         | -        | -       | -                |
| 31  | CLA  | J     | 105 | X         | -        | -       | -                |
| 31  | CLA  | K     | 205 | X         | -        | -       | -                |
| 31  | CLA  | L     | 307 | X         | -        | -       | -                |
| 31  | CLA  | O     | 202 | X         | -        | -       | -                |
| 31  | CLA  | O     | 203 | X         | -        | -       | -                |
| 31  | CLA  | O     | 204 | X         | -        | -       | -                |
| 31  | CLA  | a     | 309 | X         | -        | -       | -                |
| 31  | CLA  | a     | 310 | X         | -        | -       | -                |
| 31  | CLA  | a     | 311 | X         | -        | -       | -                |
| 31  | CLA  | a     | 312 | X         | -        | -       | -                |
| 31  | CLA  | a     | 313 | X         | -        | -       | -                |
| 31  | CLA  | a     | 314 | X         | -        | -       | -                |
| 31  | CLA  | a     | 315 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | CLA  | a     | 319 | X         | -        | -       | -                |
| 31  | CLA  | a     | 322 | X         | -        | -       | -                |
| 31  | CLA  | b     | 302 | X         | -        | -       | -                |
| 31  | CLA  | b     | 303 | X         | -        | -       | -                |
| 31  | CLA  | b     | 304 | X         | -        | -       | -                |
| 31  | CLA  | b     | 305 | X         | -        | -       | -                |
| 31  | CLA  | b     | 307 | X         | -        | -       | -                |
| 31  | CLA  | b     | 310 | X         | -        | -       | -                |
| 31  | CLA  | b     | 311 | X         | -        | -       | -                |
| 31  | CLA  | b     | 313 | X         | -        | -       | -                |
| 32  | CHL  | 3     | 315 | X         | -        | -       | -                |
| 32  | CHL  | 4     | 310 | X         | -        | -       | -                |
| 32  | CHL  | 4     | 313 | X         | -        | -       | -                |
| 32  | CHL  | 4     | 317 | X         | -        | -       | -                |
| 32  | CHL  | 5     | 316 | X         | -        | -       | -                |
| 32  | CHL  | 5     | 317 | X         | -        | -       | -                |
| 32  | CHL  | 5     | 319 | X         | -        | -       | -                |
| 32  | CHL  | 5     | 322 | X         | -        | -       | -                |
| 32  | CHL  | 6     | 309 | X         | -        | -       | -                |
| 32  | CHL  | 6     | 317 | X         | -        | -       | -                |
| 32  | CHL  | 6     | 318 | X         | -        | -       | -                |
| 32  | CHL  | 6     | 319 | X         | -        | -       | -                |
| 32  | CHL  | 6     | 320 | X         | -        | -       | -                |
| 32  | CHL  | 6     | 321 | X         | -        | -       | -                |
| 32  | CHL  | 7     | 317 | X         | -        | -       | -                |
| 32  | CHL  | 7     | 318 | X         | -        | -       | -                |
| 32  | CHL  | 7     | 319 | X         | -        | -       | -                |
| 32  | CHL  | 7     | 320 | X         | -        | -       | -                |
| 32  | CHL  | 7     | 324 | X         | -        | -       | -                |
| 32  | CHL  | 8     | 316 | X         | -        | -       | -                |
| 32  | CHL  | 8     | 319 | X         | -        | -       | -                |
| 32  | CHL  | 9     | 320 | X         | -        | -       | -                |
| 32  | CHL  | 9     | 322 | X         | -        | -       | -                |
| 32  | CHL  | A     | 831 | X         | -        | -       | -                |
| 32  | CHL  | A     | 839 | X         | -        | -       | -                |
| 32  | CHL  | A     | 840 | X         | -        | -       | -                |
| 32  | CHL  | K     | 201 | X         | -        | -       | -                |
| 32  | CHL  | a     | 317 | X         | -        | -       | -                |
| 32  | CHL  | a     | 318 | X         | -        | -       | -                |
| 32  | CHL  | a     | 320 | X         | -        | -       | -                |
| 32  | CHL  | b     | 309 | X         | -        | -       | -                |
| 36  | LUT  | 4     | 302 | -         | X        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 36  | LUT  | 6     | 303 | -         | X        | -       | -                |
| 36  | LUT  | 9     | 302 | -         | X        | -       | -                |
| 36  | LUT  | 9     | 305 | -         | X        | -       | -                |
| 36  | LUT  | F     | 304 | -         | X        | -       | -                |
| 36  | LUT  | a     | 305 | -         | X        | -       | -                |

## 2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 52991 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 Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 1   | A     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5814  | 3800 | 992 | 1004 | 18 |         |       |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 732      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5808  | 3812 | 985 | 998 | 13 |         |       |

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 596   | 365 | 103 | 117 | 11 |         |       |

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1110  | 711 | 193 | 203 | 3 |         |       |

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | E     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 490   | 316 | 83 | 90 | 1 |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1264  | 805 | 223 | 234 | 2 |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 767   | 488 | 132 | 146 | 1 |         |       |

- Molecule 8 is a protein called Photosystem I reaction centre subunit VI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 706   | 449 | 120 | 137 |   |         |       |

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | I     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 248   | 171 | 34 | 41 | 2 |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 39       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 319   | 220 | 46 | 52 | 1 |         |       |

- Molecule 11 is a protein called PSI-K.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 11  | K     | 81       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 560   | 356 | 96 | 107 | 1 |         |       |

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | M     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 237   | 160 | 35 | 41 | 1 |         |       |

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | a     | 195      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 944 | 245 | 267 | 2 |         |       |
| 13  | b     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 952   | 606 | 168 | 176 | 2 |         |       |

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | 3     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1580  | 1036 | 255 | 286 | 3 |         |       |

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | 7     | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 1059 | 276 | 296 | 2 |         |       |

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 8     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1112 | 276 | 310 | 3 |         |       |

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | 9     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1414  | 915 | 238 | 258 | 3 |         |       |

- Molecule 18 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | L     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 723 | 183 | 194 | 2 |         |       |

- Molecule 19 is a protein called Photosystem I PsaO.

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 19  | O     | 78       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 605   | 403 | 98 | 104 |         |       |

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic/Lhca2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | 2     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1606  | 1046 | 270 | 286 | 4 |         |       |

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | 4     | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 984 | 246 | 273 | 3 |         |       |

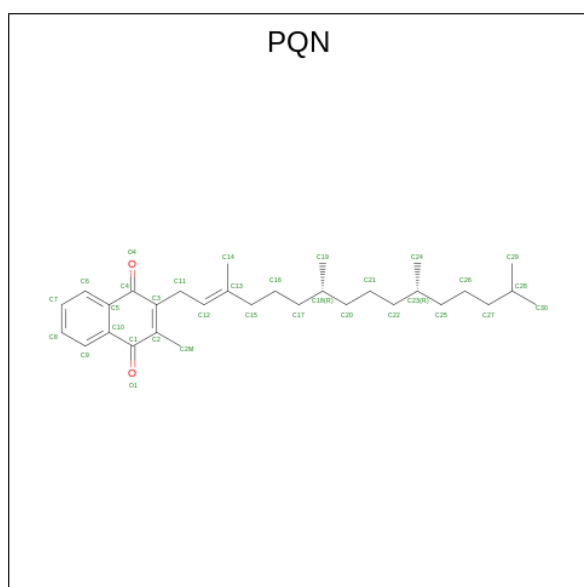
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | 5     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1766  | 1152 | 303 | 307 | 4 |         |       |

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | 6     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1658  | 1088 | 276 | 287 | 7 |         |       |

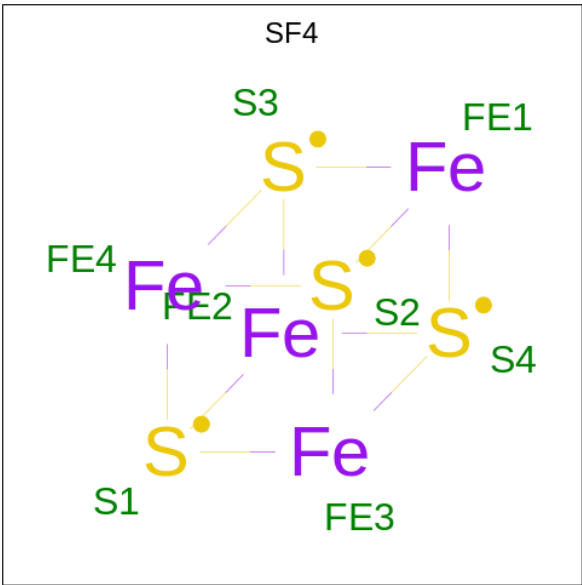
- Molecule 24 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 24  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

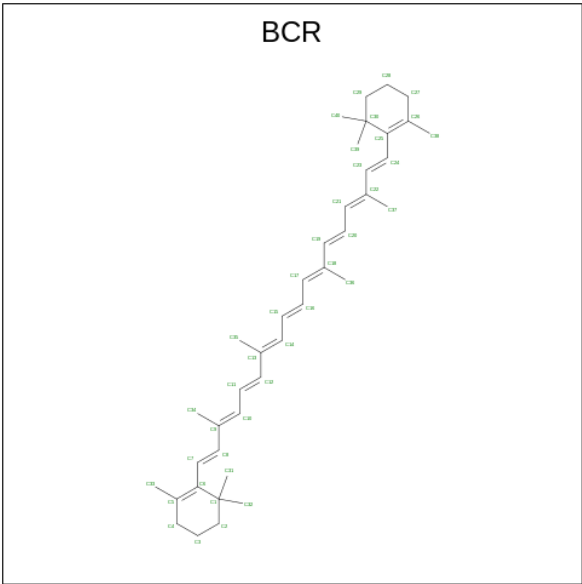
- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 25  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 25  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



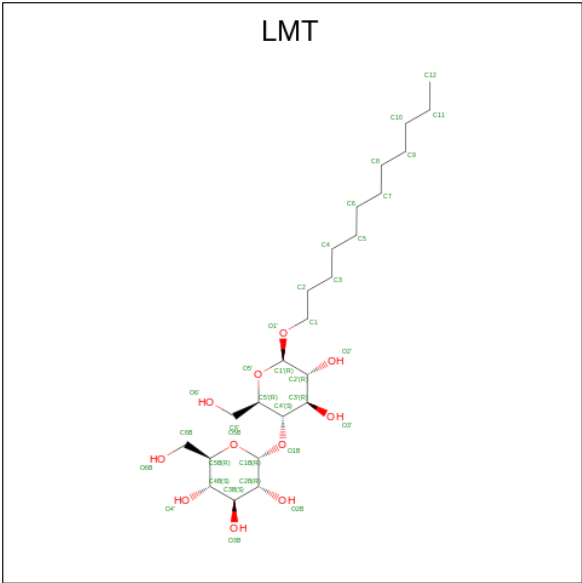
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 26  | A     | 1        | Total C<br>40 40 | 0       |
| 26  | A     | 1        | Total C<br>40 40 | 0       |
| 26  | A     | 1        | Total C<br>40 40 | 0       |
| 26  | A     | 1        | Total C<br>40 40 | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       |
| 26  | B     | 1        | Total C<br>40 40 | 0       |
| 26  | F     | 1        | Total C<br>40 40 | 0       |
| 26  | G     | 1        | Total C<br>40 40 | 0       |
| 26  | G     | 1        | Total C<br>40 40 | 0       |
| 26  | I     | 1        | Total C<br>40 40 | 0       |
| 26  | J     | 1        | Total C<br>40 40 | 0       |
| 26  | K     | 1        | Total C<br>40 40 | 0       |
| 26  | K     | 1        | Total C<br>40 40 | 0       |
| 26  | M     | 1        | Total C<br>40 40 | 0       |
| 26  | 3     | 1        | Total C<br>40 40 | 0       |
| 26  | 3     | 1        | Total C<br>40 40 | 0       |
| 26  | 3     | 1        | Total C<br>40 40 | 0       |
| 26  | 7     | 1        | Total C<br>40 40 | 0       |
| 26  | 8     | 1        | Total C<br>40 40 | 0       |

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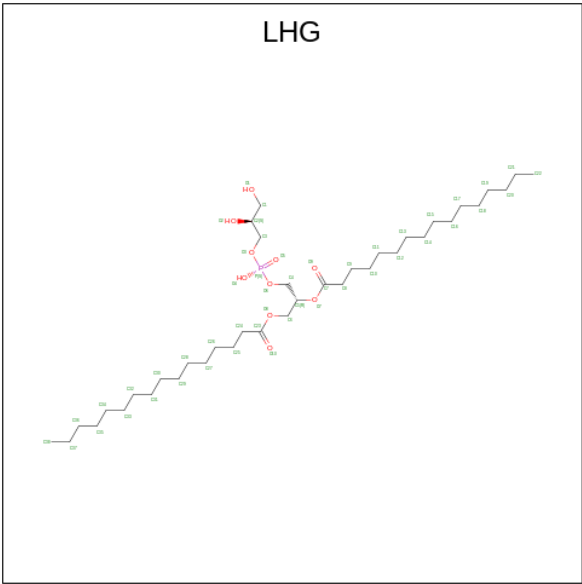
| Mol | Chain | Residues | Atoms |      | AltConf |
|-----|-------|----------|-------|------|---------|
| 26  | L     | 1        | Total | C 40 | 0       |
| 26  | L     | 1        | Total | C 40 | 0       |
| 26  | L     | 1        | Total | C 40 | 0       |
| 26  | O     | 1        | Total | C 40 | 0       |
| 26  | 2     | 1        | Total | C 40 | 0       |
| 26  | 5     | 1        | Total | C 40 | 0       |
| 26  | 6     | 1        | Total | C 40 | 0       |

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |      |      | AltConf |
|-----|-------|----------|-------|------|------|---------|
| 27  | A     | 1        | Total | C 35 | O 24 | 0       |
| 27  | A     | 1        | Total | C 35 | O 24 | 0       |
| 27  | 9     | 1        | Total | C 35 | O 24 | 0       |
| 27  | 5     | 1        | Total | C 35 | O 24 | 0       |

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ) (labeled as "Ligand of Interest" by depositor).

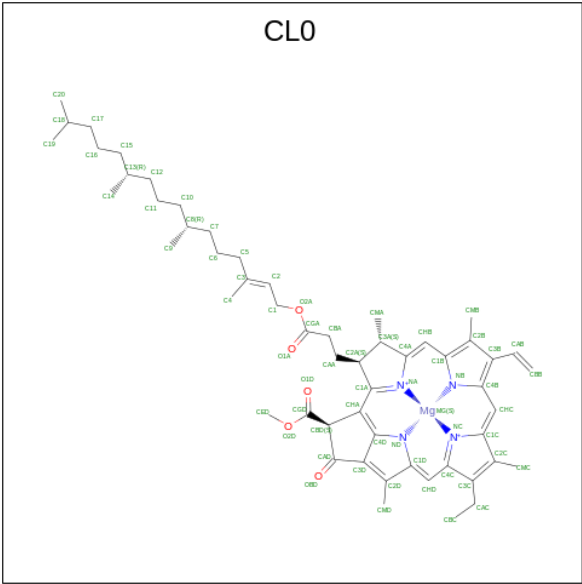


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 28  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 28  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 31 | 10 | 1 |         |
| 28  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |
| 28  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 7     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |
| 28  | 8     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 28  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 35    | 24 | 10 | 1 |         |
| 28  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 16 | 10 | 1 |         |
| 28  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 32    | 21 | 10 | 1 |         |

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

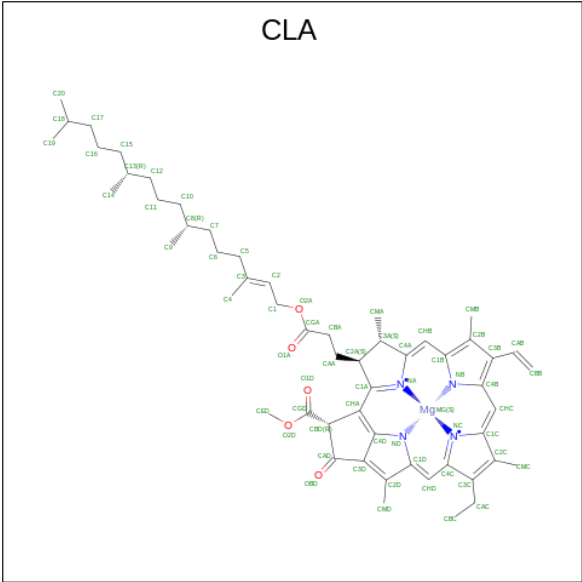
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 29  | A     | 2        | Total | C  | 0       |
|     |       |          | 20    | 20 |         |
| 29  | B     | 2        | Total | C  | 0       |
|     |       |          | 24    | 24 |         |
| 29  | a     | 2        | Total | C  | 0       |
|     |       |          | 27    | 27 |         |
| 29  | 3     | 1        | Total | C  | 0       |
|     |       |          | 11    | 11 |         |
| 29  | 7     | 1        | Total | C  | 0       |
|     |       |          | 8     | 8  |         |
| 29  | 8     | 1        | Total | C  | 0       |
|     |       |          | 18    | 18 |         |
| 29  | 9     | 6        | Total | C  | 0       |
|     |       |          | 81    | 81 |         |
| 29  | 2     | 1        | Total | C  | 0       |
|     |       |          | 11    | 11 |         |
| 29  | 4     | 1        | Total | C  | 0       |
|     |       |          | 13    | 13 |         |

- Molecule 30 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 30  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 31 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 51 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | B     | 1        | Total<br>62 | C<br>52 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | F     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | F     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | F     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | G     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | H     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | K     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | a     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>61 | C<br>51 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 3     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 7     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 62    | 52 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | 8     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 9     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | O     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | O     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | O     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>57 | C<br>47 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 2     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 4     | 1        | Total<br>52 | C<br>42 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 31  | 4     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

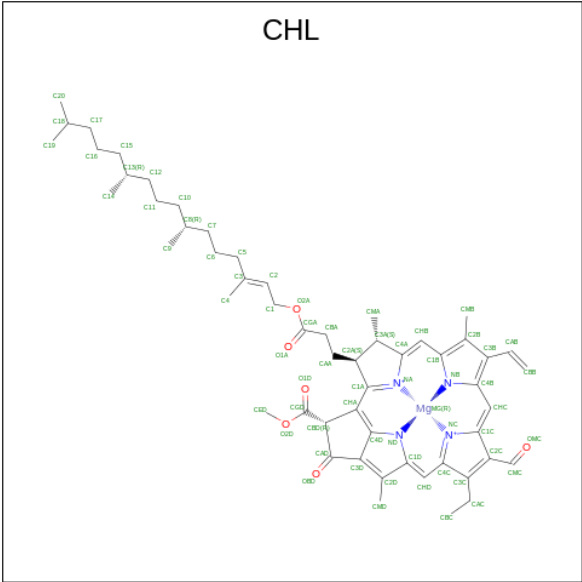
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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 31  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |

- Molecule 32 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).





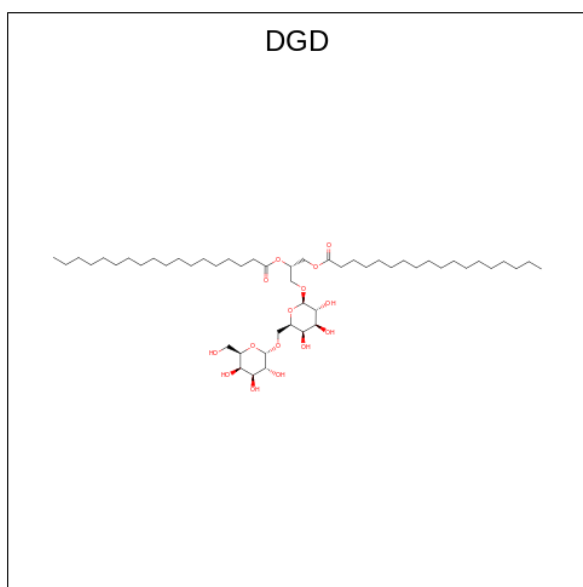
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 32  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 47 | 1  | 4 | 6 |         |
| 32  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 32  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 32  | K     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 32  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 32  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 32  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 32  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 46 | 1  | 4 | 6 |         |
| 32  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 32  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 61    | 50 | 1  | 4 | 6 |         |
| 32  | 7     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 32  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |

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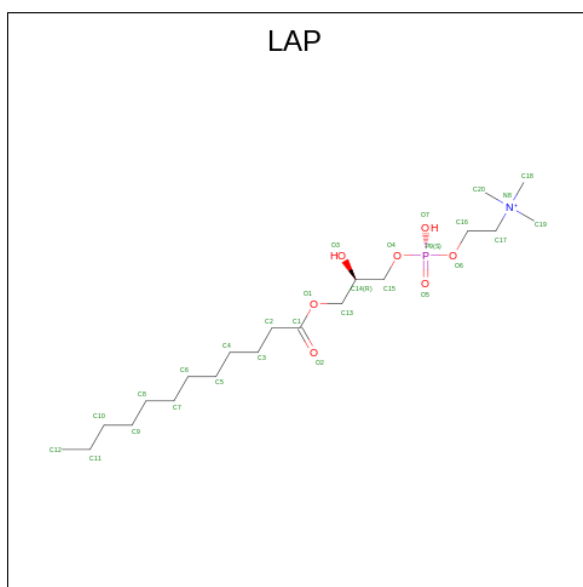
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 32  | 8     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 32  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 32  | 9     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 48    | 37 | 1  | 4 | 6 |         |
| 32  | 4     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 32  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 45 | 1  | 4 | 6 |         |
| 32  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 66    | 55 | 1  | 4 | 6 |         |
| 32  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 32  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |
| 32  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



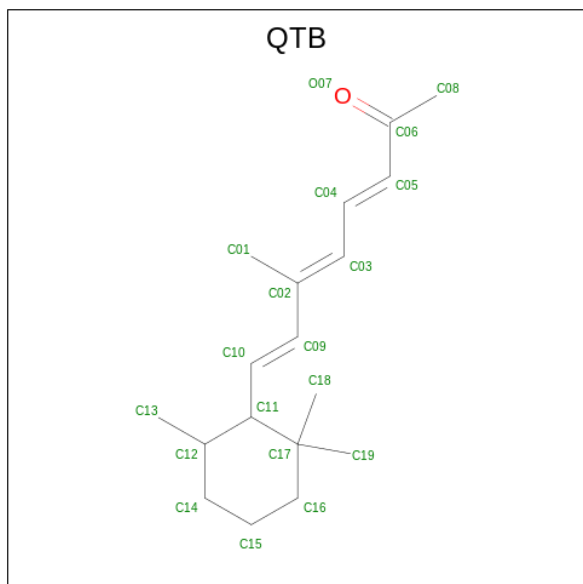
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 33  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 61    | 46 | 15 |         |
| 33  | 7     | 1        | Total | C  | O  | 0       |
|     |       |          | 52    | 37 | 15 |         |

- Molecule 34 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (three-letter code: LAP) (formula: C<sub>20</sub>H<sub>43</sub>NO<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



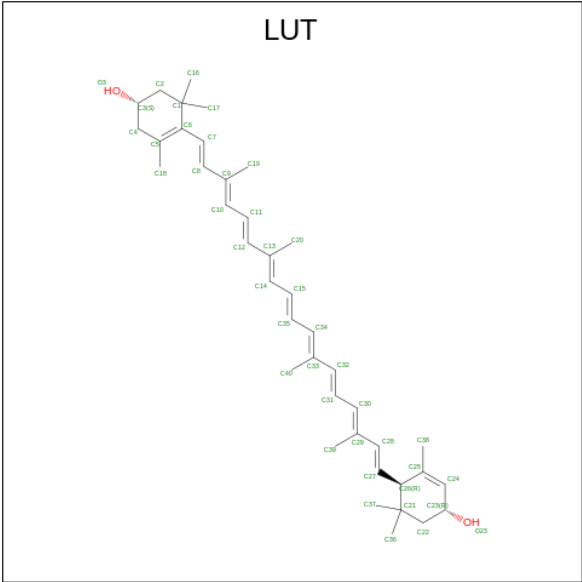
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 34  | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 20 | 1 | 7 | 1 |         |

- Molecule 35 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula: C<sub>18</sub>H<sub>28</sub>O) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 35  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 19    | 18 | 1 |         |
| 35  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 19    | 18 | 1 |         |
| 35  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 19    | 18 | 1 |         |
| 35  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 19    | 18 | 1 |         |

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



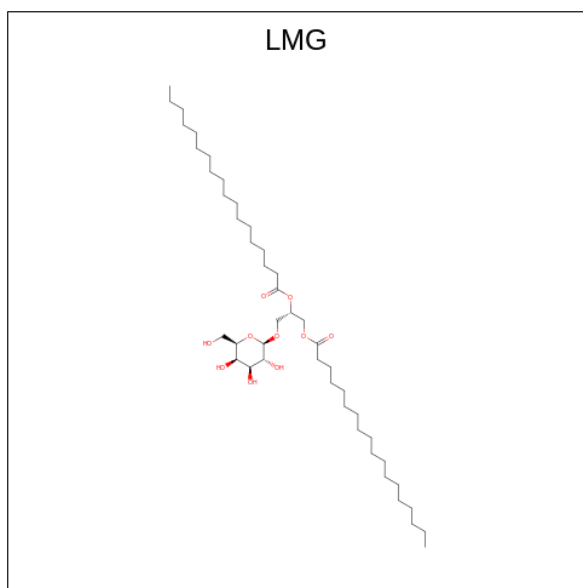
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | F     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 9     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | L     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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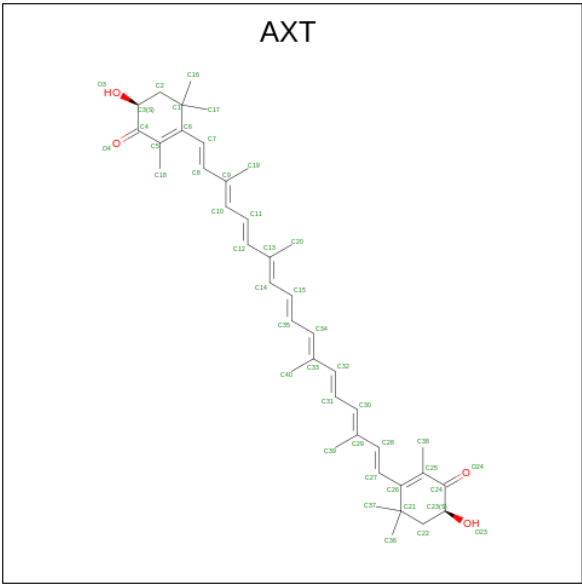
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 36  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 4     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 36  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



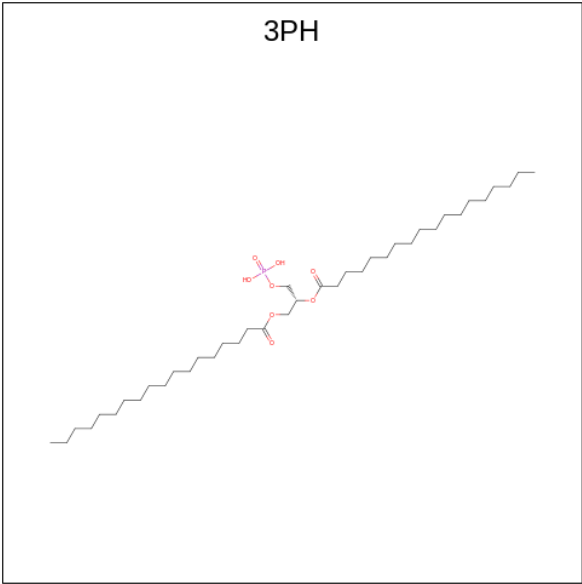
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 37  | G     | 1        | Total | C  | O  | 0       |
|     |       |          | 44    | 34 | 10 |         |
| 37  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 49    | 39 | 10 |         |
| 37  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 29    | 19 | 10 |         |
| 37  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 42    | 32 | 10 |         |

- Molecule 38 is ASTAXANTHIN (three-letter code: AXT) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



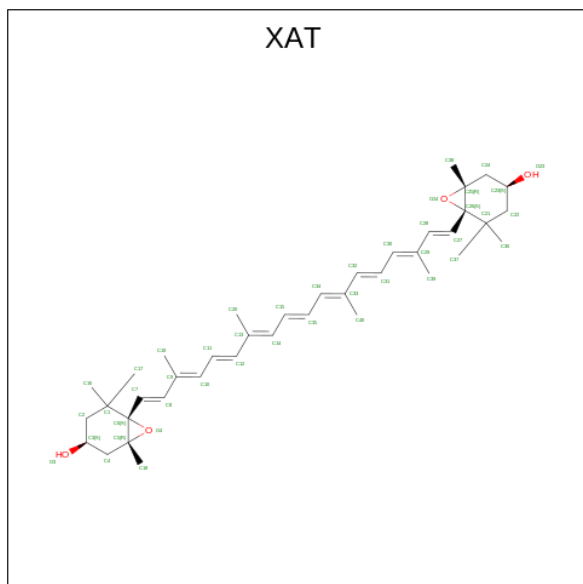
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 38  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 40 | 3 |         |

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



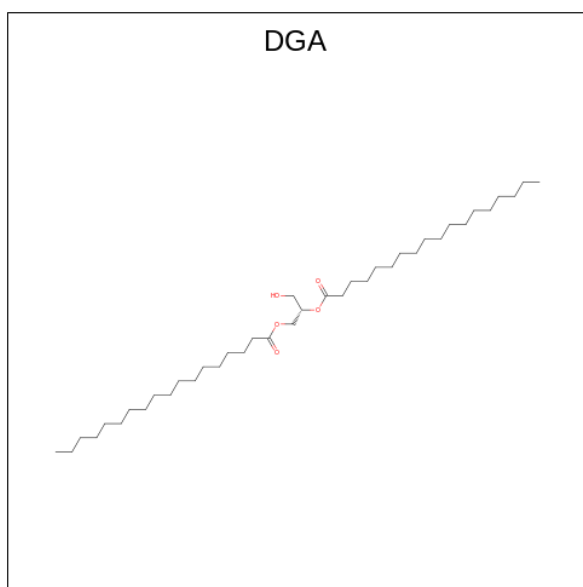
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 39  | 7     | 1        | Total | C  | O | P | 0       |
|     |       |          | 33    | 24 | 8 | 1 |         |

- Molecule 40 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 40  | 7     | 1        | Total | C  | O | 0       |
|     |       |          | 44    | 40 | 4 |         |

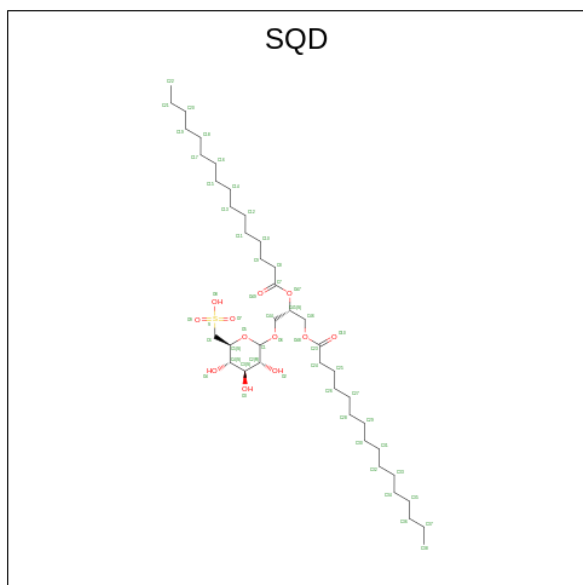
- Molecule 41 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ) (labeled as "Ligand of Interest" by depositor).





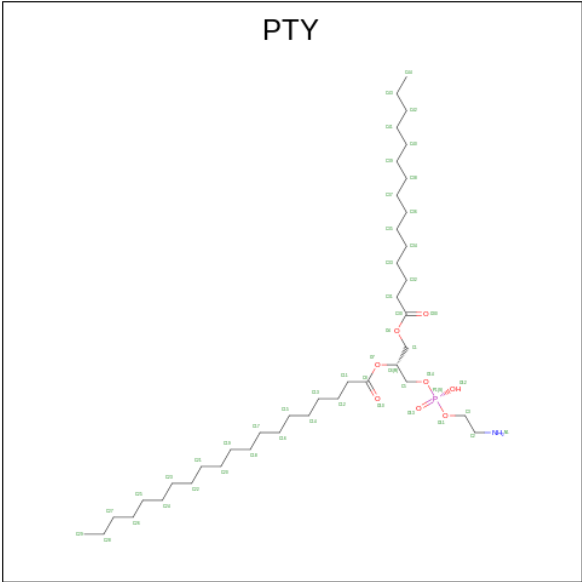
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 41  | 8     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 23 | 5 |         |

- Molecule 42 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 42  | 4     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 35    | 22 | 12 | 1 |         |

- Molecule 43 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 43  | 5     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |

- Molecule 44 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 44  | A     | 297      | Total | O   | 0       |
|     |       |          | 297   | 297 |         |
| 44  | B     | 311      | Total | O   | 0       |
|     |       |          | 311   | 311 |         |
| 44  | C     | 60       | Total | O   | 0       |
|     |       |          | 60    | 60  |         |
| 44  | D     | 53       | Total | O   | 0       |
|     |       |          | 53    | 53  |         |
| 44  | E     | 28       | Total | O   | 0       |
|     |       |          | 28    | 28  |         |
| 44  | F     | 57       | Total | O   | 0       |
|     |       |          | 57    | 57  |         |
| 44  | G     | 18       | Total | O   | 0       |
|     |       |          | 18    | 18  |         |
| 44  | H     | 6        | Total | O   | 0       |
|     |       |          | 6     | 6   |         |
| 44  | I     | 6        | Total | O   | 0       |
|     |       |          | 6     | 6   |         |
| 44  | J     | 16       | Total | O   | 0       |
|     |       |          | 16    | 16  |         |
| 44  | K     | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |

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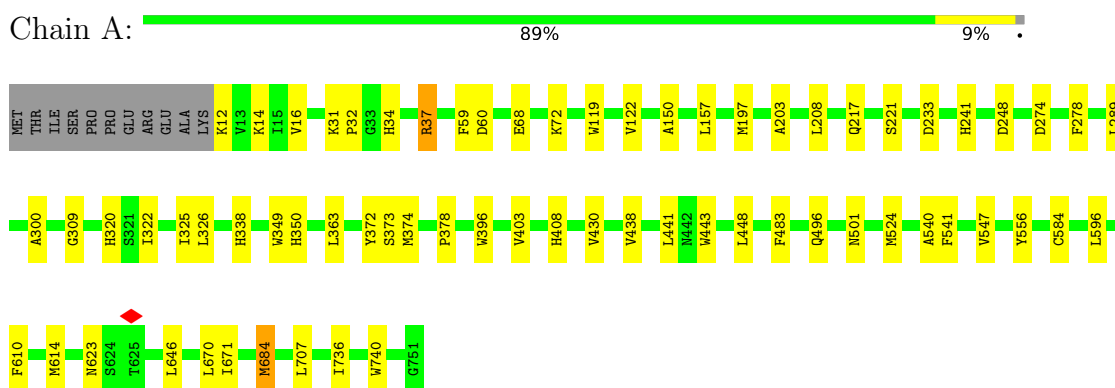
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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 44  | M     | 5        | Total<br>5  | O<br>5  | 0       |
| 44  | a     | 34       | Total<br>34 | O<br>34 | 0       |
| 44  | 3     | 32       | Total<br>32 | O<br>32 | 0       |
| 44  | 7     | 39       | Total<br>39 | O<br>39 | 0       |
| 44  | 8     | 37       | Total<br>37 | O<br>37 | 0       |
| 44  | 9     | 21       | Total<br>21 | O<br>21 | 0       |
| 44  | L     | 17       | Total<br>17 | O<br>17 | 0       |
| 44  | O     | 4        | Total<br>4  | O<br>4  | 0       |
| 44  | 2     | 3        | Total<br>3  | O<br>3  | 0       |
| 44  | 4     | 1        | Total<br>1  | O<br>1  | 0       |
| 44  | 5     | 11       | Total<br>11 | O<br>11 | 0       |
| 44  | 6     | 2        | Total<br>2  | O<br>2  | 0       |

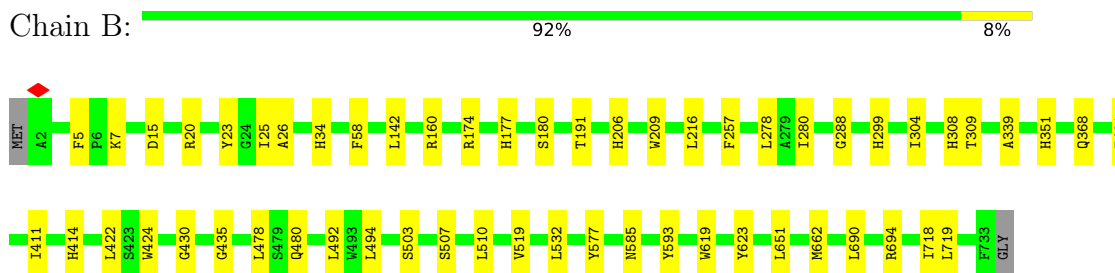
### 3 Residue-property plots

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

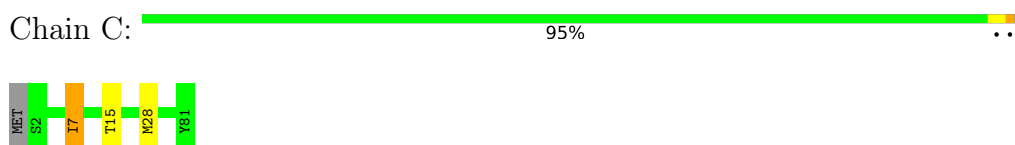
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

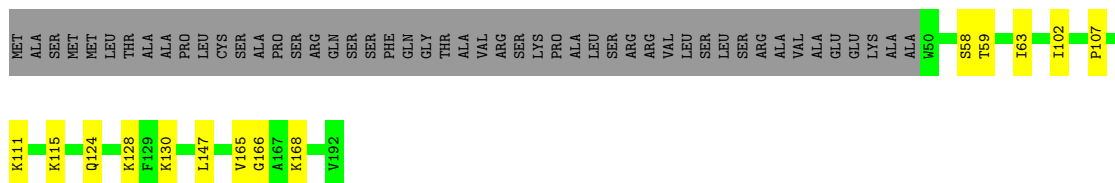


- Molecule 3: Photosystem I iron-sulfur center

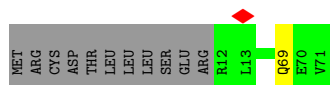
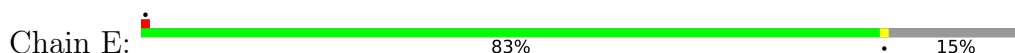


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

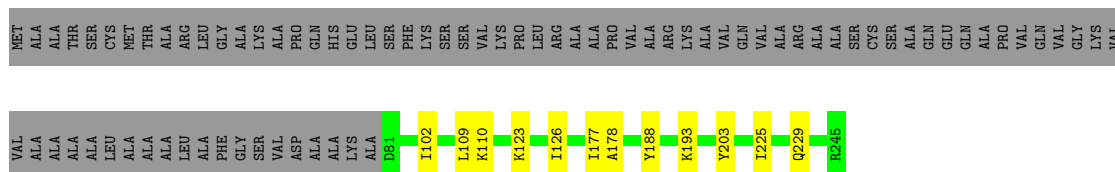




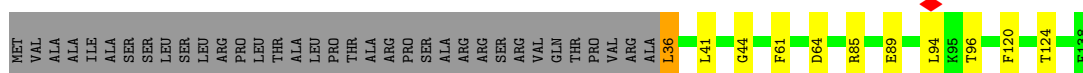
- Molecule 5: Photosystem I reaction centre subunit IV/PsaE



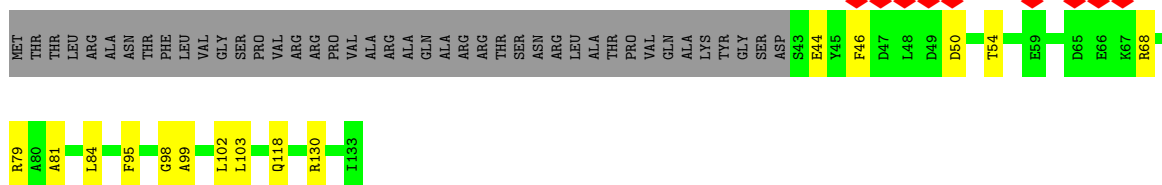
- Molecule 6: Photosystem I reaction center subunit III



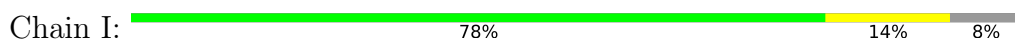
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic




- Molecule 8: Photosystem I reaction centre subunit VI



- Molecule 9: Photosystem I reaction center subunit VIII



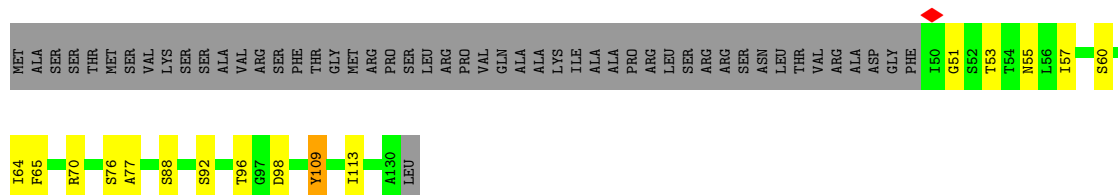
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  78% 17% 5%



- Molecule 11: PSI-K

Chain K:  50% 11% 38%




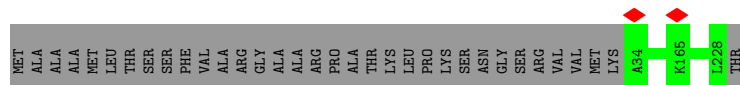
- Molecule 12: Photosystem I reaction center subunit XII

Chain M:  87% 13%



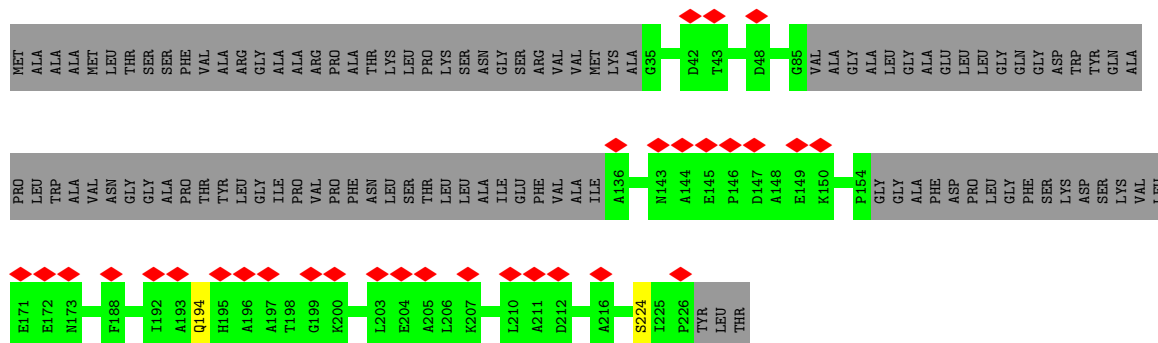
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain a:  85% 15%



- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

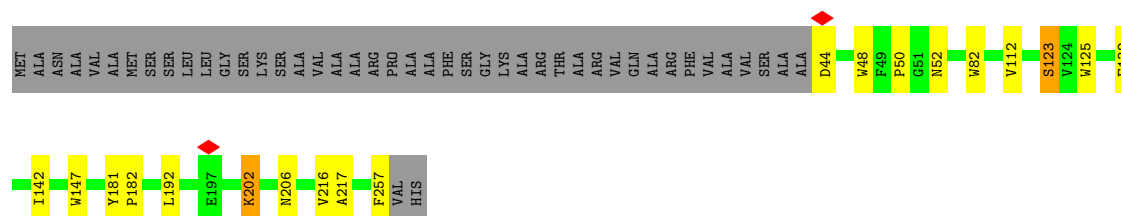
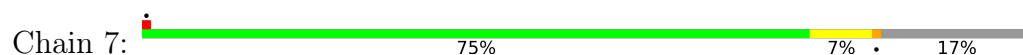
Chain b:  14% 54% 45%



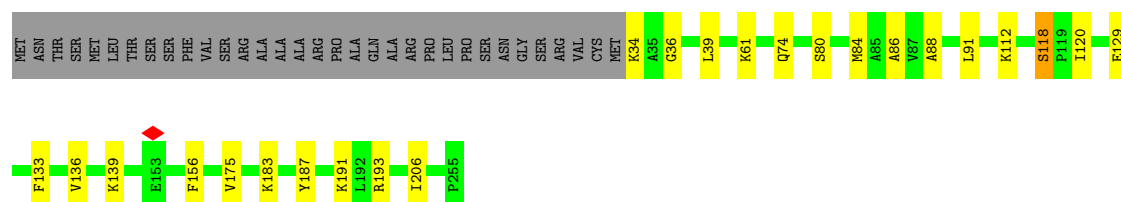
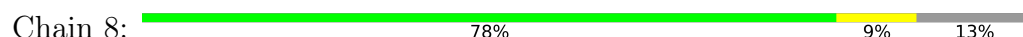
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 3:  72% 10% 17%

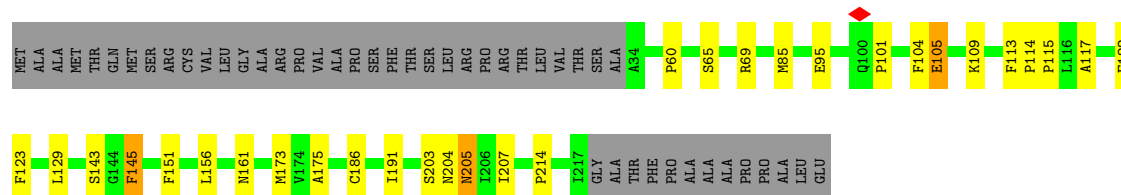
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



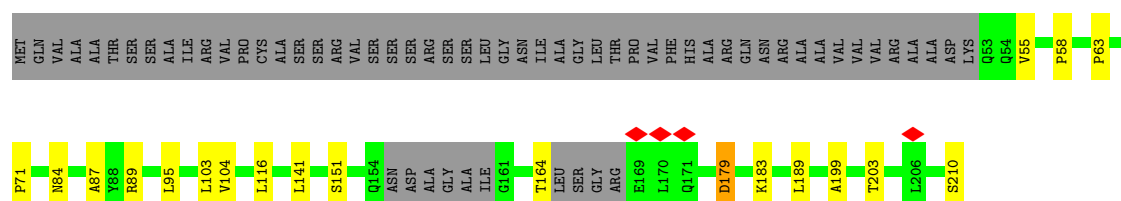
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



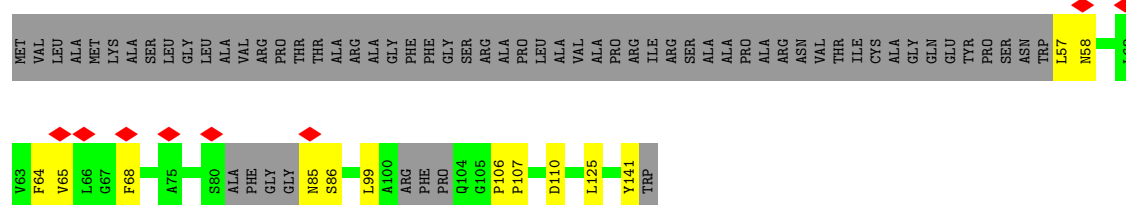
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



- Molecule 18: PSI subunit V



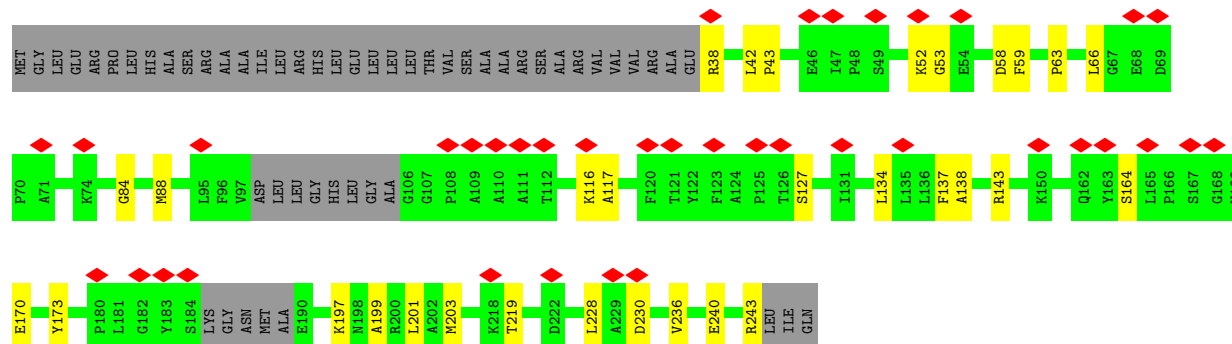
- Molecule 19: Photosystem I PsaO



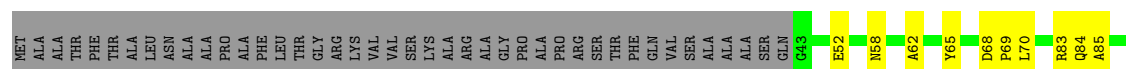
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic/Lhca2



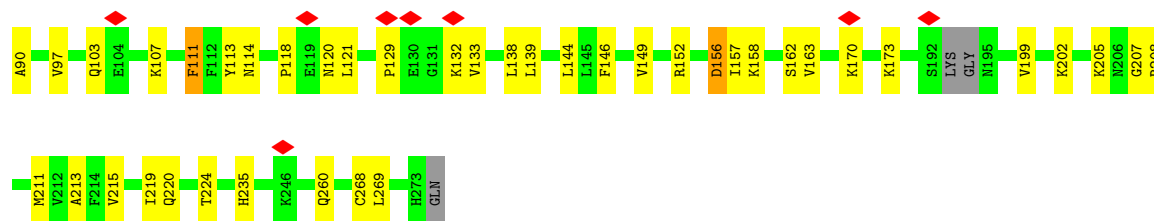
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



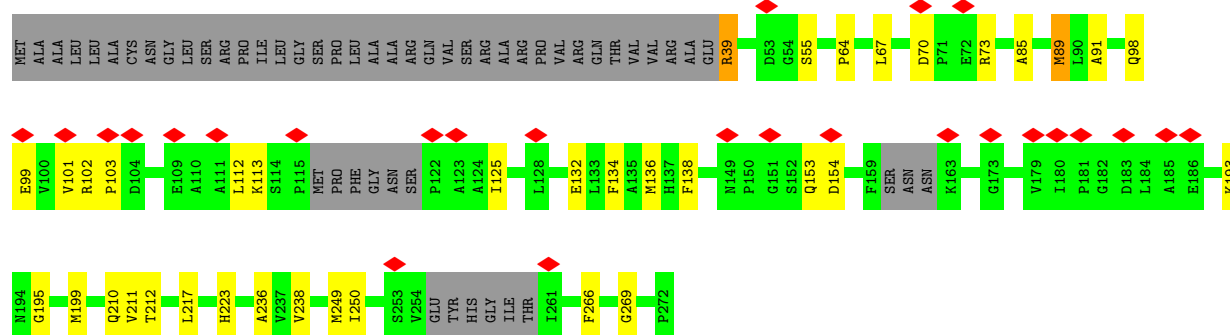
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic







- Molecule 23: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 224674                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 165000                                  | Depositor |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.393                                   | Depositor |
| Minimum map value                    | -0.655                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.018                                   | Depositor |
| Recommended contour level            | 0.085                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 436.2, 436.2, 436.2                     | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.727, 0.727, 0.727                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, CLA, AXT, PQN, BCR, UNL, DGA, QTB, DGD, LUT, CHL, XAT, PTY, LAP, LHG, LMT, 3PH, SF4, SQD, LMG

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     | 0.30         | 0/6012      | 0.50        | 1/8202 (0.0%)  |
| 2   | B     | 0.30         | 0/6017      | 0.51        | 0/8218         |
| 3   | C     | 0.30         | 0/606       | 0.64        | 0/822          |
| 4   | D     | 0.29         | 0/1136      | 0.53        | 0/1537         |
| 5   | E     | 0.31         | 0/502       | 0.57        | 0/686          |
| 6   | F     | 0.29         | 0/1288      | 0.51        | 0/1737         |
| 7   | G     | 0.27         | 0/783       | 0.50        | 0/1063         |
| 8   | H     | 0.29         | 0/722       | 0.56        | 0/972          |
| 9   | I     | 0.34         | 0/254       | 0.54        | 0/347          |
| 10  | J     | 0.29         | 0/330       | 0.47        | 0/452          |
| 11  | K     | 0.28         | 0/568       | 0.49        | 0/773          |
| 12  | M     | 0.29         | 0/240       | 0.41        | 0/325          |
| 13  | a     | 0.30         | 0/1501      | 0.51        | 0/2045         |
| 13  | b     | 0.25         | 0/977       | 0.46        | 0/1322         |
| 14  | 3     | 0.32         | 0/1629      | 0.50        | 0/2217         |
| 15  | 7     | 0.29         | 0/1684      | 0.47        | 0/2298         |
| 16  | 8     | 0.30         | 0/1752      | 0.46        | 0/2379         |
| 17  | 9     | 0.29         | 0/1451      | 0.50        | 0/1964         |
| 18  | L     | 0.29         | 0/1129      | 0.50        | 0/1542         |
| 19  | O     | 0.27         | 0/619       | 0.53        | 1/839 (0.1%)   |
| 20  | 2     | 0.29         | 0/1654      | 0.62        | 2/2254 (0.1%)  |
| 21  | 4     | 0.28         | 0/1553      | 0.47        | 0/2113         |
| 22  | 5     | 0.30         | 0/1820      | 0.54        | 2/2477 (0.1%)  |
| 23  | 6     | 0.28         | 0/1709      | 0.47        | 0/2328         |
| All | All   | 0.29         | 0/35936     | 0.51        | 6/48912 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 23  | 6     | 0                   | 1                   |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 20  | 2     | 66  | PRO  | CA-N-CD   | -8.31 | 99.87       | 111.50   |
| 22  | 5     | 129 | PRO  | N-CD-CG   | -7.27 | 92.30       | 103.20   |
| 20  | 2     | 65  | GLU  | C-N-CD    | 6.92  | 142.93      | 128.40   |
| 1   | A     | 233 | ASP  | CB-CG-OD1 | 5.66  | 123.39      | 118.30   |
| 22  | 5     | 156 | ASP  | CB-CG-OD1 | 5.35  | 123.11      | 118.30   |
| 19  | O     | 125 | LEU  | CA-CB-CG  | 5.11  | 127.05      | 115.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 23  | 6     | 39  | ARG  | Sidechain |

## 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     | 5814  | 0        | 5649     | 51      | 0            |
| 2   | B     | 5808  | 0        | 5584     | 38      | 0            |
| 3   | C     | 596   | 0        | 573      | 3       | 0            |
| 4   | D     | 1110  | 0        | 1131     | 9       | 0            |
| 5   | E     | 490   | 0        | 482      | 0       | 0            |
| 6   | F     | 1264  | 0        | 1300     | 9       | 0            |
| 7   | G     | 767   | 0        | 749      | 6       | 0            |
| 8   | H     | 706   | 0        | 687      | 12      | 0            |
| 9   | I     | 248   | 0        | 269      | 4       | 0            |
| 10  | J     | 319   | 0        | 326      | 7       | 0            |
| 11  | K     | 560   | 0        | 583      | 8       | 0            |
| 12  | M     | 237   | 0        | 260      | 2       | 0            |
| 13  | a     | 1458  | 0        | 1423     | 0       | 0            |
| 13  | b     | 952   | 0        | 917      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | 3     | 1580  | 0        | 1546     | 24      | 0            |
| 15  | 7     | 1633  | 0        | 1579     | 17      | 0            |
| 16  | 8     | 1701  | 0        | 1683     | 14      | 0            |
| 17  | 9     | 1414  | 0        | 1405     | 20      | 0            |
| 18  | L     | 1102  | 0        | 1129     | 15      | 0            |
| 19  | O     | 605   | 0        | 616      | 7       | 0            |
| 20  | 2     | 1606  | 0        | 1578     | 37      | 0            |
| 21  | 4     | 1506  | 0        | 1468     | 26      | 0            |
| 22  | 5     | 1766  | 0        | 1746     | 36      | 0            |
| 23  | 6     | 1658  | 0        | 1657     | 28      | 0            |
| 24  | A     | 33    | 0        | 46       | 1       | 0            |
| 24  | B     | 33    | 0        | 46       | 2       | 0            |
| 25  | A     | 8     | 0        | 0        | 0       | 0            |
| 25  | C     | 16    | 0        | 0        | 0       | 0            |
| 26  | 2     | 40    | 0        | 56       | 3       | 0            |
| 26  | 3     | 120   | 0        | 168      | 9       | 0            |
| 26  | 5     | 40    | 0        | 56       | 2       | 0            |
| 26  | 6     | 40    | 0        | 56       | 2       | 0            |
| 26  | 7     | 40    | 0        | 56       | 6       | 0            |
| 26  | 8     | 40    | 0        | 56       | 2       | 0            |
| 26  | A     | 160   | 0        | 224      | 12      | 0            |
| 26  | B     | 200   | 0        | 280      | 16      | 0            |
| 26  | F     | 40    | 0        | 56       | 2       | 0            |
| 26  | G     | 80    | 0        | 112      | 2       | 0            |
| 26  | I     | 40    | 0        | 56       | 1       | 0            |
| 26  | J     | 40    | 0        | 56       | 1       | 0            |
| 26  | K     | 80    | 0        | 112      | 8       | 0            |
| 26  | L     | 120   | 0        | 168      | 6       | 0            |
| 26  | M     | 40    | 0        | 56       | 3       | 0            |
| 26  | O     | 40    | 0        | 56       | 2       | 0            |
| 27  | 5     | 35    | 0        | 44       | 2       | 0            |
| 27  | 9     | 35    | 0        | 44       | 0       | 0            |
| 27  | A     | 70    | 0        | 89       | 4       | 0            |
| 28  | 5     | 35    | 0        | 40       | 2       | 0            |
| 28  | 6     | 59    | 0        | 58       | 4       | 0            |
| 28  | 7     | 86    | 0        | 118      | 10      | 0            |
| 28  | 8     | 49    | 0        | 74       | 0       | 0            |
| 28  | A     | 133   | 0        | 188      | 8       | 0            |
| 28  | B     | 32    | 0        | 34       | 0       | 0            |
| 28  | a     | 49    | 0        | 74       | 0       | 0            |
| 29  | 2     | 11    | 0        | 0        | 0       | 0            |
| 29  | 3     | 11    | 0        | 0        | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | 4     | 13    | 0        | 0        | 1       | 0            |
| 29  | 7     | 8     | 0        | 0        | 0       | 0            |
| 29  | 8     | 18    | 0        | 0        | 0       | 0            |
| 29  | 9     | 81    | 0        | 0        | 0       | 0            |
| 29  | A     | 20    | 0        | 0        | 0       | 0            |
| 29  | B     | 24    | 0        | 0        | 0       | 0            |
| 29  | a     | 27    | 0        | 0        | 0       | 0            |
| 30  | A     | 65    | 0        | 72       | 3       | 0            |
| 31  | 2     | 574   | 0        | 442      | 19      | 0            |
| 31  | 3     | 736   | 0        | 697      | 19      | 0            |
| 31  | 4     | 685   | 0        | 550      | 27      | 0            |
| 31  | 5     | 678   | 0        | 588      | 26      | 0            |
| 31  | 6     | 545   | 0        | 436      | 16      | 0            |
| 31  | 7     | 523   | 0        | 445      | 15      | 0            |
| 31  | 8     | 692   | 0        | 606      | 25      | 0            |
| 31  | 9     | 524   | 0        | 452      | 7       | 0            |
| 31  | A     | 2450  | 0        | 2472     | 113     | 0            |
| 31  | B     | 2382  | 0        | 2381     | 76      | 0            |
| 31  | F     | 161   | 0        | 144      | 5       | 0            |
| 31  | G     | 141   | 0        | 105      | 6       | 0            |
| 31  | H     | 138   | 0        | 99       | 11      | 0            |
| 31  | J     | 42    | 0        | 31       | 1       | 0            |
| 31  | K     | 142   | 0        | 105      | 1       | 0            |
| 31  | L     | 150   | 0        | 125      | 7       | 0            |
| 31  | O     | 134   | 0        | 98       | 0       | 0            |
| 31  | a     | 601   | 0        | 547      | 0       | 0            |
| 31  | b     | 520   | 0        | 389      | 0       | 0            |
| 32  | 3     | 56    | 0        | 46       | 2       | 0            |
| 32  | 4     | 141   | 0        | 92       | 17      | 0            |
| 32  | 5     | 197   | 0        | 136      | 14      | 0            |
| 32  | 6     | 296   | 0        | 217      | 19      | 0            |
| 32  | 7     | 297   | 0        | 272      | 31      | 0            |
| 32  | 8     | 111   | 0        | 99       | 10      | 0            |
| 32  | 9     | 95    | 0        | 62       | 6       | 0            |
| 32  | A     | 180   | 0        | 165      | 10      | 0            |
| 32  | K     | 47    | 0        | 31       | 2       | 0            |
| 32  | a     | 157   | 0        | 120      | 0       | 0            |
| 32  | b     | 47    | 0        | 30       | 0       | 0            |
| 33  | 7     | 52    | 0        | 65       | 1       | 0            |
| 33  | B     | 61    | 0        | 83       | 4       | 0            |
| 34  | B     | 29    | 0        | 42       | 4       | 0            |
| 35  | 7     | 19    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | 9     | 19    | 0        | 0        | 0       | 0            |
| 35  | F     | 19    | 0        | 0        | 0       | 0            |
| 35  | a     | 19    | 0        | 0        | 0       | 0            |
| 36  | 2     | 42    | 0        | 56       | 4       | 0            |
| 36  | 3     | 84    | 0        | 111      | 10      | 0            |
| 36  | 4     | 84    | 0        | 111      | 12      | 0            |
| 36  | 5     | 84    | 0        | 111      | 9       | 0            |
| 36  | 6     | 84    | 0        | 111      | 5       | 0            |
| 36  | 7     | 42    | 0        | 56       | 3       | 0            |
| 36  | 8     | 84    | 0        | 112      | 7       | 0            |
| 36  | 9     | 126   | 0        | 165      | 9       | 0            |
| 36  | F     | 42    | 0        | 55       | 2       | 0            |
| 36  | J     | 42    | 0        | 54       | 3       | 0            |
| 36  | L     | 42    | 0        | 55       | 1       | 0            |
| 36  | a     | 84    | 0        | 109      | 0       | 0            |
| 36  | b     | 42    | 0        | 56       | 0       | 0            |
| 37  | G     | 44    | 0        | 58       | 4       | 0            |
| 37  | J     | 78    | 0        | 99       | 4       | 0            |
| 37  | a     | 42    | 0        | 54       | 0       | 0            |
| 38  | a     | 43    | 0        | 52       | 0       | 0            |
| 39  | 7     | 33    | 0        | 39       | 1       | 0            |
| 40  | 7     | 44    | 0        | 56       | 0       | 0            |
| 41  | 8     | 28    | 0        | 38       | 2       | 0            |
| 42  | 4     | 35    | 0        | 34       | 1       | 0            |
| 43  | 5     | 31    | 0        | 35       | 1       | 0            |
| 44  | 2     | 3     | 0        | 0        | 0       | 0            |
| 44  | 3     | 32    | 0        | 0        | 0       | 0            |
| 44  | 4     | 1     | 0        | 0        | 0       | 0            |
| 44  | 5     | 11    | 0        | 0        | 0       | 0            |
| 44  | 6     | 2     | 0        | 0        | 0       | 0            |
| 44  | 7     | 39    | 0        | 0        | 0       | 0            |
| 44  | 8     | 37    | 0        | 0        | 0       | 0            |
| 44  | 9     | 21    | 0        | 0        | 0       | 0            |
| 44  | A     | 297   | 0        | 0        | 1       | 0            |
| 44  | B     | 311   | 0        | 0        | 2       | 0            |
| 44  | C     | 60    | 0        | 0        | 0       | 0            |
| 44  | D     | 53    | 0        | 0        | 0       | 0            |
| 44  | E     | 28    | 0        | 0        | 0       | 0            |
| 44  | F     | 57    | 0        | 0        | 0       | 0            |
| 44  | G     | 18    | 0        | 0        | 0       | 0            |
| 44  | H     | 6     | 0        | 0        | 1       | 0            |
| 44  | I     | 6     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | J     | 16    | 0        | 0        | 0       | 0            |
| 44  | K     | 2     | 0        | 0        | 0       | 0            |
| 44  | L     | 17    | 0        | 0        | 0       | 0            |
| 44  | M     | 5     | 0        | 0        | 1       | 0            |
| 44  | O     | 4     | 0        | 0        | 0       | 0            |
| 44  | a     | 34    | 0        | 0        | 0       | 0            |
| All | All   | 52991 | 0        | 50690    | 709     | 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 8.

All (709) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:H:902:CLA:HAA1 | 20:2:153:LEU:HD23 | 1.31                     | 1.06              |
| 14:3:241:PHE:CD2  | 29:3:306:UNL:C2   | 2.39                     | 1.05              |
| 31:A:829:CLA:HBA2 | 28:7:302:LHG:H242 | 1.39                     | 1.02              |
| 31:H:902:CLA:O1A  | 20:2:153:LEU:HD21 | 1.61                     | 0.99              |
| 20:2:243:ALA:O    | 20:2:247:ILE:HG13 | 1.64                     | 0.96              |
| 14:3:241:PHE:CE2  | 29:3:306:UNL:C2   | 2.56                     | 0.88              |
| 26:2:302:BCR:H12C | 31:2:304:CLA:HAB  | 1.58                     | 0.86              |
| 1:A:241:HIS:NE2   | 31:A:829:CLA:HMD3 | 1.92                     | 0.84              |
| 31:A:825:CLA:H2   | 14:3:49:LEU:HD13  | 1.60                     | 0.83              |
| 31:A:827:CLA:H62  | 31:A:829:CLA:HMB2 | 1.61                     | 0.82              |
| 31:H:902:CLA:O1A  | 20:2:153:LEU:CD2  | 2.28                     | 0.80              |
| 14:3:241:PHE:HD2  | 29:3:306:UNL:C2   | 1.93                     | 0.77              |
| 31:H:902:CLA:CAA  | 20:2:153:LEU:HD23 | 2.14                     | 0.75              |
| 31:2:312:CLA:HBB1 | 31:2:314:CLA:HBB1 | 1.70                     | 0.74              |
| 31:B:829:CLA:HMD2 | 26:G:201:BCR:HC7  | 1.71                     | 0.72              |
| 1:A:350:HIS:HD2   | 1:A:408:HIS:HD1   | 1.36                     | 0.72              |
| 26:M:101:BCR:H23C | 31:2:315:CLA:HBB1 | 1.71                     | 0.72              |
| 31:5:318:CLA:MG   | 31:5:318:CLA:ND   | 1.48                     | 0.71              |
| 12:M:24:ARG:NH1   | 44:M:201:HOH:O    | 2.22                     | 0.71              |
| 32:8:316:CHL:H92  | 32:8:316:CHL:H41  | 1.73                     | 0.70              |
| 32:5:316:CHL:HAB  | 32:5:319:CHL:HBB2 | 1.74                     | 0.70              |
| 31:B:834:CLA:HBB2 | 31:B:850:CLA:HBA2 | 1.74                     | 0.69              |
| 36:6:303:LUT:H32  | 31:6:307:CLA:HMC2 | 1.74                     | 0.69              |
| 14:3:49:LEU:HD12  | 36:3:305:LUT:H222 | 1.72                     | 0.69              |
| 2:B:209:TRP:HB3   | 34:B:851:LAP:H202 | 1.75                     | 0.68              |
| 31:A:835:CLA:HMD2 | 26:K:202:BCR:H24C | 1.76                     | 0.68              |
| 1:A:31:LYS:NZ     | 44:A:903:HOH:O    | 2.28                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:2:104:ARG:HH22 | 31:2:304:CLA:HED2 | 1.59                     | 0.67              |
| 31:A:837:CLA:H201 | 31:A:837:CLA:HAB  | 1.77                     | 0.66              |
| 20:2:66:PRO:HD2   | 20:2:66:PRO:O     | 1.96                     | 0.66              |
| 23:6:210:GLN:HE22 | 23:6:266:PHE:H    | 1.41                     | 0.66              |
| 16:8:84:MET:HB3   | 31:8:308:CLA:HMC3 | 1.78                     | 0.65              |
| 33:7:308:DGD:HGB3 | 32:7:319:CHL:HMB2 | 1.78                     | 0.65              |
| 1:A:483:PHE:HB3   | 31:A:850:CLA:H2   | 1.78                     | 0.65              |
| 31:A:829:CLA:CBA  | 28:7:302:LHG:H242 | 2.22                     | 0.65              |
| 16:8:193:ARG:HG3  | 31:8:313:CLA:HED2 | 1.80                     | 0.64              |
| 20:2:149:ALA:O    | 20:2:153:LEU:HG   | 1.98                     | 0.64              |
| 31:A:823:CLA:HMD2 | 31:3:311:CLA:H102 | 1.80                     | 0.64              |
| 32:5:317:CHL:HAB  | 32:5:322:CHL:CMC  | 2.28                     | 0.64              |
| 2:B:15:ASP:HB3    | 2:B:20:ARG:HB2    | 1.81                     | 0.63              |
| 36:3:305:LUT:H393 | 31:3:319:CLA:H151 | 1.81                     | 0.63              |
| 14:3:75:ALA:HB1   | 14:3:200:GLY:HA3  | 1.81                     | 0.62              |
| 1:A:16:VAL:HG12   | 14:3:56:GLY:HA3   | 1.81                     | 0.62              |
| 31:A:832:CLA:H141 | 32:A:840:CHL:H202 | 1.81                     | 0.62              |
| 21:4:143:ARG:HE   | 31:4:315:CLA:HMC3 | 1.64                     | 0.62              |
| 32:7:320:CHL:HBB1 | 32:7:320:CHL:HMB1 | 1.80                     | 0.62              |
| 31:H:901:CLA:HMB2 | 31:H:903:CLA:HAA2 | 1.82                     | 0.62              |
| 21:4:88:MET:CE    | 31:4:305:CLA:HHC  | 2.29                     | 0.62              |
| 22:5:208:ARG:HH22 | 31:5:310:CLA:HED3 | 1.65                     | 0.61              |
| 1:A:350:HIS:CD2   | 1:A:408:HIS:HD1   | 2.18                     | 0.61              |
| 32:4:310:CHL:HAA1 | 32:4:317:CHL:HHD  | 1.83                     | 0.61              |
| 1:A:32:PRO:HB3    | 31:A:816:CLA:HAC1 | 1.82                     | 0.61              |
| 31:A:851:CLA:H191 | 31:L:305:CLA:H93  | 1.81                     | 0.61              |
| 31:A:816:CLA:HHC  | 31:A:816:CLA:HBB1 | 1.82                     | 0.61              |
| 26:A:803:BCR:H21C | 27:A:807:LMT:H123 | 1.83                     | 0.61              |
| 14:3:195:LYS:NZ   | 31:3:308:CLA:O1D  | 2.33                     | 0.61              |
| 1:A:241:HIS:CD2   | 31:A:829:CLA:HMD3 | 2.35                     | 0.60              |
| 20:2:242:ILE:O    | 20:2:246:THR:HG23 | 2.01                     | 0.60              |
| 41:8:305:DGA:HG11 | 31:8:321:CLA:HED2 | 1.83                     | 0.60              |
| 32:A:839:CHL:HMA2 | 32:A:840:CHL:O1D  | 2.01                     | 0.60              |
| 14:3:161:LEU:HD22 | 26:3:302:BCR:HC32 | 1.83                     | 0.60              |
| 31:B:831:CLA:HAB  | 31:B:838:CLA:HMD2 | 1.83                     | 0.60              |
| 31:B:843:CLA:HED3 | 31:G:206:CLA:HMA3 | 1.84                     | 0.60              |
| 7:G:124:THR:HG22  | 31:G:206:CLA:HED2 | 1.84                     | 0.60              |
| 36:4:302:LUT:H392 | 31:4:305:CLA:HBC3 | 1.83                     | 0.60              |
| 32:7:318:CHL:HMC  | 32:7:318:CHL:HBC2 | 1.84                     | 0.60              |
| 20:2:145:HIS:HD2  | 31:2:314:CLA:HBB2 | 1.66                     | 0.59              |
| 1:A:197:MET:HB2   | 31:A:826:CLA:HBC2 | 1.82                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:A:806:BCR:H23C | 31:A:815:CLA:H111 | 1.84                     | 0.59              |
| 31:A:830:CLA:CHD  | 32:A:831:CHL:HBB2 | 2.32                     | 0.59              |
| 31:3:309:CLA:H192 | 15:7:52:ASN:HD22  | 1.66                     | 0.59              |
| 31:A:825:CLA:H51  | 31:3:319:CLA:H8   | 1.84                     | 0.59              |
| 31:7:315:CLA:HMB2 | 27:5:301:LMT:H21  | 1.84                     | 0.59              |
| 16:8:112:LYS:HB2  | 32:8:316:CHL:HED2 | 1.83                     | 0.59              |
| 31:4:311:CLA:NB   | 28:6:301:LHG:O4   | 2.35                     | 0.59              |
| 33:B:808:DGD:HA91 | 31:B:813:CLA:HBC1 | 1.84                     | 0.58              |
| 23:6:85:ALA:HB1   | 23:6:195:GLY:HA3  | 1.84                     | 0.58              |
| 31:A:833:CLA:C2   | 14:3:48:PRO:HB2   | 2.33                     | 0.58              |
| 26:7:304:BCR:H21C | 32:7:320:CHL:C2   | 2.33                     | 0.58              |
| 31:B:825:CLA:H12  | 31:G:206:CLA:HED1 | 1.83                     | 0.58              |
| 15:7:181:TYR:HB3  | 31:7:309:CLA:HED3 | 1.84                     | 0.58              |
| 23:6:210:GLN:HA   | 23:6:250:ILE:HD12 | 1.85                     | 0.58              |
| 14:3:137:GLN:NE2  | 31:3:309:CLA:O1D  | 2.37                     | 0.58              |
| 17:9:101:PRO:HG2  | 17:9:109:LYS:HD2  | 1.86                     | 0.58              |
| 31:2:306:CLA:H101 | 31:2:306:CLA:HAB  | 1.84                     | 0.58              |
| 26:B:804:BCR:HC31 | 37:G:202:LMG:H391 | 1.85                     | 0.58              |
| 32:9:320:CHL:C1C  | 32:9:322:CHL:HMC  | 2.34                     | 0.58              |
| 2:B:216:LEU:HD11  | 17:9:214:PRO:HA   | 1.86                     | 0.57              |
| 36:9:303:LUT:H393 | 31:9:314:CLA:H121 | 1.87                     | 0.57              |
| 1:A:217:GLN:HA    | 1:A:221:SER:HB2   | 1.86                     | 0.57              |
| 31:H:903:CLA:HAC1 | 18:L:84:ASN:HB3   | 1.87                     | 0.57              |
| 32:7:324:CHL:HMA3 | 16:8:39:LEU:HD13  | 1.85                     | 0.57              |
| 22:5:146:PHE:HA   | 22:5:149:VAL:HG22 | 1.87                     | 0.57              |
| 15:7:257:PHE:HE1  | 31:7:322:CLA:HAB  | 1.69                     | 0.57              |
| 21:4:138:ALA:HA   | 31:4:316:CLA:HBB1 | 1.84                     | 0.57              |
| 26:A:804:BCR:HC8  | 31:A:818:CLA:H72  | 1.85                     | 0.57              |
| 26:3:302:BCR:HC7  | 32:3:315:CHL:HMB2 | 1.87                     | 0.57              |
| 26:5:302:BCR:H372 | 32:5:316:CHL:HBB1 | 1.86                     | 0.57              |
| 31:B:820:CLA:HBB2 | 31:B:822:CLA:HMA3 | 1.85                     | 0.57              |
| 31:A:823:CLA:H12  | 31:A:825:CLA:H43  | 1.85                     | 0.57              |
| 20:2:82:PRO:HD2   | 36:2:301:LUT:H3   | 1.85                     | 0.57              |
| 32:4:310:CHL:HAA1 | 32:4:317:CHL:CHD  | 2.35                     | 0.57              |
| 27:A:807:LMT:O3'  | 31:A:828:CLA:O1D  | 2.22                     | 0.57              |
| 36:4:303:LUT:H193 | 31:4:314:CLA:HBA2 | 1.86                     | 0.57              |
| 36:5:304:LUT:H363 | 31:5:315:CLA:H43  | 1.86                     | 0.57              |
| 11:K:77:ALA:O     | 11:K:92:SER:OG    | 2.22                     | 0.56              |
| 22:5:65:TYR:HB2   | 31:5:310:CLA:HMD1 | 1.87                     | 0.56              |
| 31:6:306:CLA:HMB2 | 31:6:322:CLA:C2D  | 2.35                     | 0.56              |
| 31:A:853:CLA:H111 | 31:A:853:CLA:HAB  | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:5:317:CHL:OMC  | 32:5:322:CHL:HMC  | 2.06                     | 0.56              |
| 10:J:24:GLY:HA3   | 31:J:105:CLA:HAB  | 1.88                     | 0.56              |
| 19:O:65:VAL:HA    | 19:O:68:PHE:HB2   | 1.87                     | 0.56              |
| 31:H:902:CLA:HAA1 | 20:2:153:LEU:CD2  | 2.21                     | 0.56              |
| 22:5:90:ALA:HB1   | 22:5:207:GLY:HA3  | 1.88                     | 0.56              |
| 1:A:540:ALA:HB1   | 31:A:851:CLA:HMB3 | 1.87                     | 0.56              |
| 31:3:309:CLA:HBA2 | 32:7:317:CHL:H102 | 1.88                     | 0.56              |
| 22:5:114:ASN:O    | 22:5:120:ASN:ND2  | 2.39                     | 0.55              |
| 14:3:241:PHE:CD2  | 29:3:306:UNL:C3   | 2.89                     | 0.55              |
| 31:3:309:CLA:H111 | 15:7:48:TRP:HH2   | 1.71                     | 0.55              |
| 15:7:192:LEU:HD21 | 23:6:67:LEU:HD23  | 1.88                     | 0.55              |
| 21:4:59:PHE:CD2   | 32:4:313:CHL:HMC  | 2.41                     | 0.55              |
| 26:A:805:BCR:H291 | 31:A:849:CLA:HMB1 | 1.88                     | 0.55              |
| 20:2:65:GLU:HB3   | 20:2:255:LYS:HE2  | 1.89                     | 0.55              |
| 31:4:312:CLA:HED2 | 23:6:134:PHE:HE2  | 1.70                     | 0.55              |
| 23:6:102:ARG:NH1  | 31:6:314:CLA:OBD  | 2.38                     | 0.55              |
| 22:5:69:PRO:HD2   | 36:5:304:LUT:H23  | 1.87                     | 0.55              |
| 31:B:820:CLA:HMD2 | 31:9:315:CLA:H42  | 1.88                     | 0.55              |
| 32:7:319:CHL:HMB1 | 32:7:319:CHL:HBB1 | 1.87                     | 0.55              |
| 31:B:819:CLA:H171 | 8:H:98:GLY:HA3    | 1.88                     | 0.55              |
| 15:7:142:ILE:HG21 | 31:8:314:CLA:HMC3 | 1.89                     | 0.55              |
| 17:9:95:GLU:HB3   | 17:9:191:ILE:HD12 | 1.88                     | 0.55              |
| 1:A:59:PHE:CD2    | 31:A:818:CLA:HMC2 | 2.42                     | 0.54              |
| 28:A:811:LHG:H161 | 31:A:855:CLA:HBA2 | 1.88                     | 0.54              |
| 36:7:305:LUT:H181 | 31:7:311:CLA:HBB1 | 1.89                     | 0.54              |
| 21:4:84:GLY:HA3   | 21:4:199:ALA:HB1  | 1.89                     | 0.54              |
| 32:5:319:CHL:HED1 | 31:5:320:CLA:CGA  | 2.36                     | 0.54              |
| 23:6:91:ALA:HB2   | 36:6:304:LUT:H192 | 1.90                     | 0.54              |
| 31:A:845:CLA:HMB1 | 31:A:857:CLA:HAA2 | 1.88                     | 0.54              |
| 17:9:173:MET:HB3  | 36:9:303:LUT:H402 | 1.89                     | 0.54              |
| 1:A:119:TRP:HB3   | 36:J:103:LUT:H42  | 1.89                     | 0.54              |
| 31:A:814:CLA:HHB  | 31:B:811:CLA:H202 | 1.90                     | 0.54              |
| 2:B:424:TRP:HZ3   | 31:B:845:CLA:HBC2 | 1.71                     | 0.54              |
| 17:9:105:GLU:HA   | 32:9:320:CHL:HED1 | 1.90                     | 0.54              |
| 36:5:304:LUT:H382 | 31:5:310:CLA:H2   | 1.90                     | 0.54              |
| 28:A:811:LHG:H223 | 31:A:819:CLA:HED3 | 1.88                     | 0.54              |
| 31:A:841:CLA:H201 | 26:J:102:BCR:H15C | 1.89                     | 0.54              |
| 31:F:301:CLA:HMC2 | 26:F:302:BCR:H381 | 1.90                     | 0.54              |
| 32:4:310:CHL:HMA2 | 32:4:317:CHL:HAC2 | 1.90                     | 0.54              |
| 2:B:507:SER:HA    | 2:B:510:LEU:HD21  | 1.90                     | 0.54              |
| 7:G:44:GLY:HA3    | 31:G:204:CLA:H2   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:A:845:CLA:H8   | 31:L:305:CLA:H91  | 1.90                     | 0.53              |
| 31:7:311:CLA:H52  | 32:7:317:CHL:H92  | 1.89                     | 0.53              |
| 22:5:118:PRO:HA   | 22:5:121:LEU:HD12 | 1.89                     | 0.53              |
| 32:6:318:CHL:C4C  | 32:6:320:CHL:HMC  | 2.38                     | 0.53              |
| 1:A:363:LEU:HD11  | 31:A:832:CLA:H51  | 1.90                     | 0.53              |
| 31:B:844:CLA:H93  | 31:B:845:CLA:HBC1 | 1.91                     | 0.53              |
| 32:8:316:CHL:H41  | 32:8:316:CHL:C9   | 2.38                     | 0.53              |
| 6:F:102:ILE:HD12  | 6:F:126:ILE:HG23  | 1.89                     | 0.53              |
| 12:M:10:ILE:HD11  | 20:2:235:THR:OG1  | 2.09                     | 0.53              |
| 15:7:82:TRP:CE2   | 32:7:319:CHL:HED3 | 2.44                     | 0.53              |
| 32:7:324:CHL:HBB1 | 32:7:324:CHL:HMB1 | 1.89                     | 0.53              |
| 22:5:260:GLN:HG3  | 26:5:302:BCR:H311 | 1.91                     | 0.53              |
| 32:4:317:CHL:HMB1 | 32:4:317:CHL:HBB1 | 1.91                     | 0.52              |
| 17:9:117:ALA:HB1  | 31:2:311:CLA:HED1 | 1.92                     | 0.52              |
| 4:D:124:GLN:HG3   | 4:D:128:LYS:HE3   | 1.91                     | 0.52              |
| 26:3:301:BCR:HC42 | 32:7:317:CHL:HMD2 | 1.91                     | 0.52              |
| 28:A:811:LHG:H332 | 31:A:819:CLA:H72  | 1.91                     | 0.52              |
| 2:B:26:ALA:HA     | 31:B:837:CLA:H42  | 1.90                     | 0.52              |
| 26:A:803:BCR:H392 | 26:K:202:BCR:HC8  | 1.92                     | 0.52              |
| 31:B:828:CLA:HMB2 | 31:B:832:CLA:HMA3 | 1.91                     | 0.52              |
| 4:D:63:ILE:HB     | 4:D:102:ILE:HB    | 1.92                     | 0.52              |
| 36:8:302:LUT:H31  | 31:8:308:CLA:H112 | 1.91                     | 0.52              |
| 36:5:304:LUT:H193 | 32:5:316:CHL:HAB  | 1.92                     | 0.52              |
| 15:7:123:SER:HB2  | 32:7:318:CHL:HED2 | 1.92                     | 0.52              |
| 32:5:316:CHL:H8   | 32:6:309:CHL:CED  | 2.40                     | 0.52              |
| 21:4:63:PRO:HD2   | 36:4:303:LUT:H23  | 1.91                     | 0.52              |
| 31:B:820:CLA:H201 | 31:B:823:CLA:H92  | 1.91                     | 0.51              |
| 19:O:85:ASN:OD1   | 19:O:85:ASN:N     | 2.42                     | 0.51              |
| 28:6:305:LHG:HC82 | 28:6:305:LHG:H262 | 1.91                     | 0.51              |
| 36:4:302:LUT:C32  | 31:4:305:CLA:HMC2 | 2.40                     | 0.51              |
| 32:4:310:CHL:HBC2 | 32:4:310:CHL:HHD  | 1.91                     | 0.51              |
| 10:J:16:LEU:HD13  | 36:J:103:LUT:H30  | 1.92                     | 0.51              |
| 17:9:145:PHE:H    | 17:9:151:PHE:HB2  | 1.76                     | 0.51              |
| 1:A:740:TRP:NE1   | 31:A:841:CLA:O1A  | 2.38                     | 0.51              |
| 1:A:241:HIS:CE1   | 31:A:829:CLA:C2D  | 2.94                     | 0.51              |
| 31:7:313:CLA:HMC3 | 32:7:318:CHL:H13  | 1.92                     | 0.51              |
| 36:8:302:LUT:H32  | 31:8:308:CLA:HMC2 | 1.91                     | 0.51              |
| 36:8:302:LUT:H27  | 31:8:317:CLA:H42  | 1.93                     | 0.51              |
| 1:A:322:ILE:HG21  | 31:A:838:CLA:HAC1 | 1.93                     | 0.51              |
| 31:A:846:CLA:H102 | 31:B:846:CLA:H51  | 1.92                     | 0.51              |
| 31:B:831:CLA:HBB2 | 31:B:848:CLA:H52  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:7:317:CHL:O1D  | 32:7:317:CHL:HAA1 | 2.11                     | 0.51              |
| 3:C:7:ILE:O       | 4:D:168:LYS:N     | 2.42                     | 0.51              |
| 22:5:97:VAL:HG11  | 36:5:303:LUT:H10  | 1.93                     | 0.51              |
| 31:3:309:CLA:HED3 | 32:7:317:CHL:HMB2 | 1.93                     | 0.51              |
| 21:4:138:ALA:CA   | 31:4:316:CLA:HBB1 | 2.41                     | 0.51              |
| 31:4:307:CLA:H71  | 31:4:307:CLA:HMC2 | 1.92                     | 0.51              |
| 22:5:156:ASP:HB2  | 32:5:317:CHL:HAC1 | 1.93                     | 0.51              |
| 31:A:845:CLA:H2   | 31:L:305:CLA:H43  | 1.92                     | 0.50              |
| 2:B:351:HIS:ND1   | 31:B:850:CLA:OBD  | 2.43                     | 0.50              |
| 31:5:323:CLA:HED2 | 32:6:317:CHL:H3A  | 1.92                     | 0.50              |
| 23:6:249:MET:SD   | 23:6:249:MET:N    | 2.84                     | 0.50              |
| 31:A:856:CLA:HBB1 | 31:A:856:CLA:HMB1 | 1.93                     | 0.50              |
| 8:H:84:LEU:HD13   | 18:L:189:LEU:HD23 | 1.93                     | 0.50              |
| 18:L:71:PRO:HB3   | 19:O:57:LEU:HG    | 1.92                     | 0.50              |
| 23:6:211:VAL:HG23 | 23:6:212:THR:HG23 | 1.93                     | 0.50              |
| 31:A:836:CLA:HAB  | 31:A:854:CLA:HAB  | 1.93                     | 0.50              |
| 4:D:59:THR:HG23   | 4:D:107:PRO:HB2   | 1.92                     | 0.50              |
| 21:4:137:PHE:CZ   | 32:4:317:CHL:HMB3 | 2.47                     | 0.50              |
| 31:A:827:CLA:C6   | 31:A:829:CLA:HMB2 | 2.39                     | 0.50              |
| 8:H:103:LEU:HD22  | 9:I:9:VAL:HG13    | 1.93                     | 0.50              |
| 1:A:501:ASN:HB2   | 31:A:849:CLA:HED2 | 1.93                     | 0.50              |
| 31:A:838:CLA:HMD2 | 31:A:838:CLA:H143 | 1.93                     | 0.50              |
| 31:A:857:CLA:H13  | 18:L:141:LEU:HD21 | 1.94                     | 0.50              |
| 14:3:52:LEU:HB2   | 31:3:319:CLA:HBA2 | 1.92                     | 0.50              |
| 28:7:307:LHG:H321 | 31:7:311:CLA:H91  | 1.94                     | 0.50              |
| 31:7:313:CLA:HAC1 | 32:7:318:CHL:HBB2 | 1.93                     | 0.50              |
| 20:2:218:ASP:HB3  | 20:2:226:ASN:HD22 | 1.77                     | 0.50              |
| 36:4:302:LUT:C39  | 31:4:305:CLA:HBC3 | 2.42                     | 0.50              |
| 26:7:304:BCR:H21C | 32:7:320:CHL:H61  | 1.93                     | 0.50              |
| 36:8:303:LUT:H393 | 31:8:310:CLA:H13  | 1.94                     | 0.50              |
| 1:A:373:SER:HB2   | 32:A:840:CHL:HMC  | 1.94                     | 0.49              |
| 26:B:804:BCR:H323 | 37:G:202:LMG:H361 | 1.94                     | 0.49              |
| 10:J:12:PRO:HB2   | 36:J:103:LUT:H363 | 1.94                     | 0.49              |
| 2:B:368:GLN:NE2   | 44:B:918:HOH:O    | 2.45                     | 0.49              |
| 1:A:349:TRP:HB3   | 31:A:818:CLA:HAC1 | 1.94                     | 0.49              |
| 1:A:448:LEU:HB3   | 1:A:541:PHE:HB2   | 1.94                     | 0.49              |
| 31:A:814:CLA:H121 | 31:A:841:CLA:H151 | 1.94                     | 0.49              |
| 31:B:813:CLA:H193 | 31:B:813:CLA:HMC2 | 1.93                     | 0.49              |
| 10:J:29:ILE:HG12  | 37:J:101:LMG:H341 | 1.93                     | 0.49              |
| 22:5:213:ALA:HB2  | 36:5:303:LUT:H192 | 1.94                     | 0.49              |
| 31:4:314:CLA:C3D  | 32:4:317:CHL:HMC  | 2.43                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:6:70:ASP:HB2   | 23:6:73:ARG:HB2   | 1.95                     | 0.49              |
| 1:A:119:TRP:CD2   | 31:A:822:CLA:HED3 | 2.47                     | 0.49              |
| 31:A:828:CLA:H191 | 36:3:305:LUT:H8   | 1.94                     | 0.49              |
| 2:B:422:LEU:HD13  | 2:B:532:LEU:HA    | 1.94                     | 0.49              |
| 2:B:690:LEU:HD11  | 18:L:87:ALA:HB1   | 1.94                     | 0.49              |
| 16:8:133:PHE:HA   | 16:8:136:VAL:HG22 | 1.94                     | 0.49              |
| 31:4:318:CLA:HAA2 | 31:4:318:CLA:HED2 | 1.94                     | 0.49              |
| 2:B:339:ALA:HB2   | 26:B:805:BCR:H372 | 1.95                     | 0.49              |
| 14:3:228:HIS:CD2  | 31:3:320:CLA:NC   | 2.80                     | 0.49              |
| 28:5:305:LHG:H281 | 31:5:315:CLA:HMA3 | 1.94                     | 0.49              |
| 1:A:68:GLU:HG3    | 1:A:72:LYS:HE2    | 1.94                     | 0.49              |
| 7:G:85:ARG:NH1    | 17:9:65:SER:OG    | 2.44                     | 0.49              |
| 26:7:304:BCR:C21  | 32:7:320:CHL:H61  | 2.43                     | 0.49              |
| 31:5:318:CLA:H143 | 32:6:309:CHL:H2   | 1.94                     | 0.49              |
| 20:2:152:GLU:OE2  | 31:2:314:CLA:NB   | 2.45                     | 0.49              |
| 23:6:64:PRO:HD2   | 36:6:304:LUT:H23  | 1.95                     | 0.49              |
| 31:B:849:CLA:HBB1 | 31:B:849:CLA:HMB1 | 1.95                     | 0.49              |
| 31:5:318:CLA:H191 | 31:6:308:CLA:HBC1 | 1.95                     | 0.49              |
| 18:L:87:ALA:HB2   | 31:L:305:CLA:HMD1 | 1.95                     | 0.48              |
| 17:9:156:LEU:O    | 17:9:161:ASN:ND2  | 2.45                     | 0.48              |
| 21:4:138:ALA:HB2  | 31:4:316:CLA:CBB  | 2.43                     | 0.48              |
| 23:6:132:GLU:OE1  | 32:6:318:CHL:HMC  | 2.13                     | 0.48              |
| 24:A:801:PQN:H202 | 31:F:301:CLA:HAB  | 1.95                     | 0.48              |
| 31:H:901:CLA:HBB2 | 26:L:303:BCR:H311 | 1.94                     | 0.48              |
| 32:5:317:CHL:HAA1 | 32:5:317:CHL:CGD  | 2.43                     | 0.48              |
| 31:6:306:CLA:HBA2 | 31:6:306:CLA:H3A  | 1.45                     | 0.48              |
| 26:A:806:BCR:H24C | 31:B:841:CLA:HMC2 | 1.95                     | 0.48              |
| 28:A:810:LHG:H302 | 31:A:837:CLA:H172 | 1.95                     | 0.48              |
| 30:A:813:CL0:H33  | 31:A:856:CLA:C1D  | 2.44                     | 0.48              |
| 34:B:851:LAP:H32  | 17:9:104:PHE:CD2  | 2.49                     | 0.48              |
| 21:4:170:GLU:HB2  | 21:4:173:TYR:HB2  | 1.95                     | 0.48              |
| 2:B:25:ILE:HA     | 31:B:813:CLA:HMD3 | 1.94                     | 0.48              |
| 8:H:130:ARG:NH1   | 44:H:1002:HOH:O   | 2.37                     | 0.48              |
| 17:9:60:PRO:HD2   | 36:9:303:LUT:H23  | 1.96                     | 0.48              |
| 32:4:313:CHL:H11  | 23:6:134:PHE:HD1  | 1.79                     | 0.48              |
| 31:6:306:CLA:HMB2 | 31:6:322:CLA:C3D  | 2.43                     | 0.48              |
| 31:A:829:CLA:HAB  | 28:7:302:LHG:H322 | 1.95                     | 0.48              |
| 2:B:5:PHE:HB2     | 9:I:30:ILE:HA     | 1.95                     | 0.48              |
| 31:7:315:CLA:HMB2 | 27:5:301:LMT:H42  | 1.95                     | 0.48              |
| 16:8:34:LYS:NZ    | 16:8:36:GLY:O     | 2.40                     | 0.48              |
| 31:3:314:CLA:HMB2 | 28:7:302:LHG:HC5  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:7:182:PRO:HB3  | 31:7:321:CLA:HBC2 | 1.95                     | 0.48              |
| 16:8:80:SER:O     | 16:8:84:MET:HB2   | 2.13                     | 0.48              |
| 17:9:175:ALA:HB2  | 36:9:302:LUT:H192 | 1.96                     | 0.48              |
| 20:2:66:PRO:O     | 20:2:66:PRO:CD    | 2.61                     | 0.48              |
| 9:I:19:PRO:O      | 9:I:23:MET:HG3    | 2.14                     | 0.48              |
| 21:4:197:LYS:HD3  | 28:6:301:LHG:HC61 | 1.96                     | 0.48              |
| 31:4:318:CLA:HBA1 | 31:4:318:CLA:H3A  | 1.66                     | 0.48              |
| 32:7:318:CHL:H51  | 32:7:318:CHL:H93  | 1.96                     | 0.47              |
| 32:A:840:CHL:HMB1 | 32:A:840:CHL:HBB1 | 1.95                     | 0.47              |
| 10:J:36:PRO:HB2   | 37:J:101:LMG:H112 | 1.96                     | 0.47              |
| 20:2:103:GLY:O    | 20:2:107:MET:HG2  | 2.13                     | 0.47              |
| 31:A:814:CLA:HBC2 | 2:B:585:ASN:HB2   | 1.96                     | 0.47              |
| 31:A:819:CLA:H71  | 31:A:843:CLA:HBC3 | 1.96                     | 0.47              |
| 31:A:848:CLA:H41  | 31:A:848:CLA:H61  | 1.62                     | 0.47              |
| 8:H:95:PHE:CE1    | 9:I:21:ILE:HD11   | 2.49                     | 0.47              |
| 14:3:111:VAL:HG21 | 36:3:305:LUT:H172 | 1.96                     | 0.47              |
| 20:2:152:GLU:HA   | 20:2:155:ARG:HB2  | 1.96                     | 0.47              |
| 36:4:303:LUT:H172 | 31:4:314:CLA:HBB  | 1.96                     | 0.47              |
| 22:5:111:PHE:HB3  | 22:5:114:ASN:HB2  | 1.95                     | 0.47              |
| 36:5:303:LUT:H30  | 31:5:307:CLA:H61  | 1.96                     | 0.47              |
| 1:A:396:TRP:HB3   | 31:A:841:CLA:HMC3 | 1.96                     | 0.47              |
| 32:A:831:CHL:HBB1 | 32:A:831:CHL:H92  | 1.95                     | 0.47              |
| 22:5:107:LYS:HB3  | 22:5:107:LYS:HE3  | 1.73                     | 0.47              |
| 32:6:321:CHL:HBC2 | 32:6:321:CHL:HMC  | 1.96                     | 0.47              |
| 26:A:806:BCR:H362 | 31:A:814:CLA:H2   | 1.96                     | 0.47              |
| 11:K:113:ILE:HD11 | 26:K:202:BCR:H23C | 1.97                     | 0.47              |
| 1:A:241:HIS:CG    | 31:A:829:CLA:C1D  | 2.98                     | 0.47              |
| 27:A:807:LMT:H122 | 26:3:303:BCR:H331 | 1.96                     | 0.47              |
| 21:4:38:ARG:NH2   | 21:4:58:ASP:OD1   | 2.48                     | 0.47              |
| 21:4:117:ALA:HB1  | 32:4:310:CHL:HED1 | 1.95                     | 0.47              |
| 22:5:139:LEU:HD21 | 31:5:318:CLA:H171 | 1.95                     | 0.47              |
| 15:7:202:LYS:HD3  | 31:7:315:CLA:HED1 | 1.97                     | 0.47              |
| 18:L:199:ALA:O    | 18:L:203:THR:HG23 | 2.15                     | 0.47              |
| 23:6:210:GLN:HE22 | 23:6:266:PHE:N    | 2.12                     | 0.47              |
| 1:A:610:PHE:O     | 1:A:614:MET:HG2   | 2.15                     | 0.47              |
| 31:A:823:CLA:HBB2 | 31:A:826:CLA:HMA3 | 1.97                     | 0.47              |
| 26:3:302:BCR:HC31 | 22:5:70:LEU:HD22  | 1.97                     | 0.47              |
| 22:5:235:HIS:CG   | 31:5:309:CLA:HAA2 | 2.49                     | 0.47              |
| 1:A:684:MET:HB2   | 31:A:815:CLA:C1C  | 2.45                     | 0.47              |
| 32:7:318:CHL:HBA2 | 32:7:318:CHL:H3A  | 1.69                     | 0.47              |
| 32:8:316:CHL:H93  | 32:8:316:CHL:H51  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:5:138:LEU:HD12 | 22:5:138:LEU:HA   | 1.77                     | 0.47              |
| 2:B:411:ILE:HA    | 2:B:414:HIS:CE1   | 2.50                     | 0.46              |
| 32:K:201:CHL:HMA3 | 26:K:203:BCR:H392 | 1.96                     | 0.46              |
| 32:7:324:CHL:O1D  | 32:7:324:CHL:HAA2 | 2.15                     | 0.46              |
| 20:2:107:MET:HG3  | 31:2:304:CLA:HMC3 | 1.97                     | 0.46              |
| 31:4:305:CLA:HBC2 | 31:4:315:CLA:O2A  | 2.15                     | 0.46              |
| 30:A:813:CL0:H33  | 31:A:856:CLA:CHD  | 2.45                     | 0.46              |
| 2:B:718:ILE:HG22  | 31:B:835:CLA:H52  | 1.96                     | 0.46              |
| 3:C:7:ILE:N       | 4:D:166:GLY:O     | 2.40                     | 0.46              |
| 32:9:322:CHL:HAA2 | 32:9:322:CHL:CGD  | 2.45                     | 0.46              |
| 6:F:177:ILE:HG23  | 31:F:306:CLA:HAA1 | 1.98                     | 0.46              |
| 17:9:69:ARG:HD2   | 17:9:69:ARG:HA    | 1.63                     | 0.46              |
| 22:5:138:LEU:HD11 | 32:5:319:CHL:C2D  | 2.45                     | 0.46              |
| 31:6:306:CLA:HBB1 | 31:6:306:CLA:HMB1 | 1.98                     | 0.46              |
| 31:6:306:CLA:HBB2 | 31:6:322:CLA:HBC3 | 1.98                     | 0.46              |
| 31:A:830:CLA:H41  | 31:A:830:CLA:H62  | 1.54                     | 0.46              |
| 31:A:835:CLA:H2   | 31:A:835:CLA:H62  | 1.70                     | 0.46              |
| 22:5:268:CYS:HB2  | 43:5:306:PTY:HN12 | 1.80                     | 0.46              |
| 31:B:844:CLA:HMB1 | 31:B:844:CLA:HBB1 | 1.98                     | 0.46              |
| 20:2:154:LYS:HB3  | 20:2:154:LYS:HE3  | 1.77                     | 0.46              |
| 22:5:144:LEU:HD11 | 31:6:316:CLA:HBD  | 1.97                     | 0.46              |
| 1:A:203:ALA:HB2   | 1:A:309:GLY:HA3   | 1.98                     | 0.46              |
| 2:B:719:LEU:HD23  | 31:B:835:CLA:H41  | 1.97                     | 0.46              |
| 31:B:832:CLA:H91  | 31:B:832:CLA:HMB3 | 1.98                     | 0.46              |
| 14:3:206:ALA:HB2  | 36:3:304:LUT:H192 | 1.96                     | 0.46              |
| 1:A:157:LEU:HD12  | 31:A:829:CLA:HED3 | 1.97                     | 0.46              |
| 2:B:58:PHE:HD1    | 2:B:142:LEU:HD22  | 1.81                     | 0.46              |
| 23:6:223:HIS:CG   | 31:6:311:CLA:HAA2 | 2.51                     | 0.46              |
| 28:A:810:LHG:H362 | 28:A:810:LHG:H332 | 1.75                     | 0.46              |
| 2:B:191:THR:HG21  | 2:B:278:LEU:HB2   | 1.98                     | 0.46              |
| 26:F:302:BCR:HC32 | 37:J:101:LMG:H142 | 1.97                     | 0.45              |
| 18:L:104:VAL:HG21 | 31:L:305:CLA:HED3 | 1.98                     | 0.45              |
| 31:L:305:CLA:H92  | 31:L:305:CLA:H61  | 1.75                     | 0.45              |
| 22:5:219:ILE:HG22 | 31:5:309:CLA:HMD3 | 1.98                     | 0.45              |
| 31:5:321:CLA:HMC2 | 32:6:309:CHL:H202 | 1.97                     | 0.45              |
| 1:A:34:HIS:HE1    | 31:A:824:CLA:HED2 | 1.81                     | 0.45              |
| 28:A:809:LHG:H132 | 31:A:847:CLA:HMB3 | 1.99                     | 0.45              |
| 2:B:177:HIS:CG    | 31:B:822:CLA:HMC2 | 2.52                     | 0.45              |
| 31:7:309:CLA:HMD2 | 31:7:321:CLA:HBA2 | 1.99                     | 0.45              |
| 1:A:208:LEU:HD21  | 31:A:833:CLA:HMC1 | 1.98                     | 0.45              |
| 31:B:816:CLA:H102 | 26:I:801:BCR:HC41 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:5:84:GLN:HG3   | 22:5:157:ILE:HG12 | 1.98                     | 0.45              |
| 22:5:207:GLY:O    | 22:5:211:MET:HG3  | 2.16                     | 0.45              |
| 31:B:822:CLA:H92  | 31:B:832:CLA:H11  | 1.98                     | 0.45              |
| 20:2:228:ILE:N    | 31:2:306:CLA:O1A  | 2.49                     | 0.45              |
| 21:4:230:ASP:OD1  | 21:4:230:ASP:N    | 2.48                     | 0.45              |
| 32:A:839:CHL:H3A  | 32:A:839:CHL:HBA2 | 1.63                     | 0.45              |
| 36:6:304:LUT:H31  | 31:6:312:CLA:H151 | 1.97                     | 0.45              |
| 32:6:309:CHL:HAA2 | 32:6:309:CHL:HED2 | 1.99                     | 0.45              |
| 32:7:319:CHL:HBC2 | 32:7:320:CHL:H122 | 1.99                     | 0.45              |
| 36:9:303:LUT:H31  | 31:9:314:CLA:H142 | 1.98                     | 0.45              |
| 20:2:244:ILE:HA   | 20:2:247:ILE:HD12 | 1.98                     | 0.45              |
| 4:D:130:LYS:HA    | 4:D:130:LYS:HD3   | 1.83                     | 0.45              |
| 11:K:60:SER:O     | 11:K:64:ILE:HG13  | 2.17                     | 0.45              |
| 31:8:311:CLA:HMB1 | 31:8:311:CLA:HBB1 | 1.97                     | 0.45              |
| 20:2:126:SER:OG   | 20:2:130:ARG:NH1  | 2.49                     | 0.45              |
| 19:O:107:PRO:HD2  | 19:O:110:ASP:HB2  | 1.98                     | 0.45              |
| 31:A:834:CLA:H122 | 31:A:837:CLA:H93  | 1.98                     | 0.45              |
| 26:B:804:BCR:H20C | 26:B:804:BCR:H361 | 1.83                     | 0.45              |
| 14:3:137:GLN:HE22 | 31:3:309:CLA:C1A  | 2.30                     | 0.45              |
| 15:7:217:ALA:HB2  | 36:7:305:LUT:H192 | 1.99                     | 0.45              |
| 32:7:318:CHL:H91  | 32:7:318:CHL:H112 | 1.71                     | 0.45              |
| 18:L:103:LEU:HD22 | 26:L:303:BCR:H10C | 1.99                     | 0.45              |
| 31:A:833:CLA:H3A  | 31:A:833:CLA:HBA2 | 1.59                     | 0.45              |
| 31:A:851:CLA:H112 | 31:A:851:CLA:HMC2 | 1.99                     | 0.45              |
| 2:B:478:LEU:HD22  | 2:B:494:LEU:HD11  | 1.97                     | 0.45              |
| 24:B:801:PQN:H241 | 31:B:847:CLA:HBA2 | 1.99                     | 0.45              |
| 31:B:842:CLA:H143 | 31:B:842:CLA:H112 | 1.90                     | 0.45              |
| 10:J:33:PHE:HB3   | 37:J:101:LMG:HC2  | 1.99                     | 0.45              |
| 32:4:310:CHL:HBA1 | 31:4:319:CLA:HBB  | 1.99                     | 0.45              |
| 23:6:101:VAL:HG12 | 23:6:102:ARG:HG2  | 1.98                     | 0.45              |
| 31:A:829:CLA:HMC2 | 28:7:302:LHG:H301 | 1.99                     | 0.44              |
| 31:A:853:CLA:H18  | 31:F:301:CLA:H72  | 1.99                     | 0.44              |
| 2:B:308:HIS:HA    | 31:B:848:CLA:HMD1 | 1.99                     | 0.44              |
| 21:4:137:PHE:CE1  | 32:4:317:CHL:HMB3 | 2.52                     | 0.44              |
| 32:4:313:CHL:HMD2 | 28:6:301:LHG:HC12 | 1.99                     | 0.44              |
| 22:5:215:VAL:HG11 | 31:5:310:CLA:H192 | 1.99                     | 0.44              |
| 36:5:304:LUT:H162 | 31:5:312:CLA:HMB3 | 1.98                     | 0.44              |
| 28:5:305:LHG:H132 | 28:5:305:LHG:H102 | 1.78                     | 0.44              |
| 31:A:820:CLA:HMB1 | 31:A:820:CLA:HBB1 | 1.99                     | 0.44              |
| 11:K:51:GLY:H     | 11:K:55:ASN:HD22  | 1.66                     | 0.44              |
| 23:6:193:LYS:NZ   | 31:6:315:CLA:O1D  | 2.40                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:23:TYR:CE2    | 33:B:808:DGD:HG32 | 2.52                     | 0.44              |
| 31:B:815:CLA:H93  | 31:B:815:CLA:H61  | 1.86                     | 0.44              |
| 8:H:79:ARG:NE     | 31:H:902:CLA:OBD  | 2.38                     | 0.44              |
| 32:7:317:CHL:H41  | 32:7:317:CHL:H62  | 1.62                     | 0.44              |
| 26:B:805:BCR:H313 | 31:B:842:CLA:HAB  | 1.98                     | 0.44              |
| 31:B:826:CLA:H43  | 17:9:60:PRO:HG3   | 2.00                     | 0.44              |
| 32:7:317:CHL:H41  | 32:7:317:CHL:C10  | 2.46                     | 0.44              |
| 36:9:302:LUT:H3   | 31:9:318:CLA:HMA3 | 1.99                     | 0.44              |
| 21:4:236:VAL:HG22 | 31:4:318:CLA:HBC3 | 1.99                     | 0.44              |
| 31:5:309:CLA:HMA1 | 31:5:314:CLA:HBC3 | 2.00                     | 0.44              |
| 26:A:804:BCR:H20C | 26:A:804:BCR:H361 | 1.75                     | 0.44              |
| 31:A:851:CLA:H102 | 31:A:851:CLA:H62  | 1.76                     | 0.44              |
| 31:B:814:CLA:H112 | 31:B:814:CLA:HBD  | 2.00                     | 0.44              |
| 31:2:304:CLA:HBA2 | 31:2:304:CLA:H3A  | 1.74                     | 0.44              |
| 23:6:98:GLN:HG2   | 31:6:314:CLA:HED3 | 1.98                     | 0.44              |
| 28:A:809:LHG:H242 | 18:L:116:LEU:HD21 | 2.00                     | 0.44              |
| 31:A:850:CLA:HBB1 | 31:A:850:CLA:HMB1 | 1.98                     | 0.44              |
| 31:B:812:CLA:H141 | 31:B:819:CLA:HBC1 | 1.98                     | 0.44              |
| 36:3:304:LUT:H201 | 36:3:304:LUT:H15  | 1.73                     | 0.44              |
| 31:8:310:CLA:H152 | 31:8:310:CLA:H112 | 1.75                     | 0.44              |
| 31:8:311:CLA:H61  | 31:8:311:CLA:H41  | 1.72                     | 0.44              |
| 17:9:85:MET:HE3   | 31:9:311:CLA:HMC3 | 2.00                     | 0.44              |
| 2:B:23:TYR:CZ     | 33:B:808:DGD:HG11 | 2.53                     | 0.44              |
| 32:K:201:CHL:HED2 | 26:K:203:BCR:H391 | 1.99                     | 0.44              |
| 1:A:320:HIS:HB3   | 1:A:325:ILE:HD11  | 1.99                     | 0.44              |
| 26:A:805:BCR:H12C | 31:A:834:CLA:H71  | 2.00                     | 0.44              |
| 31:B:843:CLA:HAB  | 31:B:843:CLA:HHC  | 1.78                     | 0.44              |
| 31:8:309:CLA:HBC1 | 29:4:301:UNL:C13  | 2.48                     | 0.44              |
| 32:8:316:CHL:H51  | 32:8:316:CHL:C3B  | 2.48                     | 0.44              |
| 21:4:203:MET:HB3  | 36:4:303:LUT:H402 | 1.99                     | 0.44              |
| 32:6:317:CHL:H3A  | 32:6:317:CHL:HBA2 | 1.49                     | 0.44              |
| 31:3:313:CLA:H92  | 31:3:313:CLA:H62  | 1.90                     | 0.44              |
| 39:7:301:3PH:H252 | 39:7:301:3PH:H221 | 1.84                     | 0.44              |
| 36:8:302:LUT:H15  | 36:8:302:LUT:H201 | 1.79                     | 0.44              |
| 18:L:179:ASP:O    | 18:L:183:LYS:HG3  | 2.18                     | 0.44              |
| 31:6:313:CLA:HAB  | 31:6:313:CLA:HHC  | 1.82                     | 0.44              |
| 26:A:806:BCR:H20C | 26:A:806:BCR:H361 | 1.76                     | 0.43              |
| 31:A:855:CLA:H41  | 31:A:855:CLA:H62  | 1.68                     | 0.43              |
| 26:B:802:BCR:H282 | 31:B:836:CLA:ND   | 2.33                     | 0.43              |
| 20:2:239:LEU:HD23 | 20:2:239:LEU:HA   | 1.87                     | 0.43              |
| 26:B:805:BCR:H352 | 31:B:845:CLA:H12  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:B:840:CLA:H2   | 31:B:840:CLA:H62  | 1.74                     | 0.43              |
| 8:H:68:ARG:HD2    | 18:L:89:ARG:HG3   | 2.00                     | 0.43              |
| 26:K:203:BCR:H24C | 26:K:203:BCR:H371 | 1.78                     | 0.43              |
| 36:9:303:LUT:H12  | 31:9:315:CLA:HBC3 | 1.99                     | 0.43              |
| 26:O:201:BCR:H15C | 26:O:201:BCR:H351 | 1.90                     | 0.43              |
| 2:B:180:SER:HB3   | 2:B:288:GLY:HA3   | 1.99                     | 0.43              |
| 31:B:833:CLA:HMB1 | 31:B:833:CLA:HBB1 | 2.01                     | 0.43              |
| 11:K:53:THR:O     | 11:K:57:ILE:HD12  | 2.18                     | 0.43              |
| 20:2:44:SER:N     | 20:2:164:GLU:OE1  | 2.51                     | 0.43              |
| 31:4:314:CLA:C4D  | 32:4:317:CHL:HMC  | 2.47                     | 0.43              |
| 22:5:68:ASP:OD1   | 36:5:304:LUT:O23  | 2.33                     | 0.43              |
| 31:5:310:CLA:H72  | 31:5:310:CLA:H111 | 1.80                     | 0.43              |
| 1:A:32:PRO:HG2    | 6:F:203:TYR:HE2   | 1.82                     | 0.43              |
| 31:A:827:CLA:H62  | 31:A:829:CLA:CMB  | 2.40                     | 0.43              |
| 31:A:843:CLA:H102 | 31:A:855:CLA:HAA1 | 1.99                     | 0.43              |
| 2:B:422:LEU:HG    | 31:B:845:CLA:CBB  | 2.49                     | 0.43              |
| 15:7:50:PRO:HD2   | 32:7:317:CHL:HED3 | 2.00                     | 0.43              |
| 21:4:66:LEU:HD23  | 21:4:66:LEU:HA    | 1.86                     | 0.43              |
| 1:A:547:VAL:HG11  | 31:A:852:CLA:HMB3 | 2.01                     | 0.43              |
| 31:A:846:CLA:H51  | 26:B:806:BCR:H372 | 1.99                     | 0.43              |
| 31:B:841:CLA:H41  | 31:B:841:CLA:H62  | 1.70                     | 0.43              |
| 7:G:61:PHE:HE1    | 37:G:202:LMG:HC1  | 1.83                     | 0.43              |
| 31:3:308:CLA:HED3 | 31:3:313:CLA:H8   | 2.01                     | 0.43              |
| 16:8:118:SER:OG   | 16:8:120:ILE:O    | 2.34                     | 0.43              |
| 31:L:305:CLA:H61  | 31:L:305:CLA:H2   | 1.86                     | 0.43              |
| 31:A:853:CLA:H193 | 6:F:188:TYR:HB2   | 1.99                     | 0.43              |
| 31:A:856:CLA:H122 | 26:B:806:BCR:H12C | 2.00                     | 0.43              |
| 26:B:802:BCR:H16C | 31:B:820:CLA:H142 | 2.01                     | 0.43              |
| 31:B:839:CLA:H91  | 31:B:839:CLA:H112 | 1.86                     | 0.43              |
| 15:7:125:TRP:CZ2  | 32:7:320:CHL:HMD3 | 2.53                     | 0.43              |
| 26:L:302:BCR:H15C | 26:L:302:BCR:H351 | 1.86                     | 0.43              |
| 23:6:236:ALA:O    | 32:6:309:CHL:HBB1 | 2.18                     | 0.43              |
| 31:A:836:CLA:H61  | 31:A:836:CLA:H41  | 1.71                     | 0.43              |
| 31:B:813:CLA:HBA2 | 31:B:813:CLA:H142 | 1.99                     | 0.43              |
| 26:L:301:BCR:H403 | 26:L:301:BCR:H23C | 2.00                     | 0.43              |
| 20:2:104:ARG:HG2  | 31:2:304:CLA:C4C  | 2.49                     | 0.43              |
| 31:A:822:CLA:HMB1 | 31:A:822:CLA:HBB1 | 2.00                     | 0.43              |
| 26:3:301:BCR:H24C | 26:3:301:BCR:H371 | 1.91                     | 0.43              |
| 4:D:115:LYS:HE3   | 4:D:147:LEU:HD13  | 2.01                     | 0.43              |
| 31:2:306:CLA:H41  | 31:2:306:CLA:H62  | 1.69                     | 0.43              |
| 23:6:89:MET:SD    | 31:6:307:CLA:HAB  | 2.59                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:225:ILE:O     | 6:F:229:GLN:HG3   | 2.19                     | 0.43              |
| 8:H:99:ALA:O      | 8:H:103:LEU:HG    | 2.19                     | 0.43              |
| 36:7:305:LUT:H15  | 36:7:305:LUT:H201 | 1.79                     | 0.43              |
| 23:6:195:GLY:O    | 23:6:199:MET:HG3  | 2.19                     | 0.43              |
| 32:6:319:CHL:HMC  | 32:6:321:CHL:HMC  | 2.01                     | 0.43              |
| 1:A:122:VAL:HB    | 31:B:841:CLA:HMD1 | 2.00                     | 0.42              |
| 28:A:809:LHG:H241 | 28:A:809:LHG:H271 | 1.88                     | 0.42              |
| 2:B:34:HIS:HE1    | 31:B:813:CLA:HED1 | 1.84                     | 0.42              |
| 31:B:840:CLA:H8   | 6:F:178:ALA:HB1   | 2.00                     | 0.42              |
| 6:F:109:LEU:HD21  | 6:F:123:LYS:HZ3   | 1.84                     | 0.42              |
| 15:7:206:ASN:ND2  | 31:7:315:CLA:OBD  | 2.41                     | 0.42              |
| 32:7:324:CHL:H3A  | 32:7:324:CHL:HBA2 | 1.83                     | 0.42              |
| 16:8:86:ALA:HB2   | 36:8:303:LUT:H192 | 2.01                     | 0.42              |
| 31:8:308:CLA:H162 | 31:8:308:CLA:H202 | 1.85                     | 0.42              |
| 36:2:301:LUT:H31  | 31:2:308:CLA:HAC2 | 2.01                     | 0.42              |
| 1:A:274:ASP:OD1   | 1:A:274:ASP:N     | 2.51                     | 0.42              |
| 31:A:822:CLA:HAB  | 31:A:822:CLA:HHC  | 1.84                     | 0.42              |
| 26:3:303:BCR:H24C | 26:3:303:BCR:H371 | 1.79                     | 0.42              |
| 17:9:129:LEU:HD13 | 36:9:305:LUT:H172 | 2.01                     | 0.42              |
| 19:O:106:PRO:HA   | 19:O:107:PRO:HD3  | 1.90                     | 0.42              |
| 1:A:150:ALA:HB2   | 1:A:378:PRO:HD2   | 2.00                     | 0.42              |
| 26:B:802:BCR:H20C | 26:B:802:BCR:H361 | 1.88                     | 0.42              |
| 6:F:110:LYS:HE2   | 6:F:110:LYS:HB3   | 1.92                     | 0.42              |
| 31:H:901:CLA:HBA1 | 31:H:901:CLA:H3A  | 1.71                     | 0.42              |
| 31:3:311:CLA:HAB  | 31:3:311:CLA:HHC  | 1.81                     | 0.42              |
| 32:7:318:CHL:H151 | 32:7:318:CHL:CMB  | 2.49                     | 0.42              |
| 36:6:303:LUT:H15  | 36:6:303:LUT:H201 | 1.80                     | 0.42              |
| 1:A:646:LEU:HD22  | 2:B:651:LEU:HD21  | 2.01                     | 0.42              |
| 31:A:818:CLA:H172 | 31:A:826:CLA:H61  | 2.00                     | 0.42              |
| 31:A:857:CLA:H72  | 31:B:846:CLA:H43  | 2.01                     | 0.42              |
| 2:B:299:HIS:HB3   | 2:B:304:ILE:HD11  | 2.00                     | 0.42              |
| 31:B:818:CLA:H93  | 31:B:818:CLA:H61  | 1.83                     | 0.42              |
| 20:2:195:MET:HG3  | 31:2:307:CLA:HMC3 | 2.00                     | 0.42              |
| 22:5:202:LYS:HD3  | 31:5:308:CLA:HBD  | 2.01                     | 0.42              |
| 31:5:323:CLA:H92  | 31:5:323:CLA:H62  | 1.88                     | 0.42              |
| 31:A:821:CLA:H93  | 31:A:821:CLA:H61  | 1.86                     | 0.42              |
| 2:B:494:LEU:HD23  | 2:B:494:LEU:HA    | 1.86                     | 0.42              |
| 26:G:201:BCR:H20C | 26:G:201:BCR:H361 | 1.87                     | 0.42              |
| 22:5:85:ALA:HB2   | 31:5:318:CLA:HED2 | 2.01                     | 0.42              |
| 32:5:322:CHL:HBA2 | 32:5:322:CHL:H3A  | 1.57                     | 0.42              |
| 31:A:834:CLA:HBB1 | 31:A:834:CLA:HMB1 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:A:835:CLA:HBB2 | 31:A:836:CLA:HBC2 | 2.02                     | 0.42              |
| 31:A:841:CLA:HMB1 | 31:A:841:CLA:HBB1 | 2.02                     | 0.42              |
| 33:B:808:DGD:HBW2 | 31:B:837:CLA:H93  | 2.01                     | 0.42              |
| 3:C:15:THR:HG22   | 3:C:28:MET:HG3    | 2.00                     | 0.42              |
| 32:7:318:CHL:HBC3 | 32:7:320:CHL:C1C  | 2.49                     | 0.42              |
| 32:8:319:CHL:HMB1 | 32:8:319:CHL:HBB1 | 2.01                     | 0.42              |
| 31:8:321:CLA:HMB1 | 31:8:321:CLA:HBB1 | 2.01                     | 0.42              |
| 17:9:205:ASN:HD22 | 17:9:207:ILE:H    | 1.68                     | 0.42              |
| 23:6:125:ILE:HD11 | 32:6:318:CHL:HBC1 | 2.01                     | 0.42              |
| 23:6:132:GLU:O    | 23:6:136:MET:HB2  | 2.19                     | 0.42              |
| 2:B:435:GLY:HA3   | 31:B:841:CLA:HAB  | 2.01                     | 0.42              |
| 15:7:216:VAL:HG21 | 28:7:307:LHG:H281 | 2.02                     | 0.42              |
| 16:8:129:GLU:OE1  | 32:8:316:CHL:HMC  | 2.20                     | 0.42              |
| 31:8:308:CLA:HBB1 | 31:8:308:CLA:HMB1 | 2.01                     | 0.42              |
| 26:6:302:BCR:H402 | 32:6:318:CHL:HBA2 | 2.02                     | 0.42              |
| 31:A:834:CLA:HMB2 | 31:A:838:CLA:HMA3 | 2.02                     | 0.42              |
| 26:K:203:BCR:H20C | 26:K:203:BCR:H361 | 1.87                     | 0.42              |
| 14:3:74:HIS:HD2   | 36:3:305:LUT:H15  | 1.84                     | 0.42              |
| 14:3:87:ALA:HA    | 26:3:302:BCR:H272 | 2.01                     | 0.42              |
| 32:8:316:CHL:H3A  | 32:8:316:CHL:HBA2 | 1.31                     | 0.42              |
| 32:8:316:CHL:HBB1 | 32:8:316:CHL:HMB1 | 2.02                     | 0.42              |
| 31:8:320:CLA:H91  | 31:8:320:CLA:H111 | 1.80                     | 0.42              |
| 32:9:320:CHL:HMC  | 32:9:320:CHL:HBC2 | 2.02                     | 0.42              |
| 32:9:322:CHL:HMB1 | 32:9:322:CHL:HBB1 | 2.01                     | 0.42              |
| 36:4:302:LUT:H373 | 31:4:305:CLA:H11  | 2.01                     | 0.42              |
| 22:5:158:LYS:HB2  | 22:5:158:LYS:HE3  | 1.85                     | 0.42              |
| 34:B:851:LAP:H52  | 34:B:851:LAP:H82  | 1.30                     | 0.42              |
| 4:D:111:LYS:HE2   | 8:H:44:GLU:HB3    | 2.02                     | 0.42              |
| 26:M:101:BCR:H24C | 26:M:101:BCR:H371 | 1.82                     | 0.42              |
| 28:7:307:LHG:H311 | 31:7:315:CLA:HAC1 | 2.01                     | 0.42              |
| 16:8:139:LYS:HB3  | 31:8:317:CLA:HMC3 | 2.01                     | 0.42              |
| 41:8:305:DGA:HA52 | 31:8:321:CLA:HBA2 | 2.02                     | 0.42              |
| 31:5:323:CLA:HBA2 | 31:5:323:CLA:H3A  | 1.76                     | 0.42              |
| 1:A:289:LEU:HD21  | 1:A:374:MET:HB3   | 2.01                     | 0.42              |
| 26:B:802:BCR:H15C | 26:B:802:BCR:H351 | 1.90                     | 0.42              |
| 26:B:803:BCR:H24C | 26:B:803:BCR:H371 | 1.90                     | 0.42              |
| 31:B:825:CLA:H52  | 7:G:120:PHE:HD1   | 1.85                     | 0.42              |
| 31:B:842:CLA:H13  | 31:G:206:CLA:HBB1 | 2.01                     | 0.42              |
| 11:K:65:PHE:HE1   | 31:K:206:CLA:HAB  | 1.84                     | 0.42              |
| 14:3:181:LEU:HD23 | 36:3:304:LUT:H23  | 2.02                     | 0.42              |
| 20:2:83:PHE:HD2   | 36:2:301:LUT:C2   | 2.32                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:5:113:TYR:CD1  | 32:5:316:CHL:HMA2 | 2.55                     | 0.42              |
| 22:5:205:LYS:HE2  | 31:5:313:CLA:C4D  | 2.49                     | 0.42              |
| 23:6:238:VAL:HB   | 32:6:309:CHL:C1C  | 2.50                     | 0.42              |
| 1:A:300:ALA:HA    | 31:A:830:CLA:HMC3 | 2.01                     | 0.41              |
| 31:A:814:CLA:H171 | 31:A:814:CLA:H13  | 1.78                     | 0.41              |
| 31:B:814:CLA:H203 | 31:B:814:CLA:H162 | 1.88                     | 0.41              |
| 31:B:814:CLA:HMB1 | 31:B:814:CLA:HBB1 | 2.02                     | 0.41              |
| 4:D:111:LYS:NZ    | 8:H:54:THR:O      | 2.46                     | 0.41              |
| 31:8:307:CLA:C1C  | 31:8:318:CLA:HMB2 | 2.50                     | 0.41              |
| 26:O:201:BCR:H371 | 26:O:201:BCR:H24C | 1.77                     | 0.41              |
| 20:2:124:TRP:HE3  | 36:2:301:LUT:H221 | 1.84                     | 0.41              |
| 31:4:308:CLA:HAB  | 31:4:308:CLA:HHC  | 1.82                     | 0.41              |
| 22:5:62:ALA:O     | 22:5:83:ARG:NH2   | 2.51                     | 0.41              |
| 23:6:99:GLU:HG2   | 23:6:217:LEU:HD12 | 2.01                     | 0.41              |
| 1:A:443:TRP:CD1   | 31:A:846:CLA:HED2 | 2.55                     | 0.41              |
| 1:A:670:LEU:HD13  | 31:A:822:CLA:HMC1 | 2.01                     | 0.41              |
| 2:B:174:ARG:HB2   | 31:B:822:CLA:HBC2 | 2.00                     | 0.41              |
| 31:B:844:CLA:HAB  | 31:B:844:CLA:HHC  | 1.80                     | 0.41              |
| 31:3:309:CLA:HED2 | 31:3:309:CLA:H11  | 2.02                     | 0.41              |
| 31:8:308:CLA:HAB  | 31:8:308:CLA:HHC  | 1.87                     | 0.41              |
| 18:L:58:PRO:HB3   | 18:L:63:PRO:HA    | 2.02                     | 0.41              |
| 31:2:313:CLA:H2A  | 31:2:313:CLA:HED3 | 2.01                     | 0.41              |
| 22:5:113:TYR:CD1  | 32:5:316:CHL:HED1 | 2.55                     | 0.41              |
| 22:5:152:ARG:NH1  | 32:6:317:CHL:OBD  | 2.52                     | 0.41              |
| 32:5:319:CHL:OBD  | 32:5:319:CHL:HED2 | 2.20                     | 0.41              |
| 31:A:815:CLA:O1A  | 2:B:430:GLY:HA3   | 2.21                     | 0.41              |
| 31:B:834:CLA:H191 | 31:B:848:CLA:H152 | 2.02                     | 0.41              |
| 8:H:81:ALA:HB3    | 18:L:95:LEU:HD11  | 2.01                     | 0.41              |
| 14:3:144:TRP:CE2  | 14:3:148:ARG:HD2  | 2.56                     | 0.41              |
| 16:8:206:ILE:HG21 | 31:8:310:CLA:H202 | 2.01                     | 0.41              |
| 31:8:311:CLA:H52  | 31:8:311:CLA:H12  | 1.87                     | 0.41              |
| 26:L:302:BCR:H20C | 26:L:302:BCR:H361 | 1.86                     | 0.41              |
| 36:L:304:LUT:H7   | 36:L:304:LUT:H161 | 1.76                     | 0.41              |
| 36:4:302:LUT:H201 | 36:4:302:LUT:H15  | 1.77                     | 0.41              |
| 31:A:852:CLA:HMB1 | 31:A:852:CLA:HBB1 | 2.02                     | 0.41              |
| 7:G:36:LEU:HD11   | 7:G:41:LEU:HD13   | 2.03                     | 0.41              |
| 11:K:109:TYR:CE1  | 26:K:202:BCR:H382 | 2.55                     | 0.41              |
| 14:3:114:PRO:HG2  | 31:3:314:CLA:HAB  | 2.03                     | 0.41              |
| 32:4:313:CHL:HBA1 | 23:6:138:PHE:HA   | 2.02                     | 0.41              |
| 22:5:269:LEU:HD23 | 22:5:269:LEU:HA   | 1.94                     | 0.41              |
| 31:6:313:CLA:HBB1 | 31:6:313:CLA:HMB1 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:441:LEU:HD21  | 1:A:547:VAL:HG12  | 2.01                     | 0.41              |
| 31:B:817:CLA:HAB  | 31:B:818:CLA:HAA2 | 2.02                     | 0.41              |
| 31:B:837:CLA:H52  | 31:B:837:CLA:H8   | 1.95                     | 0.41              |
| 6:F:225:ILE:HD12  | 31:8:311:CLA:H43  | 2.02                     | 0.41              |
| 36:F:304:LUT:H193 | 36:F:304:LUT:H7   | 1.87                     | 0.41              |
| 32:3:315:CHL:H61  | 32:3:315:CHL:H41  | 1.70                     | 0.41              |
| 32:8:316:CHL:H142 | 32:8:316:CHL:H112 | 1.63                     | 0.41              |
| 26:L:303:BCR:H15C | 26:L:303:BCR:H351 | 1.90                     | 0.41              |
| 20:2:78:ARG:HB2   | 31:2:307:CLA:HMD1 | 2.02                     | 0.41              |
| 22:5:199:VAL:HG22 | 31:5:307:CLA:HHB  | 2.01                     | 0.41              |
| 20:2:43:PRO:HB2   | 20:2:46:LEU:HD12  | 2.02                     | 0.41              |
| 20:2:78:ARG:CZ    | 20:2:189:ARG:HH21 | 2.33                     | 0.41              |
| 21:4:134:LEU:HD12 | 21:4:134:LEU:HA   | 1.92                     | 0.41              |
| 31:A:821:CLA:HAA1 | 31:A:841:CLA:HED2 | 2.03                     | 0.41              |
| 31:A:845:CLA:HMB1 | 31:A:845:CLA:HBB1 | 2.03                     | 0.41              |
| 31:B:833:CLA:HED2 | 31:B:834:CLA:HBD  | 2.01                     | 0.41              |
| 31:H:903:CLA:H3A  | 31:H:903:CLA:HBA2 | 1.83                     | 0.41              |
| 16:8:88:ALA:HB2   | 36:8:302:LUT:H401 | 2.02                     | 0.41              |
| 21:4:43:PRO:HB2   | 23:6:153:GLN:HE22 | 1.86                     | 0.41              |
| 36:4:302:LUT:H11  | 36:4:302:LUT:H191 | 1.86                     | 0.41              |
| 32:6:318:CHL:HBA2 | 32:6:318:CHL:H3A  | 1.43                     | 0.41              |
| 1:A:671:ILE:HG12  | 31:A:841:CLA:H142 | 2.03                     | 0.41              |
| 30:A:813:CL0:H36  | 30:A:813:CL0:CED  | 2.50                     | 0.41              |
| 31:A:838:CLA:HBB1 | 31:A:838:CLA:HMB1 | 2.01                     | 0.41              |
| 31:B:813:CLA:H162 | 31:B:813:CLA:H141 | 1.83                     | 0.41              |
| 31:B:825:CLA:CHD  | 31:B:850:CLA:HBB2 | 2.50                     | 0.41              |
| 31:F:301:CLA:H42  | 10:J:15:ALA:HA    | 2.02                     | 0.41              |
| 14:3:123:LEU:HG   | 14:3:127:SER:HB2  | 2.02                     | 0.41              |
| 15:7:147:TRP:CZ2  | 26:7:304:BCR:HC8  | 2.56                     | 0.41              |
| 17:9:114:PRO:HA   | 17:9:115:PRO:HD3  | 1.97                     | 0.41              |
| 18:L:55:VAL:HG12  | 19:O:58:ASN:HB2   | 2.03                     | 0.41              |
| 20:2:245:THR:HA   | 31:2:313:CLA:HAB  | 2.02                     | 0.41              |
| 21:4:243:ARG:HG2  | 31:4:318:CLA:HAB  | 2.03                     | 0.41              |
| 26:6:302:BCR:H20C | 26:6:302:BCR:H361 | 1.78                     | 0.41              |
| 1:A:430:VAL:HG11  | 31:A:834:CLA:H193 | 2.01                     | 0.41              |
| 1:A:438:VAL:HG21  | 1:A:556:TYR:HE1   | 1.85                     | 0.41              |
| 1:A:707:LEU:HD13  | 36:F:304:LUT:H383 | 2.02                     | 0.41              |
| 31:A:814:CLA:HBB1 | 31:A:814:CLA:HMB1 | 2.03                     | 0.41              |
| 31:A:820:CLA:HAB  | 31:A:820:CLA:HHC  | 1.81                     | 0.41              |
| 32:A:839:CHL:H43  | 31:A:851:CLA:HBA1 | 2.03                     | 0.41              |
| 2:B:519:VAL:HG21  | 2:B:593:TYR:HB2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:B:801:PQN:H141 | 31:B:846:CLA:HBB2 | 2.01                     | 0.41              |
| 31:B:829:CLA:HMB1 | 37:G:202:LMG:H371 | 2.03                     | 0.41              |
| 31:B:837:CLA:H72  | 31:B:847:CLA:HED1 | 2.03                     | 0.41              |
| 31:B:842:CLA:H72  | 31:B:842:CLA:H111 | 1.85                     | 0.41              |
| 36:3:305:LUT:H11  | 36:3:305:LUT:H191 | 1.90                     | 0.41              |
| 16:8:187:TYR:CZ   | 16:8:191:LYS:HE3  | 2.56                     | 0.41              |
| 20:2:249:ILE:HD12 | 20:2:249:ILE:HA   | 1.93                     | 0.41              |
| 26:2:302:BCR:H15C | 26:2:302:BCR:H351 | 1.90                     | 0.41              |
| 21:4:201:LEU:HG   | 36:4:302:LUT:H11  | 2.03                     | 0.41              |
| 42:4:304:SQD:H91  | 31:4:316:CLA:HBA1 | 2.02                     | 0.41              |
| 31:5:311:CLA:HED2 | 32:6:309:CHL:H142 | 2.02                     | 0.41              |
| 32:6:319:CHL:H3A  | 32:6:319:CHL:HBA2 | 1.49                     | 0.41              |
| 26:A:805:BCR:H10C | 31:A:834:CLA:H101 | 2.03                     | 0.41              |
| 32:A:831:CHL:HMD2 | 32:A:840:CHL:HMB2 | 2.02                     | 0.41              |
| 31:A:837:CLA:H162 | 31:A:837:CLA:H121 | 1.78                     | 0.41              |
| 32:A:839:CHL:H52  | 31:A:850:CLA:H11  | 2.02                     | 0.41              |
| 2:B:619:TRP:O     | 2:B:623:TYR:HB3   | 2.21                     | 0.41              |
| 26:B:804:BCR:H24C | 26:B:804:BCR:H371 | 1.88                     | 0.41              |
| 31:B:837:CLA:HBB1 | 31:B:837:CLA:HMB1 | 2.03                     | 0.41              |
| 15:7:112:VAL:HG21 | 23:6:269:GLY:HA2  | 2.03                     | 0.41              |
| 28:7:307:LHG:HC31 | 31:7:315:CLA:C1B  | 2.50                     | 0.41              |
| 20:2:167:LEU:HD12 | 31:2:304:CLA:HMD2 | 2.03                     | 0.41              |
| 26:2:302:BCR:H11C | 26:2:302:BCR:H341 | 1.89                     | 0.41              |
| 21:4:240:GLU:HB3  | 31:4:318:CLA:C1C  | 2.51                     | 0.41              |
| 1:A:403:VAL:HG11  | 1:A:596:LEU:HG    | 2.02                     | 0.40              |
| 31:A:834:CLA:H2   | 31:A:834:CLA:H61  | 1.87                     | 0.40              |
| 26:B:805:BCR:H24C | 26:B:805:BCR:H371 | 1.88                     | 0.40              |
| 11:K:70:ARG:NH2   | 11:K:98:ASP:OD1   | 2.49                     | 0.40              |
| 31:3:310:CLA:H62  | 31:3:310:CLA:H2   | 1.80                     | 0.40              |
| 26:7:304:BCR:H15C | 26:7:304:BCR:H351 | 1.91                     | 0.40              |
| 26:8:301:BCR:H20C | 26:8:301:BCR:H361 | 1.91                     | 0.40              |
| 21:4:228:LEU:HD23 | 21:4:228:LEU:HA   | 1.90                     | 0.40              |
| 1:A:37:ARG:HD3    | 1:A:37:ARG:HA     | 1.86                     | 0.40              |
| 31:A:842:CLA:HMB1 | 31:A:842:CLA:HBB1 | 2.02                     | 0.40              |
| 31:B:830:CLA:HMB3 | 31:B:848:CLA:C1D  | 2.51                     | 0.40              |
| 31:G:205:CLA:HED3 | 31:9:313:CLA:HED2 | 2.03                     | 0.40              |
| 26:M:101:BCR:H20C | 26:M:101:BCR:H361 | 1.85                     | 0.40              |
| 26:7:304:BCR:H20C | 26:7:304:BCR:H361 | 1.89                     | 0.40              |
| 26:8:301:BCR:H11C | 26:8:301:BCR:H341 | 1.92                     | 0.40              |
| 21:4:42:LEU:HD12  | 21:4:42:LEU:HA    | 1.84                     | 0.40              |
| 31:4:314:CLA:CAD  | 32:4:317:CHL:HMC  | 2.50                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:B:805:BCR:H15C | 26:B:805:BCR:H351 | 1.86                     | 0.40              |
| 34:B:851:LAP:H51  | 17:9:104:PHE:HB2  | 2.03                     | 0.40              |
| 14:3:207:VAL:HG11 | 36:3:305:LUT:H12  | 2.04                     | 0.40              |
| 17:9:122:GLU:HA   | 32:9:322:CHL:HMA3 | 2.03                     | 0.40              |
| 36:4:302:LUT:H401 | 36:4:302:LUT:H35  | 1.83                     | 0.40              |
| 31:4:321:CLA:HAA1 | 31:4:321:CLA:H2   | 2.03                     | 0.40              |
| 32:6:309:CHL:H92  | 32:6:309:CHL:H62  | 1.76                     | 0.40              |
| 27:A:807:LMT:H81  | 28:7:302:LHG:H372 | 2.03                     | 0.40              |
| 2:B:206:HIS:ND1   | 44:B:906:HOH:O    | 2.35                     | 0.40              |
| 2:B:662:MET:HB2   | 31:B:812:CLA:C1C  | 2.52                     | 0.40              |
| 8:H:102:LEU:HA    | 8:H:102:LEU:HD23  | 1.89                     | 0.40              |
| 26:3:302:BCR:H20C | 26:3:302:BCR:H361 | 1.89                     | 0.40              |
| 20:2:45:TRP:NE1   | 20:2:97:GLU:OE2   | 2.54                     | 0.40              |
| 32:4:310:CHL:H3A  | 32:4:317:CHL:C4C  | 2.51                     | 0.40              |
| 22:5:220:GLN:O    | 22:5:224:THR:OG1  | 2.34                     | 0.40              |
| 1:A:326:LEU:O     | 1:A:338:HIS:HB2   | 2.21                     | 0.40              |
| 1:A:736:ILE:HG21  | 31:A:841:CLA:HMC2 | 2.04                     | 0.40              |
| 26:A:803:BCR:H20C | 26:A:803:BCR:H361 | 1.82                     | 0.40              |
| 2:B:492:LEU:HD22  | 31:B:825:CLA:HED2 | 2.04                     | 0.40              |
| 31:B:814:CLA:HBA1 | 31:B:814:CLA:H3A  | 1.90                     | 0.40              |
| 31:B:839:CLA:HMB1 | 31:B:839:CLA:HBB1 | 2.03                     | 0.40              |
| 32:7:324:CHL:H41  | 31:8:315:CLA:H42  | 2.02                     | 0.40              |
| 31:8:311:CLA:HAB  | 31:8:311:CLA:HHC  | 1.90                     | 0.40              |
| 36:9:303:LUT:H161 | 36:9:303:LUT:H8   | 2.04                     | 0.40              |
| 19:O:85:ASN:HB2   | 19:O:86:SER:H     | 1.70                     | 0.40              |
| 21:4:53:GLY:HA2   | 21:4:58:ASP:HB3   | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 738/751 (98%)   | 721 (98%)  | 17 (2%)  | 0        | 100         | 100 |
| 2   | B     | 730/734 (100%)  | 719 (98%)  | 11 (2%)  | 0        | 100         | 100 |
| 3   | C     | 78/81 (96%)     | 77 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 4   | D     | 141/192 (73%)   | 138 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 5   | E     | 58/71 (82%)     | 56 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 6   | F     | 163/245 (66%)   | 160 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 7   | G     | 101/138 (73%)   | 99 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 8   | H     | 89/133 (67%)    | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 9   | I     | 31/36 (86%)     | 31 (100%)  | 0        | 0        | 100         | 100 |
| 10  | J     | 37/41 (90%)     | 37 (100%)  | 0        | 0        | 100         | 100 |
| 11  | K     | 79/131 (60%)    | 79 (100%)  | 0        | 0        | 100         | 100 |
| 12  | M     | 29/31 (94%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 13  | a     | 193/229 (84%)   | 191 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 13  | b     | 120/229 (52%)   | 119 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 14  | 3     | 201/246 (82%)   | 194 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 15  | 7     | 212/259 (82%)   | 209 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 16  | 8     | 220/255 (86%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 17  | 9     | 182/230 (79%)   | 179 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 18  | L     | 142/210 (68%)   | 139 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 19  | O     | 72/142 (51%)    | 71 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 20  | 2     | 198/273 (72%)   | 184 (93%)  | 14 (7%)  | 0        | 100         | 100 |
| 21  | 4     | 187/246 (76%)   | 180 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 22  | 5     | 225/274 (82%)   | 216 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 23  | 6     | 211/272 (78%)   | 206 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| All | All   | 4437/5449 (81%) | 4336 (98%) | 101 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 603/613 (98%)   | 591 (98%)  | 12 (2%)  | 50          | 36  |
| 2   | B     | 592/593 (100%)  | 582 (98%)  | 10 (2%)  | 56          | 45  |
| 3   | C     | 68/69 (99%)     | 67 (98%)   | 1 (2%)   | 60          | 49  |
| 4   | D     | 118/156 (76%)   | 116 (98%)  | 2 (2%)   | 56          | 45  |
| 5   | E     | 56/67 (84%)     | 55 (98%)   | 1 (2%)   | 54          | 42  |
| 6   | F     | 131/183 (72%)   | 130 (99%)  | 1 (1%)   | 79          | 74  |
| 7   | G     | 78/106 (74%)    | 73 (94%)   | 5 (6%)   | 14          | 4   |
| 8   | H     | 71/105 (68%)    | 68 (96%)   | 3 (4%)   | 25          | 11  |
| 9   | I     | 26/28 (93%)     | 26 (100%)  | 0        | 100         | 100 |
| 10  | J     | 35/37 (95%)     | 35 (100%)  | 0        | 100         | 100 |
| 11  | K     | 59/100 (59%)    | 55 (93%)   | 4 (7%)   | 13          | 3   |
| 12  | M     | 26/26 (100%)    | 24 (92%)   | 2 (8%)   | 10          | 2   |
| 13  | a     | 141/166 (85%)   | 141 (100%) | 0        | 100         | 100 |
| 13  | b     | 92/166 (55%)    | 90 (98%)   | 2 (2%)   | 47          | 32  |
| 14  | 3     | 162/197 (82%)   | 158 (98%)  | 4 (2%)   | 42          | 27  |
| 15  | 7     | 166/195 (85%)   | 162 (98%)  | 4 (2%)   | 44          | 28  |
| 16  | 8     | 175/202 (87%)   | 168 (96%)  | 7 (4%)   | 27          | 12  |
| 17  | 9     | 143/177 (81%)   | 134 (94%)  | 9 (6%)   | 15          | 4   |
| 18  | L     | 115/161 (71%)   | 111 (96%)  | 4 (4%)   | 31          | 15  |
| 19  | O     | 65/110 (59%)    | 62 (95%)   | 3 (5%)   | 23          | 9   |
| 20  | 2     | 166/225 (74%)   | 154 (93%)  | 12 (7%)  | 12          | 3   |
| 21  | 4     | 155/195 (80%)   | 150 (97%)  | 5 (3%)   | 34          | 17  |
| 22  | 5     | 178/208 (86%)   | 168 (94%)  | 10 (6%)  | 17          | 5   |
| 23  | 6     | 170/212 (80%)   | 163 (96%)  | 7 (4%)   | 26          | 11  |
| All | All   | 3591/4297 (84%) | 3483 (97%) | 108 (3%) | 37          | 19  |

All (108) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | LYS  |
| 1   | A     | 14  | LYS  |
| 1   | A     | 37  | ARG  |
| 1   | A     | 60  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 248 | ASP  |
| 1   | A     | 278 | PHE  |
| 1   | A     | 372 | TYR  |
| 1   | A     | 496 | GLN  |
| 1   | A     | 524 | MET  |
| 1   | A     | 584 | CYS  |
| 1   | A     | 623 | ASN  |
| 1   | A     | 684 | MET  |
| 2   | B     | 7   | LYS  |
| 2   | B     | 160 | ARG  |
| 2   | B     | 257 | PHE  |
| 2   | B     | 280 | ILE  |
| 2   | B     | 309 | THR  |
| 2   | B     | 401 | GLU  |
| 2   | B     | 480 | GLN  |
| 2   | B     | 503 | SER  |
| 2   | B     | 577 | TYR  |
| 2   | B     | 694 | ARG  |
| 3   | C     | 7   | ILE  |
| 4   | D     | 58  | SER  |
| 4   | D     | 165 | VAL  |
| 5   | E     | 69  | GLN  |
| 6   | F     | 193 | LYS  |
| 7   | G     | 36  | LEU  |
| 7   | G     | 64  | ASP  |
| 7   | G     | 89  | GLU  |
| 7   | G     | 94  | LEU  |
| 7   | G     | 96  | THR  |
| 8   | H     | 46  | PHE  |
| 8   | H     | 50  | ASP  |
| 8   | H     | 118 | GLN  |
| 11  | K     | 76  | SER  |
| 11  | K     | 88  | SER  |
| 11  | K     | 96  | THR  |
| 11  | K     | 109 | TYR  |
| 12  | M     | 6   | SER  |
| 12  | M     | 31  | SER  |
| 14  | 3     | 55  | GLU  |
| 14  | 3     | 120 | LYS  |
| 14  | 3     | 223 | LYS  |
| 14  | 3     | 241 | PHE  |
| 15  | 7     | 44  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 7     | 123 | SER  |
| 15  | 7     | 132 | PHE  |
| 15  | 7     | 202 | LYS  |
| 16  | 8     | 61  | LYS  |
| 16  | 8     | 74  | GLN  |
| 16  | 8     | 91  | LEU  |
| 16  | 8     | 118 | SER  |
| 16  | 8     | 156 | PHE  |
| 16  | 8     | 175 | VAL  |
| 16  | 8     | 183 | LYS  |
| 17  | 9     | 105 | GLU  |
| 17  | 9     | 113 | PHE  |
| 17  | 9     | 123 | PHE  |
| 17  | 9     | 143 | SER  |
| 17  | 9     | 145 | PHE  |
| 17  | 9     | 186 | CYS  |
| 17  | 9     | 203 | SER  |
| 17  | 9     | 204 | ASN  |
| 17  | 9     | 205 | ASN  |
| 18  | L     | 151 | SER  |
| 18  | L     | 164 | THR  |
| 18  | L     | 179 | ASP  |
| 18  | L     | 210 | SER  |
| 19  | O     | 64  | PHE  |
| 19  | O     | 99  | LEU  |
| 19  | O     | 141 | TYR  |
| 13  | b     | 194 | GLN  |
| 13  | b     | 224 | SER  |
| 20  | 2     | 44  | SER  |
| 20  | 2     | 52  | ARG  |
| 20  | 2     | 73  | SER  |
| 20  | 2     | 78  | ARG  |
| 20  | 2     | 101 | TYR  |
| 20  | 2     | 167 | LEU  |
| 20  | 2     | 170 | PHE  |
| 20  | 2     | 178 | MET  |
| 20  | 2     | 180 | ASP  |
| 20  | 2     | 183 | LYS  |
| 20  | 2     | 186 | SER  |
| 20  | 2     | 257 | LEU  |
| 21  | 4     | 52  | LYS  |
| 21  | 4     | 116 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 4     | 127 | SER  |
| 21  | 4     | 164 | SER  |
| 21  | 4     | 219 | THR  |
| 22  | 5     | 52  | GLU  |
| 22  | 5     | 58  | ASN  |
| 22  | 5     | 103 | GLN  |
| 22  | 5     | 111 | PHE  |
| 22  | 5     | 132 | LYS  |
| 22  | 5     | 133 | VAL  |
| 22  | 5     | 162 | SER  |
| 22  | 5     | 163 | VAL  |
| 22  | 5     | 170 | LYS  |
| 22  | 5     | 173 | LYS  |
| 23  | 6     | 39  | ARG  |
| 23  | 6     | 55  | SER  |
| 23  | 6     | 89  | MET  |
| 23  | 6     | 103 | PRO  |
| 23  | 6     | 112 | LEU  |
| 23  | 6     | 113 | LYS  |
| 23  | 6     | 154 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 350 | HIS  |
| 1   | A     | 659 | GLN  |
| 2   | B     | 235 | GLN  |
| 5   | E     | 69  | GLN  |
| 6   | F     | 229 | GLN  |
| 8   | H     | 118 | GLN  |
| 11  | K     | 55  | ASN  |
| 13  | a     | 69  | GLN  |
| 13  | a     | 102 | GLN  |
| 14  | 3     | 68  | GLN  |
| 15  | 7     | 78  | GLN  |
| 17  | 9     | 135 | GLN  |
| 17  | 9     | 205 | ASN  |
| 18  | L     | 57  | GLN  |
| 18  | L     | 182 | GLN  |
| 19  | O     | 85  | ASN  |
| 19  | O     | 131 | GLN  |
| 20  | 2     | 227 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 4     | 77  | GLN  |
| 23  | 6     | 153 | GLN  |
| 23  | 6     | 210 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 354 ligands modelled in this entry, 17 are unknown - leaving 337 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 | $\# Z  > 2$ |
| 31  | CLA  | 5     | 310 | 22   | 65,73,73     | 2.63 | 18 (27%)    | 76,113,113  | 2.22 | 25 (32%)    |
| 31  | CLA  | 9     | 311 | 17   | 55,63,73     | 4.29 | 18 (32%)    | 64,101,113  | 2.27 | 27 (42%)    |
| 31  | CLA  | 4     | 306 | 21   | 45,53,73     | 3.31 | 20 (44%)    | 52,89,113   | 2.44 | 21 (40%)    |
| 37  | LMG  | G     | 202 | -    | 44,44,55     | 0.87 | 1 (2%)      | 52,52,63    | 1.30 | 5 (9%)      |
| 32  | CHL  | a     | 317 | 13   | 61,69,74     | 2.12 | 15 (24%)    | 67,108,114  | 2.07 | 25 (37%)    |
| 31  | CLA  | a     | 310 | 13   | 45,53,73     | 3.28 | 19 (42%)    | 52,89,113   | 2.55 | 20 (38%)    |
| 31  | CLA  | 8     | 312 | 44   | 50,58,73     | 2.83 | 18 (36%)    | 58,95,113   | 2.40 | 21 (36%)    |
| 31  | CLA  | A     | 837 | 1    | 65,73,73     | 2.46 | 17 (26%)    | 76,113,113  | 2.12 | 19 (25%)    |
| 31  | CLA  | 7     | 311 | 15   | 65,73,73     | 2.47 | 18 (27%)    | 76,113,113  | 2.18 | 19 (25%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | BCR  | O     | 201 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.25 | 5 (8%)   |
| 31  | CLA  | L     | 305 | 18   | 60,68,73     | 2.58 | 17 (28%) | 70,107,113  | 2.28 | 21 (30%) |
| 27  | LMT  | 5     | 301 | -    | 36,36,36     | 1.22 | 5 (13%)  | 47,47,47    | 0.96 | 2 (4%)   |
| 31  | CLA  | 2     | 309 | -    | 46,54,73     | 2.72 | 18 (39%) | 53,90,113   | 2.38 | 18 (33%) |
| 31  | CLA  | A     | 828 | 1    | 65,73,73     | 2.55 | 18 (27%) | 76,113,113  | 2.23 | 22 (28%) |
| 31  | CLA  | O     | 203 | 44   | 55,63,73     | 2.71 | 20 (36%) | 64,101,113  | 2.31 | 24 (37%) |
| 41  | DGA  | 8     | 305 | -    | 27,27,43     | 0.25 | 0        | 29,29,45    | 0.17 | 0        |
| 36  | LUT  | a     | 305 | -    | 42,43,43     | 5.74 | 20 (47%) | 51,60,60    | 5.70 | 29 (56%) |
| 31  | CLA  | 4     | 319 | -    | 42,50,73     | 4.22 | 19 (45%) | 48,85,113   | 2.55 | 19 (39%) |
| 32  | CHL  | 5     | 319 | -    | 47,55,74     | 3.36 | 17 (36%) | 50,91,114   | 2.26 | 17 (34%) |
| 35  | QTB  | F     | 303 | -    | 19,19,19     | 1.31 | 3 (15%)  | 20,26,26    | 1.32 | 4 (20%)  |
| 31  | CLA  | 8     | 320 | 16   | 65,73,73     | 2.56 | 19 (29%) | 76,113,113  | 2.13 | 23 (30%) |
| 31  | CLA  | 5     | 315 | 22   | 65,73,73     | 3.73 | 20 (30%) | 76,113,113  | 4.33 | 24 (31%) |
| 31  | CLA  | a     | 314 | 44   | 50,58,73     | 3.72 | 19 (38%) | 58,95,113   | 2.47 | 22 (37%) |
| 31  | CLA  | 9     | 319 | 17   | 46,54,73     | 5.19 | 19 (41%) | 53,90,113   | 2.55 | 21 (39%) |
| 31  | CLA  | 4     | 314 | -    | 45,53,73     | 3.87 | 19 (42%) | 52,89,113   | 2.64 | 22 (42%) |
| 31  | CLA  | 4     | 311 | 28   | 46,54,73     | 5.85 | 20 (43%) | 53,90,113   | 2.41 | 19 (35%) |
| 31  | CLA  | 7     | 315 | 28   | 55,63,73     | 3.66 | 19 (34%) | 63,100,113  | 2.29 | 21 (33%) |
| 36  | LUT  | 7     | 305 | -    | 42,43,43     | 5.55 | 20 (47%) | 51,60,60    | 5.71 | 31 (60%) |
| 36  | LUT  | L     | 304 | 31   | 42,43,43     | 5.64 | 20 (47%) | 51,60,60    | 5.75 | 33 (64%) |
| 31  | CLA  | 6     | 316 | 23   | 50,58,73     | 4.45 | 19 (38%) | 58,95,113   | 2.49 | 23 (39%) |
| 25  | SF4  | A     | 802 | 1,2  | 0,12,12      | -    | -        | -           | -    | -        |
| 31  | CLA  | 3     | 319 | 14   | 61,69,73     | 2.71 | 17 (27%) | 71,108,113  | 2.33 | 25 (35%) |
| 28  | LHG  | 8     | 304 | 31   | 48,48,48     | 0.63 | 1 (2%)   | 51,54,54    | 1.24 | 6 (11%)  |
| 36  | LUT  | 6     | 304 | -    | 42,43,43     | 5.62 | 19 (45%) | 51,60,60    | 5.35 | 31 (60%) |
| 26  | BCR  | K     | 203 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.27 | 6 (10%)  |
| 31  | CLA  | B     | 828 | 44   | 60,68,73     | 2.44 | 18 (30%) | 70,107,113  | 2.27 | 23 (32%) |
| 31  | CLA  | K     | 205 | 11   | 46,54,73     | 3.28 | 18 (39%) | 53,90,113   | 2.51 | 19 (35%) |
| 31  | CLA  | 5     | 321 | 22   | 46,54,73     | 3.45 | 18 (39%) | 53,90,113   | 2.53 | 20 (37%) |
| 31  | CLA  | 9     | 312 | 17   | 46,54,73     | 2.95 | 18 (39%) | 53,90,113   | 2.51 | 18 (33%) |
| 27  | LMT  | A     | 807 | -    | 36,36,36     | 1.21 | 6 (16%)  | 47,47,47    | 1.06 | 3 (6%)   |
| 28  | LHG  | a     | 306 | 31   | 48,48,48     | 0.62 | 1 (2%)   | 51,54,54    | 1.23 | 5 (9%)   |
| 31  | CLA  | A     | 846 | 1    | 65,73,73     | 2.63 | 19 (29%) | 76,113,113  | 2.22 | 22 (28%) |
| 31  | CLA  | a     | 321 | 44   | 50,58,73     | 2.98 | 16 (32%) | 58,95,113   | 2.47 | 25 (43%) |
| 31  | CLA  | a     | 313 | 13   | 60,68,73     | 2.61 | 20 (33%) | 70,107,113  | 2.29 | 22 (31%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 4     | 315 | 44   | 45,53,73     | 4.54 | 20 (44%) | 52,89,113   | 2.39 | 20 (38%) |
| 31  | CLA  | H     | 901 | 8    | 46,54,73     | 2.84 | 19 (41%) | 53,90,113   | 2.39 | 20 (37%) |
| 31  | CLA  | A     | 847 | 1    | 65,73,73     | 2.54 | 17 (26%) | 76,113,113  | 2.24 | 22 (28%) |
| 31  | CLA  | B     | 842 | 2    | 61,69,73     | 2.65 | 17 (27%) | 71,108,113  | 2.25 | 24 (33%) |
| 26  | BCR  | G     | 201 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.19 | 4 (7%)   |
| 31  | CLA  | A     | 843 | 1    | 65,73,73     | 2.85 | 18 (27%) | 76,113,113  | 2.16 | 21 (27%) |
| 31  | CLA  | 9     | 315 | 17   | 54,62,73     | 2.77 | 19 (35%) | 62,99,113   | 2.41 | 25 (40%) |
| 31  | CLA  | B     | 845 | 2    | 50,58,73     | 2.75 | 17 (34%) | 58,95,113   | 2.60 | 22 (37%) |
| 39  | 3PH  | 7     | 301 | -    | 32,32,47     | 0.75 | 1 (3%)   | 36,37,52    | 0.73 | 1 (2%)   |
| 31  | CLA  | 3     | 318 | 14   | 51,59,73     | 3.35 | 18 (35%) | 59,96,113   | 2.43 | 23 (38%) |
| 31  | CLA  | 6     | 308 | 44   | 47,55,73     | 3.07 | 19 (40%) | 54,91,113   | 2.52 | 19 (35%) |
| 31  | CLA  | 3     | 317 | 44   | 51,59,73     | 3.17 | 17 (33%) | 59,96,113   | 2.51 | 23 (38%) |
| 27  | LMT  | A     | 808 | -    | 36,36,36     | 1.21 | 5 (13%)  | 47,47,47    | 0.99 | 2 (4%)   |
| 31  | CLA  | A     | 819 | 1    | 65,73,73     | 2.33 | 19 (29%) | 76,113,113  | 2.25 | 24 (31%) |
| 31  | CLA  | B     | 835 | 2    | 57,65,73     | 3.06 | 18 (31%) | 66,103,113  | 2.36 | 21 (31%) |
| 31  | CLA  | 4     | 318 | 21   | 45,53,73     | 3.25 | 19 (42%) | 52,89,113   | 2.46 | 20 (38%) |
| 31  | CLA  | K     | 206 | 11   | 46,54,73     | 3.18 | 18 (39%) | 53,90,113   | 2.51 | 19 (35%) |
| 31  | CLA  | 3     | 316 | 44   | 50,58,73     | 2.64 | 18 (36%) | 58,95,113   | 2.35 | 23 (39%) |
| 25  | SF4  | C     | 102 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 24  | PQN  | B     | 801 | -    | 34,34,34     | 0.51 | 0        | 42,45,45    | 0.75 | 1 (2%)   |
| 31  | CLA  | 9     | 313 | 17   | 45,53,73     | 4.07 | 19 (42%) | 52,89,113   | 2.59 | 19 (36%) |
| 31  | CLA  | B     | 816 | 2    | 61,69,73     | 2.87 | 18 (29%) | 71,108,113  | 2.34 | 22 (30%) |
| 36  | LUT  | 3     | 305 | -    | 42,43,43     | 5.47 | 19 (45%) | 51,60,60    | 5.76 | 32 (62%) |
| 26  | BCR  | L     | 301 | -    | 41,41,41     | 0.98 | 1 (2%)   | 56,56,56    | 1.19 | 5 (8%)   |
| 31  | CLA  | 5     | 318 | 22   | 65,73,73     | 4.40 | 19 (29%) | 76,113,113  | 2.12 | 23 (30%) |
| 31  | CLA  | 7     | 313 | 15   | 43,52,73     | 3.07 | 20 (46%) | 49,88,113   | 2.41 | 18 (36%) |
| 26  | BCR  | B     | 803 | -    | 41,41,41     | 1.08 | 2 (4%)   | 56,56,56    | 1.16 | 2 (3%)   |
| 31  | CLA  | B     | 849 | 2    | 50,58,73     | 3.06 | 17 (34%) | 58,95,113   | 2.43 | 21 (36%) |
| 31  | CLA  | 2     | 313 | 20   | 46,54,73     | 3.22 | 18 (39%) | 53,90,113   | 2.41 | 18 (33%) |
| 31  | CLA  | 8     | 313 | 28   | 46,54,73     | 3.50 | 20 (43%) | 53,90,113   | 2.53 | 18 (33%) |
| 26  | BCR  | 3     | 302 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.17 | 4 (7%)   |
| 26  | BCR  | A     | 803 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.13 | 3 (5%)   |
| 31  | CLA  | F     | 306 | 44   | 50,58,73     | 2.85 | 18 (36%) | 58,95,113   | 2.46 | 22 (37%) |
| 31  | CLA  | A     | 850 | 1    | 51,59,73     | 2.83 | 18 (35%) | 59,96,113   | 2.53 | 24 (40%) |
| 31  | CLA  | 8     | 311 | 16   | 55,63,73     | 2.77 | 18 (32%) | 64,101,113  | 2.41 | 23 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | O     | 202 | 19   | 36,46,73     | 3.45 | 19 (52%) | 41,80,113   | 2.56 | 18 (43%) |
| 31  | CLA  | A     | 856 | 44   | 65,73,73     | 2.33 | 18 (27%) | 76,113,113  | 2.25 | 22 (28%) |
| 32  | CHL  | 7     | 320 | 44   | 61,69,74     | 2.56 | 15 (24%) | 67,108,114  | 2.10 | 23 (34%) |
| 31  | CLA  | B     | 833 | 44   | 55,63,73     | 2.42 | 18 (32%) | 64,101,113  | 2.27 | 18 (28%) |
| 32  | CHL  | 9     | 322 | 44   | 47,55,74     | 2.95 | 16 (34%) | 50,91,114   | 2.26 | 20 (40%) |
| 31  | CLA  | B     | 831 | 2    | 50,58,73     | 2.72 | 19 (38%) | 58,95,113   | 2.42 | 23 (39%) |
| 31  | CLA  | 3     | 320 | 14   | 45,53,73     | 3.62 | 20 (44%) | 52,89,113   | 2.59 | 19 (36%) |
| 32  | CHL  | a     | 318 | 44   | 48,56,74     | 2.69 | 14 (29%) | 51,92,114   | 2.35 | 18 (35%) |
| 31  | CLA  | 8     | 307 | 16   | 46,54,73     | 3.07 | 19 (41%) | 53,90,113   | 2.58 | 20 (37%) |
| 26  | BCR  | 7     | 304 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.19 | 4 (7%)   |
| 33  | DGD  | B     | 808 | -    | 62,62,67     | 1.03 | 2 (3%)   | 76,76,81    | 1.29 | 5 (6%)   |
| 31  | CLA  | 8     | 310 | 16   | 65,73,73     | 2.48 | 18 (27%) | 76,113,113  | 2.28 | 21 (27%) |
| 31  | CLA  | 3     | 310 | 14   | 60,68,73     | 2.76 | 18 (30%) | 70,107,113  | 2.32 | 22 (31%) |
| 26  | BCR  | L     | 303 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 32  | CHL  | 4     | 310 | -    | 47,55,74     | 2.65 | 16 (34%) | 50,91,114   | 2.28 | 20 (40%) |
| 31  | CLA  | 6     | 312 | 23   | 65,73,73     | 3.05 | 19 (29%) | 76,113,113  | 2.17 | 22 (28%) |
| 31  | CLA  | 8     | 315 | 16   | 52,60,73     | 2.81 | 19 (36%) | 60,97,113   | 2.37 | 25 (41%) |
| 31  | CLA  | 2     | 312 | 20   | 46,54,73     | 3.49 | 19 (41%) | 53,90,113   | 2.55 | 20 (37%) |
| 31  | CLA  | 8     | 318 | 16   | 50,58,73     | 2.57 | 18 (36%) | 58,95,113   | 2.40 | 22 (37%) |
| 31  | CLA  | B     | 811 | 2    | 65,73,73     | 2.59 | 18 (27%) | 76,113,113  | 2.22 | 19 (25%) |
| 31  | CLA  | B     | 836 | 2    | 65,73,73     | 2.52 | 18 (27%) | 76,113,113  | 2.13 | 22 (28%) |
| 31  | CLA  | B     | 843 | 44   | 45,53,73     | 2.98 | 19 (42%) | 52,89,113   | 2.60 | 21 (40%) |
| 31  | CLA  | 6     | 311 | 23   | 55,63,73     | 3.67 | 19 (34%) | 64,101,113  | 2.35 | 23 (35%) |
| 31  | CLA  | 2     | 308 | 20   | 46,54,73     | 3.12 | 19 (41%) | 53,90,113   | 2.60 | 22 (41%) |
| 31  | CLA  | 3     | 307 | 14   | 65,73,73     | 2.96 | 20 (30%) | 76,113,113  | 2.18 | 24 (31%) |
| 31  | CLA  | a     | 311 | 44   | 60,68,73     | 2.66 | 19 (31%) | 70,107,113  | 2.32 | 23 (32%) |
| 32  | CHL  | 8     | 316 | 44   | 66,74,74     | 2.02 | 15 (22%) | 73,114,114  | 2.05 | 21 (28%) |
| 32  | CHL  | 6     | 309 | 23   | 66,74,74     | 2.15 | 17 (25%) | 73,114,114  | 1.93 | 21 (28%) |
| 31  | CLA  | 4     | 309 | 21   | 60,68,73     | 2.48 | 19 (31%) | 70,107,113  | 2.30 | 27 (38%) |
| 31  | CLA  | B     | 829 | 2    | 55,63,73     | 2.59 | 18 (32%) | 64,101,113  | 2.49 | 21 (32%) |
| 31  | CLA  | A     | 829 | -    | 50,58,73     | 2.67 | 17 (34%) | 58,95,113   | 3.34 | 24 (41%) |
| 32  | CHL  | 7     | 318 | 44   | 66,74,74     | 2.27 | 15 (22%) | 73,114,114  | 2.15 | 21 (28%) |
| 26  | BCR  | B     | 804 | -    | 41,41,41     | 1.03 | 2 (4%)   | 56,56,56    | 1.12 | 3 (5%)   |
| 31  | CLA  | A     | 857 | 44   | 65,73,73     | 2.23 | 17 (26%) | 76,113,113  | 2.30 | 23 (30%) |
| 36  | LUT  | 6     | 303 | -    | 42,43,43     | 5.57 | 19 (45%) | 51,60,60    | 5.78 | 34 (66%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | BCR  | F     | 302 | -    | 41,41,41     | 0.98 | 2 (4%)   | 56,56,56    | 1.02 | 2 (3%)   |
| 36  | LUT  | 9     | 302 | -    | 42,43,43     | 5.49 | 20 (47%) | 51,60,60    | 5.76 | 33 (64%) |
| 31  | CLA  | A     | 815 | -    | 65,73,73     | 2.61 | 18 (27%) | 76,113,113  | 2.19 | 21 (27%) |
| 26  | BCR  | G     | 203 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.18 | 4 (7%)   |
| 32  | CHL  | 5     | 316 | 44   | 56,64,74     | 2.30 | 14 (25%) | 61,102,114  | 2.27 | 23 (37%) |
| 26  | BCR  | B     | 802 | -    | 41,41,41     | 1.06 | 2 (4%)   | 56,56,56    | 1.16 | 4 (7%)   |
| 26  | BCR  | L     | 302 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.14 | 6 (10%)  |
| 31  | CLA  | O     | 204 | -    | 41,49,73     | 3.03 | 19 (46%) | 47,84,113   | 2.58 | 21 (44%) |
| 31  | CLA  | A     | 838 | 44   | 65,73,73     | 2.56 | 19 (29%) | 76,113,113  | 2.32 | 22 (28%) |
| 31  | CLA  | 7     | 310 | 15   | 44,52,73     | 3.36 | 19 (43%) | 51,88,113   | 2.56 | 19 (37%) |
| 31  | CLA  | A     | 844 | 1    | 50,58,73     | 3.11 | 19 (38%) | 58,95,113   | 2.44 | 22 (37%) |
| 36  | LUT  | 5     | 303 | -    | 42,43,43     | 5.56 | 19 (45%) | 51,60,60    | 5.70 | 33 (64%) |
| 32  | CHL  | b     | 309 | 13   | 47,55,74     | 2.41 | 16 (34%) | 50,91,114   | 2.23 | 19 (38%) |
| 31  | CLA  | 4     | 321 | 21   | 50,58,73     | 3.35 | 19 (38%) | 58,95,113   | 2.42 | 25 (43%) |
| 31  | CLA  | 3     | 313 | -    | 60,68,73     | 2.81 | 18 (30%) | 70,107,113  | 2.35 | 23 (32%) |
| 36  | LUT  | a     | 303 | -    | 42,43,43     | 5.61 | 19 (45%) | 51,60,60    | 5.48 | 34 (66%) |
| 31  | CLA  | A     | 816 | 1    | 65,73,73     | 2.33 | 17 (26%) | 76,113,113  | 2.23 | 21 (27%) |
| 31  | CLA  | 2     | 307 | 20   | 57,65,73     | 2.89 | 18 (31%) | 66,103,113  | 2.33 | 24 (36%) |
| 31  | CLA  | 4     | 305 | -    | 52,60,73     | 2.43 | 16 (30%) | 60,97,113   | 4.39 | 30 (50%) |
| 30  | CL0  | A     | 813 | 1    | 65,73,73     | 1.82 | 13 (20%) | 76,113,113  | 3.07 | 28 (36%) |
| 31  | CLA  | b     | 304 | 13   | 46,54,73     | 3.49 | 20 (43%) | 53,90,113   | 2.45 | 20 (37%) |
| 31  | CLA  | 2     | 310 | 20   | 45,53,73     | 6.25 | 20 (44%) | 52,89,113   | 2.53 | 20 (38%) |
| 31  | CLA  | A     | 848 | 1    | 57,65,73     | 2.70 | 18 (31%) | 66,103,113  | 2.21 | 21 (31%) |
| 42  | SQD  | 4     | 304 | -    | 34,35,54     | 1.80 | 7 (20%)  | 43,46,65    | 1.54 | 6 (13%)  |
| 31  | CLA  | 5     | 313 | 28   | 46,54,73     | 3.76 | 23 (50%) | 53,90,113   | 2.54 | 17 (32%) |
| 31  | CLA  | 9     | 318 | 44   | 65,73,73     | 2.94 | 18 (27%) | 76,113,113  | 2.14 | 22 (28%) |
| 31  | CLA  | B     | 840 | 2    | 65,73,73     | 2.46 | 19 (29%) | 76,113,113  | 2.18 | 21 (27%) |
| 31  | CLA  | 6     | 313 | 23   | 46,54,73     | 3.05 | 20 (43%) | 53,90,113   | 2.62 | 22 (41%) |
| 31  | CLA  | A     | 853 | 1    | 65,73,73     | 2.68 | 18 (27%) | 76,113,113  | 2.20 | 24 (31%) |
| 24  | PQN  | A     | 801 | -    | 34,34,34     | 0.35 | 0        | 42,45,45    | 0.58 | 0        |
| 31  | CLA  | 9     | 316 | 17   | 50,58,73     | 3.02 | 18 (36%) | 58,95,113   | 2.45 | 20 (34%) |
| 31  | CLA  | B     | 844 | 2    | 65,73,73     | 2.43 | 18 (27%) | 76,113,113  | 2.15 | 21 (27%) |
| 31  | CLA  | 2     | 306 | 20   | 60,68,73     | 3.12 | 20 (33%) | 70,107,113  | 2.18 | 21 (30%) |
| 31  | CLA  | B     | 815 | 2    | 65,73,73     | 2.30 | 17 (26%) | 76,113,113  | 2.17 | 21 (27%) |
| 38  | AXT  | a     | 304 | -    | 44,44,45     | 0.70 | 1 (2%)   | 55,62,64    | 0.91 | 1 (1%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | A     | 823 | 1    | 55,63,73     | 2.81 | 17 (30%) | 64,101,113  | 2.25 | 20 (31%) |
| 32  | CHL  | A     | 831 | 1    | 58,66,74     | 2.23 | 16 (27%) | 63,104,114  | 2.46 | 24 (38%) |
| 31  | CLA  | A     | 826 | 1    | 65,73,73     | 2.55 | 18 (27%) | 76,113,113  | 2.18 | 23 (30%) |
| 31  | CLA  | B     | 814 | 2    | 65,73,73     | 2.75 | 18 (27%) | 76,113,113  | 2.19 | 21 (27%) |
| 31  | CLA  | A     | 822 | 1    | 55,63,73     | 2.61 | 18 (32%) | 64,101,113  | 2.45 | 24 (37%) |
| 31  | CLA  | A     | 832 | 1    | 65,73,73     | 2.32 | 17 (26%) | 76,113,113  | 2.13 | 22 (28%) |
| 32  | CHL  | 6     | 320 | -    | 47,55,74     | 3.14 | 15 (31%) | 50,91,114   | 2.19 | 17 (34%) |
| 31  | CLA  | B     | 824 | 2    | 57,65,73     | 2.95 | 19 (33%) | 66,103,113  | 2.35 | 24 (36%) |
| 36  | LUT  | 3     | 304 | -    | 42,43,43     | 5.56 | 20 (47%) | 51,60,60    | 5.67 | 33 (64%) |
| 26  | BCR  | M     | 101 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.16 | 3 (5%)   |
| 31  | CLA  | A     | 814 | 44   | 65,73,73     | 2.60 | 18 (27%) | 76,113,113  | 2.18 | 22 (28%) |
| 32  | CHL  | 6     | 318 | 44   | 46,54,74     | 3.48 | 16 (34%) | 49,90,114   | 2.27 | 20 (40%) |
| 36  | LUT  | 8     | 302 | -    | 42,43,43     | 5.50 | 19 (45%) | 51,60,60    | 5.63 | 31 (60%) |
| 32  | CHL  | a     | 320 | 44   | 48,56,74     | 2.15 | 16 (33%) | 51,92,114   | 2.35 | 18 (35%) |
| 26  | BCR  | 3     | 303 | -    | 41,41,41     | 1.08 | 3 (7%)   | 56,56,56    | 1.25 | 5 (8%)   |
| 31  | CLA  | 8     | 317 | 44   | 50,58,73     | 2.86 | 16 (32%) | 58,95,113   | 2.58 | 22 (37%) |
| 32  | CHL  | A     | 840 | 1    | 66,74,74     | 2.02 | 14 (21%) | 73,114,114  | 1.95 | 21 (28%) |
| 31  | CLA  | b     | 310 | -    | 46,54,73     | 2.86 | 17 (36%) | 53,90,113   | 2.41 | 19 (35%) |
| 31  | CLA  | B     | 822 | 2    | 65,73,73     | 2.64 | 18 (27%) | 76,113,113  | 2.13 | 20 (26%) |
| 31  | CLA  | F     | 301 | 44   | 65,73,73     | 2.45 | 19 (29%) | 76,113,113  | 2.25 | 25 (32%) |
| 32  | CHL  | 7     | 319 | 15   | 47,55,74     | 2.51 | 15 (31%) | 50,91,114   | 2.74 | 16 (32%) |
| 26  | BCR  | 8     | 301 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 27  | LMT  | 9     | 306 | -    | 36,36,36     | 1.26 | 6 (16%)  | 47,47,47    | 0.95 | 2 (4%)   |
| 31  | CLA  | B     | 820 | 2    | 65,73,73     | 2.74 | 20 (30%) | 76,113,113  | 2.19 | 22 (28%) |
| 31  | CLA  | 5     | 309 | 22   | 47,55,73     | 3.58 | 19 (40%) | 54,91,113   | 2.45 | 20 (37%) |
| 31  | CLA  | A     | 852 | 1    | 51,59,73     | 3.31 | 18 (35%) | 59,96,113   | 2.55 | 21 (35%) |
| 31  | CLA  | b     | 313 | 13   | 60,68,73     | 3.23 | 18 (30%) | 70,107,113  | 2.15 | 22 (31%) |
| 31  | CLA  | L     | 307 | 36   | 45,53,73     | 4.01 | 18 (40%) | 52,89,113   | 2.52 | 19 (36%) |
| 31  | CLA  | B     | 825 | 2    | 60,68,73     | 2.70 | 19 (31%) | 70,107,113  | 2.32 | 22 (31%) |
| 31  | CLA  | a     | 309 | 13   | 60,68,73     | 4.19 | 20 (33%) | 70,107,113  | 2.31 | 26 (37%) |
| 32  | CHL  | 5     | 322 | 22   | 47,55,74     | 2.81 | 17 (36%) | 50,91,114   | 2.23 | 20 (40%) |
| 28  | LHG  | 7     | 302 | -    | 48,48,48     | 0.58 | 0        | 51,54,54    | 1.26 | 5 (9%)   |
| 31  | CLA  | A     | 836 | 1    | 60,68,73     | 2.61 | 20 (33%) | 70,107,113  | 2.31 | 21 (30%) |
| 31  | CLA  | a     | 316 | 13   | 45,53,73     | 3.31 | 18 (40%) | 52,89,113   | 2.44 | 21 (40%) |
| 31  | CLA  | b     | 311 | 13   | 46,54,73     | 3.26 | 20 (43%) | 53,90,113   | 2.49 | 20 (37%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | G     | 204 | 7    | 50,58,73     | 3.00 | 18 (36%) | 58,95,113   | 2.39 | 23 (39%) |
| 28  | LHG  | A     | 809 | -    | 41,41,48     | 0.72 | 2 (4%)   | 44,47,54    | 1.29 | 6 (13%)  |
| 26  | BCR  | B     | 805 | -    | 41,41,41     | 1.05 | 2 (4%)   | 56,56,56    | 1.29 | 5 (8%)   |
| 28  | LHG  | 7     | 307 | 31   | 36,36,48     | 0.77 | 1 (2%)   | 39,42,54    | 1.24 | 4 (10%)  |
| 31  | CLA  | A     | 845 | 1    | 56,64,73     | 2.60 | 18 (32%) | 65,102,113  | 2.37 | 21 (32%) |
| 32  | CHL  | 4     | 313 | 21   | 48,56,74     | 3.77 | 16 (33%) | 51,92,114   | 2.21 | 20 (39%) |
| 31  | CLA  | A     | 824 | 1,31 | 62,70,73     | 2.76 | 17 (27%) | 72,109,113  | 2.19 | 22 (30%) |
| 31  | CLA  | b     | 305 | 13   | 46,54,73     | 3.08 | 20 (43%) | 53,90,113   | 2.43 | 23 (43%) |
| 26  | BCR  | 3     | 301 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.27 | 6 (10%)  |
| 31  | CLA  | A     | 854 | 28   | 46,54,73     | 2.90 | 17 (36%) | 53,90,113   | 2.60 | 19 (35%) |
| 31  | CLA  | b     | 308 | 13   | 46,54,73     | 3.51 | 20 (43%) | 53,90,113   | 2.37 | 19 (35%) |
| 36  | LUT  | J     | 103 | -    | 42,43,43     | 5.66 | 20 (47%) | 51,60,60    | 5.75 | 31 (60%) |
| 31  | CLA  | B     | 826 | 2    | 50,58,73     | 2.84 | 17 (34%) | 58,95,113   | 2.59 | 22 (37%) |
| 31  | CLA  | b     | 306 | -    | 46,54,73     | 4.09 | 19 (41%) | 53,90,113   | 2.45 | 18 (33%) |
| 31  | CLA  | 5     | 312 | 44   | 50,58,73     | 2.71 | 19 (38%) | 58,95,113   | 2.49 | 23 (39%) |
| 31  | CLA  | 6     | 322 | 23   | 46,54,73     | 3.09 | 19 (41%) | 53,90,113   | 2.42 | 21 (39%) |
| 31  | CLA  | 8     | 321 | 16   | 46,54,73     | 3.10 | 16 (34%) | 53,90,113   | 2.57 | 18 (33%) |
| 31  | CLA  | a     | 312 | 13   | 65,73,73     | 3.07 | 19 (29%) | 76,113,113  | 2.26 | 21 (27%) |
| 35  | QTB  | 9     | 304 | -    | 19,19,19     | 1.29 | 2 (10%)  | 20,26,26    | 1.46 | 2 (10%)  |
| 31  | CLA  | A     | 849 | 1    | 46,54,73     | 3.35 | 19 (41%) | 53,90,113   | 2.43 | 20 (37%) |
| 32  | CHL  | 8     | 319 | 44   | 45,53,74     | 2.66 | 15 (33%) | 47,88,114   | 2.41 | 17 (36%) |
| 28  | LHG  | A     | 810 | 31   | 41,41,48     | 0.72 | 1 (2%)   | 44,47,54    | 1.14 | 4 (9%)   |
| 31  | CLA  | B     | 827 | 2    | 60,68,73     | 2.44 | 18 (30%) | 70,107,113  | 2.28 | 23 (32%) |
| 31  | CLA  | H     | 903 | 18   | 46,54,73     | 3.12 | 18 (39%) | 53,90,113   | 2.43 | 17 (32%) |
| 31  | CLA  | b     | 307 | -    | 46,54,73     | 5.48 | 20 (43%) | 53,90,113   | 2.63 | 20 (37%) |
| 31  | CLA  | J     | 105 | 10   | 42,50,73     | 3.06 | 17 (40%) | 48,85,113   | 2.67 | 17 (35%) |
| 31  | CLA  | B     | 841 | 2    | 55,63,73     | 2.67 | 16 (29%) | 64,101,113  | 2.39 | 24 (37%) |
| 31  | CLA  | G     | 205 | 7    | 46,54,73     | 2.94 | 19 (41%) | 53,90,113   | 2.52 | 18 (33%) |
| 32  | CHL  | A     | 839 | 44   | 56,64,74     | 2.13 | 14 (25%) | 61,102,114  | 2.74 | 23 (37%) |
| 36  | LUT  | F     | 304 | -    | 42,43,43     | 5.43 | 20 (47%) | 51,60,60    | 6.02 | 35 (68%) |
| 31  | CLA  | 5     | 314 | 22   | 45,53,73     | 3.30 | 20 (44%) | 52,89,113   | 2.53 | 19 (36%) |
| 36  | LUT  | 4     | 303 | -    | 42,43,43     | 5.65 | 19 (45%) | 51,60,60    | 5.53 | 31 (60%) |
| 31  | CLA  | A     | 833 | 1    | 47,55,73     | 3.19 | 19 (40%) | 54,91,113   | 2.65 | 20 (37%) |
| 31  | CLA  | 5     | 307 | 22   | 55,63,73     | 3.54 | 19 (34%) | 64,101,113  | 2.31 | 26 (40%) |
| 34  | LAP  | B     | 851 | -    | 28,28,28     | 0.34 | 0        | 33,35,35    | 0.38 | 0        |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 7     | 316 | 15   | 46,54,73     | 3.36 | 19 (41%) | 53,90,113   | 2.51 | 19 (35%) |
| 31  | CLA  | A     | 830 | 1    | 60,68,73     | 2.81 | 19 (31%) | 70,107,113  | 2.31 | 24 (34%) |
| 31  | CLA  | B     | 839 | 2    | 60,68,73     | 2.49 | 18 (30%) | 70,107,113  | 2.23 | 24 (34%) |
| 31  | CLA  | B     | 850 | 2    | 62,70,73     | 2.60 | 18 (29%) | 72,109,113  | 2.15 | 21 (29%) |
| 31  | CLA  | 2     | 304 | 20   | 46,54,73     | 3.18 | 19 (41%) | 53,90,113   | 2.42 | 18 (33%) |
| 31  | CLA  | 3     | 308 | 14   | 46,54,73     | 3.62 | 19 (41%) | 53,90,113   | 2.57 | 19 (35%) |
| 32  | CHL  | 3     | 315 | 44   | 56,64,74     | 2.32 | 14 (25%) | 61,102,114  | 2.47 | 21 (34%) |
| 31  | CLA  | 3     | 314 | 14   | 52,60,73     | 3.06 | 17 (32%) | 60,97,113   | 2.37 | 22 (36%) |
| 31  | CLA  | L     | 306 | 44   | 45,53,73     | 2.80 | 19 (42%) | 52,89,113   | 2.52 | 20 (38%) |
| 37  | LMG  | J     | 101 | -    | 49,49,55     | 0.83 | 3 (6%)   | 57,57,63    | 1.23 | 2 (3%)   |
| 31  | CLA  | K     | 204 | 44   | 50,58,73     | 3.41 | 19 (38%) | 58,95,113   | 2.44 | 19 (32%) |
| 31  | CLA  | 6     | 314 | 23   | 47,55,73     | 4.29 | 19 (40%) | 54,91,113   | 2.52 | 20 (37%) |
| 31  | CLA  | 6     | 306 | 23   | 46,54,73     | 3.37 | 22 (47%) | 53,90,113   | 2.69 | 16 (30%) |
| 32  | CHL  | 5     | 317 | 44   | 47,55,74     | 3.03 | 15 (31%) | 50,91,114   | 2.42 | 19 (38%) |
| 32  | CHL  | 6     | 317 | 23   | 47,55,74     | 2.82 | 16 (34%) | 50,91,114   | 2.21 | 19 (38%) |
| 31  | CLA  | 3     | 312 | 44   | 65,73,73     | 2.74 | 18 (27%) | 76,113,113  | 2.17 | 25 (32%) |
| 31  | CLA  | 5     | 311 | 22   | 46,54,73     | 2.84 | 18 (39%) | 53,90,113   | 2.53 | 23 (43%) |
| 31  | CLA  | B     | 832 | 44   | 65,73,73     | 2.33 | 18 (27%) | 76,113,113  | 2.35 | 25 (32%) |
| 31  | CLA  | B     | 837 | 2    | 55,63,73     | 2.94 | 18 (32%) | 64,101,113  | 2.26 | 23 (35%) |
| 26  | BCR  | B     | 806 | -    | 41,41,41     | 1.04 | 2 (4%)   | 56,56,56    | 1.05 | 5 (8%)   |
| 31  | CLA  | B     | 846 | 44   | 65,73,73     | 2.44 | 18 (27%) | 76,113,113  | 2.12 | 22 (28%) |
| 36  | LUT  | 4     | 302 | -    | 42,43,43     | 5.65 | 19 (45%) | 51,60,60    | 5.74 | 34 (66%) |
| 32  | CHL  | 6     | 321 | 23   | 43,51,74     | 3.73 | 15 (34%) | 45,86,114   | 2.31 | 18 (40%) |
| 31  | CLA  | A     | 820 | 1    | 55,63,73     | 2.98 | 19 (34%) | 64,101,113  | 2.43 | 21 (32%) |
| 43  | PTY  | 5     | 306 | -    | 30,30,49     | 0.54 | 0        | 33,35,54    | 0.80 | 1 (3%)   |
| 31  | CLA  | 7     | 322 | 15   | 46,54,73     | 3.10 | 19 (41%) | 53,90,113   | 2.42 | 17 (32%) |
| 31  | CLA  | B     | 838 | 2    | 46,54,73     | 3.02 | 20 (43%) | 53,90,113   | 2.38 | 20 (37%) |
| 32  | CHL  | 6     | 319 | -    | 47,55,74     | 4.65 | 16 (34%) | 50,91,114   | 2.36 | 23 (46%) |
| 31  | CLA  | B     | 812 | -    | 65,73,73     | 2.21 | 18 (27%) | 76,113,113  | 2.19 | 22 (28%) |
| 31  | CLA  | A     | 827 | 1    | 55,63,73     | 2.86 | 17 (30%) | 64,101,113  | 2.34 | 20 (31%) |
| 36  | LUT  | b     | 301 | -    | 42,43,43     | 5.67 | 19 (45%) | 51,60,60    | 5.69 | 33 (64%) |
| 31  | CLA  | 6     | 310 | 23   | 47,55,73     | 4.13 | 20 (42%) | 54,91,113   | 2.48 | 21 (38%) |
| 26  | BCR  | 6     | 302 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.30 | 6 (10%)  |
| 31  | CLA  | B     | 848 | 28   | 65,73,73     | 2.27 | 17 (26%) | 76,113,113  | 2.19 | 20 (26%) |
| 26  | BCR  | 2     | 302 | -    | 41,41,41     | 1.10 | 3 (7%)   | 56,56,56    | 1.27 | 7 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 2     | 315 | 44   | 46,54,73     | 3.25 | 19 (41%) | 53,90,113   | 2.53 | 18 (33%) |
| 31  | CLA  | B     | 818 | 2    | 55,63,73     | 2.42 | 17 (30%) | 64,101,113  | 2.39 | 23 (35%) |
| 31  | CLA  | A     | 835 | 1    | 55,63,73     | 2.82 | 19 (34%) | 64,101,113  | 2.31 | 19 (29%) |
| 32  | CHL  | 7     | 317 | 15   | 57,65,74     | 2.19 | 16 (28%) | 62,103,114  | 2.16 | 22 (35%) |
| 31  | CLA  | A     | 821 | 1    | 65,73,73     | 2.57 | 16 (24%) | 76,113,113  | 2.27 | 23 (30%) |
| 26  | BCR  | J     | 102 | -    | 41,41,41     | 0.99 | 2 (4%)   | 56,56,56    | 1.20 | 3 (5%)   |
| 26  | BCR  | A     | 805 | -    | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |
| 31  | CLA  | F     | 305 | 6    | 46,54,73     | 2.92 | 19 (41%) | 53,90,113   | 2.60 | 22 (41%) |
| 36  | LUT  | 8     | 303 | -    | 42,43,43     | 5.52 | 20 (47%) | 51,60,60    | 5.71 | 34 (66%) |
| 35  | QTB  | 7     | 303 | -    | 19,19,19     | 1.28 | 2 (10%)  | 20,26,26    | 1.53 | 4 (20%)  |
| 31  | CLA  | A     | 842 | 1    | 65,73,73     | 2.66 | 18 (27%) | 76,113,113  | 2.27 | 22 (28%) |
| 35  | QTB  | a     | 302 | -    | 19,19,19     | 1.28 | 2 (10%)  | 20,26,26    | 1.69 | 4 (20%)  |
| 31  | CLA  | 4     | 308 | 21   | 60,68,73     | 2.43 | 18 (30%) | 70,107,113  | 2.32 | 25 (35%) |
| 28  | LHG  | 5     | 305 | 31   | 34,34,48     | 0.33 | 0        | 37,40,54    | 0.40 | 0        |
| 31  | CLA  | B     | 813 | 2    | 65,73,73     | 2.76 | 19 (29%) | 76,113,113  | 2.30 | 23 (30%) |
| 31  | CLA  | a     | 319 | 13   | 65,73,73     | 2.47 | 17 (26%) | 76,113,113  | 2.24 | 21 (27%) |
| 36  | LUT  | 5     | 304 | -    | 42,43,43     | 5.61 | 19 (45%) | 51,60,60    | 5.48 | 31 (60%) |
| 31  | CLA  | 8     | 309 | 16   | 50,58,73     | 3.12 | 19 (38%) | 58,95,113   | 2.51 | 25 (43%) |
| 31  | CLA  | 4     | 312 | 21   | 47,55,73     | 2.98 | 20 (42%) | 54,91,113   | 2.46 | 20 (37%) |
| 31  | CLA  | 2     | 314 | 20   | 46,54,73     | 4.36 | 19 (41%) | 53,90,113   | 2.43 | 21 (39%) |
| 31  | CLA  | 7     | 314 | 44   | 54,62,73     | 2.80 | 19 (35%) | 63,100,113  | 2.37 | 23 (36%) |
| 31  | CLA  | 6     | 307 | 23   | 50,58,73     | 3.79 | 19 (38%) | 58,95,113   | 2.39 | 23 (39%) |
| 31  | CLA  | A     | 817 | 1,31 | 55,63,73     | 2.77 | 17 (30%) | 64,101,113  | 2.38 | 21 (32%) |
| 31  | CLA  | G     | 206 | 44   | 45,53,73     | 3.28 | 17 (37%) | 52,89,113   | 2.41 | 18 (34%) |
| 31  | CLA  | 4     | 316 | -    | 47,55,73     | 3.39 | 19 (40%) | 54,91,113   | 2.91 | 17 (31%) |
| 33  | DGD  | 7     | 308 | -    | 53,53,67     | 1.05 | 4 (7%)   | 67,67,81    | 1.53 | 12 (17%) |
| 32  | CHL  | 9     | 320 | 44   | 48,56,74     | 2.34 | 14 (29%) | 51,92,114   | 2.17 | 20 (39%) |
| 31  | CLA  | 5     | 320 | 22   | 46,54,73     | 4.96 | 21 (45%) | 53,90,113   | 2.54 | 22 (41%) |
| 31  | CLA  | 8     | 314 | 44   | 52,60,73     | 2.70 | 18 (34%) | 60,97,113   | 2.42 | 26 (43%) |
| 31  | CLA  | 4     | 320 | 21   | 45,53,73     | 3.44 | 20 (44%) | 52,89,113   | 2.52 | 20 (38%) |
| 26  | BCR  | K     | 202 | -    | 41,41,41     | 1.07 | 2 (4%)   | 56,56,56    | 1.25 | 8 (14%)  |
| 26  | BCR  | A     | 804 | -    | 41,41,41     | 1.09 | 2 (4%)   | 56,56,56    | 1.14 | 4 (7%)   |
| 31  | CLA  | a     | 315 | 28   | 55,63,73     | 2.61 | 18 (32%) | 64,101,113  | 2.44 | 21 (32%) |
| 31  | CLA  | B     | 830 | 2    | 60,68,73     | 2.68 | 19 (31%) | 70,107,113  | 2.21 | 24 (34%) |
| 31  | CLA  | 3     | 311 | 14   | 65,73,73     | 2.76 | 19 (29%) | 76,113,113  | 2.14 | 24 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | b     | 312 | 13   | 46,54,73     | 4.30 | 19 (41%) | 53,90,113   | 2.42 | 20 (37%) |
| 31  | CLA  | 7     | 321 | 44   | 47,55,73     | 3.26 | 18 (38%) | 54,91,113   | 2.55 | 22 (40%) |
| 37  | LMG  | a     | 301 | -    | 42,42,55     | 0.83 | 0        | 50,50,63    | 1.26 | 4 (8%)   |
| 31  | CLA  | B     | 817 | 2    | 65,73,73     | 2.31 | 17 (26%) | 76,113,113  | 2.24 | 20 (26%) |
| 31  | CLA  | b     | 303 | -    | 46,54,73     | 3.42 | 19 (41%) | 53,90,113   | 2.53 | 20 (37%) |
| 31  | CLA  | B     | 823 | 2    | 55,63,73     | 2.72 | 18 (32%) | 64,101,113  | 2.38 | 22 (34%) |
| 31  | CLA  | A     | 855 | 1    | 65,73,73     | 2.74 | 18 (27%) | 76,113,113  | 2.27 | 22 (28%) |
| 31  | CLA  | 2     | 305 | 20   | 45,53,73     | 4.19 | 19 (42%) | 52,89,113   | 2.57 | 19 (36%) |
| 36  | LUT  | 9     | 303 | -    | 42,43,43     | 5.55 | 19 (45%) | 51,60,60    | 5.53 | 30 (58%) |
| 31  | CLA  | B     | 821 | 2    | 58,66,73     | 2.72 | 16 (27%) | 67,104,113  | 2.28 | 20 (29%) |
| 26  | BCR  | 5     | 302 | -    | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.29 | 8 (14%)  |
| 31  | CLA  | 9     | 317 | -    | 47,55,73     | 3.52 | 23 (48%) | 54,91,113   | 2.58 | 17 (31%) |
| 31  | CLA  | B     | 819 | 2    | 65,73,73     | 2.53 | 19 (29%) | 76,113,113  | 2.27 | 25 (32%) |
| 31  | CLA  | A     | 834 | 44   | 65,73,73     | 2.31 | 18 (27%) | 76,113,113  | 2.14 | 21 (27%) |
| 32  | CHL  | K     | 201 | 11   | 47,55,74     | 2.24 | 15 (31%) | 50,91,114   | 2.94 | 19 (38%) |
| 37  | LMG  | J     | 104 | -    | 29,29,55     | 1.03 | 1 (3%)   | 37,37,63    | 1.19 | 3 (8%)   |
| 28  | LHG  | 6     | 301 | 31   | 26,26,48     | 0.78 | 0        | 29,32,54    | 1.22 | 2 (6%)   |
| 31  | CLA  | A     | 818 | 1    | 65,73,73     | 2.24 | 18 (27%) | 76,113,113  | 2.19 | 22 (28%) |
| 31  | CLA  | 4     | 307 | 21   | 56,64,73     | 2.68 | 19 (33%) | 65,102,113  | 2.24 | 23 (35%) |
| 31  | CLA  | b     | 302 | 13   | 46,54,73     | 3.05 | 19 (41%) | 53,90,113   | 2.53 | 21 (39%) |
| 28  | LHG  | A     | 811 | -    | 48,48,48     | 0.72 | 1 (2%)   | 51,54,54    | 1.26 | 5 (9%)   |
| 32  | CHL  | 7     | 324 | 16   | 66,74,74     | 1.81 | 14 (21%) | 73,114,114  | 2.02 | 23 (31%) |
| 25  | SF4  | C     | 101 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 36  | LUT  | 9     | 305 | -    | 42,43,43     | 5.68 | 19 (45%) | 51,60,60    | 5.95 | 32 (62%) |
| 31  | CLA  | 7     | 309 | 15   | 60,68,73     | 2.33 | 19 (31%) | 70,107,113  | 2.25 | 23 (32%) |
| 31  | CLA  | 3     | 309 | 14   | 65,73,73     | 2.34 | 19 (29%) | 76,113,113  | 2.20 | 23 (30%) |
| 31  | CLA  | B     | 834 | 2    | 65,73,73     | 2.91 | 18 (27%) | 76,113,113  | 2.22 | 23 (30%) |
| 31  | CLA  | 5     | 308 | 22   | 46,54,73     | 3.49 | 19 (41%) | 53,90,113   | 2.49 | 19 (35%) |
| 31  | CLA  | H     | 902 | 44   | 46,54,73     | 3.88 | 20 (43%) | 53,90,113   | 2.44 | 20 (37%) |
| 40  | XAT  | 7     | 306 | -    | 39,47,47     | 1.60 | 8 (20%)  | 54,74,74    | 1.55 | 9 (16%)  |
| 31  | CLA  | 9     | 314 | 17   | 60,68,73     | 3.31 | 18 (30%) | 70,107,113  | 2.30 | 23 (32%) |
| 28  | LHG  | B     | 807 | 31   | 31,31,48     | 0.81 | 1 (3%)   | 34,37,54    | 1.27 | 4 (11%)  |
| 32  | CHL  | 4     | 317 | -    | 46,54,74     | 2.66 | 16 (34%) | 49,90,114   | 2.30 | 18 (36%) |
| 31  | CLA  | B     | 847 | 2    | 65,73,73     | 2.81 | 18 (27%) | 76,113,113  | 2.27 | 17 (22%) |
| 31  | CLA  | a     | 322 | 13   | 46,54,73     | 3.28 | 18 (39%) | 53,90,113   | 2.36 | 19 (35%) |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | CLA  | 2     | 311 | 20   | 45,53,73     | 4.92 | 20 (44%) | 52,89,113   | 2.46 | 18 (34%) |
| 31  | CLA  | A     | 841 | 1    | 65,73,73     | 2.49 | 17 (26%) | 76,113,113  | 2.33 | 24 (31%) |
| 31  | CLA  | A     | 851 | 1    | 65,73,73     | 2.76 | 18 (27%) | 76,113,113  | 2.17 | 20 (26%) |
| 31  | CLA  | 5     | 323 | 22   | 56,64,73     | 3.08 | 17 (30%) | 65,102,113  | 2.42 | 23 (35%) |
| 36  | LUT  | 2     | 301 | -    | 42,43,43     | 5.53 | 19 (45%) | 51,60,60    | 5.77 | 32 (62%) |
| 26  | BCR  | A     | 806 | -    | 41,41,41     | 1.01 | 2 (4%)   | 56,56,56    | 1.10 | 5 (8%)   |
| 31  | CLA  | 9     | 321 | 17   | 56,64,73     | 2.53 | 19 (33%) | 65,102,113  | 2.35 | 22 (33%) |
| 28  | LHG  | 6     | 305 | 31   | 31,31,48     | 0.74 | 1 (3%)   | 34,37,54    | 1.29 | 4 (11%)  |
| 31  | CLA  | 6     | 315 | 28   | 46,54,73     | 5.53 | 20 (43%) | 53,90,113   | 2.53 | 19 (35%) |
| 26  | BCR  | I     | 801 | -    | 41,41,41     | 1.05 | 1 (2%)   | 56,56,56    | 1.18 | 4 (7%)   |
| 31  | CLA  | A     | 825 | 1    | 54,62,73     | 2.73 | 19 (35%) | 62,99,113   | 2.48 | 23 (37%) |
| 31  | CLA  | 8     | 308 | 16   | 65,73,73     | 2.61 | 20 (30%) | 76,113,113  | 2.21 | 23 (30%) |
| 31  | CLA  | 7     | 312 | 15   | 62,70,73     | 2.63 | 19 (30%) | 72,109,113  | 2.21 | 23 (31%) |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 5     | 310 | 22   | 1/1/15/20 | 6/37/115/115  | -       |
| 31  | CLA  | 9     | 311 | 17   | 1/1/13/20 | 5/25/103/115  | -       |
| 31  | CLA  | 4     | 306 | 21   | 1/1/11/20 | 4/13/91/115   | -       |
| 37  | LMG  | G     | 202 | -    | -         | 23/39/59/70   | 0/1/1/1 |
| 32  | CHL  | a     | 317 | 13   | 2/2/19/26 | 15/33/131/137 | -       |
| 31  | CLA  | a     | 310 | 13   | 1/1/11/20 | 6/13/91/115   | -       |
| 31  | CLA  | 8     | 312 | 44   | 1/1/12/20 | 4/19/97/115   | -       |
| 31  | CLA  | A     | 837 | 1    | -         | 16/37/115/115 | -       |
| 31  | CLA  | 7     | 311 | 15   | -         | 10/37/115/115 | -       |
| 26  | BCR  | O     | 201 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 31  | CLA  | L     | 305 | 18   | -         | 10/31/109/115 | -       |
| 27  | LMT  | 5     | 301 | -    | -         | 9/21/61/61    | 0/2/2/2 |
| 31  | CLA  | 2     | 309 | -    | -         | 5/15/93/115   | -       |
| 31  | CLA  | A     | 828 | 1    | -         | 7/37/115/115  | -       |
| 31  | CLA  | O     | 203 | 44   | 1/1/13/20 | 14/25/103/115 | -       |
| 41  | DGA  | 8     | 305 | -    | -         | 18/29/29/45   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 36  | LUT  | a     | 305 | -    | -         | 22/29/67/67   | 0/2/2/2 |
| 31  | CLA  | 4     | 319 | -    | 1/1/10/20 | 5/10/88/115   | -       |
| 32  | CHL  | 5     | 319 | -    | 2/2/16/26 | 2/17/115/137  | -       |
| 35  | QTB  | F     | 303 | -    | -         | 7/11/28/28    | 1/1/1/1 |
| 31  | CLA  | 8     | 320 | 16   | -         | 10/37/115/115 | -       |
| 31  | CLA  | 5     | 315 | 22   | 1/1/15/20 | 11/37/115/115 | -       |
| 31  | CLA  | a     | 314 | 44   | 1/1/12/20 | 6/19/97/115   | -       |
| 31  | CLA  | 9     | 319 | 17   | -         | 7/15/93/115   | -       |
| 31  | CLA  | 4     | 314 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 31  | CLA  | 4     | 311 | 28   | 1/1/11/20 | 6/15/93/115   | -       |
| 31  | CLA  | 7     | 315 | 28   | 1/1/12/20 | 8/25/103/115  | -       |
| 36  | LUT  | 7     | 305 | -    | -         | 14/29/67/67   | 0/2/2/2 |
| 36  | LUT  | L     | 304 | 31   | -         | 15/29/67/67   | 0/2/2/2 |
| 31  | CLA  | 6     | 316 | 23   | 1/1/12/20 | 3/19/97/115   | -       |
| 31  | CLA  | 3     | 319 | 14   | 1/1/14/20 | 7/33/111/115  | -       |
| 25  | SF4  | A     | 802 | 1,2  | -         | -             | 0/6/5/5 |
| 28  | LHG  | 8     | 304 | 31   | -         | 15/53/53/53   | -       |
| 36  | LUT  | 6     | 304 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 26  | BCR  | K     | 203 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 31  | CLA  | B     | 828 | 44   | 1/1/14/20 | 2/31/109/115  | -       |
| 31  | CLA  | K     | 205 | 11   | 1/1/11/20 | 3/15/93/115   | -       |
| 31  | CLA  | 5     | 321 | 22   | -         | 4/15/93/115   | -       |
| 31  | CLA  | 9     | 312 | 17   | 1/1/11/20 | 2/15/93/115   | -       |
| 27  | LMT  | A     | 807 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 28  | LHG  | a     | 306 | 31   | -         | 19/53/53/53   | -       |
| 31  | CLA  | A     | 846 | 1    | -         | 5/37/115/115  | -       |
| 31  | CLA  | 4     | 315 | 44   | 1/1/11/20 | 5/13/91/115   | -       |
| 31  | CLA  | a     | 313 | 13   | 1/1/14/20 | 7/31/109/115  | -       |
| 31  | CLA  | a     | 321 | 44   | -         | 4/19/97/115   | -       |
| 31  | CLA  | H     | 901 | 8    | 1/1/11/20 | 7/15/93/115   | -       |
| 31  | CLA  | B     | 842 | 2    | 1/1/14/20 | 8/33/111/115  | -       |
| 31  | CLA  | A     | 847 | 1    | -         | 7/37/115/115  | -       |
| 26  | BCR  | G     | 201 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 843 | 1    | -         | 9/37/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 9     | 315 | 17   | 1/1/12/20 | 9/24/102/115  | -       |
| 31  | CLA  | B     | 845 | 2    | -         | 1/19/97/115   | -       |
| 39  | 3PH  | 7     | 301 | -    | -         | 15/34/34/49   | -       |
| 31  | CLA  | 3     | 318 | 14   | -         | 7/21/99/115   | -       |
| 31  | CLA  | 6     | 308 | 44   | 1/1/11/20 | 5/16/94/115   | -       |
| 31  | CLA  | 3     | 317 | 44   | 1/1/12/20 | 8/21/99/115   | -       |
| 27  | LMT  | A     | 808 | -    | -         | 6/21/61/61    | 0/2/2/2 |
| 31  | CLA  | A     | 819 | 1    | 1/1/15/20 | 8/37/115/115  | -       |
| 31  | CLA  | B     | 835 | 2    | 1/1/13/20 | 8/28/106/115  | -       |
| 31  | CLA  | 4     | 318 | 21   | 1/1/11/20 | 5/13/91/115   | -       |
| 31  | CLA  | K     | 206 | 11   | -         | 5/15/93/115   | -       |
| 31  | CLA  | 3     | 316 | 44   | 1/1/12/20 | 4/19/97/115   | -       |
| 25  | SF4  | C     | 102 | 3    | -         | -             | 0/6/5/5 |
| 24  | PQN  | B     | 801 | -    | -         | 4/23/43/43    | 0/2/2/2 |
| 31  | CLA  | 9     | 313 | 17   | 1/1/11/20 | 6/13/91/115   | -       |
| 31  | CLA  | B     | 816 | 2    | -         | 5/33/111/115  | -       |
| 36  | LUT  | 3     | 305 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 26  | BCR  | L     | 301 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 5     | 318 | 22   | 1/1/15/20 | 11/37/115/115 | -       |
| 31  | CLA  | 7     | 313 | 15   | 1/1/11/20 | 4/11/89/115   | -       |
| 26  | BCR  | B     | 803 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | B     | 849 | 2    | 1/1/12/20 | 4/19/97/115   | -       |
| 31  | CLA  | 2     | 313 | 20   | 1/1/11/20 | 8/15/93/115   | -       |
| 31  | CLA  | 8     | 313 | 28   | 1/1/11/20 | 6/15/93/115   | -       |
| 26  | BCR  | 3     | 302 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 26  | BCR  | A     | 803 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 31  | CLA  | F     | 306 | 44   | 1/1/12/20 | 2/19/97/115   | -       |
| 31  | CLA  | A     | 850 | 1    | 1/1/12/20 | 8/21/99/115   | -       |
| 31  | CLA  | 8     | 311 | 16   | 1/1/13/20 | 10/25/103/115 | -       |
| 31  | CLA  | O     | 202 | 19   | 1/1/9/20  | 1/4/78/115    | -       |
| 31  | CLA  | A     | 856 | 44   | 1/1/15/20 | 6/37/115/115  | -       |
| 32  | CHL  | 7     | 320 | 44   | 3/3/19/26 | 12/33/131/137 | -       |
| 31  | CLA  | B     | 833 | 44   | 1/1/13/20 | 7/25/103/115  | -       |
| 32  | CHL  | 9     | 322 | 44   | 3/3/16/26 | 4/17/115/137  | -       |
| 31  | CLA  | B     | 831 | 2    | -         | 6/19/97/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | 3     | 320 | 14   | 1/1/11/20 | 2/13/91/115   | -       |
| 32  | CHL  | a     | 318 | 44   | 2/2/16/26 | 6/18/116/137  | -       |
| 31  | CLA  | 8     | 307 | 16   | 1/1/11/20 | 3/15/93/115   | -       |
| 26  | BCR  | 7     | 304 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 33  | DGD  | B     | 808 | -    | -         | 22/50/90/95   | 0/2/2/2 |
| 31  | CLA  | 8     | 310 | 16   | 1/1/15/20 | 10/37/115/115 | -       |
| 31  | CLA  | 3     | 310 | 14   | 1/1/14/20 | 8/31/109/115  | -       |
| 32  | CHL  | 4     | 310 | -    | 2/2/16/26 | 6/17/115/137  | -       |
| 26  | BCR  | L     | 303 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 6     | 312 | 23   | 1/1/15/20 | 10/37/115/115 | -       |
| 31  | CLA  | 8     | 315 | 16   | 1/1/12/20 | 5/22/100/115  | -       |
| 31  | CLA  | 2     | 312 | 20   | 1/1/11/20 | 4/15/93/115   | -       |
| 31  | CLA  | 8     | 318 | 16   | 1/1/12/20 | 2/19/97/115   | -       |
| 31  | CLA  | B     | 811 | 2    | 1/1/15/20 | 6/37/115/115  | -       |
| 31  | CLA  | B     | 836 | 2    | -         | 6/37/115/115  | -       |
| 31  | CLA  | B     | 843 | 44   | 1/1/11/20 | 5/13/91/115   | -       |
| 31  | CLA  | 6     | 311 | 23   | 1/1/13/20 | 10/25/103/115 | -       |
| 31  | CLA  | 2     | 308 | 20   | 1/1/11/20 | 3/15/93/115   | -       |
| 31  | CLA  | 3     | 307 | 14   | 1/1/15/20 | 10/37/115/115 | -       |
| 31  | CLA  | a     | 311 | 44   | 1/1/14/20 | 9/31/109/115  | -       |
| 32  | CHL  | 8     | 316 | 44   | 3/3/20/26 | 12/39/137/137 | -       |
| 32  | CHL  | 6     | 309 | 23   | 3/3/20/26 | 18/39/137/137 | -       |
| 31  | CLA  | 4     | 309 | 21   | 1/1/14/20 | 10/31/109/115 | -       |
| 31  | CLA  | B     | 829 | 2    | -         | 5/25/103/115  | -       |
| 31  | CLA  | A     | 829 | -    | -         | 5/19/97/115   | -       |
| 32  | CHL  | 7     | 318 | 44   | 3/3/20/26 | 23/39/137/137 | -       |
| 26  | BCR  | B     | 804 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 857 | 44   | 1/1/15/20 | 14/37/115/115 | -       |
| 36  | LUT  | 6     | 303 | -    | -         | 18/29/67/67   | 0/2/2/2 |
| 26  | BCR  | F     | 302 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 36  | LUT  | 9     | 302 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 31  | CLA  | A     | 815 | -    | -         | 5/37/115/115  | -       |
| 26  | BCR  | G     | 203 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 32  | CHL  | 5     | 316 | 44   | 3/3/18/26 | 12/27/125/137 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 26  | BCR  | B     | 802 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 31  | CLA  | O     | 204 | -    | 1/1/10/20 | 2/8/86/115    | -       |
| 26  | BCR  | L     | 302 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 838 | 44   | 1/1/15/20 | 11/37/115/115 | -       |
| 31  | CLA  | 7     | 310 | 15   | 1/1/11/20 | 4/11/89/115   | -       |
| 31  | CLA  | A     | 844 | 1    | -         | 3/19/97/115   | -       |
| 36  | LUT  | 5     | 303 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 32  | CHL  | b     | 309 | 13   | 2/2/16/26 | 10/17/115/137 | -       |
| 31  | CLA  | 4     | 321 | 21   | 1/1/12/20 | 6/19/97/115   | -       |
| 31  | CLA  | 3     | 313 | -    | 1/1/14/20 | 10/31/109/115 | -       |
| 36  | LUT  | a     | 303 | -    | -         | 14/29/67/67   | 0/2/2/2 |
| 31  | CLA  | A     | 816 | 1    | 1/1/15/20 | 6/37/115/115  | -       |
| 31  | CLA  | 2     | 307 | 20   | 1/1/13/20 | 9/28/106/115  | -       |
| 31  | CLA  | 4     | 305 | -    | -         | 5/22/100/115  | -       |
| 30  | CL0  | A     | 813 | 1    | 1/1/20/25 | 7/37/135/135  | -       |
| 31  | CLA  | b     | 304 | 13   | 1/1/11/20 | 5/15/93/115   | -       |
| 31  | CLA  | 2     | 310 | 20   | 1/1/11/20 | 4/13/91/115   | -       |
| 31  | CLA  | A     | 848 | 1    | -         | 11/28/106/115 | -       |
| 42  | SQD  | 4     | 304 | -    | -         | 12/30/50/69   | 0/1/1/1 |
| 31  | CLA  | 5     | 313 | 28   | -         | 4/15/93/115   | -       |
| 31  | CLA  | 9     | 318 | 44   | 1/1/15/20 | 8/37/115/115  | -       |
| 31  | CLA  | B     | 840 | 2    | 1/1/15/20 | 12/37/115/115 | -       |
| 31  | CLA  | 6     | 313 | 23   | 1/1/11/20 | 5/15/93/115   | -       |
| 31  | CLA  | A     | 853 | 1    | -         | 10/37/115/115 | -       |
| 31  | CLA  | 9     | 316 | 17   | 1/1/12/20 | 5/19/97/115   | -       |
| 24  | PQN  | A     | 801 | -    | -         | 2/23/43/43    | 0/2/2/2 |
| 31  | CLA  | B     | 844 | 2    | 1/1/15/20 | 10/37/115/115 | -       |
| 31  | CLA  | 2     | 306 | 20   | 1/1/14/20 | 9/31/109/115  | -       |
| 31  | CLA  | B     | 815 | 2    | 1/1/15/20 | 15/37/115/115 | -       |
| 38  | AXT  | a     | 304 | -    | -         | 2/29/71/75    | 0/2/2/2 |
| 31  | CLA  | A     | 823 | 1    | -         | 7/25/103/115  | -       |
| 32  | CHL  | A     | 831 | 1    | 2/2/18/26 | 11/30/128/137 | -       |
| 31  | CLA  | A     | 826 | 1    | 1/1/15/20 | 14/37/115/115 | -       |
| 31  | CLA  | B     | 814 | 2    | 1/1/15/20 | 16/37/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | A     | 822 | 1    | -         | 9/25/103/115  | -       |
| 31  | CLA  | A     | 832 | 1    | -         | 6/37/115/115  | -       |
| 32  | CHL  | 6     | 320 | -    | 3/3/16/26 | 10/17/115/137 | -       |
| 31  | CLA  | B     | 824 | 2    | -         | 10/28/106/115 | -       |
| 36  | LUT  | 3     | 304 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 26  | BCR  | M     | 101 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 814 | 44   | 1/1/15/20 | 10/37/115/115 | -       |
| 32  | CHL  | 6     | 318 | 44   | 3/3/16/26 | 9/15/113/137  | -       |
| 36  | LUT  | 8     | 302 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 32  | CHL  | a     | 320 | 44   | 3/3/16/26 | 7/18/116/137  | -       |
| 26  | BCR  | 3     | 303 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 8     | 317 | 44   | -         | 2/19/97/115   | -       |
| 32  | CHL  | A     | 840 | 1    | 2/2/20/26 | 13/39/137/137 | -       |
| 31  | CLA  | b     | 310 | -    | 1/1/11/20 | 6/15/93/115   | -       |
| 31  | CLA  | B     | 822 | 2    | 1/1/15/20 | 17/37/115/115 | -       |
| 31  | CLA  | F     | 301 | 44   | 1/1/15/20 | 7/37/115/115  | -       |
| 32  | CHL  | 7     | 319 | 15   | 3/3/16/26 | 1/17/115/137  | -       |
| 26  | BCR  | 8     | 301 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 27  | LMT  | 9     | 306 | -    | -         | 10/21/61/61   | 0/2/2/2 |
| 31  | CLA  | B     | 820 | 2    | -         | 11/37/115/115 | -       |
| 31  | CLA  | 5     | 309 | 22   | -         | 5/16/94/115   | -       |
| 31  | CLA  | A     | 852 | 1    | -         | 2/21/99/115   | -       |
| 31  | CLA  | b     | 313 | 13   | 1/1/14/20 | 12/31/109/115 | -       |
| 31  | CLA  | L     | 307 | 36   | 1/1/11/20 | 7/13/91/115   | -       |
| 31  | CLA  | B     | 825 | 2    | -         | 8/31/109/115  | -       |
| 31  | CLA  | a     | 309 | 13   | 1/1/14/20 | 6/31/109/115  | -       |
| 32  | CHL  | 5     | 322 | 22   | 3/3/16/26 | 5/17/115/137  | -       |
| 28  | LHG  | 7     | 302 | -    | -         | 32/53/53/53   | -       |
| 31  | CLA  | A     | 836 | 1    | -         | 6/31/109/115  | -       |
| 31  | CLA  | a     | 316 | 13   | -         | 9/13/91/115   | -       |
| 31  | CLA  | b     | 311 | 13   | 1/1/11/20 | 5/15/93/115   | -       |
| 31  | CLA  | G     | 204 | 7    | 1/1/12/20 | 5/19/97/115   | -       |
| 28  | LHG  | A     | 809 | -    | -         | 20/46/46/53   | -       |
| 26  | BCR  | B     | 805 | -    | -         | 7/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 28  | LHG  | 7     | 307 | 31   | -         | 21/41/41/53   | -       |
| 31  | CLA  | A     | 845 | 1    | -         | 7/27/105/115  | -       |
| 32  | CHL  | 4     | 313 | 21   | 2/2/16/26 | 8/18/116/137  | -       |
| 31  | CLA  | A     | 824 | 1,31 | 1/1/14/20 | 8/34/112/115  | -       |
| 31  | CLA  | b     | 305 | 13   | 1/1/11/20 | 6/15/93/115   | -       |
| 26  | BCR  | 3     | 301 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 854 | 28   | 1/1/11/20 | 6/15/93/115   | -       |
| 31  | CLA  | b     | 308 | 13   | -         | 5/15/93/115   | -       |
| 36  | LUT  | J     | 103 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 31  | CLA  | B     | 826 | 2    | -         | 9/19/97/115   | -       |
| 31  | CLA  | b     | 306 | -    | -         | 5/15/93/115   | -       |
| 31  | CLA  | 5     | 312 | 44   | 1/1/12/20 | 8/19/97/115   | -       |
| 31  | CLA  | 6     | 322 | 23   | -         | 5/15/93/115   | -       |
| 31  | CLA  | 8     | 321 | 16   | 1/1/11/20 | 3/15/93/115   | -       |
| 31  | CLA  | a     | 312 | 13   | 1/1/15/20 | 13/37/115/115 | -       |
| 35  | QTB  | 9     | 304 | -    | -         | 6/11/28/28    | 0/1/1/1 |
| 31  | CLA  | A     | 849 | 1    | 1/1/11/20 | 7/15/93/115   | -       |
| 32  | CHL  | 8     | 319 | 44   | 3/3/15/26 | 3/14/112/137  | -       |
| 28  | LHG  | A     | 810 | 31   | -         | 18/46/46/53   | -       |
| 31  | CLA  | B     | 827 | 2    | 1/1/14/20 | 9/31/109/115  | -       |
| 31  | CLA  | H     | 903 | 18   | -         | 5/15/93/115   | -       |
| 31  | CLA  | b     | 307 | -    | 1/1/11/20 | 5/15/93/115   | -       |
| 31  | CLA  | J     | 105 | 10   | 1/1/10/20 | 4/10/88/115   | -       |
| 31  | CLA  | B     | 841 | 2    | -         | 10/25/103/115 | -       |
| 31  | CLA  | G     | 205 | 7    | 1/1/11/20 | 6/15/93/115   | -       |
| 32  | CHL  | A     | 839 | 44   | 2/2/18/26 | 6/27/125/137  | -       |
| 36  | LUT  | F     | 304 | -    | -         | 17/29/67/67   | 0/2/2/2 |
| 31  | CLA  | 5     | 314 | 22   | -         | 5/13/91/115   | -       |
| 36  | LUT  | 4     | 303 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 31  | CLA  | A     | 833 | 1    | -         | 7/16/94/115   | -       |
| 31  | CLA  | 5     | 307 | 22   | 1/1/13/20 | 5/25/103/115  | -       |
| 34  | LAP  | B     | 851 | -    | -         | 16/30/30/30   | -       |
| 31  | CLA  | 7     | 316 | 15   | 1/1/11/20 | 3/15/93/115   | -       |
| 31  | CLA  | A     | 830 | 1    | -         | 11/31/109/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | B     | 839 | 2    | -         | 10/31/109/115 | -       |
| 31  | CLA  | B     | 850 | 2    | -         | 6/34/112/115  | -       |
| 31  | CLA  | 2     | 304 | 20   | -         | 11/15/93/115  | -       |
| 31  | CLA  | 3     | 308 | 14   | 1/1/11/20 | 5/15/93/115   | -       |
| 32  | CHL  | 3     | 315 | 44   | 2/2/18/26 | 7/27/125/137  | -       |
| 31  | CLA  | 3     | 314 | 14   | -         | 7/22/100/115  | -       |
| 31  | CLA  | L     | 306 | 44   | -         | 4/13/91/115   | -       |
| 37  | LMG  | J     | 101 | -    | -         | 20/44/64/70   | 0/1/1/1 |
| 31  | CLA  | K     | 204 | 44   | -         | 3/19/97/115   | -       |
| 31  | CLA  | 6     | 314 | 23   | -         | 4/16/94/115   | -       |
| 31  | CLA  | 6     | 306 | 23   | -         | 5/15/93/115   | -       |
| 32  | CHL  | 5     | 317 | 44   | 2/2/16/26 | 6/17/115/137  | -       |
| 32  | CHL  | 6     | 317 | 23   | 2/2/16/26 | 8/17/115/137  | -       |
| 31  | CLA  | 3     | 312 | 44   | 1/1/15/20 | 9/37/115/115  | -       |
| 31  | CLA  | 5     | 311 | 22   | 1/1/11/20 | 5/15/93/115   | -       |
| 31  | CLA  | B     | 832 | 44   | 1/1/15/20 | 9/37/115/115  | -       |
| 31  | CLA  | B     | 837 | 2    | -         | 6/25/103/115  | -       |
| 26  | BCR  | B     | 806 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 31  | CLA  | B     | 846 | 44   | -         | 8/37/115/115  | -       |
| 36  | LUT  | 4     | 302 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 32  | CHL  | 6     | 321 | 23   | 3/3/15/26 | 7/12/110/137  | -       |
| 31  | CLA  | A     | 820 | 1    | -         | 4/25/103/115  | -       |
| 43  | PTY  | 5     | 306 | -    | -         | 17/34/34/53   | -       |
| 31  | CLA  | 7     | 322 | 15   | 1/1/11/20 | 4/15/93/115   | -       |
| 31  | CLA  | B     | 838 | 2    | -         | 3/15/93/115   | -       |
| 32  | CHL  | 6     | 319 | -    | 1/1/16/26 | 6/17/115/137  | -       |
| 31  | CLA  | B     | 812 | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 31  | CLA  | A     | 827 | 1    | -         | 9/25/103/115  | -       |
| 36  | LUT  | b     | 301 | -    | -         | 14/29/67/67   | 0/2/2/2 |
| 31  | CLA  | 6     | 310 | 23   | 1/1/11/20 | 4/16/94/115   | -       |
| 26  | BCR  | 6     | 302 | -    | -         | 15/29/63/63   | 0/2/2/2 |
| 31  | CLA  | B     | 848 | 28   | 1/1/15/20 | 9/37/115/115  | -       |
| 26  | BCR  | 2     | 302 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 2     | 315 | 44   | 1/1/11/20 | 6/15/93/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | B     | 818 | 2    | 1/1/13/20 | 5/25/103/115  | -       |
| 31  | CLA  | A     | 835 | 1    | -         | 5/25/103/115  | -       |
| 32  | CHL  | 7     | 317 | 15   | 3/3/18/26 | 10/29/127/137 | -       |
| 31  | CLA  | A     | 821 | 1    | 1/1/15/20 | 12/37/115/115 | -       |
| 26  | BCR  | J     | 102 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 26  | BCR  | A     | 805 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 31  | CLA  | F     | 305 | 6    | 1/1/11/20 | 4/15/93/115   | -       |
| 36  | LUT  | 8     | 303 | -    | -         | 14/29/67/67   | 0/2/2/2 |
| 35  | QTB  | 7     | 303 | -    | -         | 10/11/28/28   | 1/1/1/1 |
| 31  | CLA  | A     | 842 | 1    | -         | 5/37/115/115  | -       |
| 35  | QTB  | a     | 302 | -    | -         | 5/11/28/28    | 0/1/1/1 |
| 31  | CLA  | 4     | 308 | 21   | 1/1/14/20 | 8/31/109/115  | -       |
| 28  | LHG  | 5     | 305 | 31   | -         | 24/39/39/53   | -       |
| 31  | CLA  | B     | 813 | 2    | -         | 8/37/115/115  | -       |
| 31  | CLA  | a     | 319 | 13   | 1/1/15/20 | 11/37/115/115 | -       |
| 36  | LUT  | 5     | 304 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 31  | CLA  | 8     | 309 | 16   | 1/1/12/20 | 6/19/97/115   | -       |
| 31  | CLA  | 4     | 312 | 21   | 1/1/11/20 | 7/16/94/115   | -       |
| 31  | CLA  | 2     | 314 | 20   | 1/1/11/20 | 2/15/93/115   | -       |
| 31  | CLA  | 7     | 314 | 44   | -         | 7/23/101/115  | -       |
| 31  | CLA  | 6     | 307 | 23   | 1/1/12/20 | 5/19/97/115   | -       |
| 31  | CLA  | A     | 817 | 1,31 | 1/1/13/20 | 6/25/103/115  | -       |
| 31  | CLA  | G     | 206 | 44   | 1/1/11/20 | 2/13/91/115   | -       |
| 31  | CLA  | 4     | 316 | -    | -         | 6/16/94/115   | -       |
| 33  | DGD  | 7     | 308 | -    | -         | 14/41/81/95   | 0/2/2/2 |
| 32  | CHL  | 9     | 320 | 44   | 3/3/16/26 | 7/18/116/137  | -       |
| 31  | CLA  | 5     | 320 | 22   | -         | 3/15/93/115   | -       |
| 31  | CLA  | 8     | 314 | 44   | 1/1/12/20 | 4/22/100/115  | -       |
| 31  | CLA  | 4     | 320 | 21   | 1/1/11/20 | 7/13/91/115   | -       |
| 26  | BCR  | K     | 202 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 26  | BCR  | A     | 804 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 31  | CLA  | a     | 315 | 28   | 1/1/13/20 | 7/25/103/115  | -       |
| 31  | CLA  | B     | 830 | 2    | -         | 7/31/109/115  | -       |
| 31  | CLA  | 3     | 311 | 14   | 1/1/15/20 | 11/37/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | b     | 312 | 13   | -         | 3/15/93/115   | -       |
| 31  | CLA  | 7     | 321 | 44   | -         | 7/16/94/115   | -       |
| 37  | LMG  | a     | 301 | -    | -         | 21/37/57/70   | 0/1/1/1 |
| 31  | CLA  | B     | 817 | 2    | 1/1/15/20 | 11/37/115/115 | -       |
| 31  | CLA  | b     | 303 | -    | 1/1/11/20 | 5/15/93/115   | -       |
| 31  | CLA  | B     | 823 | 2    | 1/1/13/20 | 9/25/103/115  | -       |
| 31  | CLA  | A     | 855 | 1    | -         | 13/37/115/115 | -       |
| 31  | CLA  | 2     | 305 | 20   | 1/1/11/20 | 5/13/91/115   | -       |
| 36  | LUT  | 9     | 303 | -    | -         | 16/29/67/67   | 0/2/2/2 |
| 31  | CLA  | B     | 821 | 2    | -         | 4/29/107/115  | -       |
| 26  | BCR  | 5     | 302 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 31  | CLA  | 9     | 317 | -    | -         | 6/16/94/115   | -       |
| 31  | CLA  | B     | 819 | 2    | 1/1/15/20 | 6/37/115/115  | -       |
| 31  | CLA  | A     | 834 | 44   | 1/1/15/20 | 10/37/115/115 | -       |
| 32  | CHL  | K     | 201 | 11   | 3/3/16/26 | 7/17/115/137  | -       |
| 37  | LMG  | J     | 104 | -    | -         | 11/24/44/70   | 0/1/1/1 |
| 31  | CLA  | A     | 818 | 1    | 1/1/15/20 | 10/37/115/115 | -       |
| 28  | LHG  | 6     | 301 | 31   | -         | 16/31/31/53   | -       |
| 31  | CLA  | 4     | 307 | 21   | 1/1/13/20 | 8/27/105/115  | -       |
| 31  | CLA  | b     | 302 | 13   | 1/1/11/20 | 6/15/93/115   | -       |
| 28  | LHG  | A     | 811 | -    | -         | 19/53/53/53   | -       |
| 32  | CHL  | 7     | 324 | 16   | 2/2/20/26 | 14/39/137/137 | -       |
| 25  | SF4  | C     | 101 | 3    | -         | -             | 0/6/5/5 |
| 36  | LUT  | 9     | 305 | -    | -         | 18/29/67/67   | 0/2/2/2 |
| 31  | CLA  | 7     | 309 | 15   | 1/1/14/20 | 4/31/109/115  | -       |
| 31  | CLA  | 3     | 309 | 14   | 1/1/15/20 | 14/37/115/115 | -       |
| 31  | CLA  | B     | 834 | 2    | 1/1/15/20 | 5/37/115/115  | -       |
| 31  | CLA  | 5     | 308 | 22   | 1/1/11/20 | 2/15/93/115   | -       |
| 31  | CLA  | H     | 902 | 44   | 1/1/11/20 | 3/15/93/115   | -       |
| 40  | XAT  | 7     | 306 | -    | -         | 4/31/93/93    | 0/4/4/4 |
| 31  | CLA  | 9     | 314 | 17   | 1/1/14/20 | 10/31/109/115 | -       |
| 28  | LHG  | B     | 807 | 31   | -         | 7/36/36/53    | -       |
| 32  | CHL  | 4     | 317 | -    | 3/3/16/26 | 10/15/113/137 | -       |
| 31  | CLA  | B     | 847 | 2    | -         | 9/37/115/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 31  | CLA  | a     | 322 | 13   | 1/1/11/20 | 6/15/93/115   | -       |
| 31  | CLA  | 2     | 311 | 20   | 1/1/11/20 | 6/13/91/115   | -       |
| 31  | CLA  | A     | 841 | 1    | 1/1/15/20 | 13/37/115/115 | -       |
| 31  | CLA  | A     | 851 | 1    | 1/1/15/20 | 9/37/115/115  | -       |
| 31  | CLA  | 5     | 323 | 22   | 1/1/13/20 | 9/27/105/115  | -       |
| 36  | LUT  | 2     | 301 | -    | -         | 13/29/67/67   | 0/2/2/2 |
| 26  | BCR  | A     | 806 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 31  | CLA  | 9     | 321 | 17   | 1/1/13/20 | 12/27/105/115 | -       |
| 28  | LHG  | 6     | 305 | 31   | -         | 8/36/36/53    | -       |
| 31  | CLA  | 6     | 315 | 28   | 1/1/11/20 | 3/15/93/115   | -       |
| 26  | BCR  | I     | 801 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 31  | CLA  | A     | 825 | 1    | -         | 2/24/102/115  | -       |
| 31  | CLA  | 8     | 308 | 16   | 1/1/15/20 | 13/37/115/115 | -       |
| 31  | CLA  | 7     | 312 | 15   | 1/1/14/20 | 11/34/112/115 | -       |

All (5056) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 31  | 2     | 310 | CLA  | MG-NA | 30.68  | 2.79        | 2.06     |
| 31  | b     | 307 | CLA  | MG-NA | 29.70  | 2.76        | 2.06     |
| 31  | 6     | 315 | CLA  | MG-NA | 29.56  | 2.76        | 2.06     |
| 31  | 5     | 318 | CLA  | MG-ND | -28.84 | 1.48        | 2.05     |
| 31  | 9     | 319 | CLA  | MG-NA | 28.29  | 2.73        | 2.06     |
| 31  | 4     | 311 | CLA  | MG-ND | -26.69 | 1.52        | 2.05     |
| 31  | 2     | 311 | CLA  | MG-NA | 25.66  | 2.67        | 2.06     |
| 31  | 4     | 311 | CLA  | MG-NA | 23.77  | 2.62        | 2.06     |
| 31  | 5     | 320 | CLA  | MG-NC | 23.37  | 2.61        | 2.06     |
| 31  | 6     | 314 | CLA  | MG-NA | 22.99  | 2.60        | 2.06     |
| 31  | 2     | 305 | CLA  | MG-NA | 22.11  | 2.58        | 2.06     |
| 31  | 5     | 315 | CLA  | MG-ND | -21.91 | 1.62        | 2.05     |
| 32  | 6     | 319 | CHL  | MG-NA | 21.90  | 2.58        | 2.06     |
| 31  | 4     | 315 | CLA  | MG-ND | -21.88 | 1.62        | 2.05     |
| 31  | 9     | 311 | CLA  | MG-ND | -21.75 | 1.62        | 2.05     |
| 31  | 6     | 316 | CLA  | MG-NA | 21.34  | 2.57        | 2.06     |
| 31  | 2     | 310 | CLA  | MG-ND | 20.99  | 2.47        | 2.05     |
| 31  | 2     | 314 | CLA  | MG-ND | -20.98 | 1.64        | 2.05     |
| 31  | L     | 307 | CLA  | MG-NA | 20.83  | 2.55        | 2.06     |
| 31  | 4     | 319 | CLA  | MG-NA | 20.75  | 2.55        | 2.06     |
| 31  | a     | 309 | CLA  | MG-ND | -20.29 | 1.65        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | 6     | 307 | CLA  | MG-NA   | 19.39  | 2.52        | 2.06     |
| 31  | H     | 902 | CLA  | MG-NA   | 19.39  | 2.52        | 2.06     |
| 31  | a     | 309 | CLA  | MG-NA   | 19.29  | 2.52        | 2.06     |
| 32  | 4     | 313 | CHL  | MG-NC   | 19.09  | 2.51        | 2.06     |
| 31  | b     | 312 | CLA  | MG-ND   | 19.04  | 2.43        | 2.05     |
| 31  | 6     | 311 | CLA  | MG-NA   | 18.85  | 2.51        | 2.06     |
| 31  | 7     | 315 | CLA  | MG-NA   | 18.75  | 2.50        | 2.06     |
| 31  | 5     | 307 | CLA  | MG-ND   | -18.32 | 1.69        | 2.05     |
| 31  | a     | 314 | CLA  | MG-NC   | 17.92  | 2.48        | 2.06     |
| 32  | 6     | 321 | CHL  | MG-NA   | 17.65  | 2.48        | 2.06     |
| 31  | 6     | 310 | CLA  | MG-ND   | 17.47  | 2.40        | 2.05     |
| 31  | B     | 834 | CLA  | MG-NA   | 17.28  | 2.47        | 2.06     |
| 36  | 9     | 305 | LUT  | C24-C25 | 17.28  | 1.54        | 1.33     |
| 31  | 3     | 320 | CLA  | MG-NA   | 17.26  | 2.47        | 2.06     |
| 31  | 9     | 313 | CLA  | MG-NA   | 17.23  | 2.47        | 2.06     |
| 31  | 9     | 318 | CLA  | MG-NA   | 17.18  | 2.47        | 2.06     |
| 36  | 8     | 303 | LUT  | C24-C25 | 16.98  | 1.54        | 1.33     |
| 36  | a     | 305 | LUT  | C24-C25 | 16.97  | 1.54        | 1.33     |
| 36  | 6     | 303 | LUT  | C24-C25 | 16.93  | 1.54        | 1.33     |
| 36  | a     | 303 | LUT  | C24-C25 | 16.91  | 1.54        | 1.33     |
| 36  | 3     | 305 | LUT  | C24-C25 | 16.86  | 1.54        | 1.33     |
| 36  | 4     | 302 | LUT  | C24-C25 | 16.85  | 1.54        | 1.33     |
| 31  | 5     | 321 | CLA  | MG-NC   | 16.81  | 2.46        | 2.06     |
| 36  | J     | 103 | LUT  | C24-C25 | 16.80  | 1.54        | 1.33     |
| 32  | 6     | 319 | CHL  | MG-NC   | -16.72 | 1.66        | 2.06     |
| 31  | 5     | 320 | CLA  | MG-ND   | -16.69 | 1.72        | 2.05     |
| 36  | 5     | 303 | LUT  | C24-C25 | 16.66  | 1.53        | 1.33     |
| 36  | b     | 301 | LUT  | C24-C25 | 16.66  | 1.53        | 1.33     |
| 36  | 7     | 305 | LUT  | C24-C25 | 16.63  | 1.53        | 1.33     |
| 31  | 8     | 313 | CLA  | MG-NA   | 16.63  | 2.45        | 2.06     |
| 36  | F     | 304 | LUT  | C24-C25 | 16.63  | 1.53        | 1.33     |
| 31  | 3     | 308 | CLA  | MG-NA   | 16.62  | 2.45        | 2.06     |
| 31  | b     | 306 | CLA  | MG-NA   | 16.60  | 2.45        | 2.06     |
| 31  | 9     | 311 | CLA  | MG-NA   | 16.60  | 2.45        | 2.06     |
| 36  | 9     | 302 | LUT  | C24-C25 | 16.59  | 1.53        | 1.33     |
| 36  | 8     | 302 | LUT  | C24-C25 | 16.59  | 1.53        | 1.33     |
| 36  | 4     | 303 | LUT  | C24-C25 | 16.56  | 1.53        | 1.33     |
| 36  | L     | 304 | LUT  | C24-C25 | 16.55  | 1.53        | 1.33     |
| 31  | a     | 312 | CLA  | MG-NA   | 16.54  | 2.45        | 2.06     |
| 36  | 5     | 304 | LUT  | C24-C25 | 16.50  | 1.53        | 1.33     |
| 31  | 5     | 323 | CLA  | MG-NA   | 16.41  | 2.45        | 2.06     |
| 36  | 9     | 303 | LUT  | C24-C25 | 16.38  | 1.53        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | A     | 852 | CLA  | MG-NC   | 16.38  | 2.45        | 2.06     |
| 36  | 3     | 304 | LUT  | C24-C25 | 16.37  | 1.53        | 1.33     |
| 31  | 4     | 314 | CLA  | MG-ND   | -16.37 | 1.73        | 2.05     |
| 36  | 6     | 304 | LUT  | C24-C25 | 16.36  | 1.53        | 1.33     |
| 31  | 3     | 318 | CLA  | MG-NA   | 16.31  | 2.45        | 2.06     |
| 31  | B     | 835 | CLA  | MG-NA   | 16.24  | 2.44        | 2.06     |
| 36  | 2     | 301 | LUT  | C24-C25 | 16.23  | 1.53        | 1.33     |
| 32  | 5     | 319 | CHL  | MG-NC   | 16.19  | 2.44        | 2.06     |
| 31  | 6     | 312 | CLA  | MG-NA   | 16.11  | 2.44        | 2.06     |
| 31  | K     | 204 | CLA  | MG-NC   | 15.99  | 2.44        | 2.06     |
| 31  | 7     | 316 | CLA  | MG-NA   | 15.73  | 2.43        | 2.06     |
| 31  | 7     | 321 | CLA  | MG-NA   | 15.62  | 2.43        | 2.06     |
| 31  | 3     | 317 | CLA  | MG-NC   | 15.61  | 2.43        | 2.06     |
| 31  | 6     | 316 | CLA  | MG-ND   | 15.45  | 2.36        | 2.05     |
| 31  | 5     | 309 | CLA  | MG-NA   | 15.24  | 2.42        | 2.06     |
| 31  | 2     | 312 | CLA  | MG-NA   | 15.07  | 2.42        | 2.06     |
| 31  | a     | 322 | CLA  | MG-NA   | 15.01  | 2.41        | 2.06     |
| 31  | 3     | 314 | CLA  | MG-NA   | 14.95  | 2.41        | 2.06     |
| 31  | A     | 844 | CLA  | MG-NC   | 14.93  | 2.41        | 2.06     |
| 31  | b     | 306 | CLA  | MG-ND   | 14.92  | 2.35        | 2.05     |
| 31  | 2     | 315 | CLA  | MG-NC   | 14.78  | 2.41        | 2.06     |
| 31  | K     | 205 | CLA  | MG-NA   | 14.71  | 2.41        | 2.06     |
| 31  | A     | 843 | CLA  | MG-NA   | 14.68  | 2.41        | 2.06     |
| 31  | B     | 816 | CLA  | MG-NC   | 14.66  | 2.41        | 2.06     |
| 31  | 2     | 306 | CLA  | MG-ND   | -14.56 | 1.76        | 2.05     |
| 31  | 4     | 320 | CLA  | MG-NC   | 14.55  | 2.40        | 2.06     |
| 31  | 9     | 314 | CLA  | MG-ND   | -14.48 | 1.77        | 2.05     |
| 31  | 4     | 306 | CLA  | MG-NA   | 14.47  | 2.40        | 2.06     |
| 31  | 3     | 312 | CLA  | MG-NA   | 14.44  | 2.40        | 2.06     |
| 31  | 3     | 311 | CLA  | MG-NA   | 14.42  | 2.40        | 2.06     |
| 31  | 3     | 313 | CLA  | MG-NA   | 14.27  | 2.40        | 2.06     |
| 31  | a     | 310 | CLA  | MG-NA   | 14.22  | 2.40        | 2.06     |
| 31  | A     | 824 | CLA  | MG-NA   | 14.09  | 2.39        | 2.06     |
| 36  | 4     | 303 | LUT  | C30-C29 | 14.08  | 1.54        | 1.35     |
| 36  | b     | 301 | LUT  | C14-C13 | 14.01  | 1.54        | 1.35     |
| 36  | a     | 305 | LUT  | C30-C29 | 13.99  | 1.54        | 1.35     |
| 31  | 7     | 310 | CLA  | MG-NA   | 13.91  | 2.39        | 2.06     |
| 31  | B     | 849 | CLA  | MG-NC   | 13.91  | 2.39        | 2.06     |
| 36  | 5     | 304 | LUT  | C14-C13 | 13.88  | 1.54        | 1.35     |
| 36  | b     | 301 | LUT  | C30-C29 | 13.88  | 1.54        | 1.35     |
| 36  | 2     | 301 | LUT  | C30-C29 | 13.86  | 1.54        | 1.35     |
| 31  | K     | 206 | CLA  | MG-NA   | 13.86  | 2.39        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | a     | 316 | CLA  | MG-NA   | 13.85  | 2.39        | 2.06     |
| 36  | 6     | 304 | LUT  | C30-C29 | 13.84  | 1.54        | 1.35     |
| 31  | A     | 827 | CLA  | MG-NA   | 13.83  | 2.39        | 2.06     |
| 36  | 9     | 305 | LUT  | C30-C29 | 13.83  | 1.54        | 1.35     |
| 36  | 6     | 304 | LUT  | C14-C13 | 13.81  | 1.54        | 1.35     |
| 31  | 5     | 310 | CLA  | MG-NA   | 13.80  | 2.39        | 2.06     |
| 31  | 9     | 314 | CLA  | MG-NA   | 13.79  | 2.39        | 2.06     |
| 31  | 2     | 304 | CLA  | MG-NA   | 13.76  | 2.39        | 2.06     |
| 31  | 8     | 309 | CLA  | MG-NA   | 13.76  | 2.38        | 2.06     |
| 36  | 3     | 305 | LUT  | C30-C29 | 13.75  | 1.54        | 1.35     |
| 36  | 9     | 303 | LUT  | C14-C13 | 13.74  | 1.54        | 1.35     |
| 36  | 9     | 303 | LUT  | C30-C29 | 13.72  | 1.54        | 1.35     |
| 31  | b     | 307 | CLA  | MG-NC   | -13.69 | 1.73        | 2.06     |
| 31  | a     | 321 | CLA  | MG-NA   | 13.68  | 2.38        | 2.06     |
| 36  | 4     | 302 | LUT  | C10-C9  | 13.68  | 1.53        | 1.35     |
| 36  | 9     | 305 | LUT  | C34-C33 | 13.65  | 1.53        | 1.35     |
| 36  | 4     | 303 | LUT  | C14-C13 | 13.64  | 1.53        | 1.35     |
| 31  | 9     | 316 | CLA  | MG-NC   | 13.63  | 2.38        | 2.06     |
| 36  | 4     | 303 | LUT  | C10-C9  | 13.63  | 1.53        | 1.35     |
| 31  | 5     | 313 | CLA  | MG-NC   | 13.61  | 2.38        | 2.06     |
| 31  | b     | 304 | CLA  | MG-ND   | 13.61  | 2.32        | 2.05     |
| 36  | 4     | 302 | LUT  | C30-C29 | 13.61  | 1.53        | 1.35     |
| 36  | J     | 103 | LUT  | C30-C29 | 13.61  | 1.53        | 1.35     |
| 31  | b     | 313 | CLA  | MG-NC   | 13.61  | 2.38        | 2.06     |
| 36  | 6     | 304 | LUT  | C10-C9  | 13.60  | 1.53        | 1.35     |
| 36  | 6     | 303 | LUT  | C30-C29 | 13.60  | 1.53        | 1.35     |
| 36  | 8     | 303 | LUT  | C14-C13 | 13.60  | 1.53        | 1.35     |
| 36  | a     | 305 | LUT  | C10-C9  | 13.59  | 1.53        | 1.35     |
| 36  | b     | 301 | LUT  | C34-C33 | 13.59  | 1.53        | 1.35     |
| 36  | J     | 103 | LUT  | C10-C9  | 13.59  | 1.53        | 1.35     |
| 36  | 9     | 303 | LUT  | C10-C9  | 13.58  | 1.53        | 1.35     |
| 36  | L     | 304 | LUT  | C30-C29 | 13.57  | 1.53        | 1.35     |
| 36  | J     | 103 | LUT  | C14-C13 | 13.55  | 1.53        | 1.35     |
| 36  | 6     | 303 | LUT  | C14-C13 | 13.55  | 1.53        | 1.35     |
| 36  | 3     | 304 | LUT  | C10-C9  | 13.54  | 1.53        | 1.35     |
| 36  | 8     | 303 | LUT  | C10-C9  | 13.54  | 1.53        | 1.35     |
| 36  | 5     | 303 | LUT  | C14-C13 | 13.54  | 1.53        | 1.35     |
| 31  | A     | 821 | CLA  | MG-NA   | 13.53  | 2.38        | 2.06     |
| 36  | 5     | 304 | LUT  | C10-C9  | 13.51  | 1.53        | 1.35     |
| 36  | L     | 304 | LUT  | C10-C9  | 13.51  | 1.53        | 1.35     |
| 31  | 3     | 307 | CLA  | MG-ND   | -13.50 | 1.79        | 2.05     |
| 36  | a     | 303 | LUT  | C10-C9  | 13.49  | 1.53        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | a     | 305 | LUT  | C34-C33 | 13.49 | 1.53        | 1.35     |
| 31  | A     | 820 | CLA  | MG-NC   | 13.48 | 2.38        | 2.06     |
| 36  | 9     | 305 | LUT  | C10-C9  | 13.48 | 1.53        | 1.35     |
| 36  | a     | 305 | LUT  | C14-C13 | 13.46 | 1.53        | 1.35     |
| 31  | 9     | 313 | CLA  | MG-ND   | 13.45 | 2.32        | 2.05     |
| 36  | 5     | 303 | LUT  | C10-C9  | 13.45 | 1.53        | 1.35     |
| 36  | 5     | 304 | LUT  | C30-C29 | 13.45 | 1.53        | 1.35     |
| 31  | A     | 842 | CLA  | MG-NA   | 13.43 | 2.38        | 2.06     |
| 36  | 8     | 303 | LUT  | C30-C29 | 13.42 | 1.53        | 1.35     |
| 32  | 6     | 320 | CHL  | MG-NA   | 13.42 | 2.38        | 2.06     |
| 36  | a     | 303 | LUT  | C30-C29 | 13.39 | 1.53        | 1.35     |
| 36  | a     | 303 | LUT  | C14-C13 | 13.39 | 1.53        | 1.35     |
| 36  | b     | 301 | LUT  | C10-C9  | 13.37 | 1.53        | 1.35     |
| 36  | L     | 304 | LUT  | C14-C13 | 13.36 | 1.53        | 1.35     |
| 36  | 7     | 305 | LUT  | C30-C29 | 13.34 | 1.53        | 1.35     |
| 36  | 4     | 303 | LUT  | C34-C33 | 13.34 | 1.53        | 1.35     |
| 31  | 2     | 313 | CLA  | MG-NC   | 13.33 | 2.37        | 2.06     |
| 36  | 4     | 302 | LUT  | C14-C13 | 13.33 | 1.53        | 1.35     |
| 36  | J     | 103 | LUT  | C34-C33 | 13.31 | 1.53        | 1.35     |
| 36  | L     | 304 | LUT  | C34-C33 | 13.31 | 1.53        | 1.35     |
| 36  | 3     | 304 | LUT  | C5-C6   | 13.28 | 1.57        | 1.34     |
| 36  | 9     | 302 | LUT  | C34-C33 | 13.28 | 1.53        | 1.35     |
| 36  | 3     | 304 | LUT  | C14-C13 | 13.26 | 1.53        | 1.35     |
| 31  | B     | 824 | CLA  | MG-NA   | 13.26 | 2.37        | 2.06     |
| 36  | 7     | 305 | LUT  | C5-C6   | 13.25 | 1.57        | 1.34     |
| 36  | 6     | 303 | LUT  | C10-C9  | 13.25 | 1.53        | 1.35     |
| 36  | 3     | 304 | LUT  | C30-C29 | 13.25 | 1.53        | 1.35     |
| 31  | 2     | 308 | CLA  | MG-NC   | 13.24 | 2.37        | 2.06     |
| 36  | 2     | 301 | LUT  | C14-C13 | 13.24 | 1.53        | 1.35     |
| 36  | 8     | 302 | LUT  | C14-C13 | 13.24 | 1.53        | 1.35     |
| 36  | 9     | 302 | LUT  | C30-C29 | 13.20 | 1.53        | 1.35     |
| 36  | 5     | 303 | LUT  | C30-C29 | 13.20 | 1.53        | 1.35     |
| 36  | 9     | 302 | LUT  | C10-C9  | 13.18 | 1.53        | 1.35     |
| 36  | 9     | 305 | LUT  | C14-C13 | 13.18 | 1.53        | 1.35     |
| 32  | 6     | 318 | CHL  | MG-NA   | 13.18 | 2.37        | 2.06     |
| 36  | 6     | 304 | LUT  | C34-C33 | 13.17 | 1.53        | 1.35     |
| 36  | 8     | 302 | LUT  | C34-C33 | 13.16 | 1.53        | 1.35     |
| 36  | 3     | 305 | LUT  | C14-C13 | 13.14 | 1.53        | 1.35     |
| 36  | 3     | 305 | LUT  | C10-C9  | 13.13 | 1.53        | 1.35     |
| 36  | 7     | 305 | LUT  | C10-C9  | 13.13 | 1.53        | 1.35     |
| 36  | 2     | 301 | LUT  | C10-C9  | 13.13 | 1.53        | 1.35     |
| 36  | 4     | 302 | LUT  | C34-C33 | 13.12 | 1.53        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 31  | B     | 820 | CLA  | MG-NA   | 13.12  | 2.37        | 2.06     |
| 31  | 8     | 307 | CLA  | MG-NA   | 13.10  | 2.37        | 2.06     |
| 36  | 8     | 302 | LUT  | C10-C9  | 13.07  | 1.53        | 1.35     |
| 36  | F     | 304 | LUT  | C30-C29 | 13.06  | 1.53        | 1.35     |
| 36  | a     | 303 | LUT  | C34-C33 | 13.02  | 1.53        | 1.35     |
| 36  | 7     | 305 | LUT  | C14-C13 | 13.02  | 1.53        | 1.35     |
| 36  | 8     | 302 | LUT  | C30-C29 | 13.00  | 1.53        | 1.35     |
| 36  | 6     | 303 | LUT  | C34-C33 | 12.97  | 1.53        | 1.35     |
| 36  | F     | 304 | LUT  | C10-C9  | 12.93  | 1.52        | 1.35     |
| 31  | 2     | 314 | CLA  | MG-NA   | 12.93  | 2.37        | 2.06     |
| 36  | 2     | 301 | LUT  | C34-C33 | 12.92  | 1.52        | 1.35     |
| 32  | 6     | 318 | CHL  | MG-ND   | -12.91 | 1.80        | 2.05     |
| 31  | 4     | 316 | CLA  | MG-NC   | 12.91  | 2.36        | 2.06     |
| 31  | b     | 313 | CLA  | MG-ND   | -12.87 | 1.80        | 2.05     |
| 31  | B     | 821 | CLA  | MG-NA   | 12.86  | 2.36        | 2.06     |
| 36  | 5     | 304 | LUT  | C34-C33 | 12.84  | 1.52        | 1.35     |
| 36  | 9     | 303 | LUT  | C34-C33 | 12.82  | 1.52        | 1.35     |
| 36  | 5     | 303 | LUT  | C34-C33 | 12.81  | 1.52        | 1.35     |
| 31  | 4     | 315 | CLA  | MG-NA   | 12.81  | 2.36        | 2.06     |
| 36  | F     | 304 | LUT  | C14-C13 | 12.80  | 1.52        | 1.35     |
| 36  | F     | 304 | LUT  | C34-C33 | 12.75  | 1.52        | 1.35     |
| 31  | 5     | 314 | CLA  | MG-NA   | 12.75  | 2.36        | 2.06     |
| 31  | 4     | 321 | CLA  | MG-ND   | 12.69  | 2.30        | 2.05     |
| 32  | 5     | 317 | CHL  | MG-NC   | 12.67  | 2.36        | 2.06     |
| 31  | B     | 837 | CLA  | MG-NA   | 12.67  | 2.36        | 2.06     |
| 31  | A     | 817 | CLA  | MG-NA   | 12.67  | 2.36        | 2.06     |
| 36  | a     | 305 | LUT  | C5-C6   | 12.64  | 1.56        | 1.34     |
| 36  | 3     | 305 | LUT  | C34-C33 | 12.63  | 1.52        | 1.35     |
| 36  | 5     | 304 | LUT  | C5-C6   | 12.62  | 1.56        | 1.34     |
| 31  | 6     | 315 | CLA  | MG-NC   | -12.62 | 1.76        | 2.06     |
| 31  | H     | 903 | CLA  | MG-NA   | 12.52  | 2.36        | 2.06     |
| 31  | 8     | 317 | CLA  | MG-NA   | 12.47  | 2.35        | 2.06     |
| 31  | 7     | 312 | CLA  | MG-NA   | 12.46  | 2.35        | 2.06     |
| 31  | 6     | 310 | CLA  | MG-NC   | 12.45  | 2.35        | 2.06     |
| 36  | L     | 304 | LUT  | C5-C6   | 12.43  | 1.56        | 1.34     |
| 36  | J     | 103 | LUT  | C5-C6   | 12.43  | 1.56        | 1.34     |
| 36  | 5     | 303 | LUT  | C5-C6   | 12.39  | 1.55        | 1.34     |
| 36  | 9     | 302 | LUT  | C5-C6   | 12.37  | 1.55        | 1.34     |
| 36  | 3     | 304 | LUT  | C34-C33 | 12.37  | 1.52        | 1.35     |
| 36  | a     | 303 | LUT  | C5-C6   | 12.37  | 1.55        | 1.34     |
| 31  | 9     | 317 | CLA  | MG-NC   | 12.35  | 2.35        | 2.06     |
| 36  | 2     | 301 | LUT  | C5-C6   | 12.34  | 1.55        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 36  | 9     | 302 | LUT  | C14-C13 | 12.34  | 1.52        | 1.35     |
| 36  | 7     | 305 | LUT  | C34-C33 | 12.32  | 1.52        | 1.35     |
| 36  | 4     | 302 | LUT  | C5-C6   | 12.31  | 1.55        | 1.34     |
| 31  | O     | 202 | CLA  | MG-NC   | 12.30  | 2.35        | 2.06     |
| 36  | 8     | 302 | LUT  | C5-C6   | 12.24  | 1.55        | 1.34     |
| 36  | 6     | 304 | LUT  | C5-C6   | 12.24  | 1.55        | 1.34     |
| 31  | A     | 830 | CLA  | MG-NA   | 12.18  | 2.35        | 2.06     |
| 31  | A     | 815 | CLA  | MG-NC   | 12.07  | 2.34        | 2.06     |
| 31  | 8     | 320 | CLA  | MG-NA   | 12.04  | 2.34        | 2.06     |
| 36  | b     | 301 | LUT  | C5-C6   | 12.04  | 1.55        | 1.34     |
| 36  | 8     | 303 | LUT  | C34-C33 | 12.04  | 1.51        | 1.35     |
| 31  | A     | 814 | CLA  | MG-NA   | 12.02  | 2.34        | 2.06     |
| 31  | B     | 830 | CLA  | MG-NA   | 12.00  | 2.34        | 2.06     |
| 36  | 9     | 305 | LUT  | C5-C6   | 11.98  | 1.55        | 1.34     |
| 31  | A     | 849 | CLA  | MG-NA   | 11.98  | 2.34        | 2.06     |
| 32  | 6     | 317 | CHL  | MG-NC   | 11.97  | 2.34        | 2.06     |
| 31  | A     | 828 | CLA  | MG-NC   | 11.87  | 2.34        | 2.06     |
| 31  | b     | 305 | CLA  | MG-NA   | 11.87  | 2.34        | 2.06     |
| 31  | 9     | 315 | CLA  | MG-NA   | 11.85  | 2.34        | 2.06     |
| 32  | 5     | 322 | CHL  | MG-ND   | -11.83 | 1.82        | 2.05     |
| 31  | B     | 841 | CLA  | MG-NA   | 11.83  | 2.34        | 2.06     |
| 31  | G     | 204 | CLA  | MG-NC   | 11.78  | 2.34        | 2.06     |
| 31  | B     | 814 | CLA  | MG-NA   | 11.76  | 2.34        | 2.06     |
| 31  | 5     | 308 | CLA  | MG-ND   | -11.76 | 1.82        | 2.05     |
| 31  | F     | 306 | CLA  | MG-NA   | 11.76  | 2.34        | 2.06     |
| 31  | A     | 854 | CLA  | MG-NA   | 11.70  | 2.34        | 2.06     |
| 32  | a     | 318 | CHL  | MG-ND   | 11.69  | 2.29        | 2.05     |
| 36  | F     | 304 | LUT  | C5-C6   | 11.67  | 1.54        | 1.34     |
| 31  | 5     | 313 | CLA  | MG-NA   | 11.67  | 2.34        | 2.06     |
| 31  | a     | 319 | CLA  | MG-NA   | 11.65  | 2.33        | 2.06     |
| 31  | 5     | 318 | CLA  | MG-NC   | 11.64  | 2.33        | 2.06     |
| 36  | 4     | 303 | LUT  | C5-C6   | 11.64  | 1.54        | 1.34     |
| 31  | 5     | 315 | CLA  | MG-NA   | 11.60  | 2.33        | 2.06     |
| 31  | b     | 312 | CLA  | MG-NA   | 11.58  | 2.33        | 2.06     |
| 36  | 6     | 303 | LUT  | C5-C6   | 11.43  | 1.54        | 1.34     |
| 31  | A     | 841 | CLA  | MG-NA   | 11.39  | 2.33        | 2.06     |
| 36  | 8     | 303 | LUT  | C5-C6   | 11.38  | 1.54        | 1.34     |
| 31  | 7     | 314 | CLA  | MG-NC   | 11.38  | 2.33        | 2.06     |
| 31  | B     | 819 | CLA  | MG-NC   | 11.36  | 2.33        | 2.06     |
| 31  | 2     | 307 | CLA  | MG-NA   | 11.36  | 2.33        | 2.06     |
| 31  | 7     | 311 | CLA  | MG-NA   | 11.32  | 2.33        | 2.06     |
| 36  | 9     | 303 | LUT  | C5-C6   | 11.30  | 1.54        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 31  | B     | 842 | CLA  | MG-NC  | 11.29  | 2.33        | 2.06     |
| 31  | b     | 303 | CLA  | MG-ND  | 11.28  | 2.28        | 2.05     |
| 31  | 8     | 311 | CLA  | MG-NC  | 11.27  | 2.33        | 2.06     |
| 31  | 8     | 315 | CLA  | MG-NA  | 11.26  | 2.33        | 2.06     |
| 31  | A     | 826 | CLA  | MG-NC  | 11.26  | 2.33        | 2.06     |
| 31  | a     | 313 | CLA  | MG-NC  | 11.26  | 2.33        | 2.06     |
| 31  | 8     | 321 | CLA  | MG-NA  | 11.22  | 2.32        | 2.06     |
| 31  | 7     | 322 | CLA  | MG-NC  | 11.21  | 2.32        | 2.06     |
| 31  | b     | 308 | CLA  | MG-ND  | 11.19  | 2.28        | 2.05     |
| 31  | 6     | 322 | CLA  | MG-NA  | 11.13  | 2.32        | 2.06     |
| 31  | 6     | 306 | CLA  | MG-NC  | 11.11  | 2.32        | 2.06     |
| 31  | 8     | 308 | CLA  | MG-NA  | 11.08  | 2.32        | 2.06     |
| 32  | 7     | 318 | CHL  | MG-NA  | 11.07  | 2.32        | 2.06     |
| 31  | B     | 836 | CLA  | MG-NA  | 11.06  | 2.32        | 2.06     |
| 31  | B     | 847 | CLA  | MG-NC  | 11.03  | 2.32        | 2.06     |
| 32  | 4     | 313 | CHL  | MG-NA  | -11.02 | 1.80        | 2.06     |
| 31  | 6     | 313 | CLA  | MG-NC  | 11.01  | 2.32        | 2.06     |
| 31  | 3     | 307 | CLA  | MG-NA  | 11.01  | 2.32        | 2.06     |
| 31  | b     | 311 | CLA  | MG-ND  | 11.00  | 2.27        | 2.05     |
| 31  | 7     | 315 | CLA  | MG-ND  | -11.00 | 1.84        | 2.05     |
| 36  | 3     | 305 | LUT  | C5-C6  | 11.00  | 1.53        | 1.34     |
| 31  | G     | 206 | CLA  | MG-ND  | -10.96 | 1.84        | 2.05     |
| 31  | 3     | 310 | CLA  | MG-ND  | -10.91 | 1.84        | 2.05     |
| 31  | 6     | 311 | CLA  | MG-ND  | 10.86  | 2.27        | 2.05     |
| 32  | 8     | 319 | CHL  | MG-NC  | 10.86  | 2.32        | 2.06     |
| 31  | 4     | 305 | CLA  | C1D-ND | 10.86  | 1.51        | 1.37     |
| 31  | J     | 105 | CLA  | MG-NC  | 10.82  | 2.32        | 2.06     |
| 31  | A     | 850 | CLA  | MG-NA  | 10.82  | 2.32        | 2.06     |
| 31  | B     | 846 | CLA  | MG-NA  | 10.80  | 2.31        | 2.06     |
| 31  | b     | 302 | CLA  | MG-NC  | 10.77  | 2.31        | 2.06     |
| 31  | B     | 843 | CLA  | MG-NC  | 10.76  | 2.31        | 2.06     |
| 31  | 8     | 312 | CLA  | MG-NA  | 10.75  | 2.31        | 2.06     |
| 31  | A     | 825 | CLA  | MG-NA  | 10.73  | 2.31        | 2.06     |
| 31  | B     | 838 | CLA  | MG-NC  | 10.73  | 2.31        | 2.06     |
| 31  | B     | 822 | CLA  | MG-NA  | 10.73  | 2.31        | 2.06     |
| 31  | 6     | 315 | CLA  | MG-ND  | -10.72 | 1.84        | 2.05     |
| 31  | 8     | 314 | CLA  | MG-NA  | 10.63  | 2.31        | 2.06     |
| 32  | 7     | 320 | CHL  | MG-NA  | 10.61  | 2.31        | 2.06     |
| 31  | A     | 846 | CLA  | MG-NC  | 10.60  | 2.31        | 2.06     |
| 31  | G     | 206 | CLA  | MG-NA  | 10.60  | 2.31        | 2.06     |
| 31  | a     | 311 | CLA  | MG-NA  | 10.58  | 2.31        | 2.06     |
| 31  | A     | 849 | CLA  | MG-ND  | -10.56 | 1.84        | 2.05     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 31  | 2     | 310 | CLA  | MG-NC | -10.52 | 1.81        | 2.06     |
| 31  | A     | 848 | CLA  | MG-NA | 10.51  | 2.31        | 2.06     |
| 31  | G     | 205 | CLA  | MG-NA | 10.48  | 2.31        | 2.06     |
| 32  | 6     | 321 | CHL  | MG-NC | -10.44 | 1.81        | 2.06     |
| 32  | 9     | 322 | CHL  | MG-NA | 10.31  | 2.30        | 2.06     |
| 31  | 4     | 318 | CLA  | MG-ND | 10.29  | 2.26        | 2.05     |
| 32  | 3     | 315 | CHL  | MG-NA | 10.26  | 2.30        | 2.06     |
| 32  | 9     | 322 | CHL  | MG-ND | 10.25  | 2.26        | 2.05     |
| 31  | b     | 310 | CLA  | MG-NC | 10.22  | 2.30        | 2.06     |
| 31  | B     | 826 | CLA  | MG-NA | 10.20  | 2.30        | 2.06     |
| 31  | A     | 853 | CLA  | MG-NC | 10.15  | 2.30        | 2.06     |
| 31  | b     | 303 | CLA  | MG-NA | 10.14  | 2.30        | 2.06     |
| 31  | B     | 845 | CLA  | MG-NA | 10.10  | 2.30        | 2.06     |
| 31  | A     | 835 | CLA  | MG-NC | 10.08  | 2.30        | 2.06     |
| 31  | A     | 855 | CLA  | MG-NC | 10.04  | 2.30        | 2.06     |
| 31  | B     | 850 | CLA  | MG-NC | 10.02  | 2.30        | 2.06     |
| 31  | 9     | 317 | CLA  | MG-NA | 10.00  | 2.30        | 2.06     |
| 31  | A     | 816 | CLA  | MG-NC | 10.00  | 2.30        | 2.06     |
| 31  | B     | 825 | CLA  | MG-NA | 10.00  | 2.30        | 2.06     |
| 31  | 5     | 309 | CLA  | MG-ND | 9.96   | 2.25        | 2.05     |
| 31  | B     | 823 | CLA  | MG-NC | 9.96   | 2.29        | 2.06     |
| 31  | B     | 844 | CLA  | MG-NC | 9.96   | 2.29        | 2.06     |
| 31  | 9     | 312 | CLA  | MG-NA | 9.95   | 2.29        | 2.06     |
| 32  | 7     | 320 | CHL  | MG-ND | 9.91   | 2.25        | 2.05     |
| 31  | A     | 833 | CLA  | MG-NA | 9.91   | 2.29        | 2.06     |
| 31  | A     | 838 | CLA  | MG-NA | 9.89   | 2.29        | 2.06     |
| 31  | A     | 855 | CLA  | MG-NA | 9.84   | 2.29        | 2.06     |
| 31  | F     | 301 | CLA  | MG-NC | 9.83   | 2.29        | 2.06     |
| 31  | B     | 813 | CLA  | MG-NA | 9.83   | 2.29        | 2.06     |
| 31  | 3     | 319 | CLA  | MG-NC | 9.81   | 2.29        | 2.06     |
| 31  | 9     | 319 | CLA  | MG-ND | 9.80   | 2.25        | 2.05     |
| 31  | 6     | 308 | CLA  | MG-NC | 9.79   | 2.29        | 2.06     |
| 31  | a     | 314 | CLA  | MG-ND | 9.78   | 2.25        | 2.05     |
| 31  | A     | 823 | CLA  | MG-NA | 9.78   | 2.29        | 2.06     |
| 32  | 5     | 316 | CHL  | MG-ND | 9.78   | 2.25        | 2.05     |
| 31  | A     | 851 | CLA  | MG-NC | 9.77   | 2.29        | 2.06     |
| 31  | B     | 827 | CLA  | MG-NA | 9.76   | 2.29        | 2.06     |
| 32  | 6     | 309 | CHL  | MG-NA | 9.76   | 2.29        | 2.06     |
| 31  | 2     | 306 | CLA  | MG-NA | 9.74   | 2.29        | 2.06     |
| 31  | 4     | 314 | CLA  | MG-NC | 9.72   | 2.29        | 2.06     |
| 31  | O     | 203 | CLA  | MG-NC | 9.68   | 2.29        | 2.06     |
| 31  | 3     | 319 | CLA  | MG-ND | 9.64   | 2.24        | 2.05     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 31  | B     | 839 | CLA  | MG-NA  | 9.62  | 2.29        | 2.06     |
| 31  | 4     | 312 | CLA  | MG-NA  | 9.59  | 2.29        | 2.06     |
| 31  | a     | 315 | CLA  | MG-NA  | 9.58  | 2.29        | 2.06     |
| 31  | b     | 308 | CLA  | MG-NA  | 9.55  | 2.28        | 2.06     |
| 31  | 2     | 311 | CLA  | MG-NC  | -9.52 | 1.83        | 2.06     |
| 31  | A     | 847 | CLA  | MG-NC  | 9.51  | 2.28        | 2.06     |
| 31  | A     | 833 | CLA  | MG-ND  | -9.50 | 1.87        | 2.05     |
| 31  | A     | 851 | CLA  | MG-NA  | 9.46  | 2.28        | 2.06     |
| 31  | A     | 845 | CLA  | MG-NA  | 9.37  | 2.28        | 2.06     |
| 31  | A     | 853 | CLA  | MG-ND  | 9.36  | 2.24        | 2.05     |
| 31  | A     | 829 | CLA  | C1D-ND | 9.35  | 1.49        | 1.37     |
| 31  | 5     | 308 | CLA  | MG-NC  | 9.32  | 2.28        | 2.06     |
| 31  | B     | 811 | CLA  | MG-NA  | 9.25  | 2.28        | 2.06     |
| 31  | b     | 312 | CLA  | MG-NC  | 9.24  | 2.28        | 2.06     |
| 31  | B     | 832 | CLA  | MG-NA  | 9.16  | 2.28        | 2.06     |
| 31  | A     | 847 | CLA  | MG-NA  | 9.15  | 2.28        | 2.06     |
| 31  | 4     | 321 | CLA  | MG-NC  | 9.15  | 2.28        | 2.06     |
| 32  | 5     | 317 | CHL  | MG-NA  | -9.15 | 1.84        | 2.06     |
| 31  | A     | 836 | CLA  | MG-NA  | 9.02  | 2.27        | 2.06     |
| 31  | a     | 312 | CLA  | MG-ND  | -9.01 | 1.87        | 2.05     |
| 31  | 2     | 307 | CLA  | MG-ND  | -9.00 | 1.87        | 2.05     |
| 31  | 5     | 307 | CLA  | MG-NA  | 8.98  | 2.27        | 2.06     |
| 31  | 9     | 319 | CLA  | MG-NC  | -8.98 | 1.84        | 2.06     |
| 31  | B     | 814 | CLA  | MG-ND  | -8.96 | 1.88        | 2.05     |
| 31  | A     | 819 | CLA  | MG-NA  | 8.91  | 2.27        | 2.06     |
| 31  | 5     | 312 | CLA  | MG-NC  | 8.89  | 2.27        | 2.06     |
| 31  | O     | 204 | CLA  | MG-NC  | 8.88  | 2.27        | 2.06     |
| 31  | 6     | 310 | CLA  | MG-NA  | 8.87  | 2.27        | 2.06     |
| 31  | L     | 305 | CLA  | MG-NA  | 8.86  | 2.27        | 2.06     |
| 31  | 3     | 309 | CLA  | MG-NC  | 8.83  | 2.27        | 2.06     |
| 32  | 4     | 310 | CHL  | MG-ND  | 8.83  | 2.23        | 2.05     |
| 31  | B     | 840 | CLA  | MG-NC  | 8.82  | 2.27        | 2.06     |
| 31  | B     | 813 | CLA  | MG-ND  | 8.75  | 2.23        | 2.05     |
| 31  | B     | 847 | CLA  | MG-ND  | 8.74  | 2.23        | 2.05     |
| 31  | b     | 308 | CLA  | MG-NC  | 8.69  | 2.26        | 2.06     |
| 31  | B     | 825 | CLA  | MG-NC  | 8.69  | 2.26        | 2.06     |
| 31  | B     | 848 | CLA  | MG-NA  | 8.68  | 2.26        | 2.06     |
| 31  | A     | 846 | CLA  | MG-NA  | 8.65  | 2.26        | 2.06     |
| 31  | 7     | 313 | CLA  | MG-NA  | 8.64  | 2.26        | 2.06     |
| 31  | A     | 834 | CLA  | MG-NA  | 8.64  | 2.26        | 2.06     |
| 31  | 5     | 308 | CLA  | MG-NA  | 8.64  | 2.26        | 2.06     |
| 31  | A     | 837 | CLA  | MG-NC  | 8.58  | 2.26        | 2.06     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 31  | A     | 823 | CLA  | MG-NC | 8.56  | 2.26        | 2.06     |
| 31  | A     | 830 | CLA  | MG-NC | 8.51  | 2.26        | 2.06     |
| 31  | 6     | 312 | CLA  | MG-ND | -8.50 | 1.88        | 2.05     |
| 32  | 6     | 319 | CHL  | MG-ND | -8.49 | 1.89        | 2.05     |
| 31  | B     | 847 | CLA  | MG-NA | 8.47  | 2.26        | 2.06     |
| 31  | 3     | 310 | CLA  | MG-NC | 8.47  | 2.26        | 2.06     |
| 31  | 8     | 310 | CLA  | MG-NA | 8.44  | 2.26        | 2.06     |
| 32  | 5     | 319 | CHL  | MG-NA | -8.42 | 1.86        | 2.06     |
| 32  | b     | 309 | CHL  | MG-NC | 8.41  | 2.26        | 2.06     |
| 31  | 2     | 311 | CLA  | MG-ND | -8.38 | 1.89        | 2.05     |
| 31  | B     | 822 | CLA  | MG-NC | 8.36  | 2.26        | 2.06     |
| 31  | B     | 813 | CLA  | MG-NC | 8.33  | 2.26        | 2.06     |
| 31  | B     | 817 | CLA  | MG-NC | 8.29  | 2.26        | 2.06     |
| 31  | 4     | 309 | CLA  | MG-NA | 8.25  | 2.25        | 2.06     |
| 31  | F     | 305 | CLA  | MG-NC | 8.23  | 2.25        | 2.06     |
| 31  | A     | 837 | CLA  | MG-NA | 8.20  | 2.25        | 2.06     |
| 31  | B     | 850 | CLA  | MG-NA | 8.19  | 2.25        | 2.06     |
| 32  | A     | 840 | CHL  | MG-NA | 8.19  | 2.25        | 2.06     |
| 31  | 4     | 316 | CLA  | MG-NA | 8.17  | 2.25        | 2.06     |
| 32  | A     | 831 | CHL  | MG-NC | 8.15  | 2.25        | 2.06     |
| 32  | 4     | 317 | CHL  | MG-NC | 8.13  | 2.25        | 2.06     |
| 31  | B     | 815 | CLA  | MG-NC | 8.12  | 2.25        | 2.06     |
| 31  | 6     | 314 | CLA  | MG-NC | -8.09 | 1.87        | 2.06     |
| 31  | A     | 832 | CLA  | MG-NA | 8.07  | 2.25        | 2.06     |
| 32  | a     | 317 | CHL  | MG-NC | 8.07  | 2.25        | 2.06     |
| 31  | A     | 836 | CLA  | MG-NC | 8.06  | 2.25        | 2.06     |
| 31  | 2     | 312 | CLA  | MG-ND | 8.06  | 2.21        | 2.05     |
| 32  | 7     | 319 | CHL  | MG-ND | 8.04  | 2.21        | 2.05     |
| 31  | b     | 311 | CLA  | MG-NC | 8.02  | 2.25        | 2.06     |
| 31  | B     | 818 | CLA  | MG-NC | 8.02  | 2.25        | 2.06     |
| 31  | 5     | 311 | CLA  | MG-NC | 8.00  | 2.25        | 2.06     |
| 31  | B     | 829 | CLA  | MG-NC | 7.98  | 2.25        | 2.06     |
| 31  | B     | 831 | CLA  | MG-NC | 7.97  | 2.25        | 2.06     |
| 31  | 4     | 318 | CLA  | MG-NA | 7.97  | 2.25        | 2.06     |
| 31  | 3     | 308 | CLA  | MG-ND | 7.95  | 2.21        | 2.05     |
| 31  | 8     | 321 | CLA  | MG-ND | 7.92  | 2.21        | 2.05     |
| 31  | L     | 306 | CLA  | MG-NC | 7.91  | 2.25        | 2.06     |
| 31  | 6     | 307 | CLA  | MG-ND | 7.77  | 2.21        | 2.05     |
| 32  | 4     | 317 | CHL  | MG-ND | -7.76 | 1.90        | 2.05     |
| 31  | B     | 840 | CLA  | MG-NA | 7.74  | 2.24        | 2.06     |
| 32  | 7     | 317 | CHL  | MG-ND | 7.71  | 2.21        | 2.05     |
| 31  | B     | 811 | CLA  | MG-ND | 7.68  | 2.21        | 2.05     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 31  | B     | 829 | CLA  | MG-NA  | 7.67  | 2.24        | 2.06     |
| 31  | F     | 305 | CLA  | MG-NA  | 7.67  | 2.24        | 2.06     |
| 31  | L     | 305 | CLA  | MG-NC  | 7.65  | 2.24        | 2.06     |
| 31  | B     | 837 | CLA  | MG-NC  | 7.64  | 2.24        | 2.06     |
| 31  | 6     | 306 | CLA  | MG-NA  | 7.64  | 2.24        | 2.06     |
| 31  | b     | 304 | CLA  | MG-NC  | 7.61  | 2.24        | 2.06     |
| 31  | A     | 838 | CLA  | MG-NC  | 7.57  | 2.24        | 2.06     |
| 31  | 4     | 319 | CLA  | MG-NC  | -7.56 | 1.88        | 2.06     |
| 31  | 8     | 308 | CLA  | MG-ND  | -7.54 | 1.90        | 2.05     |
| 31  | A     | 822 | CLA  | MG-NC  | 7.50  | 2.24        | 2.06     |
| 31  | 5     | 311 | CLA  | MG-NA  | 7.49  | 2.24        | 2.06     |
| 31  | 5     | 314 | CLA  | MG-ND  | 7.48  | 2.20        | 2.05     |
| 31  | A     | 851 | CLA  | MG-ND  | 7.46  | 2.20        | 2.05     |
| 31  | 4     | 321 | CLA  | MG-NA  | 7.45  | 2.24        | 2.06     |
| 32  | 6     | 320 | CHL  | MG-NC  | -7.43 | 1.88        | 2.06     |
| 31  | 8     | 318 | CLA  | MG-NA  | 7.42  | 2.23        | 2.06     |
| 31  | A     | 856 | CLA  | MG-NC  | 7.41  | 2.23        | 2.06     |
| 31  | 8     | 310 | CLA  | MG-ND  | -7.41 | 1.91        | 2.05     |
| 31  | B     | 828 | CLA  | MG-NC  | 7.36  | 2.23        | 2.06     |
| 31  | H     | 901 | CLA  | MG-NA  | 7.35  | 2.23        | 2.06     |
| 31  | 3     | 316 | CLA  | MG-NA  | 7.34  | 2.23        | 2.06     |
| 31  | A     | 829 | CLA  | MG-NC  | 7.34  | 2.23        | 2.06     |
| 31  | 7     | 322 | CLA  | MG-ND  | -7.31 | 1.91        | 2.05     |
| 31  | 7     | 313 | CLA  | MG-NC  | 7.29  | 2.23        | 2.06     |
| 31  | 6     | 308 | CLA  | MG-ND  | -7.27 | 1.91        | 2.05     |
| 32  | 4     | 310 | CHL  | MG-NA  | 7.24  | 2.23        | 2.06     |
| 31  | B     | 838 | CLA  | MG-NA  | 7.23  | 2.23        | 2.06     |
| 31  | b     | 304 | CLA  | MG-NA  | 7.21  | 2.23        | 2.06     |
| 32  | 8     | 316 | CHL  | MG-ND  | -7.14 | 1.91        | 2.05     |
| 31  | 4     | 307 | CLA  | MG-NA  | 7.12  | 2.23        | 2.06     |
| 31  | A     | 850 | CLA  | MG-NC  | 7.12  | 2.23        | 2.06     |
| 31  | B     | 842 | CLA  | MG-ND  | 7.07  | 2.19        | 2.05     |
| 31  | B     | 820 | CLA  | MG-NC  | 7.04  | 2.23        | 2.06     |
| 31  | b     | 302 | CLA  | MG-NA  | 7.03  | 2.23        | 2.06     |
| 31  | K     | 204 | CLA  | MG-ND  | -7.02 | 1.91        | 2.05     |
| 30  | A     | 813 | CL0  | C1D-ND | 7.02  | 1.46        | 1.37     |
| 31  | 4     | 308 | CLA  | MG-NC  | 7.02  | 2.22        | 2.06     |
| 31  | G     | 204 | CLA  | MG-NA  | 6.98  | 2.22        | 2.06     |
| 31  | A     | 815 | CLA  | MG-NA  | 6.98  | 2.22        | 2.06     |
| 31  | A     | 820 | CLA  | MG-NA  | 6.97  | 2.22        | 2.06     |
| 31  | 4     | 312 | CLA  | MG-NC  | 6.97  | 2.22        | 2.06     |
| 31  | 2     | 309 | CLA  | MG-NC  | 6.94  | 2.22        | 2.06     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 31  | B     | 833 | CLA  | MG-NC  | 6.90  | 2.22        | 2.06     |
| 31  | B     | 817 | CLA  | MG-NA  | 6.89  | 2.22        | 2.06     |
| 31  | 4     | 318 | CLA  | MG-NC  | 6.86  | 2.22        | 2.06     |
| 31  | A     | 835 | CLA  | MG-ND  | -6.82 | 1.92        | 2.05     |
| 31  | B     | 811 | CLA  | MG-NC  | 6.81  | 2.22        | 2.06     |
| 31  | 4     | 307 | CLA  | MG-NC  | 6.80  | 2.22        | 2.06     |
| 31  | A     | 857 | CLA  | MG-NC  | 6.79  | 2.22        | 2.06     |
| 31  | 9     | 321 | CLA  | MG-NC  | 6.73  | 2.22        | 2.06     |
| 31  | 4     | 316 | CLA  | C1D-ND | 6.73  | 1.46        | 1.37     |
| 31  | 7     | 309 | CLA  | MG-NC  | 6.70  | 2.22        | 2.06     |
| 31  | 5     | 313 | CLA  | C4D-ND | 6.68  | 1.46        | 1.37     |
| 31  | A     | 814 | CLA  | MG-ND  | 6.64  | 2.19        | 2.05     |
| 31  | A     | 833 | CLA  | MG-NC  | 6.64  | 2.22        | 2.06     |
| 31  | A     | 855 | CLA  | MG-ND  | 6.63  | 2.18        | 2.05     |
| 32  | 7     | 319 | CHL  | MG-NC  | 6.63  | 2.22        | 2.06     |
| 31  | b     | 307 | CLA  | MG-ND  | -6.62 | 1.92        | 2.05     |
| 32  | 9     | 320 | CHL  | MG-NC  | 6.61  | 2.22        | 2.06     |
| 31  | 4     | 309 | CLA  | MG-NC  | 6.60  | 2.21        | 2.06     |
| 31  | B     | 831 | CLA  | MG-NA  | 6.59  | 2.21        | 2.06     |
| 31  | B     | 824 | CLA  | MG-NC  | 6.57  | 2.21        | 2.06     |
| 31  | 4     | 308 | CLA  | MG-NA  | 6.56  | 2.21        | 2.06     |
| 31  | B     | 823 | CLA  | MG-NA  | 6.53  | 2.21        | 2.06     |
| 31  | A     | 822 | CLA  | MG-ND  | -6.53 | 1.92        | 2.05     |
| 31  | 4     | 314 | CLA  | MG-NA  | 6.53  | 2.21        | 2.06     |
| 31  | 9     | 312 | CLA  | MG-NC  | 6.52  | 2.21        | 2.06     |
| 31  | 3     | 318 | CLA  | MG-ND  | -6.50 | 1.92        | 2.05     |
| 31  | 6     | 306 | CLA  | C4D-ND | 6.49  | 1.46        | 1.37     |
| 31  | 9     | 317 | CLA  | C4D-ND | 6.42  | 1.46        | 1.37     |
| 31  | J     | 105 | CLA  | MG-ND  | 6.40  | 2.18        | 2.05     |
| 32  | A     | 839 | CHL  | MG-ND  | 6.37  | 2.18        | 2.05     |
| 31  | A     | 818 | CLA  | MG-NA  | 6.36  | 2.21        | 2.06     |
| 31  | 4     | 307 | CLA  | MG-ND  | -6.34 | 1.93        | 2.05     |
| 32  | 6     | 320 | CHL  | MG-ND  | -6.34 | 1.93        | 2.05     |
| 31  | B     | 815 | CLA  | MG-NA  | 6.31  | 2.21        | 2.06     |
| 31  | B     | 826 | CLA  | MG-NC  | 6.29  | 2.21        | 2.06     |
| 31  | b     | 303 | CLA  | MG-NC  | 6.23  | 2.21        | 2.06     |
| 31  | B     | 819 | CLA  | MG-NA  | 6.16  | 2.20        | 2.06     |
| 31  | A     | 832 | CLA  | MG-NC  | 6.15  | 2.20        | 2.06     |
| 31  | 6     | 313 | CLA  | MG-NA  | 6.15  | 2.20        | 2.06     |
| 31  | H     | 901 | CLA  | MG-NC  | 6.14  | 2.20        | 2.06     |
| 31  | b     | 311 | CLA  | MG-NA  | 6.13  | 2.20        | 2.06     |
| 32  | 6     | 317 | CHL  | MG-NA  | -6.13 | 1.91        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 316 | CLA  | MG-NC   | 6.11  | 2.20        | 2.06     |
| 31  | 5     | 320 | CLA  | MG-NA   | -6.10 | 1.91        | 2.06     |
| 31  | O     | 202 | CLA  | C3C-C2C | 6.08  | 1.48        | 1.36     |
| 31  | A     | 857 | CLA  | MG-NA   | 6.05  | 2.20        | 2.06     |
| 31  | 4     | 320 | CLA  | MG-ND   | -6.03 | 1.93        | 2.05     |
| 31  | A     | 845 | CLA  | MG-NC   | 6.02  | 2.20        | 2.06     |
| 31  | 7     | 313 | CLA  | MG-ND   | -6.02 | 1.93        | 2.05     |
| 31  | a     | 316 | CLA  | MG-ND   | 6.01  | 2.17        | 2.05     |
| 31  | 6     | 306 | CLA  | C3B-C2B | 5.99  | 1.48        | 1.40     |
| 32  | 9     | 320 | CHL  | MG-ND   | 5.97  | 2.17        | 2.05     |
| 31  | A     | 818 | CLA  | MG-NC   | 5.95  | 2.20        | 2.06     |
| 31  | H     | 902 | CLA  | MG-NC   | -5.90 | 1.92        | 2.06     |
| 31  | 3     | 311 | CLA  | MG-ND   | -5.88 | 1.94        | 2.05     |
| 31  | 7     | 314 | CLA  | C3C-C2C | 5.88  | 1.48        | 1.36     |
| 31  | B     | 836 | CLA  | MG-NC   | 5.87  | 2.20        | 2.06     |
| 31  | A     | 848 | CLA  | MG-ND   | 5.86  | 2.17        | 2.05     |
| 31  | 7     | 310 | CLA  | C3C-C2C | 5.84  | 1.48        | 1.36     |
| 31  | A     | 843 | CLA  | MG-ND   | 5.84  | 2.17        | 2.05     |
| 32  | A     | 831 | CHL  | MG-ND   | 5.84  | 2.17        | 2.05     |
| 31  | 9     | 321 | CLA  | MG-NA   | 5.83  | 2.20        | 2.06     |
| 31  | B     | 845 | CLA  | MG-NC   | 5.82  | 2.20        | 2.06     |
| 31  | B     | 830 | CLA  | MG-NC   | 5.80  | 2.20        | 2.06     |
| 31  | 9     | 313 | CLA  | C3B-C2B | 5.80  | 1.48        | 1.40     |
| 31  | 8     | 321 | CLA  | C3B-C2B | 5.80  | 1.48        | 1.40     |
| 32  | 8     | 316 | CHL  | MG-NA   | 5.79  | 2.20        | 2.06     |
| 31  | A     | 856 | CLA  | MG-NA   | 5.79  | 2.20        | 2.06     |
| 31  | B     | 812 | CLA  | MG-NC   | 5.78  | 2.20        | 2.06     |
| 31  | 6     | 322 | CLA  | MG-NC   | 5.77  | 2.20        | 2.06     |
| 31  | A     | 825 | CLA  | C3B-C2B | 5.75  | 1.48        | 1.40     |
| 31  | K     | 205 | CLA  | C3B-C2B | 5.75  | 1.48        | 1.40     |
| 31  | A     | 820 | CLA  | C3B-C2B | 5.74  | 1.48        | 1.40     |
| 31  | 3     | 317 | CLA  | C3B-C2B | 5.74  | 1.48        | 1.40     |
| 31  | 8     | 311 | CLA  | MG-NA   | 5.73  | 2.19        | 2.06     |
| 31  | 2     | 308 | CLA  | C3B-C2B | 5.71  | 1.48        | 1.40     |
| 31  | 2     | 313 | CLA  | MG-ND   | 5.71  | 2.17        | 2.05     |
| 31  | B     | 840 | CLA  | C3B-C2B | 5.70  | 1.48        | 1.40     |
| 31  | 5     | 320 | CLA  | C3B-C2B | 5.70  | 1.48        | 1.40     |
| 31  | 3     | 319 | CLA  | C3B-C2B | 5.68  | 1.48        | 1.40     |
| 31  | B     | 826 | CLA  | C3B-C2B | 5.67  | 1.48        | 1.40     |
| 31  | B     | 828 | CLA  | MG-NA   | 5.67  | 2.19        | 2.06     |
| 31  | 6     | 313 | CLA  | C3B-C2B | 5.66  | 1.48        | 1.40     |
| 31  | b     | 311 | CLA  | C3C-C2C | 5.65  | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 316 | CLA  | C3B-C2B | 5.65  | 1.48        | 1.40     |
| 31  | b     | 310 | CLA  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 31  | 6     | 315 | CLA  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 31  | 6     | 316 | CLA  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 31  | B     | 849 | CLA  | C3B-C2B | 5.63  | 1.48        | 1.40     |
| 31  | 4     | 319 | CLA  | C3C-C2C | 5.62  | 1.48        | 1.36     |
| 31  | 4     | 320 | CLA  | C3B-C2B | 5.62  | 1.48        | 1.40     |
| 31  | G     | 205 | CLA  | C3B-C2B | 5.61  | 1.48        | 1.40     |
| 31  | B     | 816 | CLA  | MG-ND   | -5.61 | 1.94        | 2.05     |
| 31  | 4     | 308 | CLA  | C3B-C2B | 5.60  | 1.48        | 1.40     |
| 31  | 4     | 320 | CLA  | C3C-C2C | 5.60  | 1.48        | 1.36     |
| 31  | B     | 832 | CLA  | MG-NC   | 5.60  | 2.19        | 2.06     |
| 31  | O     | 203 | CLA  | MG-NA   | 5.60  | 2.19        | 2.06     |
| 31  | b     | 304 | CLA  | C3B-C2B | 5.59  | 1.48        | 1.40     |
| 31  | O     | 204 | CLA  | MG-NA   | 5.59  | 2.19        | 2.06     |
| 31  | A     | 814 | CLA  | C3B-C2B | 5.59  | 1.48        | 1.40     |
| 31  | L     | 306 | CLA  | C3B-C2B | 5.59  | 1.48        | 1.40     |
| 31  | B     | 848 | CLA  | C3B-C2B | 5.59  | 1.48        | 1.40     |
| 31  | 6     | 308 | CLA  | MG-NA   | 5.58  | 2.19        | 2.06     |
| 31  | 5     | 318 | CLA  | C3C-C2C | 5.58  | 1.48        | 1.36     |
| 31  | b     | 306 | CLA  | C3C-C2C | 5.58  | 1.48        | 1.36     |
| 31  | B     | 844 | CLA  | MG-NA   | 5.57  | 2.19        | 2.06     |
| 31  | B     | 839 | CLA  | C3B-C2B | 5.57  | 1.48        | 1.40     |
| 31  | 2     | 307 | CLA  | C3B-C2B | 5.57  | 1.48        | 1.40     |
| 31  | A     | 822 | CLA  | C3B-C2B | 5.56  | 1.48        | 1.40     |
| 31  | 4     | 311 | CLA  | MG-NC   | -5.56 | 1.93        | 2.06     |
| 31  | 9     | 317 | CLA  | C3C-C2C | 5.56  | 1.48        | 1.36     |
| 31  | 3     | 310 | CLA  | C3C-C2C | 5.56  | 1.48        | 1.36     |
| 31  | L     | 305 | CLA  | C3B-C2B | 5.56  | 1.48        | 1.40     |
| 31  | 8     | 307 | CLA  | C3B-C2B | 5.55  | 1.48        | 1.40     |
| 31  | 2     | 313 | CLA  | C3C-C2C | 5.55  | 1.48        | 1.36     |
| 31  | 5     | 313 | CLA  | C3C-C2C | 5.55  | 1.48        | 1.36     |
| 31  | B     | 814 | CLA  | C3B-C2B | 5.55  | 1.48        | 1.40     |
| 31  | b     | 305 | CLA  | C3B-C2B | 5.54  | 1.48        | 1.40     |
| 31  | 4     | 316 | CLA  | C3B-C2B | 5.53  | 1.48        | 1.40     |
| 31  | 7     | 321 | CLA  | C3B-C2B | 5.53  | 1.48        | 1.40     |
| 31  | 2     | 304 | CLA  | C3B-C2B | 5.53  | 1.48        | 1.40     |
| 31  | 9     | 314 | CLA  | C3B-C2B | 5.53  | 1.48        | 1.40     |
| 31  | 3     | 307 | CLA  | C3B-C2B | 5.52  | 1.48        | 1.40     |
| 31  | b     | 313 | CLA  | C3C-C2C | 5.52  | 1.48        | 1.36     |
| 31  | 7     | 312 | CLA  | C3B-C2B | 5.52  | 1.48        | 1.40     |
| 31  | 8     | 308 | CLA  | C3B-C2B | 5.52  | 1.48        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 312 | CLA  | C3B-C2B | 5.52  | 1.48        | 1.40     |
| 31  | a     | 315 | CLA  | C3B-C2B | 5.51  | 1.48        | 1.40     |
| 31  | a     | 311 | CLA  | MG-ND   | -5.51 | 1.94        | 2.05     |
| 31  | 8     | 310 | CLA  | C3B-C2B | 5.51  | 1.48        | 1.40     |
| 31  | 6     | 306 | CLA  | C3C-C2C | 5.51  | 1.48        | 1.36     |
| 31  | B     | 841 | CLA  | C3B-C2B | 5.51  | 1.48        | 1.40     |
| 31  | b     | 303 | CLA  | C3B-C2B | 5.50  | 1.48        | 1.40     |
| 31  | A     | 842 | CLA  | C3B-C2B | 5.50  | 1.48        | 1.40     |
| 31  | B     | 831 | CLA  | C3B-C2B | 5.50  | 1.48        | 1.40     |
| 31  | H     | 901 | CLA  | C3C-C2C | 5.50  | 1.48        | 1.36     |
| 31  | A     | 823 | CLA  | C3C-C2C | 5.49  | 1.48        | 1.36     |
| 31  | 2     | 310 | CLA  | C3C-C2C | 5.49  | 1.48        | 1.36     |
| 31  | B     | 813 | CLA  | C3B-C2B | 5.49  | 1.48        | 1.40     |
| 31  | H     | 901 | CLA  | C3B-C2B | 5.49  | 1.48        | 1.40     |
| 31  | a     | 309 | CLA  | C3B-C2B | 5.49  | 1.48        | 1.40     |
| 31  | 8     | 309 | CLA  | MG-NC   | 5.48  | 2.19        | 2.06     |
| 31  | b     | 313 | CLA  | C3B-C2B | 5.48  | 1.48        | 1.40     |
| 31  | A     | 843 | CLA  | MG-NC   | 5.48  | 2.19        | 2.06     |
| 31  | A     | 818 | CLA  | C3B-C2B | 5.48  | 1.48        | 1.40     |
| 31  | 3     | 320 | CLA  | C3C-C2C | 5.48  | 1.48        | 1.36     |
| 31  | a     | 312 | CLA  | C3B-C2B | 5.47  | 1.48        | 1.40     |
| 31  | 4     | 312 | CLA  | C3C-C2C | 5.47  | 1.48        | 1.36     |
| 31  | B     | 821 | CLA  | C3C-C2C | 5.47  | 1.48        | 1.36     |
| 31  | 5     | 310 | CLA  | C3B-C2B | 5.47  | 1.48        | 1.40     |
| 31  | O     | 203 | CLA  | C3C-C2C | 5.47  | 1.48        | 1.36     |
| 31  | A     | 828 | CLA  | C3B-C2B | 5.47  | 1.48        | 1.40     |
| 31  | 8     | 314 | CLA  | C3C-C2C | 5.47  | 1.48        | 1.36     |
| 31  | 8     | 317 | CLA  | C3B-C2B | 5.46  | 1.48        | 1.40     |
| 31  | A     | 835 | CLA  | C3B-C2B | 5.46  | 1.47        | 1.40     |
| 31  | O     | 202 | CLA  | C3B-C2B | 5.46  | 1.47        | 1.40     |
| 31  | 4     | 316 | CLA  | C3C-C2C | 5.46  | 1.48        | 1.36     |
| 31  | 5     | 307 | CLA  | C3B-C2B | 5.46  | 1.47        | 1.40     |
| 31  | a     | 314 | CLA  | C3C-C2C | 5.45  | 1.48        | 1.36     |
| 32  | 6     | 318 | CHL  | MG-NC   | -5.45 | 1.93        | 2.06     |
| 31  | B     | 823 | CLA  | C3B-C2B | 5.45  | 1.47        | 1.40     |
| 31  | 4     | 314 | CLA  | C3C-C2C | 5.45  | 1.48        | 1.36     |
| 31  | A     | 850 | CLA  | C3B-C2B | 5.45  | 1.47        | 1.40     |
| 31  | 8     | 311 | CLA  | C3B-C2B | 5.45  | 1.47        | 1.40     |
| 32  | 8     | 319 | CHL  | MG-NA   | -5.45 | 1.93        | 2.06     |
| 31  | b     | 307 | CLA  | C3B-C2B | 5.44  | 1.47        | 1.40     |
| 31  | 3     | 319 | CLA  | CHC-C1C | 5.44  | 1.48        | 1.35     |
| 31  | B     | 822 | CLA  | C3C-C2C | 5.44  | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | H     | 903 | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 31  | 3     | 320 | CLA  | C3B-C2B | 5.44 | 1.47        | 1.40     |
| 31  | L     | 305 | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 31  | O     | 204 | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 31  | 2     | 312 | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 31  | 3     | 311 | CLA  | C3B-C2B | 5.44 | 1.47        | 1.40     |
| 31  | 4     | 311 | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 31  | 5     | 314 | CLA  | C3C-C2C | 5.44 | 1.48        | 1.36     |
| 31  | B     | 812 | CLA  | MG-NA   | 5.43 | 2.19        | 2.06     |
| 31  | A     | 848 | CLA  | C3C-C2C | 5.43 | 1.48        | 1.36     |
| 31  | A     | 851 | CLA  | C3C-C2C | 5.43 | 1.48        | 1.36     |
| 31  | A     | 854 | CLA  | C3B-C2B | 5.43 | 1.47        | 1.40     |
| 31  | O     | 203 | CLA  | C3B-C2B | 5.43 | 1.47        | 1.40     |
| 31  | K     | 204 | CLA  | C3B-C2B | 5.43 | 1.47        | 1.40     |
| 31  | 9     | 315 | CLA  | C3B-C2B | 5.42 | 1.47        | 1.40     |
| 31  | a     | 319 | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 31  | 5     | 320 | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 31  | 4     | 312 | CLA  | C3B-C2B | 5.42 | 1.47        | 1.40     |
| 31  | 2     | 315 | CLA  | C3B-C2B | 5.42 | 1.47        | 1.40     |
| 31  | b     | 307 | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 31  | 2     | 309 | CLA  | C3B-C2B | 5.42 | 1.47        | 1.40     |
| 31  | 8     | 310 | CLA  | CHC-C1C | 5.42 | 1.48        | 1.35     |
| 31  | 9     | 316 | CLA  | C3C-C2C | 5.42 | 1.48        | 1.36     |
| 31  | 6     | 308 | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 31  | B     | 850 | CLA  | CHC-C1C | 5.41 | 1.48        | 1.35     |
| 31  | 5     | 321 | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 31  | A     | 852 | CLA  | C3B-C2B | 5.41 | 1.47        | 1.40     |
| 31  | A     | 841 | CLA  | C3B-C2B | 5.41 | 1.47        | 1.40     |
| 31  | b     | 312 | CLA  | C3B-C2B | 5.41 | 1.47        | 1.40     |
| 31  | b     | 308 | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 31  | A     | 838 | CLA  | C3B-C2B | 5.41 | 1.47        | 1.40     |
| 31  | 9     | 312 | CLA  | C3C-C2C | 5.41 | 1.48        | 1.36     |
| 31  | 5     | 311 | CLA  | C3B-C2B | 5.40 | 1.47        | 1.40     |
| 31  | 2     | 308 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 31  | A     | 849 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 31  | 6     | 314 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 31  | 7     | 322 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 31  | 9     | 318 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 31  | L     | 307 | CLA  | C3B-C2B | 5.40 | 1.47        | 1.40     |
| 31  | b     | 302 | CLA  | C3B-C2B | 5.40 | 1.47        | 1.40     |
| 31  | 2     | 309 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |
| 31  | K     | 205 | CLA  | C3C-C2C | 5.40 | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | B     | 833 | CLA  | C3B-C2B | 5.39 | 1.47        | 1.40     |
| 31  | 2     | 311 | CLA  | C3C-C2C | 5.39 | 1.48        | 1.36     |
| 31  | 6     | 308 | CLA  | C3B-C2B | 5.39 | 1.47        | 1.40     |
| 31  | b     | 306 | CLA  | C3B-C2B | 5.39 | 1.47        | 1.40     |
| 31  | K     | 206 | CLA  | C3C-C2C | 5.39 | 1.48        | 1.36     |
| 31  | 8     | 312 | CLA  | C3C-C2C | 5.39 | 1.48        | 1.36     |
| 31  | 4     | 306 | CLA  | C3B-C2B | 5.39 | 1.47        | 1.40     |
| 31  | a     | 322 | CLA  | C3C-C2C | 5.38 | 1.48        | 1.36     |
| 31  | 5     | 320 | CLA  | CHC-C1C | 5.38 | 1.48        | 1.35     |
| 31  | b     | 304 | CLA  | CHC-C1C | 5.38 | 1.48        | 1.35     |
| 31  | 9     | 313 | CLA  | C3C-C2C | 5.38 | 1.48        | 1.36     |
| 31  | 2     | 305 | CLA  | C3C-C2C | 5.38 | 1.48        | 1.36     |
| 31  | 2     | 312 | CLA  | C3B-C2B | 5.38 | 1.47        | 1.40     |
| 31  | 3     | 316 | CLA  | C3C-C2C | 5.38 | 1.48        | 1.36     |
| 31  | 5     | 308 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 31  | b     | 310 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 31  | 6     | 316 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 31  | L     | 307 | CLA  | C3C-C2C | 5.37 | 1.48        | 1.36     |
| 31  | B     | 821 | CLA  | C3B-C2B | 5.37 | 1.47        | 1.40     |
| 31  | 8     | 314 | CLA  | C3B-C2B | 5.36 | 1.47        | 1.40     |
| 31  | A     | 822 | CLA  | MG-NA   | 5.36 | 2.19        | 2.06     |
| 31  | 3     | 317 | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 31  | A     | 821 | CLA  | C3B-C2B | 5.36 | 1.47        | 1.40     |
| 31  | 3     | 313 | CLA  | C3C-C2C | 5.36 | 1.48        | 1.36     |
| 31  | A     | 853 | CLA  | MG-NA   | 5.36 | 2.19        | 2.06     |
| 31  | A     | 845 | CLA  | C3B-C2B | 5.36 | 1.47        | 1.40     |
| 31  | b     | 303 | CLA  | CHD-C1D | 5.36 | 1.48        | 1.38     |
| 31  | 6     | 306 | CLA  | CHC-C1C | 5.36 | 1.48        | 1.35     |
| 31  | H     | 903 | CLA  | C3B-C2B | 5.36 | 1.47        | 1.40     |
| 31  | A     | 828 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | a     | 322 | CLA  | C3B-C2B | 5.35 | 1.47        | 1.40     |
| 31  | a     | 315 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | b     | 304 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | b     | 308 | CLA  | C3B-C2B | 5.35 | 1.47        | 1.40     |
| 31  | B     | 823 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | 5     | 315 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | 4     | 318 | CLA  | C3B-C2B | 5.35 | 1.47        | 1.40     |
| 31  | 8     | 315 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | 7     | 312 | CLA  | CHC-C1C | 5.35 | 1.48        | 1.35     |
| 31  | B     | 835 | CLA  | C3B-C2B | 5.35 | 1.47        | 1.40     |
| 31  | b     | 303 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |
| 31  | 5     | 312 | CLA  | C3C-C2C | 5.35 | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | b     | 313 | CLA  | CHC-C1C | 5.34 | 1.48        | 1.35     |
| 31  | B     | 831 | CLA  | C3C-C2C | 5.34 | 1.48        | 1.36     |
| 31  | 4     | 321 | CLA  | C3C-C2C | 5.34 | 1.48        | 1.36     |
| 31  | O     | 203 | CLA  | CHC-C1C | 5.34 | 1.48        | 1.35     |
| 31  | H     | 902 | CLA  | C3B-C2B | 5.34 | 1.47        | 1.40     |
| 31  | 3     | 309 | CLA  | C3C-C2C | 5.34 | 1.48        | 1.36     |
| 31  | H     | 902 | CLA  | C3C-C2C | 5.34 | 1.48        | 1.36     |
| 31  | 5     | 314 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | a     | 321 | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 31  | 9     | 318 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | O     | 204 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | 4     | 319 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | b     | 312 | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 31  | 9     | 321 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | G     | 205 | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 31  | b     | 311 | CLA  | CHC-C1C | 5.33 | 1.48        | 1.35     |
| 31  | B     | 820 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | B     | 834 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | 6     | 314 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | 4     | 321 | CLA  | O2D-CGD | 5.33 | 1.46        | 1.33     |
| 31  | b     | 305 | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 31  | b     | 312 | CLA  | CHD-C1D | 5.33 | 1.48        | 1.38     |
| 31  | 3     | 312 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | 2     | 314 | CLA  | C3B-C2B | 5.33 | 1.47        | 1.40     |
| 31  | 4     | 306 | CLA  | C3C-C2C | 5.33 | 1.48        | 1.36     |
| 31  | A     | 824 | CLA  | C3B-C2B | 5.32 | 1.47        | 1.40     |
| 31  | 4     | 307 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 31  | B     | 825 | CLA  | C3B-C2B | 5.32 | 1.47        | 1.40     |
| 31  | 2     | 314 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 31  | A     | 826 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 31  | 6     | 322 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 31  | O     | 204 | CLA  | CHC-C1C | 5.32 | 1.48        | 1.35     |
| 31  | 2     | 304 | CLA  | CHC-C1C | 5.32 | 1.48        | 1.35     |
| 31  | 5     | 307 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 31  | 3     | 320 | CLA  | O2D-CGD | 5.32 | 1.46        | 1.33     |
| 31  | 2     | 306 | CLA  | C3C-C2C | 5.32 | 1.48        | 1.36     |
| 31  | 2     | 308 | CLA  | CHC-C1C | 5.32 | 1.48        | 1.35     |
| 31  | 3     | 313 | CLA  | C3B-C2B | 5.32 | 1.47        | 1.40     |
| 31  | b     | 310 | CLA  | CHC-C1C | 5.32 | 1.48        | 1.35     |
| 31  | b     | 305 | CLA  | O2D-CGD | 5.32 | 1.46        | 1.33     |
| 31  | B     | 837 | CLA  | C3B-C2B | 5.32 | 1.47        | 1.40     |
| 31  | B     | 829 | CLA  | C3B-C2B | 5.32 | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 314 | CLA  | C3B-C2B | 5.32  | 1.47        | 1.40     |
| 31  | 2     | 305 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | 6     | 312 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |
| 31  | 2     | 311 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |
| 31  | 9     | 319 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | 3     | 307 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |
| 31  | a     | 316 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | 5     | 315 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | A     | 818 | CLA  | CHC-C1C | 5.31  | 1.48        | 1.35     |
| 31  | 4     | 309 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | A     | 836 | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 31  | 3     | 308 | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 31  | O     | 204 | CLA  | O2D-CGD | 5.31  | 1.46        | 1.33     |
| 31  | 9     | 311 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | a     | 313 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | 6     | 311 | CLA  | C3C-C2C | 5.31  | 1.48        | 1.36     |
| 31  | 2     | 312 | CLA  | O2D-CGD | 5.31  | 1.46        | 1.33     |
| 31  | B     | 846 | CLA  | C3B-C2B | 5.31  | 1.47        | 1.40     |
| 31  | H     | 901 | CLA  | CHD-C1D | 5.30  | 1.48        | 1.38     |
| 31  | 9     | 312 | CLA  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 31  | 7     | 309 | CLA  | CHC-C1C | 5.30  | 1.48        | 1.35     |
| 31  | 8     | 315 | CLA  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 31  | 7     | 316 | CLA  | CHC-C1C | 5.30  | 1.48        | 1.35     |
| 31  | 2     | 312 | CLA  | CHC-C1C | 5.30  | 1.48        | 1.35     |
| 31  | 7     | 316 | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 31  | L     | 307 | CLA  | CHD-C1D | 5.30  | 1.48        | 1.38     |
| 31  | 3     | 308 | CLA  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 31  | A     | 823 | CLA  | C3B-C2B | 5.30  | 1.47        | 1.40     |
| 31  | b     | 306 | CLA  | O2D-CGD | 5.30  | 1.46        | 1.33     |
| 31  | 7     | 311 | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 31  | b     | 308 | CLA  | CHC-C1C | 5.30  | 1.48        | 1.35     |
| 31  | A     | 835 | CLA  | C3C-C2C | 5.30  | 1.48        | 1.36     |
| 31  | 2     | 309 | CLA  | CHC-C1C | 5.30  | 1.48        | 1.35     |
| 31  | 2     | 305 | CLA  | O2D-CGD | 5.29  | 1.46        | 1.33     |
| 31  | H     | 902 | CLA  | MG-ND   | -5.29 | 1.95        | 2.05     |
| 31  | B     | 824 | CLA  | C3B-C2B | 5.29  | 1.47        | 1.40     |
| 31  | G     | 204 | CLA  | C3C-C2C | 5.29  | 1.48        | 1.36     |
| 31  | b     | 302 | CLA  | C3C-C2C | 5.29  | 1.48        | 1.36     |
| 31  | 4     | 315 | CLA  | CHC-C1C | 5.29  | 1.48        | 1.35     |
| 31  | A     | 834 | CLA  | C3C-C2C | 5.29  | 1.48        | 1.36     |
| 31  | 4     | 311 | CLA  | C3B-C2B | 5.29  | 1.47        | 1.40     |
| 31  | A     | 814 | CLA  | C3C-C2C | 5.29  | 1.48        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | a     | 313 | CLA  | C3C-C2C | 5.29 | 1.48        | 1.36     |
| 31  | 9     | 318 | CLA  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 31  | B     | 835 | CLA  | C3C-C2C | 5.29 | 1.48        | 1.36     |
| 31  | 5     | 323 | CLA  | C3C-C2C | 5.29 | 1.48        | 1.36     |
| 31  | 6     | 310 | CLA  | C3B-C2B | 5.29 | 1.47        | 1.40     |
| 31  | 3     | 318 | CLA  | C3B-C2B | 5.29 | 1.47        | 1.40     |
| 31  | A     | 819 | CLA  | MG-NC   | 5.29 | 2.18        | 2.06     |
| 31  | a     | 309 | CLA  | CHC-C1C | 5.29 | 1.48        | 1.35     |
| 31  | 4     | 319 | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 31  | 3     | 308 | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 31  | 3     | 318 | CLA  | C3C-C2C | 5.28 | 1.48        | 1.36     |
| 31  | 6     | 312 | CLA  | C3C-C2C | 5.28 | 1.48        | 1.36     |
| 31  | 4     | 314 | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 31  | 5     | 312 | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 31  | 5     | 308 | CLA  | O2D-CGD | 5.28 | 1.46        | 1.33     |
| 31  | A     | 852 | CLA  | C3C-C2C | 5.28 | 1.47        | 1.36     |
| 31  | 6     | 313 | CLA  | C3C-C2C | 5.28 | 1.47        | 1.36     |
| 31  | A     | 851 | CLA  | C3B-C2B | 5.28 | 1.47        | 1.40     |
| 31  | 6     | 313 | CLA  | O2D-CGD | 5.28 | 1.46        | 1.33     |
| 31  | 3     | 314 | CLA  | C3C-C2C | 5.28 | 1.47        | 1.36     |
| 31  | 4     | 311 | CLA  | CHC-C1C | 5.28 | 1.48        | 1.35     |
| 31  | A     | 823 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | 3     | 312 | CLA  | C3C-C2C | 5.27 | 1.47        | 1.36     |
| 31  | A     | 830 | CLA  | C3B-C2B | 5.27 | 1.47        | 1.40     |
| 31  | 3     | 313 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | b     | 311 | CLA  | C3B-C2B | 5.27 | 1.47        | 1.40     |
| 31  | 6     | 308 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | 5     | 321 | CLA  | C3B-C2B | 5.27 | 1.47        | 1.40     |
| 31  | A     | 825 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | B     | 848 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | B     | 842 | CLA  | C3C-C2C | 5.27 | 1.47        | 1.36     |
| 31  | A     | 817 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | b     | 306 | CLA  | CHC-C1C | 5.27 | 1.48        | 1.35     |
| 31  | 5     | 309 | CLA  | C3C-C2C | 5.27 | 1.47        | 1.36     |
| 31  | 3     | 312 | CLA  | CHD-C1D | 5.27 | 1.48        | 1.38     |
| 31  | 6     | 310 | CLA  | C3C-C2C | 5.27 | 1.47        | 1.36     |
| 31  | b     | 307 | CLA  | CHD-C1D | 5.27 | 1.48        | 1.38     |
| 31  | G     | 204 | CLA  | C3B-C2B | 5.26 | 1.47        | 1.40     |
| 31  | 5     | 318 | CLA  | C3B-C2B | 5.26 | 1.47        | 1.40     |
| 31  | 9     | 321 | CLA  | C3C-C2C | 5.26 | 1.47        | 1.36     |
| 31  | B     | 819 | CLA  | C3C-C2C | 5.26 | 1.47        | 1.36     |
| 31  | B     | 814 | CLA  | C3C-C2C | 5.26 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | a     | 310 | CLA  | C3C-C2C | 5.26  | 1.47        | 1.36     |
| 31  | G     | 206 | CLA  | C3B-C2B | 5.26  | 1.47        | 1.40     |
| 31  | G     | 205 | CLA  | CHC-C1C | 5.26  | 1.48        | 1.35     |
| 31  | 7     | 315 | CLA  | C3B-C2B | 5.26  | 1.47        | 1.40     |
| 31  | A     | 826 | CLA  | C3B-C2B | 5.26  | 1.47        | 1.40     |
| 31  | 9     | 314 | CLA  | C3C-C2C | 5.26  | 1.47        | 1.36     |
| 31  | 2     | 306 | CLA  | CHD-C1D | 5.26  | 1.48        | 1.38     |
| 31  | 5     | 309 | CLA  | CHD-C1D | 5.25  | 1.48        | 1.38     |
| 31  | B     | 837 | CLA  | C3C-C2C | 5.25  | 1.47        | 1.36     |
| 31  | 8     | 315 | CLA  | CHC-C1C | 5.25  | 1.48        | 1.35     |
| 31  | b     | 312 | CLA  | O2D-CGD | 5.25  | 1.46        | 1.33     |
| 31  | A     | 847 | CLA  | C3B-C2B | 5.25  | 1.47        | 1.40     |
| 31  | L     | 305 | CLA  | CHC-C1C | 5.25  | 1.48        | 1.35     |
| 31  | 2     | 313 | CLA  | CHD-C1D | 5.25  | 1.48        | 1.38     |
| 31  | H     | 901 | CLA  | O2D-CGD | 5.25  | 1.46        | 1.33     |
| 31  | a     | 309 | CLA  | C3C-C2C | 5.25  | 1.47        | 1.36     |
| 31  | 9     | 319 | CLA  | C3C-C2C | 5.25  | 1.47        | 1.36     |
| 31  | 4     | 306 | CLA  | CHC-C1C | 5.25  | 1.48        | 1.35     |
| 31  | 6     | 316 | CLA  | MG-NC   | -5.25 | 1.93        | 2.06     |
| 31  | 7     | 315 | CLA  | C3C-C2C | 5.25  | 1.47        | 1.36     |
| 31  | 4     | 307 | CLA  | CHD-C1D | 5.25  | 1.48        | 1.38     |
| 31  | A     | 842 | CLA  | C3C-C2C | 5.25  | 1.47        | 1.36     |
| 31  | 6     | 322 | CLA  | C3B-C2B | 5.25  | 1.47        | 1.40     |
| 31  | a     | 311 | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 31  | B     | 813 | CLA  | CHC-C1C | 5.24  | 1.48        | 1.35     |
| 31  | B     | 840 | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 31  | 9     | 319 | CLA  | O2D-CGD | 5.24  | 1.46        | 1.33     |
| 31  | A     | 819 | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 31  | a     | 312 | CLA  | CHC-C1C | 5.24  | 1.48        | 1.35     |
| 31  | 2     | 308 | CLA  | O2D-CGD | 5.24  | 1.46        | 1.33     |
| 31  | 5     | 318 | CLA  | CHD-C1D | 5.24  | 1.48        | 1.38     |
| 31  | 2     | 304 | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 31  | B     | 836 | CLA  | C3B-C2B | 5.24  | 1.47        | 1.40     |
| 31  | B     | 844 | CLA  | CHC-C1C | 5.24  | 1.48        | 1.35     |
| 31  | 5     | 314 | CLA  | CHC-C1C | 5.24  | 1.48        | 1.35     |
| 31  | O     | 204 | CLA  | CHD-C1D | 5.24  | 1.48        | 1.38     |
| 31  | 9     | 313 | CLA  | CHC-C1C | 5.24  | 1.48        | 1.35     |
| 31  | B     | 826 | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 31  | 5     | 307 | CLA  | CHC-C1C | 5.24  | 1.48        | 1.35     |
| 31  | 9     | 311 | CLA  | C3C-C2C | 5.24  | 1.47        | 1.36     |
| 31  | A     | 856 | CLA  | C3C-C2C | 5.23  | 1.47        | 1.36     |
| 31  | 5     | 312 | CLA  | C3B-C2B | 5.23  | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | B     | 829 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | B     | 828 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | B     | 828 | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 31  | L     | 306 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | B     | 824 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | 6     | 316 | CLA  | CHC-C1C | 5.23 | 1.48        | 1.35     |
| 31  | G     | 206 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | a     | 310 | CLA  | C3B-C2B | 5.23 | 1.47        | 1.40     |
| 31  | 4     | 318 | CLA  | O2D-CGD | 5.23 | 1.46        | 1.33     |
| 31  | 6     | 307 | CLA  | CHD-C1D | 5.23 | 1.48        | 1.38     |
| 31  | b     | 308 | CLA  | CHD-C1D | 5.23 | 1.48        | 1.38     |
| 31  | 8     | 309 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | O     | 202 | CLA  | CHD-C1D | 5.23 | 1.48        | 1.38     |
| 31  | A     | 825 | CLA  | C3C-C2C | 5.23 | 1.47        | 1.36     |
| 31  | B     | 843 | CLA  | C3C-C2C | 5.22 | 1.47        | 1.36     |
| 31  | 8     | 320 | CLA  | CHD-C1D | 5.22 | 1.48        | 1.38     |
| 31  | 8     | 313 | CLA  | C3C-C2C | 5.22 | 1.47        | 1.36     |
| 31  | A     | 815 | CLA  | C3B-C2B | 5.22 | 1.47        | 1.40     |
| 31  | H     | 901 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 31  | 4     | 321 | CLA  | C3B-C2B | 5.22 | 1.47        | 1.40     |
| 31  | 5     | 315 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 31  | 3     | 320 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 31  | 2     | 313 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 31  | B     | 833 | CLA  | C3C-C2C | 5.22 | 1.47        | 1.36     |
| 31  | 4     | 312 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 31  | 4     | 308 | CLA  | C3C-C2C | 5.22 | 1.47        | 1.36     |
| 31  | 2     | 310 | CLA  | CHC-C1C | 5.22 | 1.48        | 1.35     |
| 31  | 5     | 309 | CLA  | C3B-C2B | 5.22 | 1.47        | 1.40     |
| 31  | K     | 204 | CLA  | C3C-C2C | 5.22 | 1.47        | 1.36     |
| 31  | B     | 816 | CLA  | C3B-C2B | 5.21 | 1.47        | 1.40     |
| 31  | 3     | 311 | CLA  | C3C-C2C | 5.21 | 1.47        | 1.36     |
| 31  | b     | 307 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | A     | 849 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | O     | 202 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | B     | 840 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | 4     | 320 | CLA  | O2D-CGD | 5.21 | 1.45        | 1.33     |
| 31  | L     | 307 | CLA  | O2D-CGD | 5.21 | 1.45        | 1.33     |
| 31  | A     | 843 | CLA  | C3C-C2C | 5.21 | 1.47        | 1.36     |
| 31  | A     | 855 | CLA  | C3C-C2C | 5.21 | 1.47        | 1.36     |
| 31  | a     | 311 | CLA  | CHD-C1D | 5.21 | 1.48        | 1.38     |
| 31  | L     | 306 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | a     | 322 | CLA  | CHD-C1D | 5.21 | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | A     | 853 | CLA  | C3B-C2B | 5.21 | 1.47        | 1.40     |
| 31  | B     | 846 | CLA  | C3C-C2C | 5.21 | 1.47        | 1.36     |
| 31  | 6     | 307 | CLA  | C3C-C2C | 5.21 | 1.47        | 1.36     |
| 31  | H     | 902 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | A     | 853 | CLA  | O2D-CGD | 5.21 | 1.45        | 1.33     |
| 31  | 9     | 321 | CLA  | CHD-C1D | 5.21 | 1.48        | 1.38     |
| 31  | 4     | 320 | CLA  | CHC-C1C | 5.21 | 1.48        | 1.35     |
| 31  | A     | 833 | CLA  | C3C-C2C | 5.21 | 1.47        | 1.36     |
| 31  | B     | 830 | CLA  | C3C-C2C | 5.20 | 1.47        | 1.36     |
| 31  | A     | 852 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | a     | 314 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | 5     | 308 | CLA  | CHD-C1D | 5.20 | 1.48        | 1.38     |
| 31  | B     | 832 | CLA  | C3B-C2B | 5.20 | 1.47        | 1.40     |
| 31  | 5     | 323 | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 31  | 8     | 313 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | A     | 827 | CLA  | C3C-C2C | 5.20 | 1.47        | 1.36     |
| 31  | A     | 842 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | 8     | 314 | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 31  | 7     | 309 | CLA  | C3B-C2B | 5.20 | 1.47        | 1.40     |
| 31  | 4     | 315 | CLA  | C3C-C2C | 5.20 | 1.47        | 1.36     |
| 31  | A     | 835 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | b     | 308 | CLA  | O2D-CGD | 5.20 | 1.45        | 1.33     |
| 31  | 9     | 312 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | A     | 844 | CLA  | C3C-C2C | 5.20 | 1.47        | 1.36     |
| 31  | 6     | 311 | CLA  | CHD-C1D | 5.20 | 1.48        | 1.38     |
| 31  | 5     | 323 | CLA  | C3B-C2B | 5.20 | 1.47        | 1.40     |
| 31  | 2     | 306 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | B     | 820 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | 5     | 308 | CLA  | CHC-C1C | 5.20 | 1.48        | 1.35     |
| 31  | 2     | 307 | CLA  | O2D-CGD | 5.19 | 1.45        | 1.33     |
| 31  | A     | 846 | CLA  | C3C-C2C | 5.19 | 1.47        | 1.36     |
| 31  | B     | 818 | CLA  | MG-NA   | 5.19 | 2.18        | 2.06     |
| 31  | a     | 316 | CLA  | C3C-C2C | 5.19 | 1.47        | 1.36     |
| 31  | B     | 825 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 31  | 6     | 315 | CLA  | C3C-C2C | 5.19 | 1.47        | 1.36     |
| 31  | 6     | 322 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 31  | 8     | 308 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 31  | A     | 843 | CLA  | C3B-C2B | 5.19 | 1.47        | 1.40     |
| 31  | 8     | 312 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 31  | 3     | 310 | CLA  | C3B-C2B | 5.19 | 1.47        | 1.40     |
| 31  | 6     | 315 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 31  | 6     | 314 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | A     | 837 | CLA  | C3B-C2B | 5.19 | 1.47        | 1.40     |
| 31  | L     | 307 | CLA  | CHC-C1C | 5.19 | 1.48        | 1.35     |
| 31  | 3     | 313 | CLA  | CHD-C1D | 5.19 | 1.48        | 1.38     |
| 31  | 3     | 316 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | A     | 833 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | 3     | 309 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | J     | 105 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 31  | 2     | 310 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | 4     | 315 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | 6     | 310 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | A     | 821 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 31  | A     | 836 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | 9     | 319 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | 8     | 320 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 31  | b     | 310 | CLA  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 31  | B     | 845 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | A     | 841 | CLA  | MG-NC   | 5.18 | 2.18        | 2.06     |
| 31  | B     | 815 | CLA  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 31  | b     | 303 | CLA  | O2D-CGD | 5.18 | 1.45        | 1.33     |
| 31  | B     | 836 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 31  | 5     | 310 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | 2     | 307 | CLA  | C3C-C2C | 5.18 | 1.47        | 1.36     |
| 31  | 4     | 314 | CLA  | CHD-C1D | 5.18 | 1.48        | 1.38     |
| 31  | A     | 835 | CLA  | MG-NA   | 5.18 | 2.18        | 2.06     |
| 31  | a     | 315 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | 3     | 317 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | B     | 842 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | a     | 316 | CLA  | CHC-C1C | 5.18 | 1.48        | 1.35     |
| 31  | B     | 822 | CLA  | C3B-C2B | 5.18 | 1.47        | 1.40     |
| 31  | B     | 839 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 31  | 2     | 311 | CLA  | C3B-C2B | 5.17 | 1.47        | 1.40     |
| 31  | 5     | 314 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 31  | 7     | 313 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 31  | A     | 832 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 31  | 4     | 319 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |
| 31  | 9     | 314 | CLA  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 31  | A     | 847 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 31  | B     | 820 | CLA  | C3C-C2C | 5.17 | 1.47        | 1.36     |
| 31  | a     | 322 | CLA  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 31  | 2     | 307 | CLA  | CHC-C1C | 5.17 | 1.48        | 1.35     |
| 31  | B     | 842 | CLA  | C3B-C2B | 5.17 | 1.47        | 1.40     |
| 31  | 6     | 307 | CLA  | O2D-CGD | 5.17 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 5     | 312 | CLA  | CHD-C1D | 5.17 | 1.48        | 1.38     |
| 31  | O     | 203 | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 31  | 5     | 315 | CLA  | CHD-C1D | 5.16 | 1.48        | 1.38     |
| 31  | 6     | 316 | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 31  | 7     | 321 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 31  | 5     | 318 | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 31  | J     | 105 | CLA  | C3B-C2B | 5.16 | 1.47        | 1.40     |
| 31  | B     | 822 | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 31  | A     | 841 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 31  | 5     | 311 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 31  | a     | 321 | CLA  | C3B-C2B | 5.16 | 1.47        | 1.40     |
| 31  | A     | 856 | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 31  | L     | 306 | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 31  | B     | 831 | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 31  | b     | 305 | CLA  | CHC-C1C | 5.16 | 1.48        | 1.35     |
| 31  | 8     | 307 | CLA  | C3C-C2C | 5.16 | 1.47        | 1.36     |
| 31  | 6     | 311 | CLA  | O2D-CGD | 5.16 | 1.45        | 1.33     |
| 31  | 9     | 316 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | b     | 312 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | 7     | 322 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 31  | B     | 839 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | F     | 305 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 31  | B     | 812 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 31  | B     | 849 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | 3     | 309 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | 7     | 321 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | 4     | 307 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | F     | 306 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 31  | 4     | 309 | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 31  | A     | 851 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | 8     | 321 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 31  | A     | 834 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 31  | A     | 846 | CLA  | C3B-C2B | 5.15 | 1.47        | 1.40     |
| 31  | 8     | 318 | CLA  | C3C-C2C | 5.15 | 1.47        | 1.36     |
| 31  | 6     | 314 | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 31  | K     | 205 | CLA  | CHD-C1D | 5.15 | 1.48        | 1.38     |
| 31  | 7     | 314 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | b     | 313 | CLA  | O2D-CGD | 5.15 | 1.45        | 1.33     |
| 31  | 3     | 316 | CLA  | CHC-C1C | 5.15 | 1.48        | 1.35     |
| 31  | 5     | 308 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 31  | K     | 205 | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 31  | 2     | 309 | CLA  | MG-NA   | 5.14 | 2.18        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | B     | 844 | CLA  | C3C-C2C | 5.14 | 1.47        | 1.36     |
| 31  | 8     | 312 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 31  | 7     | 311 | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 31  | 2     | 311 | CLA  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 31  | 5     | 321 | CLA  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 32  | 5     | 322 | CHL  | MG-NA   | 5.14 | 2.18        | 2.06     |
| 31  | 4     | 308 | CLA  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 31  | 2     | 306 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 31  | 2     | 305 | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 31  | 6     | 307 | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 31  | B     | 844 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 31  | 8     | 315 | CLA  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 31  | 4     | 312 | CLA  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 31  | 4     | 315 | CLA  | CHD-C1D | 5.14 | 1.48        | 1.38     |
| 31  | A     | 824 | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 31  | 5     | 321 | CLA  | CHC-C1C | 5.14 | 1.48        | 1.35     |
| 31  | B     | 847 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 31  | B     | 843 | CLA  | C3B-C2B | 5.14 | 1.47        | 1.40     |
| 31  | 6     | 310 | CLA  | O2D-CGD | 5.14 | 1.45        | 1.33     |
| 31  | b     | 311 | CLA  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 31  | 3     | 310 | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 31  | 7     | 314 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 31  | A     | 824 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 31  | A     | 823 | CLA  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 31  | 8     | 321 | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 31  | B     | 811 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 31  | H     | 903 | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 31  | B     | 826 | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 31  | 2     | 313 | CLA  | C3B-C2B | 5.13 | 1.47        | 1.40     |
| 31  | B     | 849 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 31  | H     | 903 | CLA  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 31  | 2     | 304 | CLA  | O2D-CGD | 5.13 | 1.45        | 1.33     |
| 31  | 3     | 317 | CLA  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 31  | b     | 310 | CLA  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 31  | B     | 815 | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 31  | K     | 204 | CLA  | CHC-C1C | 5.13 | 1.48        | 1.35     |
| 31  | A     | 849 | CLA  | CHD-C1D | 5.13 | 1.48        | 1.38     |
| 31  | 8     | 308 | CLA  | C3C-C2C | 5.13 | 1.47        | 1.36     |
| 31  | A     | 827 | CLA  | CHC-C1C | 5.12 | 1.48        | 1.35     |
| 31  | 3     | 314 | CLA  | C3B-C2B | 5.12 | 1.47        | 1.40     |
| 31  | 6     | 311 | CLA  | C3B-C2B | 5.12 | 1.47        | 1.40     |
| 31  | B     | 847 | CLA  | C3C-C2C | 5.12 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | K     | 206 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 31  | 2     | 314 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | b     | 302 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | B     | 819 | CLA  | C3B-C2B | 5.12  | 1.47        | 1.40     |
| 31  | G     | 204 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | G     | 204 | CLA  | CHD-C1D | 5.12  | 1.48        | 1.38     |
| 31  | 5     | 323 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | 7     | 314 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 31  | B     | 838 | CLA  | C3C-C2C | 5.12  | 1.47        | 1.36     |
| 31  | A     | 855 | CLA  | C3B-C2B | 5.12  | 1.47        | 1.40     |
| 31  | B     | 846 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | F     | 301 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | B     | 843 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 31  | b     | 304 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 31  | B     | 833 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | 6     | 312 | CLA  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 31  | B     | 845 | CLA  | C3C-C2C | 5.12  | 1.47        | 1.36     |
| 31  | B     | 811 | CLA  | CHC-C1C | 5.12  | 1.48        | 1.35     |
| 31  | a     | 315 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 31  | 5     | 309 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | a     | 319 | CLA  | C3B-C2B | 5.11  | 1.47        | 1.40     |
| 31  | 2     | 309 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 31  | B     | 824 | CLA  | MG-ND   | -5.11 | 1.95        | 2.05     |
| 31  | A     | 822 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | 2     | 315 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | F     | 306 | CLA  | C3B-C2B | 5.11  | 1.47        | 1.40     |
| 31  | 5     | 321 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 31  | 7     | 310 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 31  | 2     | 309 | CLA  | CHD-C1D | 5.11  | 1.48        | 1.38     |
| 31  | 4     | 318 | CLA  | C3C-C2C | 5.11  | 1.47        | 1.36     |
| 31  | 7     | 310 | CLA  | C3B-C2B | 5.11  | 1.47        | 1.40     |
| 31  | 9     | 311 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | 6     | 322 | CLA  | CHD-C1D | 5.11  | 1.48        | 1.38     |
| 31  | 4     | 318 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | 4     | 309 | CLA  | C3C-C2C | 5.11  | 1.47        | 1.36     |
| 31  | 4     | 307 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 31  | 5     | 309 | CLA  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 31  | A     | 837 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | 3     | 314 | CLA  | CHC-C1C | 5.11  | 1.48        | 1.35     |
| 31  | 4     | 311 | CLA  | O2D-CGD | 5.10  | 1.45        | 1.33     |
| 31  | 5     | 310 | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |
| 31  | A     | 838 | CLA  | C3C-C2C | 5.10  | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 2     | 314 | CLA  | CHD-C1D | 5.10 | 1.48        | 1.38     |
| 31  | B     | 814 | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 31  | K     | 206 | CLA  | CHD-C1D | 5.10 | 1.48        | 1.38     |
| 31  | B     | 835 | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 31  | A     | 838 | CLA  | CHD-C1D | 5.10 | 1.48        | 1.38     |
| 31  | 3     | 318 | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 31  | B     | 813 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 31  | A     | 820 | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 31  | A     | 824 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 31  | b     | 307 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 31  | 7     | 309 | CLA  | MG-NA   | 5.10 | 2.18        | 2.06     |
| 31  | 8     | 307 | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 31  | 7     | 309 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 31  | B     | 837 | CLA  | CHC-C1C | 5.10 | 1.48        | 1.35     |
| 31  | A     | 837 | CLA  | O2D-CGD | 5.10 | 1.45        | 1.33     |
| 31  | 9     | 315 | CLA  | C3C-C2C | 5.10 | 1.47        | 1.36     |
| 31  | a     | 313 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | 2     | 314 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 31  | 4     | 315 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 31  | 4     | 321 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | A     | 854 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 31  | 6     | 322 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 31  | G     | 206 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | B     | 834 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | 3     | 318 | CLA  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 31  | 7     | 314 | CLA  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 31  | A     | 845 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | F     | 305 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 31  | A     | 814 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | O     | 203 | CLA  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 31  | A     | 828 | CLA  | CHC-C1C | 5.09 | 1.48        | 1.35     |
| 31  | a     | 321 | CLA  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 31  | a     | 314 | CLA  | O2D-CGD | 5.09 | 1.45        | 1.33     |
| 31  | 2     | 307 | CLA  | CHD-C1D | 5.09 | 1.48        | 1.38     |
| 31  | 3     | 318 | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 31  | 4     | 306 | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 31  | A     | 834 | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 31  | 4     | 314 | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 31  | A     | 817 | CLA  | C3C-C2C | 5.08 | 1.47        | 1.36     |
| 31  | a     | 321 | CLA  | CHC-C1C | 5.08 | 1.48        | 1.35     |
| 31  | 5     | 315 | CLA  | O2D-CGD | 5.08 | 1.45        | 1.33     |
| 31  | a     | 314 | CLA  | CHD-C1D | 5.08 | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 321 | CLA  | CHC-C1C | 5.08  | 1.48        | 1.35     |
| 31  | 3     | 312 | CLA  | CHC-C1C | 5.08  | 1.48        | 1.35     |
| 31  | a     | 309 | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 31  | 3     | 319 | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 31  | B     | 831 | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 31  | A     | 822 | CLA  | C3C-C2C | 5.08  | 1.47        | 1.36     |
| 31  | 9     | 314 | CLA  | O2D-CGD | 5.08  | 1.45        | 1.33     |
| 31  | 8     | 314 | CLA  | CHC-C1C | 5.08  | 1.48        | 1.35     |
| 31  | 6     | 322 | CLA  | MG-ND   | 5.08  | 2.15        | 2.05     |
| 31  | 8     | 310 | CLA  | MG-NC   | 5.08  | 2.18        | 2.06     |
| 31  | b     | 306 | CLA  | CHD-C1D | 5.07  | 1.48        | 1.38     |
| 31  | b     | 303 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 31  | 2     | 310 | CLA  | CHD-C1D | 5.07  | 1.48        | 1.38     |
| 31  | 2     | 305 | CLA  | MG-NC   | -5.07 | 1.94        | 2.06     |
| 31  | 8     | 318 | CLA  | C3B-C2B | 5.07  | 1.47        | 1.40     |
| 31  | a     | 310 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 31  | b     | 311 | CLA  | CHD-C1D | 5.07  | 1.48        | 1.38     |
| 31  | A     | 826 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 31  | 7     | 322 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 31  | A     | 845 | CLA  | C3C-C2C | 5.07  | 1.47        | 1.36     |
| 31  | 8     | 309 | CLA  | C3B-C2B | 5.07  | 1.47        | 1.40     |
| 31  | 8     | 312 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 31  | A     | 820 | CLA  | C3C-C2C | 5.07  | 1.47        | 1.36     |
| 31  | 4     | 309 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 31  | B     | 830 | CLA  | CHC-C1C | 5.07  | 1.48        | 1.35     |
| 31  | 7     | 312 | CLA  | C3C-C2C | 5.07  | 1.47        | 1.36     |
| 31  | 3     | 307 | CLA  | C3C-C2C | 5.07  | 1.47        | 1.36     |
| 31  | 6     | 315 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 31  | 8     | 315 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 31  | a     | 319 | CLA  | CHD-C1D | 5.07  | 1.48        | 1.38     |
| 31  | G     | 205 | CLA  | O2D-CGD | 5.07  | 1.45        | 1.33     |
| 31  | 4     | 311 | CLA  | CHD-C1D | 5.06  | 1.48        | 1.38     |
| 31  | 6     | 313 | CLA  | CHC-C1C | 5.06  | 1.48        | 1.35     |
| 31  | 9     | 315 | CLA  | MG-NC   | 5.06  | 2.18        | 2.06     |
| 31  | B     | 838 | CLA  | CHD-C1D | 5.06  | 1.48        | 1.38     |
| 31  | B     | 821 | CLA  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 31  | 7     | 322 | CLA  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 31  | a     | 311 | CLA  | MG-NC   | 5.06  | 2.18        | 2.06     |
| 31  | 2     | 315 | CLA  | C3C-C2C | 5.06  | 1.47        | 1.36     |
| 31  | 9     | 319 | CLA  | CHD-C1D | 5.06  | 1.48        | 1.38     |
| 31  | 7     | 316 | CLA  | CHD-C1D | 5.06  | 1.48        | 1.38     |
| 31  | 3     | 313 | CLA  | O2D-CGD | 5.06  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | B     | 843 | CLA  | CHD-C1D | 5.06 | 1.48        | 1.38     |
| 31  | 5     | 311 | CLA  | O2D-CGD | 5.06 | 1.45        | 1.33     |
| 31  | 3     | 320 | CLA  | CHD-C1D | 5.06 | 1.48        | 1.38     |
| 31  | A     | 815 | CLA  | C3C-C2C | 5.06 | 1.47        | 1.36     |
| 31  | 7     | 316 | CLA  | C3B-C2B | 5.06 | 1.47        | 1.40     |
| 31  | 2     | 312 | CLA  | CHD-C1D | 5.06 | 1.48        | 1.38     |
| 31  | 8     | 311 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 31  | 4     | 308 | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 31  | 5     | 313 | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 31  | F     | 301 | CLA  | MG-NA   | 5.05 | 2.18        | 2.06     |
| 31  | 5     | 318 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 31  | A     | 855 | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 31  | L     | 306 | CLA  | CHD-C1D | 5.05 | 1.48        | 1.38     |
| 31  | B     | 817 | CLA  | C3C-C2C | 5.05 | 1.47        | 1.36     |
| 31  | 9     | 311 | CLA  | CHD-C1D | 5.05 | 1.48        | 1.38     |
| 31  | J     | 105 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 31  | 9     | 311 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 31  | 8     | 313 | CLA  | C3B-C2B | 5.05 | 1.47        | 1.40     |
| 31  | A     | 853 | CLA  | CHC-C1C | 5.05 | 1.47        | 1.35     |
| 31  | 6     | 312 | CLA  | CHD-C1D | 5.05 | 1.48        | 1.38     |
| 31  | A     | 826 | CLA  | MG-NA   | 5.05 | 2.18        | 2.06     |
| 31  | 9     | 317 | CLA  | O2D-CGD | 5.05 | 1.45        | 1.33     |
| 31  | a     | 316 | CLA  | CHD-C1D | 5.05 | 1.48        | 1.38     |
| 31  | b     | 302 | CLA  | CHD-C1D | 5.04 | 1.48        | 1.38     |
| 31  | 6     | 314 | CLA  | CHD-C1D | 5.04 | 1.48        | 1.38     |
| 31  | A     | 827 | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 31  | 9     | 312 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 31  | B     | 815 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 31  | B     | 850 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 31  | B     | 816 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 31  | A     | 821 | CLA  | CHC-C1C | 5.04 | 1.47        | 1.35     |
| 31  | a     | 319 | CLA  | CHC-C1C | 5.04 | 1.47        | 1.35     |
| 31  | A     | 819 | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 31  | 9     | 317 | CLA  | CHC-C1C | 5.04 | 1.47        | 1.35     |
| 31  | 3     | 317 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 31  | 3     | 311 | CLA  | CHC-C1C | 5.04 | 1.47        | 1.35     |
| 31  | A     | 817 | CLA  | C3B-C2B | 5.04 | 1.47        | 1.40     |
| 31  | A     | 849 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 31  | A     | 837 | CLA  | C3C-C2C | 5.04 | 1.47        | 1.36     |
| 31  | 5     | 312 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 31  | 5     | 313 | CLA  | O2D-CGD | 5.04 | 1.45        | 1.33     |
| 31  | 7     | 315 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 2     | 305 | CLA  | CHD-C1D | 5.03 | 1.48        | 1.38     |
| 31  | 4     | 312 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | A     | 836 | CLA  | CHD-C1D | 5.03 | 1.48        | 1.38     |
| 31  | 3     | 307 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | 7     | 310 | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 31  | K     | 205 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | 3     | 309 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | B     | 823 | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 31  | B     | 824 | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 31  | b     | 302 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | 2     | 313 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | K     | 206 | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 31  | 7     | 313 | CLA  | CHC-C1C | 5.03 | 1.47        | 1.35     |
| 31  | 7     | 309 | CLA  | O2D-CGD | 5.03 | 1.45        | 1.33     |
| 31  | 7     | 311 | CLA  | C3B-C2B | 5.03 | 1.47        | 1.40     |
| 32  | A     | 839 | CHL  | MG-NC   | 5.02 | 2.18        | 2.06     |
| 31  | 5     | 320 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 31  | 4     | 319 | CLA  | CHD-C1D | 5.02 | 1.48        | 1.38     |
| 31  | A     | 815 | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 31  | a     | 311 | CLA  | CHC-C1C | 5.02 | 1.47        | 1.35     |
| 31  | a     | 312 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 31  | 8     | 311 | CLA  | CHD-C1D | 5.02 | 1.48        | 1.38     |
| 31  | 4     | 320 | CLA  | CHD-C1D | 5.02 | 1.48        | 1.38     |
| 31  | 6     | 313 | CLA  | CHD-C1D | 5.02 | 1.48        | 1.38     |
| 31  | 3     | 316 | CLA  | CHD-C1D | 5.02 | 1.48        | 1.38     |
| 31  | 7     | 313 | CLA  | C3B-C2B | 5.02 | 1.47        | 1.40     |
| 31  | 4     | 318 | CLA  | CHD-C1D | 5.02 | 1.48        | 1.38     |
| 31  | B     | 830 | CLA  | O2D-CGD | 5.02 | 1.45        | 1.33     |
| 31  | B     | 850 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 31  | A     | 820 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 31  | 3     | 314 | CLA  | CHD-C1D | 5.01 | 1.48        | 1.38     |
| 31  | 8     | 312 | CLA  | CHD-C1D | 5.01 | 1.48        | 1.38     |
| 31  | 2     | 315 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 31  | 5     | 314 | CLA  | CHD-C1D | 5.01 | 1.48        | 1.38     |
| 31  | A     | 857 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 31  | A     | 846 | CLA  | CHC-C1C | 5.01 | 1.47        | 1.35     |
| 31  | 8     | 311 | CLA  | CHC-C1C | 5.01 | 1.47        | 1.35     |
| 31  | B     | 834 | CLA  | C3C-C2C | 5.01 | 1.47        | 1.36     |
| 31  | 3     | 308 | CLA  | CHD-C1D | 5.01 | 1.48        | 1.38     |
| 31  | 9     | 318 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 31  | A     | 832 | CLA  | CHD-C1D | 5.01 | 1.48        | 1.38     |
| 31  | B     | 816 | CLA  | CHC-C1C | 5.01 | 1.47        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 8     | 309 | CLA  | O2D-CGD | 5.01 | 1.45        | 1.33     |
| 31  | G     | 205 | CLA  | CHD-C1D | 5.01 | 1.48        | 1.38     |
| 31  | 8     | 318 | CLA  | CHC-C1C | 5.00 | 1.47        | 1.35     |
| 31  | F     | 301 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | B     | 811 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 31  | A     | 848 | CLA  | CHC-C1C | 5.00 | 1.47        | 1.35     |
| 31  | 4     | 307 | CLA  | C3B-C2B | 5.00 | 1.47        | 1.40     |
| 31  | 9     | 316 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | A     | 854 | CLA  | CHC-C1C | 5.00 | 1.47        | 1.35     |
| 31  | B     | 821 | CLA  | CHD-C1D | 5.00 | 1.48        | 1.38     |
| 31  | 5     | 307 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | B     | 841 | CLA  | CHC-C1C | 5.00 | 1.47        | 1.35     |
| 31  | 5     | 320 | CLA  | CHD-C1D | 5.00 | 1.48        | 1.38     |
| 31  | A     | 819 | CLA  | CHC-C1C | 5.00 | 1.47        | 1.35     |
| 31  | 8     | 313 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | a     | 322 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | B     | 828 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | 7     | 312 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | 9     | 313 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | 9     | 313 | CLA  | CHD-C1D | 5.00 | 1.48        | 1.38     |
| 31  | B     | 838 | CLA  | O2D-CGD | 5.00 | 1.45        | 1.33     |
| 31  | B     | 848 | CLA  | C3C-C2C | 5.00 | 1.47        | 1.36     |
| 31  | 4     | 306 | CLA  | CHD-C1D | 5.00 | 1.48        | 1.38     |
| 31  | A     | 843 | CLA  | CHD-C1D | 4.99 | 1.48        | 1.38     |
| 31  | 6     | 310 | CLA  | CHD-C1D | 4.99 | 1.48        | 1.38     |
| 31  | 8     | 310 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 31  | 8     | 320 | CLA  | CHC-C1C | 4.99 | 1.47        | 1.35     |
| 31  | b     | 305 | CLA  | CHD-C1D | 4.99 | 1.48        | 1.38     |
| 31  | J     | 105 | CLA  | CHC-C1C | 4.99 | 1.47        | 1.35     |
| 31  | A     | 828 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 31  | B     | 838 | CLA  | C3B-C2B | 4.99 | 1.47        | 1.40     |
| 31  | F     | 301 | CLA  | C3B-C2B | 4.99 | 1.47        | 1.40     |
| 31  | A     | 850 | CLA  | C3C-C2C | 4.99 | 1.47        | 1.36     |
| 31  | 3     | 308 | CLA  | O2D-CGD | 4.99 | 1.45        | 1.33     |
| 31  | 2     | 306 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 31  | B     | 812 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | B     | 838 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | 5     | 311 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | 5     | 311 | CLA  | CHD-C1D | 4.98 | 1.48        | 1.38     |
| 31  | A     | 850 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | F     | 306 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | A     | 835 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 9     | 315 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | F     | 305 | CLA  | CHD-C1D | 4.98 | 1.48        | 1.38     |
| 31  | A     | 853 | CLA  | C3C-C2C | 4.98 | 1.47        | 1.36     |
| 31  | A     | 857 | CLA  | CHC-C1C | 4.98 | 1.47        | 1.35     |
| 31  | 7     | 311 | CLA  | CHD-C1D | 4.98 | 1.48        | 1.38     |
| 31  | K     | 204 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 31  | 5     | 310 | CLA  | O2D-CGD | 4.98 | 1.45        | 1.33     |
| 31  | 8     | 308 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | F     | 306 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | B     | 830 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | F     | 305 | CLA  | CHC-C1C | 4.97 | 1.47        | 1.35     |
| 31  | a     | 319 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | a     | 321 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | 6     | 308 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | A     | 837 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | a     | 313 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | a     | 315 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | 6     | 307 | CLA  | C3B-C2B | 4.97 | 1.47        | 1.40     |
| 31  | 8     | 311 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | 8     | 321 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | A     | 834 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | H     | 902 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | 2     | 311 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | B     | 835 | CLA  | O2D-CGD | 4.97 | 1.45        | 1.33     |
| 31  | 5     | 310 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | A     | 851 | CLA  | CHD-C1D | 4.97 | 1.48        | 1.38     |
| 31  | 6     | 311 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 31  | H     | 903 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | 3     | 314 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | a     | 310 | CLA  | CHC-C1C | 4.96 | 1.47        | 1.35     |
| 31  | B     | 824 | CLA  | CHD-C1D | 4.96 | 1.48        | 1.38     |
| 31  | B     | 847 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | A     | 824 | CLA  | CHD-C1D | 4.96 | 1.48        | 1.38     |
| 31  | a     | 311 | CLA  | C3B-C2B | 4.96 | 1.47        | 1.40     |
| 31  | B     | 832 | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 31  | F     | 305 | CLA  | C3B-C2B | 4.96 | 1.47        | 1.40     |
| 31  | F     | 301 | CLA  | C3C-C2C | 4.96 | 1.47        | 1.36     |
| 31  | 8     | 318 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | A     | 848 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | 3     | 311 | CLA  | CHD-C1D | 4.96 | 1.48        | 1.38     |
| 31  | B     | 825 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | 2     | 304 | CLA  | CHD-C1D | 4.96 | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 32  | 4     | 317 | CHL  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | 4     | 316 | CLA  | O2D-CGD | 4.96 | 1.45        | 1.33     |
| 31  | B     | 822 | CLA  | CHD-C1D | 4.96 | 1.48        | 1.38     |
| 31  | 4     | 305 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 31  | A     | 830 | CLA  | CHC-C1C | 4.95 | 1.47        | 1.35     |
| 31  | 8     | 309 | CLA  | CHC-C1C | 4.95 | 1.47        | 1.35     |
| 31  | B     | 836 | CLA  | CHC-C1C | 4.95 | 1.47        | 1.35     |
| 31  | 3     | 311 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 31  | 8     | 317 | CLA  | CHC-C1C | 4.95 | 1.47        | 1.35     |
| 31  | 7     | 322 | CLA  | CHD-C1D | 4.95 | 1.48        | 1.38     |
| 31  | 7     | 315 | CLA  | CHC-C1C | 4.95 | 1.47        | 1.35     |
| 31  | a     | 316 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 31  | 2     | 310 | CLA  | O2D-CGD | 4.95 | 1.45        | 1.33     |
| 31  | A     | 844 | CLA  | C3B-C2B | 4.95 | 1.47        | 1.40     |
| 31  | 7     | 309 | CLA  | CHD-C1D | 4.95 | 1.48        | 1.38     |
| 31  | 6     | 315 | CLA  | CHD-C1D | 4.95 | 1.48        | 1.38     |
| 31  | H     | 902 | CLA  | CHD-C1D | 4.94 | 1.48        | 1.38     |
| 32  | 7     | 324 | CHL  | MG-NC   | 4.94 | 2.18        | 2.06     |
| 31  | A     | 829 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | A     | 834 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | A     | 847 | CLA  | CHD-C1D | 4.94 | 1.48        | 1.38     |
| 31  | A     | 823 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | A     | 832 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | 9     | 321 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | B     | 842 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | a     | 311 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | B     | 846 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | 3     | 316 | CLA  | O2D-CGD | 4.94 | 1.45        | 1.33     |
| 31  | A     | 848 | CLA  | CHD-C1D | 4.94 | 1.48        | 1.38     |
| 31  | B     | 841 | CLA  | C3C-C2C | 4.94 | 1.47        | 1.36     |
| 31  | 4     | 321 | CLA  | CHD-C1D | 4.93 | 1.48        | 1.38     |
| 31  | B     | 815 | CLA  | C3B-C2B | 4.93 | 1.47        | 1.40     |
| 31  | 8     | 320 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 31  | A     | 828 | CLA  | CHD-C1D | 4.93 | 1.48        | 1.38     |
| 31  | B     | 816 | CLA  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 31  | 9     | 318 | CLA  | CHD-C1D | 4.93 | 1.48        | 1.38     |
| 31  | a     | 314 | CLA  | C3B-C2B | 4.93 | 1.47        | 1.40     |
| 32  | 5     | 322 | CHL  | O2D-CGD | 4.93 | 1.45        | 1.33     |
| 31  | 5     | 313 | CLA  | C3B-C2B | 4.93 | 1.47        | 1.40     |
| 31  | 8     | 317 | CLA  | C3C-C2C | 4.93 | 1.47        | 1.36     |
| 31  | B     | 826 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | B     | 836 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | B     | 824 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | 8     | 320 | CLA  | C3B-C2B | 4.92 | 1.47        | 1.40     |
| 31  | B     | 823 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | 7     | 311 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | A     | 851 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | A     | 856 | CLA  | C3B-C2B | 4.92 | 1.47        | 1.40     |
| 31  | L     | 305 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | 7     | 315 | CLA  | CHD-C1D | 4.92 | 1.47        | 1.38     |
| 31  | A     | 815 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | 8     | 317 | CLA  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | A     | 852 | CLA  | CHD-C1D | 4.92 | 1.47        | 1.38     |
| 31  | b     | 313 | CLA  | CHD-C1D | 4.92 | 1.47        | 1.38     |
| 32  | 8     | 319 | CHL  | O2D-CGD | 4.92 | 1.45        | 1.33     |
| 31  | 3     | 312 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 32  | 6     | 321 | CHL  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 31  | A     | 835 | CLA  | CHD-C1D | 4.91 | 1.47        | 1.38     |
| 31  | b     | 304 | CLA  | CHD-C1D | 4.91 | 1.47        | 1.38     |
| 31  | a     | 313 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 31  | B     | 845 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 31  | B     | 839 | CLA  | O2D-CGD | 4.91 | 1.45        | 1.33     |
| 31  | B     | 830 | CLA  | C3B-C2B | 4.90 | 1.47        | 1.40     |
| 31  | 7     | 312 | CLA  | CHD-C1D | 4.90 | 1.47        | 1.38     |
| 31  | 8     | 313 | CLA  | CHD-C1D | 4.90 | 1.47        | 1.38     |
| 32  | 4     | 313 | CHL  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 31  | A     | 832 | CLA  | CHC-C1C | 4.90 | 1.47        | 1.35     |
| 31  | a     | 312 | CLA  | C3C-C2C | 4.90 | 1.47        | 1.36     |
| 31  | 9     | 315 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 31  | A     | 854 | CLA  | C3C-C2C | 4.90 | 1.47        | 1.36     |
| 31  | B     | 829 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 31  | A     | 830 | CLA  | CHD-C1D | 4.90 | 1.47        | 1.38     |
| 31  | B     | 844 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 31  | G     | 204 | CLA  | O2D-CGD | 4.90 | 1.45        | 1.33     |
| 31  | a     | 312 | CLA  | CHD-C1D | 4.90 | 1.47        | 1.38     |
| 31  | B     | 850 | CLA  | C3B-C2B | 4.90 | 1.47        | 1.40     |
| 31  | A     | 850 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 31  | B     | 818 | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 31  | A     | 857 | CLA  | C3C-C2C | 4.89 | 1.47        | 1.36     |
| 31  | A     | 830 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 31  | A     | 819 | CLA  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 32  | a     | 320 | CHL  | MG-NC   | 4.89 | 2.17        | 2.06     |
| 31  | 6     | 308 | CLA  | CHD-C1D | 4.89 | 1.47        | 1.38     |
| 31  | B     | 825 | CLA  | CHD-C1D | 4.89 | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 8     | 312 | CLA  | MG-NC   | 4.89 | 2.17        | 2.06     |
| 32  | A     | 840 | CHL  | MG-NC   | 4.89 | 2.17        | 2.06     |
| 31  | 3     | 309 | CLA  | CHD-C1D | 4.89 | 1.47        | 1.38     |
| 32  | b     | 309 | CHL  | O2D-CGD | 4.89 | 1.45        | 1.33     |
| 31  | B     | 825 | CLA  | C3C-C2C | 4.88 | 1.47        | 1.36     |
| 31  | 3     | 307 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | 4     | 308 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | B     | 827 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 31  | A     | 833 | CLA  | CHC-C1C | 4.88 | 1.47        | 1.35     |
| 31  | B     | 828 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 32  | K     | 201 | CHL  | CHC-C1C | 4.88 | 1.47        | 1.35     |
| 31  | 5     | 307 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | 9     | 315 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | B     | 837 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | A     | 852 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 31  | 8     | 308 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | B     | 841 | CLA  | O2D-CGD | 4.88 | 1.45        | 1.33     |
| 31  | 9     | 312 | CLA  | CHD-C1D | 4.88 | 1.47        | 1.38     |
| 31  | A     | 842 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | F     | 306 | CLA  | CHD-C1D | 4.87 | 1.47        | 1.38     |
| 32  | 6     | 320 | CHL  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | 8     | 314 | CLA  | CHD-C1D | 4.87 | 1.47        | 1.38     |
| 31  | a     | 313 | CLA  | MG-NA   | 4.87 | 2.17        | 2.06     |
| 31  | A     | 838 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | B     | 827 | CLA  | CHD-C1D | 4.87 | 1.47        | 1.38     |
| 31  | B     | 820 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | A     | 849 | CLA  | C3B-C2B | 4.87 | 1.47        | 1.40     |
| 31  | 4     | 315 | CLA  | MG-NC   | 4.87 | 2.17        | 2.06     |
| 31  | A     | 825 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | A     | 833 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | B     | 823 | CLA  | CHD-C1D | 4.87 | 1.47        | 1.38     |
| 31  | A     | 855 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | 8     | 307 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | A     | 844 | CLA  | O2D-CGD | 4.87 | 1.45        | 1.33     |
| 31  | A     | 821 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 31  | B     | 819 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 31  | B     | 839 | CLA  | CHD-C1D | 4.86 | 1.47        | 1.38     |
| 31  | A     | 827 | CLA  | CHD-C1D | 4.86 | 1.47        | 1.38     |
| 31  | 6     | 316 | CLA  | CHD-C1D | 4.86 | 1.47        | 1.38     |
| 31  | B     | 811 | CLA  | O2D-CGD | 4.86 | 1.45        | 1.33     |
| 31  | 8     | 318 | CLA  | CHD-C1D | 4.86 | 1.47        | 1.38     |
| 31  | A     | 836 | CLA  | C3B-C2B | 4.86 | 1.47        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | A     | 843 | CLA  | CHC-C1C | 4.85 | 1.47        | 1.35     |
| 31  | B     | 843 | CLA  | CHC-C1C | 4.85 | 1.47        | 1.35     |
| 31  | 6     | 306 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 31  | A     | 845 | CLA  | CHD-C1D | 4.85 | 1.47        | 1.38     |
| 31  | A     | 816 | CLA  | C3C-C2C | 4.85 | 1.47        | 1.36     |
| 31  | a     | 310 | CLA  | CHD-C1D | 4.85 | 1.47        | 1.38     |
| 31  | A     | 832 | CLA  | C3B-C2B | 4.85 | 1.47        | 1.40     |
| 31  | B     | 848 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 31  | A     | 841 | CLA  | CHC-C1C | 4.85 | 1.47        | 1.35     |
| 31  | A     | 826 | CLA  | CHD-C1D | 4.85 | 1.47        | 1.38     |
| 31  | B     | 813 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 32  | 7     | 317 | CHL  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 32  | K     | 201 | CHL  | C3B-C2B | 4.85 | 1.47        | 1.40     |
| 31  | A     | 816 | CLA  | CHC-C1C | 4.85 | 1.47        | 1.35     |
| 31  | 7     | 316 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 31  | 7     | 321 | CLA  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 32  | 6     | 317 | CHL  | O2D-CGD | 4.85 | 1.45        | 1.33     |
| 31  | G     | 206 | CLA  | CHD-C1D | 4.84 | 1.47        | 1.38     |
| 31  | 8     | 307 | CLA  | CHD-C1D | 4.84 | 1.47        | 1.38     |
| 31  | B     | 833 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 31  | 3     | 310 | CLA  | O2D-CGD | 4.84 | 1.45        | 1.33     |
| 31  | B     | 814 | CLA  | MG-NC   | 4.84 | 2.17        | 2.06     |
| 31  | A     | 853 | CLA  | CHD-C1D | 4.84 | 1.47        | 1.38     |
| 31  | 9     | 314 | CLA  | CHD-C1D | 4.84 | 1.47        | 1.38     |
| 31  | 3     | 310 | CLA  | CHD-C1D | 4.84 | 1.47        | 1.38     |
| 31  | A     | 829 | CLA  | C3C-C2C | 4.84 | 1.47        | 1.36     |
| 31  | B     | 829 | CLA  | CHD-C1D | 4.83 | 1.47        | 1.38     |
| 31  | A     | 830 | CLA  | C3C-C2C | 4.83 | 1.47        | 1.36     |
| 31  | B     | 849 | CLA  | MG-NA   | 4.83 | 2.17        | 2.06     |
| 31  | A     | 845 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 31  | B     | 827 | CLA  | C3C-C2C | 4.83 | 1.47        | 1.36     |
| 31  | A     | 817 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 31  | A     | 847 | CLA  | O2D-CGD | 4.83 | 1.45        | 1.33     |
| 31  | a     | 309 | CLA  | CHD-C1D | 4.83 | 1.47        | 1.38     |
| 31  | 7     | 321 | CLA  | CHD-C1D | 4.82 | 1.47        | 1.38     |
| 31  | 7     | 310 | CLA  | CHD-C1D | 4.82 | 1.47        | 1.38     |
| 32  | 6     | 309 | CHL  | O2D-CGD | 4.81 | 1.44        | 1.33     |
| 31  | B     | 834 | CLA  | O2D-CGD | 4.81 | 1.44        | 1.33     |
| 31  | A     | 847 | CLA  | CHC-C1C | 4.81 | 1.47        | 1.35     |
| 32  | 9     | 320 | CHL  | O2D-CGD | 4.81 | 1.44        | 1.33     |
| 31  | A     | 833 | CLA  | CHD-C1D | 4.81 | 1.47        | 1.38     |
| 31  | B     | 814 | CLA  | O2D-CGD | 4.81 | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 836 | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 31  | B     | 847 | CLA  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 31  | B     | 832 | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 32  | a     | 317 | CHL  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 31  | A     | 838 | CLA  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 31  | B     | 817 | CLA  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 32  | 5     | 319 | CHL  | O2D-CGD | 4.80  | 1.44        | 1.33     |
| 31  | 9     | 316 | CLA  | CHD-C1D | 4.80  | 1.47        | 1.38     |
| 31  | B     | 822 | CLA  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 31  | A     | 844 | CLA  | CHC-C1C | 4.79  | 1.47        | 1.35     |
| 32  | K     | 201 | CHL  | O2D-CGD | 4.79  | 1.44        | 1.33     |
| 31  | 3     | 319 | CLA  | C3C-C2C | 4.79  | 1.46        | 1.36     |
| 31  | B     | 813 | CLA  | CHD-C1D | 4.78  | 1.47        | 1.38     |
| 31  | K     | 204 | CLA  | CHD-C1D | 4.78  | 1.47        | 1.38     |
| 31  | F     | 301 | CLA  | MG-ND   | -4.78 | 1.96        | 2.05     |
| 31  | A     | 846 | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 31  | B     | 820 | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 32  | 7     | 324 | CHL  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 31  | A     | 814 | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 31  | B     | 849 | CLA  | O2D-CGD | 4.77  | 1.44        | 1.33     |
| 31  | 8     | 321 | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 31  | B     | 828 | CLA  | C3B-C2B | 4.77  | 1.47        | 1.40     |
| 31  | B     | 829 | CLA  | CHC-C1C | 4.77  | 1.47        | 1.35     |
| 31  | B     | 832 | CLA  | CHD-C1D | 4.77  | 1.47        | 1.38     |
| 31  | B     | 846 | CLA  | CHD-C1D | 4.76  | 1.47        | 1.38     |
| 31  | 5     | 323 | CLA  | CHD-C1D | 4.76  | 1.47        | 1.38     |
| 31  | H     | 903 | CLA  | MG-NC   | 4.76  | 2.17        | 2.06     |
| 31  | A     | 844 | CLA  | CHD-C1D | 4.76  | 1.47        | 1.38     |
| 32  | K     | 201 | CHL  | C3D-C4D | -4.76 | 1.33        | 1.44     |
| 31  | 2     | 315 | CLA  | CHD-C1D | 4.76  | 1.47        | 1.38     |
| 31  | B     | 827 | CLA  | CHC-C1C | 4.76  | 1.47        | 1.35     |
| 31  | A     | 827 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 31  | B     | 821 | CLA  | O2D-CGD | 4.76  | 1.44        | 1.33     |
| 31  | B     | 817 | CLA  | C3B-C2B | 4.75  | 1.47        | 1.40     |
| 31  | B     | 812 | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 31  | A     | 816 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 31  | B     | 826 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 31  | 2     | 308 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 31  | A     | 856 | CLA  | O2D-CGD | 4.75  | 1.44        | 1.33     |
| 31  | K     | 206 | CLA  | C3B-C2B | 4.75  | 1.47        | 1.40     |
| 31  | B     | 833 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 31  | B     | 819 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 847 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 31  | 7     | 310 | CLA  | MG-ND   | -4.75 | 1.96        | 2.05     |
| 31  | A     | 856 | CLA  | MG-ND   | 4.75  | 2.15        | 2.05     |
| 31  | B     | 817 | CLA  | CHC-C1C | 4.75  | 1.47        | 1.35     |
| 31  | A     | 854 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 31  | B     | 844 | CLA  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 30  | A     | 813 | CL0  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 31  | 8     | 309 | CLA  | CHD-C1D | 4.74  | 1.47        | 1.38     |
| 31  | 7     | 313 | CLA  | CHD-C1D | 4.74  | 1.47        | 1.38     |
| 31  | A     | 846 | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 31  | A     | 818 | CLA  | O2D-CGD | 4.74  | 1.44        | 1.33     |
| 31  | B     | 848 | CLA  | CHD-C1D | 4.74  | 1.47        | 1.38     |
| 31  | B     | 828 | CLA  | MG-ND   | -4.74 | 1.96        | 2.05     |
| 31  | B     | 845 | CLA  | CHD-C1D | 4.74  | 1.47        | 1.38     |
| 31  | 5     | 315 | CLA  | MG-NC   | 4.74  | 2.17        | 2.06     |
| 31  | 4     | 309 | CLA  | CHD-C1D | 4.73  | 1.47        | 1.38     |
| 31  | 8     | 310 | CLA  | C3C-C2C | 4.73  | 1.46        | 1.36     |
| 31  | A     | 816 | CLA  | C3B-C2B | 4.73  | 1.46        | 1.40     |
| 32  | 9     | 322 | CHL  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 31  | J     | 105 | CLA  | CHD-C1D | 4.73  | 1.47        | 1.38     |
| 31  | A     | 856 | CLA  | CHD-C1D | 4.73  | 1.47        | 1.38     |
| 32  | 5     | 317 | CHL  | CHC-C1C | 4.73  | 1.47        | 1.35     |
| 31  | A     | 826 | CLA  | O2D-CGD | 4.73  | 1.44        | 1.33     |
| 31  | B     | 816 | CLA  | CHD-C1D | 4.72  | 1.47        | 1.38     |
| 32  | a     | 320 | CHL  | O2D-CGD | 4.72  | 1.44        | 1.33     |
| 31  | B     | 835 | CLA  | CHD-C1D | 4.72  | 1.47        | 1.38     |
| 31  | 7     | 310 | CLA  | MG-NC   | 4.72  | 2.17        | 2.06     |
| 31  | F     | 301 | CLA  | CHD-C1D | 4.72  | 1.47        | 1.38     |
| 31  | A     | 820 | CLA  | CHD-C1D | 4.72  | 1.47        | 1.38     |
| 31  | B     | 811 | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 31  | A     | 825 | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 32  | 7     | 320 | CHL  | O2D-CGD | 4.71  | 1.44        | 1.33     |
| 31  | A     | 841 | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 31  | B     | 836 | CLA  | CHD-C1D | 4.71  | 1.47        | 1.38     |
| 31  | 5     | 313 | CLA  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 31  | B     | 837 | CLA  | O2D-CGD | 4.70  | 1.44        | 1.33     |
| 31  | A     | 818 | CLA  | C3C-C2C | 4.70  | 1.46        | 1.36     |
| 31  | A     | 819 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 31  | A     | 842 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 31  | B     | 849 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 31  | A     | 822 | CLA  | CHD-C1D | 4.69  | 1.47        | 1.38     |
| 31  | A     | 816 | CLA  | O2D-CGD | 4.69  | 1.44        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 818 | CLA  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 31  | B     | 819 | CLA  | CHC-C1C | 4.67  | 1.46        | 1.35     |
| 32  | 8     | 316 | CHL  | O2D-CGD | 4.67  | 1.44        | 1.33     |
| 31  | A     | 818 | CLA  | CHD-C1D | 4.67  | 1.47        | 1.38     |
| 31  | 8     | 313 | CLA  | MG-ND   | 4.67  | 2.15        | 2.05     |
| 31  | A     | 848 | CLA  | C3B-C2B | 4.67  | 1.46        | 1.40     |
| 31  | B     | 842 | CLA  | CHD-C1D | 4.67  | 1.47        | 1.38     |
| 31  | 4     | 316 | CLA  | CHC-C1C | 4.67  | 1.46        | 1.35     |
| 32  | 7     | 319 | CHL  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 31  | B     | 814 | CLA  | CHD-C1D | 4.66  | 1.47        | 1.38     |
| 31  | A     | 822 | CLA  | O2D-CGD | 4.66  | 1.44        | 1.33     |
| 31  | A     | 843 | CLA  | O2D-CGD | 4.66  | 1.44        | 1.33     |
| 31  | B     | 840 | CLA  | CHD-C1D | 4.66  | 1.47        | 1.38     |
| 31  | B     | 845 | CLA  | CHC-C1C | 4.66  | 1.46        | 1.35     |
| 31  | A     | 857 | CLA  | CHD-C1D | 4.66  | 1.47        | 1.38     |
| 31  | 8     | 310 | CLA  | CHD-C1D | 4.65  | 1.47        | 1.38     |
| 31  | A     | 817 | CLA  | CHD-C1D | 4.65  | 1.47        | 1.38     |
| 31  | B     | 839 | CLA  | MG-NC   | 4.65  | 2.17        | 2.06     |
| 31  | B     | 818 | CLA  | CHD-C1D | 4.65  | 1.47        | 1.38     |
| 31  | 3     | 319 | CLA  | CHD-C1D | 4.65  | 1.47        | 1.38     |
| 31  | B     | 818 | CLA  | CHC-C1C | 4.64  | 1.46        | 1.35     |
| 32  | A     | 840 | CHL  | CHC-C1C | 4.63  | 1.46        | 1.35     |
| 31  | B     | 831 | CLA  | CHD-C1D | 4.63  | 1.47        | 1.38     |
| 31  | A     | 828 | CLA  | MG-NA   | 4.63  | 2.17        | 2.06     |
| 32  | 7     | 318 | CHL  | MG-ND   | -4.63 | 1.96        | 2.05     |
| 31  | A     | 848 | CLA  | MG-NC   | 4.63  | 2.17        | 2.06     |
| 31  | A     | 814 | CLA  | CHD-C1D | 4.62  | 1.47        | 1.38     |
| 32  | 6     | 318 | CHL  | O2D-CGD | 4.62  | 1.44        | 1.33     |
| 31  | B     | 832 | CLA  | CHC-C1C | 4.62  | 1.46        | 1.35     |
| 31  | A     | 821 | CLA  | CHD-C1D | 4.61  | 1.47        | 1.38     |
| 31  | O     | 202 | CLA  | O2D-CGD | 4.61  | 1.45        | 1.30     |
| 32  | 7     | 318 | CHL  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 31  | A     | 855 | CLA  | CHD-C1D | 4.61  | 1.47        | 1.38     |
| 32  | A     | 839 | CHL  | O2D-CGD | 4.61  | 1.44        | 1.33     |
| 31  | B     | 812 | CLA  | C3C-C2C | 4.61  | 1.46        | 1.36     |
| 31  | 4     | 316 | CLA  | CHD-C4C | 4.61  | 1.49        | 1.39     |
| 31  | B     | 840 | CLA  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 32  | 5     | 317 | CHL  | O2D-CGD | 4.60  | 1.44        | 1.33     |
| 32  | 4     | 317 | CHL  | O2A-CGA | 4.59  | 1.46        | 1.30     |
| 32  | K     | 201 | CHL  | C2C-C3C | 4.59  | 1.46        | 1.36     |
| 31  | G     | 205 | CLA  | MG-NC   | 4.59  | 2.17        | 2.06     |
| 31  | 7     | 313 | CLA  | O2D-CGD | 4.59  | 1.45        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | L     | 307 | CLA  | O2A-CGA | 4.58 | 1.46        | 1.30     |
| 31  | 8     | 317 | CLA  | CHD-C1D | 4.58 | 1.47        | 1.38     |
| 32  | a     | 318 | CHL  | O2D-CGD | 4.57 | 1.44        | 1.33     |
| 31  | B     | 815 | CLA  | CHD-C1D | 4.57 | 1.47        | 1.38     |
| 32  | 6     | 321 | CHL  | CHC-C1C | 4.57 | 1.46        | 1.35     |
| 42  | 4     | 304 | SQD  | O48-C23 | 4.56 | 1.46        | 1.33     |
| 31  | A     | 838 | CLA  | MG-ND   | 4.56 | 2.14        | 2.05     |
| 32  | 5     | 316 | CHL  | O2A-CGA | 4.56 | 1.46        | 1.33     |
| 31  | b     | 305 | CLA  | MG-NC   | 4.56 | 2.17        | 2.06     |
| 31  | A     | 857 | CLA  | C3B-C2B | 4.55 | 1.46        | 1.40     |
| 32  | 5     | 316 | CHL  | O2D-CGD | 4.55 | 1.44        | 1.33     |
| 32  | A     | 840 | CHL  | O2D-CGD | 4.54 | 1.44        | 1.33     |
| 32  | b     | 309 | CHL  | CHC-C1C | 4.54 | 1.46        | 1.35     |
| 32  | a     | 318 | CHL  | CHC-C1C | 4.54 | 1.46        | 1.35     |
| 31  | B     | 850 | CLA  | CHD-C1D | 4.54 | 1.47        | 1.38     |
| 31  | B     | 827 | CLA  | C3B-C2B | 4.54 | 1.46        | 1.40     |
| 32  | 6     | 320 | CHL  | CHC-C1C | 4.53 | 1.46        | 1.35     |
| 31  | 4     | 314 | CLA  | O2A-CGA | 4.53 | 1.46        | 1.30     |
| 31  | G     | 206 | CLA  | O2A-CGA | 4.53 | 1.46        | 1.30     |
| 31  | A     | 850 | CLA  | CHD-C1D | 4.52 | 1.47        | 1.38     |
| 32  | 6     | 318 | CHL  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 31  | 5     | 314 | CLA  | O2A-CGA | 4.52 | 1.45        | 1.30     |
| 32  | 4     | 310 | CHL  | O2D-CGD | 4.52 | 1.44        | 1.33     |
| 31  | A     | 825 | CLA  | MG-NC   | 4.51 | 2.17        | 2.06     |
| 32  | A     | 831 | CHL  | CHC-C1C | 4.51 | 1.46        | 1.35     |
| 31  | 3     | 320 | CLA  | O2A-CGA | 4.51 | 1.45        | 1.30     |
| 32  | a     | 320 | CHL  | CHC-C1C | 4.51 | 1.46        | 1.35     |
| 32  | 7     | 320 | CHL  | O2A-CGA | 4.51 | 1.46        | 1.33     |
| 31  | a     | 316 | CLA  | O2A-CGA | 4.51 | 1.45        | 1.30     |
| 31  | A     | 841 | CLA  | O2D-CGD | 4.50 | 1.44        | 1.33     |
| 32  | 8     | 316 | CHL  | CHC-C1C | 4.50 | 1.46        | 1.35     |
| 31  | 4     | 318 | CLA  | O2A-CGA | 4.50 | 1.45        | 1.30     |
| 31  | 2     | 305 | CLA  | O2A-CGA | 4.50 | 1.45        | 1.30     |
| 31  | F     | 306 | CLA  | MG-NC   | 4.50 | 2.17        | 2.06     |
| 32  | 7     | 318 | CHL  | CHC-C1C | 4.49 | 1.46        | 1.35     |
| 32  | A     | 839 | CHL  | CHC-C1C | 4.49 | 1.46        | 1.35     |
| 32  | 7     | 324 | CHL  | CHC-C1C | 4.49 | 1.46        | 1.35     |
| 31  | 5     | 318 | CLA  | MG-NA   | 4.49 | 2.16        | 2.06     |
| 31  | 2     | 311 | CLA  | O2A-CGA | 4.49 | 1.45        | 1.30     |
| 31  | 4     | 320 | CLA  | O2A-CGA | 4.48 | 1.45        | 1.30     |
| 32  | 5     | 316 | CHL  | CHC-C1C | 4.47 | 1.46        | 1.35     |
| 32  | 8     | 316 | CHL  | O2A-CGA | 4.47 | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 817 | CLA  | CHD-C1D | 4.47  | 1.47        | 1.38     |
| 31  | 4     | 306 | CLA  | O2A-CGA | 4.47  | 1.45        | 1.30     |
| 31  | B     | 841 | CLA  | CHD-C1D | 4.47  | 1.47        | 1.38     |
| 32  | 6     | 319 | CHL  | O2D-CGD | 4.46  | 1.44        | 1.33     |
| 32  | 7     | 317 | CHL  | CHC-C1C | 4.46  | 1.46        | 1.35     |
| 32  | 5     | 322 | CHL  | CHC-C1C | 4.46  | 1.46        | 1.35     |
| 31  | B     | 818 | CLA  | C3B-C2B | 4.45  | 1.46        | 1.40     |
| 32  | 4     | 310 | CHL  | CHC-C1C | 4.45  | 1.46        | 1.35     |
| 31  | 2     | 310 | CLA  | O2A-CGA | 4.45  | 1.45        | 1.30     |
| 31  | A     | 825 | CLA  | O2A-CGA | 4.45  | 1.46        | 1.33     |
| 31  | 7     | 313 | CLA  | O2A-CGA | 4.44  | 1.45        | 1.30     |
| 31  | 9     | 313 | CLA  | O2A-CGA | 4.44  | 1.45        | 1.30     |
| 32  | a     | 317 | CHL  | MG-ND   | 4.44  | 2.14        | 2.05     |
| 32  | 8     | 319 | CHL  | CHC-C1C | 4.44  | 1.46        | 1.35     |
| 31  | 4     | 315 | CLA  | O2A-CGA | 4.44  | 1.45        | 1.30     |
| 31  | L     | 306 | CLA  | O2A-CGA | 4.44  | 1.45        | 1.30     |
| 31  | a     | 310 | CLA  | O2A-CGA | 4.44  | 1.45        | 1.30     |
| 31  | B     | 843 | CLA  | O2A-CGA | 4.43  | 1.45        | 1.30     |
| 32  | 3     | 315 | CHL  | CHC-C1C | 4.43  | 1.46        | 1.35     |
| 31  | 4     | 305 | CLA  | C3D-C4D | -4.43 | 1.34        | 1.44     |
| 31  | 9     | 321 | CLA  | O2A-CGA | 4.42  | 1.46        | 1.33     |
| 31  | G     | 206 | CLA  | O2D-CGD | 4.42  | 1.44        | 1.33     |
| 32  | 6     | 317 | CHL  | CHC-C1C | 4.42  | 1.46        | 1.35     |
| 32  | 5     | 319 | CHL  | CHC-C1C | 4.42  | 1.46        | 1.35     |
| 32  | 6     | 309 | CHL  | CHC-C1C | 4.41  | 1.46        | 1.35     |
| 32  | 4     | 313 | CHL  | CHC-C1C | 4.41  | 1.46        | 1.35     |
| 32  | A     | 831 | CHL  | O2D-CGD | 4.41  | 1.44        | 1.33     |
| 32  | 6     | 318 | CHL  | CHC-C1C | 4.40  | 1.46        | 1.35     |
| 31  | 4     | 316 | CLA  | C3D-C4D | -4.40 | 1.34        | 1.44     |
| 31  | L     | 305 | CLA  | CHD-C1D | 4.40  | 1.46        | 1.38     |
| 32  | a     | 317 | CHL  | CHC-C1C | 4.40  | 1.46        | 1.35     |
| 31  | 9     | 317 | CLA  | C3B-C2B | 4.39  | 1.46        | 1.40     |
| 31  | B     | 812 | CLA  | CHD-C1D | 4.39  | 1.46        | 1.38     |
| 31  | A     | 852 | CLA  | MG-ND   | 4.38  | 2.14        | 2.05     |
| 31  | 6     | 307 | CLA  | MG-NC   | -4.38 | 1.95        | 2.06     |
| 32  | 7     | 320 | CHL  | CHC-C1C | 4.38  | 1.46        | 1.35     |
| 31  | A     | 857 | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 31  | 3     | 309 | CLA  | O2A-CGA | 4.37  | 1.46        | 1.33     |
| 32  | a     | 318 | CHL  | MG-NC   | 4.37  | 2.16        | 2.06     |
| 32  | 9     | 322 | CHL  | CHC-C1C | 4.37  | 1.46        | 1.35     |
| 32  | 9     | 320 | CHL  | CHC-C1C | 4.35  | 1.46        | 1.35     |
| 31  | 9     | 317 | CLA  | C3D-C4D | -4.35 | 1.34        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | 5     | 323 | CLA  | O2A-CGA | 4.35 | 1.46        | 1.33     |
| 32  | a     | 320 | CHL  | O2A-CGA | 4.35 | 1.46        | 1.33     |
| 31  | 9     | 315 | CLA  | O2A-CGA | 4.35 | 1.46        | 1.33     |
| 31  | A     | 826 | CLA  | MG-ND   | 4.35 | 2.14        | 2.05     |
| 32  | 9     | 320 | CHL  | O2A-CGA | 4.34 | 1.46        | 1.33     |
| 31  | 5     | 313 | CLA  | CHD-C1D | 4.34 | 1.46        | 1.38     |
| 32  | a     | 317 | CHL  | O2A-CGA | 4.34 | 1.46        | 1.33     |
| 31  | 5     | 307 | CLA  | O2A-CGA | 4.33 | 1.46        | 1.33     |
| 31  | 7     | 310 | CLA  | O2A-CGA | 4.33 | 1.45        | 1.30     |
| 31  | A     | 819 | CLA  | O2A-CGA | 4.32 | 1.46        | 1.33     |
| 31  | B     | 812 | CLA  | MG-ND   | 4.32 | 2.14        | 2.05     |
| 32  | 6     | 319 | CHL  | CHC-C1C | 4.32 | 1.46        | 1.35     |
| 31  | B     | 833 | CLA  | O2A-CGA | 4.32 | 1.46        | 1.33     |
| 32  | a     | 318 | CHL  | O2A-CGA | 4.32 | 1.46        | 1.33     |
| 31  | B     | 826 | CLA  | O2A-CGA | 4.32 | 1.46        | 1.33     |
| 32  | 4     | 313 | CHL  | O2A-CGA | 4.32 | 1.46        | 1.33     |
| 31  | A     | 842 | CLA  | MG-NC   | 4.32 | 2.16        | 2.06     |
| 32  | 7     | 317 | CHL  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 31  | B     | 833 | CLA  | MG-NA   | 4.31 | 2.16        | 2.06     |
| 31  | 6     | 314 | CLA  | O2A-CGA | 4.31 | 1.45        | 1.33     |
| 32  | 3     | 315 | CHL  | O2D-CGD | 4.31 | 1.43        | 1.33     |
| 32  | 4     | 317 | CHL  | CHC-C1C | 4.31 | 1.46        | 1.35     |
| 31  | a     | 315 | CLA  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 31  | A     | 824 | CLA  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 31  | O     | 203 | CLA  | O2A-CGA | 4.30 | 1.45        | 1.33     |
| 31  | B     | 839 | CLA  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 31  | K     | 204 | CLA  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 31  | b     | 313 | CLA  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 31  | 8     | 312 | CLA  | O2A-CGA | 4.29 | 1.45        | 1.33     |
| 31  | O     | 202 | CLA  | MG-NA   | 4.29 | 2.16        | 2.06     |
| 31  | 3     | 310 | CLA  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 31  | 4     | 309 | CLA  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 31  | 3     | 319 | CLA  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 31  | 8     | 311 | CLA  | O2A-CGA | 4.28 | 1.45        | 1.33     |
| 36  | L     | 304 | LUT  | C8-C9   | 4.28 | 1.55        | 1.45     |
| 31  | 9     | 317 | CLA  | MG-ND   | 4.28 | 2.14        | 2.05     |
| 31  | 5     | 309 | CLA  | O2A-CGA | 4.27 | 1.45        | 1.33     |
| 31  | 6     | 308 | CLA  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 31  | A     | 815 | CLA  | CHD-C1D | 4.26 | 1.46        | 1.38     |
| 31  | 4     | 307 | CLA  | O2A-CGA | 4.26 | 1.45        | 1.33     |
| 31  | 9     | 317 | CLA  | CHD-C1D | 4.25 | 1.46        | 1.38     |
| 31  | 6     | 307 | CLA  | O2A-CGA | 4.25 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 816 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 32  | 3     | 315 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 31  | 8     | 320 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 31  | 5     | 312 | CLA  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 31  | b     | 308 | CLA  | CHD-C4C | 4.25  | 1.48        | 1.39     |
| 31  | 3     | 309 | CLA  | MG-NA   | 4.24  | 2.16        | 2.06     |
| 31  | 6     | 310 | CLA  | O2A-CGA | 4.24  | 1.45        | 1.33     |
| 31  | a     | 321 | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 31  | B     | 831 | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 31  | 4     | 321 | CLA  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 31  | a     | 310 | CLA  | MG-NC   | 4.23  | 2.16        | 2.06     |
| 31  | a     | 315 | CLA  | MG-NC   | 4.23  | 2.16        | 2.06     |
| 36  | 4     | 303 | LUT  | C8-C9   | 4.22  | 1.55        | 1.45     |
| 32  | 6     | 320 | CHL  | O2A-CGA | 4.22  | 1.46        | 1.33     |
| 31  | 7     | 314 | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 31  | 9     | 317 | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 31  | a     | 313 | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 31  | A     | 845 | CLA  | O2A-CGA | 4.21  | 1.45        | 1.33     |
| 31  | 6     | 308 | CLA  | CHD-C4C | 4.21  | 1.48        | 1.39     |
| 31  | B     | 848 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | 8     | 309 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | 4     | 312 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 32  | A     | 831 | CHL  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | 8     | 318 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | B     | 830 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | F     | 306 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | a     | 319 | CLA  | O2A-CGA | 4.20  | 1.45        | 1.33     |
| 31  | 6     | 316 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 31  | B     | 834 | CLA  | MG-ND   | 4.19  | 2.14        | 2.05     |
| 31  | B     | 842 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 36  | F     | 304 | LUT  | C8-C9   | 4.19  | 1.54        | 1.45     |
| 31  | 3     | 317 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 31  | B     | 847 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 31  | 9     | 311 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 31  | B     | 846 | CLA  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 32  | 9     | 322 | CHL  | O2A-CGA | 4.18  | 1.46        | 1.33     |
| 31  | 8     | 317 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 31  | 8     | 309 | CLA  | MG-ND   | -4.18 | 1.97        | 2.05     |
| 31  | a     | 311 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 31  | B     | 846 | CLA  | MG-NC   | 4.18  | 2.16        | 2.06     |
| 31  | 3     | 307 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |
| 31  | 3     | 316 | CLA  | O2A-CGA | 4.18  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 815 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 31  | B     | 818 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 32  | 6     | 309 | CHL  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 31  | F     | 305 | CLA  | MG-ND   | 4.17  | 2.14        | 2.05     |
| 31  | 5     | 315 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 36  | 8     | 302 | LUT  | C35-C34 | 4.17  | 1.56        | 1.43     |
| 31  | A     | 828 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 31  | 3     | 318 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 31  | 8     | 314 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 30  | A     | 813 | CL0  | C3D-C4D | -4.17 | 1.34        | 1.44     |
| 31  | a     | 309 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 36  | b     | 301 | LUT  | C35-C34 | 4.17  | 1.56        | 1.43     |
| 31  | A     | 851 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 31  | B     | 845 | CLA  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 32  | 7     | 318 | CHL  | O2A-CGA | 4.17  | 1.45        | 1.33     |
| 31  | G     | 204 | CLA  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 31  | A     | 823 | CLA  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 31  | 5     | 312 | CLA  | MG-NA   | 4.16  | 2.16        | 2.06     |
| 31  | 4     | 316 | CLA  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 31  | b     | 306 | CLA  | O2A-CGA | 4.16  | 1.46        | 1.33     |
| 31  | A     | 835 | CLA  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 36  | 4     | 303 | LUT  | C35-C34 | 4.16  | 1.56        | 1.43     |
| 31  | B     | 850 | CLA  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 31  | B     | 841 | CLA  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 31  | 8     | 320 | CLA  | MG-NC   | 4.15  | 2.16        | 2.06     |
| 31  | O     | 204 | CLA  | CHD-C4C | 4.15  | 1.48        | 1.39     |
| 31  | 2     | 306 | CLA  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 31  | B     | 821 | CLA  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 31  | 7     | 309 | CLA  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 31  | a     | 314 | CLA  | O2A-CGA | 4.15  | 1.45        | 1.33     |
| 32  | 5     | 317 | CHL  | O2A-CGA | 4.15  | 1.46        | 1.33     |
| 31  | 5     | 318 | CLA  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 32  | A     | 839 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 32  | 7     | 319 | CHL  | O2A-CGA | 4.14  | 1.46        | 1.33     |
| 31  | 3     | 313 | CLA  | CHD-C4C | 4.14  | 1.48        | 1.39     |
| 32  | 7     | 324 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 32  | 5     | 322 | CHL  | O2A-CGA | 4.14  | 1.46        | 1.33     |
| 32  | A     | 840 | CHL  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 31  | L     | 306 | CLA  | MG-NA   | 4.14  | 2.16        | 2.06     |
| 32  | 4     | 310 | CHL  | O2A-CGA | 4.14  | 1.46        | 1.33     |
| 31  | L     | 305 | CLA  | O2A-CGA | 4.14  | 1.45        | 1.33     |
| 31  | A     | 837 | CLA  | O2A-CGA | 4.14  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | A     | 852 | CLA  | MG-NA   | 4.14 | 2.16        | 2.06     |
| 31  | A     | 850 | CLA  | O2A-CGA | 4.14 | 1.45        | 1.33     |
| 31  | b     | 303 | CLA  | CHD-C4C | 4.13 | 1.48        | 1.39     |
| 31  | 2     | 307 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 31  | 9     | 316 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 31  | A     | 844 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 31  | B     | 837 | CLA  | O2A-CGA | 4.13 | 1.45        | 1.33     |
| 31  | 7     | 315 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | A     | 836 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | 8     | 308 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | 4     | 305 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | B     | 834 | CLA  | CHD-C1D | 4.12 | 1.46        | 1.38     |
| 31  | B     | 820 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | B     | 849 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | 5     | 310 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | 6     | 312 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | A     | 843 | CLA  | O2A-CGA | 4.12 | 1.45        | 1.33     |
| 31  | B     | 823 | CLA  | O2A-CGA | 4.11 | 1.45        | 1.33     |
| 32  | b     | 309 | CHL  | O2A-CGA | 4.11 | 1.46        | 1.33     |
| 31  | 7     | 312 | CLA  | O2A-CGA | 4.11 | 1.45        | 1.33     |
| 31  | A     | 833 | CLA  | O2A-CGA | 4.11 | 1.45        | 1.33     |
| 31  | A     | 826 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 31  | A     | 820 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 31  | 3     | 311 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 31  | A     | 855 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 31  | 8     | 315 | CLA  | CHD-C4C | 4.10 | 1.48        | 1.39     |
| 31  | A     | 829 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 31  | 3     | 312 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 31  | A     | 829 | CLA  | C3B-C2B | 4.10 | 1.46        | 1.40     |
| 36  | 5     | 304 | LUT  | C8-C9   | 4.10 | 1.54        | 1.45     |
| 31  | A     | 817 | CLA  | O2A-CGA | 4.10 | 1.45        | 1.33     |
| 32  | 6     | 319 | CHL  | O2A-CGA | 4.09 | 1.46        | 1.33     |
| 36  | J     | 103 | LUT  | C8-C9   | 4.09 | 1.54        | 1.45     |
| 31  | B     | 832 | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 31  | b     | 308 | CLA  | O2A-CGA | 4.09 | 1.46        | 1.33     |
| 31  | H     | 901 | CLA  | CHD-C4C | 4.09 | 1.48        | 1.39     |
| 31  | 6     | 307 | CLA  | CHD-C4C | 4.09 | 1.48        | 1.39     |
| 31  | A     | 856 | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 31  | 9     | 318 | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 31  | 4     | 314 | CLA  | CHD-C4C | 4.09 | 1.48        | 1.39     |
| 31  | 9     | 314 | CLA  | O2A-CGA | 4.09 | 1.45        | 1.33     |
| 36  | a     | 305 | LUT  | C8-C9   | 4.09 | 1.54        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 827 | CLA  | MG-NC   | 4.09  | 2.16        | 2.06     |
| 31  | A     | 830 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 31  | 8     | 321 | CLA  | O2A-CGA | 4.08  | 1.46        | 1.33     |
| 31  | 5     | 318 | CLA  | CHD-C4C | 4.08  | 1.48        | 1.39     |
| 31  | B     | 829 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 31  | 3     | 313 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 31  | 3     | 314 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 31  | A     | 838 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 31  | 8     | 313 | CLA  | O2A-CGA | 4.08  | 1.46        | 1.33     |
| 31  | A     | 834 | CLA  | MG-ND   | 4.08  | 2.13        | 2.05     |
| 31  | B     | 815 | CLA  | O2A-CGA | 4.08  | 1.45        | 1.33     |
| 32  | 7     | 319 | CHL  | O2D-CGD | 4.08  | 1.43        | 1.33     |
| 31  | A     | 827 | CLA  | O2A-CGA | 4.07  | 1.45        | 1.33     |
| 36  | J     | 103 | LUT  | C35-C34 | 4.07  | 1.56        | 1.43     |
| 31  | a     | 322 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 31  | 4     | 312 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 31  | 8     | 310 | CLA  | O2A-CGA | 4.07  | 1.45        | 1.33     |
| 31  | a     | 310 | CLA  | MG-ND   | -4.07 | 1.97        | 2.05     |
| 31  | B     | 828 | CLA  | CHD-C4C | 4.07  | 1.48        | 1.39     |
| 31  | A     | 852 | CLA  | O2A-CGA | 4.07  | 1.45        | 1.33     |
| 31  | 3     | 314 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 31  | 4     | 305 | CLA  | C3C-C2C | 4.06  | 1.45        | 1.36     |
| 31  | B     | 819 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 31  | G     | 205 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 31  | 4     | 308 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 31  | 2     | 309 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 31  | K     | 205 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 31  | 7     | 311 | CLA  | MG-NC   | 4.06  | 2.15        | 2.06     |
| 31  | A     | 854 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 31  | 5     | 315 | CLA  | CHD-C4C | 4.06  | 1.48        | 1.39     |
| 31  | b     | 305 | CLA  | O2A-CGA | 4.06  | 1.45        | 1.33     |
| 31  | a     | 316 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 31  | B     | 836 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | b     | 302 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | b     | 307 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | a     | 321 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 31  | 6     | 315 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | A     | 814 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | 6     | 306 | CLA  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 32  | 6     | 317 | CHL  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 32  | 6     | 321 | CHL  | C3B-C2B | 4.05  | 1.46        | 1.40     |
| 31  | A     | 848 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 2     | 309 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | 3     | 312 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 31  | 2     | 311 | CLA  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 31  | K     | 204 | CLA  | MG-NA   | -4.05 | 1.96        | 2.06     |
| 36  | 6     | 304 | LUT  | C35-C34 | 4.05  | 1.56        | 1.43     |
| 31  | A     | 846 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 31  | B     | 814 | CLA  | O2A-CGA | 4.05  | 1.45        | 1.33     |
| 32  | A     | 840 | CHL  | C3B-C2B | 4.05  | 1.46        | 1.40     |
| 31  | B     | 838 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | a     | 322 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | 4     | 307 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 31  | B     | 834 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | b     | 304 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | K     | 206 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | L     | 307 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 31  | B     | 824 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | 8     | 307 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | A     | 849 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | F     | 301 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | 2     | 312 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 31  | 2     | 314 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | K     | 205 | CLA  | CHD-C4C | 4.04  | 1.48        | 1.39     |
| 31  | 7     | 322 | CLA  | O2A-CGA | 4.04  | 1.45        | 1.33     |
| 31  | 7     | 316 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 31  | 5     | 311 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 31  | b     | 310 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 32  | K     | 201 | CHL  | CHD-C1D | 4.03  | 1.46        | 1.38     |
| 31  | A     | 847 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 31  | b     | 310 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 31  | O     | 202 | CLA  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 31  | B     | 813 | CLA  | O2A-CGA | 4.03  | 1.45        | 1.33     |
| 36  | 9     | 303 | LUT  | C35-C34 | 4.03  | 1.55        | 1.43     |
| 31  | 6     | 311 | CLA  | O2A-CGA | 4.02  | 1.45        | 1.33     |
| 31  | 5     | 313 | CLA  | O2A-CGA | 4.02  | 1.45        | 1.33     |
| 31  | 7     | 321 | CLA  | O2A-CGA | 4.02  | 1.45        | 1.33     |
| 31  | 3     | 320 | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 31  | b     | 313 | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 31  | B     | 835 | CLA  | O2A-CGA | 4.02  | 1.45        | 1.33     |
| 31  | 2     | 306 | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 31  | 5     | 320 | CLA  | CHD-C4C | 4.02  | 1.48        | 1.39     |
| 36  | 4     | 302 | LUT  | C8-C9   | 4.02  | 1.54        | 1.45     |
| 32  | K     | 201 | CHL  | O2A-CGA | 4.02  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | A     | 822 | CLA  | O2A-CGA | 4.02 | 1.45        | 1.33     |
| 31  | 9     | 321 | CLA  | CHD-C4C | 4.02 | 1.48        | 1.39     |
| 31  | 2     | 313 | CLA  | O2A-CGA | 4.02 | 1.45        | 1.33     |
| 31  | 6     | 313 | CLA  | O2A-CGA | 4.02 | 1.45        | 1.33     |
| 31  | B     | 822 | CLA  | O2A-CGA | 4.02 | 1.45        | 1.33     |
| 31  | a     | 314 | CLA  | CHD-C4C | 4.02 | 1.48        | 1.39     |
| 31  | H     | 903 | CLA  | O2A-CGA | 4.02 | 1.45        | 1.33     |
| 32  | 5     | 316 | CHL  | MG-NA   | 4.01 | 2.15        | 2.06     |
| 31  | A     | 818 | CLA  | O2A-CGA | 4.01 | 1.45        | 1.33     |
| 31  | b     | 306 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 31  | 6     | 312 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 31  | A     | 816 | CLA  | O2A-CGA | 4.01 | 1.45        | 1.33     |
| 31  | B     | 817 | CLA  | O2A-CGA | 4.01 | 1.45        | 1.33     |
| 31  | b     | 312 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 31  | B     | 825 | CLA  | O2A-CGA | 4.01 | 1.45        | 1.33     |
| 31  | 5     | 309 | CLA  | CHD-C4C | 4.01 | 1.48        | 1.39     |
| 32  | 9     | 322 | CHL  | CHD-C1D | 4.01 | 1.46        | 1.38     |
| 32  | 6     | 309 | CHL  | CHD-C1D | 4.01 | 1.46        | 1.38     |
| 32  | 5     | 319 | CHL  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | B     | 840 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | 4     | 315 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 31  | 2     | 313 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 31  | 2     | 312 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | b     | 303 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | 6     | 306 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | H     | 901 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | 4     | 318 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 31  | 5     | 320 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 30  | A     | 813 | CL0  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | K     | 206 | CLA  | MG-ND   | 4.00 | 2.13        | 2.05     |
| 31  | 7     | 316 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 36  | L     | 304 | LUT  | C35-C34 | 4.00 | 1.55        | 1.43     |
| 31  | G     | 205 | CLA  | CHD-C4C | 4.00 | 1.48        | 1.39     |
| 31  | 6     | 322 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | a     | 312 | CLA  | O2A-CGA | 4.00 | 1.45        | 1.33     |
| 31  | 2     | 315 | CLA  | O2A-CGA | 3.99 | 1.45        | 1.33     |
| 31  | A     | 853 | CLA  | O2A-CGA | 3.99 | 1.45        | 1.33     |
| 36  | 5     | 304 | LUT  | C35-C34 | 3.99 | 1.55        | 1.43     |
| 31  | 4     | 320 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 31  | 5     | 314 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 31  | 8     | 320 | CLA  | CHD-C4C | 3.99 | 1.48        | 1.39     |
| 31  | 5     | 321 | CLA  | O2A-CGA | 3.99 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 9     | 305 | LUT  | C35-C34 | 3.99  | 1.55        | 1.43     |
| 32  | 7     | 317 | CHL  | MG-NC   | 3.99  | 2.15        | 2.06     |
| 32  | 4     | 310 | CHL  | C2C-C3C | 3.99  | 1.45        | 1.36     |
| 31  | b     | 312 | CLA  | O2A-CGA | 3.99  | 1.45        | 1.33     |
| 31  | b     | 311 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 31  | b     | 305 | CLA  | MG-ND   | -3.98 | 1.97        | 2.05     |
| 31  | A     | 841 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 31  | 8     | 315 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 31  | 9     | 312 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 31  | K     | 206 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 36  | 9     | 303 | LUT  | C12-C13 | 3.98  | 1.54        | 1.45     |
| 31  | B     | 844 | CLA  | O2A-CGA | 3.98  | 1.45        | 1.33     |
| 31  | 7     | 314 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 36  | a     | 305 | LUT  | C12-C13 | 3.98  | 1.54        | 1.45     |
| 31  | 6     | 316 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 31  | 4     | 319 | CLA  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 31  | L     | 306 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 31  | 9     | 319 | CLA  | O2A-CGA | 3.97  | 1.45        | 1.33     |
| 31  | A     | 834 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 31  | B     | 812 | CLA  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 31  | B     | 839 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 31  | a     | 311 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 31  | H     | 902 | CLA  | O2A-CGA | 3.97  | 1.45        | 1.33     |
| 31  | H     | 903 | CLA  | CHD-C4C | 3.97  | 1.48        | 1.39     |
| 31  | B     | 827 | CLA  | O2A-CGA | 3.97  | 1.44        | 1.33     |
| 31  | B     | 811 | CLA  | O2A-CGA | 3.96  | 1.44        | 1.33     |
| 31  | 6     | 311 | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 31  | 5     | 308 | CLA  | O2A-CGA | 3.96  | 1.45        | 1.33     |
| 31  | A     | 823 | CLA  | CHD-C4C | 3.96  | 1.48        | 1.39     |
| 35  | 9     | 304 | QTB  | C03-C02 | 3.96  | 1.41        | 1.35     |
| 31  | 2     | 308 | CLA  | O2A-CGA | 3.96  | 1.45        | 1.33     |
| 36  | a     | 305 | LUT  | C35-C34 | 3.96  | 1.55        | 1.43     |
| 36  | 9     | 303 | LUT  | C8-C9   | 3.95  | 1.54        | 1.45     |
| 31  | 2     | 304 | CLA  | O2A-CGA | 3.95  | 1.45        | 1.33     |
| 31  | 2     | 304 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 31  | A     | 816 | CLA  | MG-NA   | 3.95  | 2.15        | 2.06     |
| 31  | 8     | 318 | CLA  | MG-NC   | 3.95  | 2.15        | 2.06     |
| 31  | A     | 846 | CLA  | MG-ND   | 3.95  | 2.13        | 2.05     |
| 31  | 9     | 318 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 31  | 5     | 312 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 31  | 4     | 311 | CLA  | O2A-CGA | 3.95  | 1.45        | 1.33     |
| 31  | a     | 315 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 832 | CLA  | O2A-CGA | 3.95  | 1.44        | 1.33     |
| 31  | A     | 849 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 36  | a     | 305 | LUT  | C28-C29 | 3.95  | 1.54        | 1.45     |
| 31  | b     | 307 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 31  | A     | 834 | CLA  | O2A-CGA | 3.95  | 1.44        | 1.33     |
| 31  | 8     | 311 | CLA  | CHD-C4C | 3.95  | 1.48        | 1.39     |
| 36  | 6     | 303 | LUT  | C35-C34 | 3.94  | 1.55        | 1.43     |
| 31  | 3     | 308 | CLA  | O2A-CGA | 3.94  | 1.45        | 1.33     |
| 31  | O     | 203 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 31  | 9     | 319 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 31  | B     | 837 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 31  | 3     | 318 | CLA  | CHD-C4C | 3.94  | 1.48        | 1.39     |
| 31  | 4     | 305 | CLA  | C3B-C2B | 3.94  | 1.45        | 1.40     |
| 32  | a     | 318 | CHL  | C3B-C2B | 3.93  | 1.45        | 1.40     |
| 32  | 6     | 321 | CHL  | C2C-C3C | 3.93  | 1.45        | 1.36     |
| 31  | A     | 827 | CLA  | MG-NC   | 3.93  | 2.15        | 2.06     |
| 36  | 6     | 304 | LUT  | C8-C9   | 3.93  | 1.54        | 1.45     |
| 32  | 7     | 318 | CHL  | C2C-C3C | 3.93  | 1.45        | 1.36     |
| 31  | 7     | 311 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 32  | 8     | 319 | CHL  | C2C-C3C | 3.93  | 1.45        | 1.36     |
| 31  | B     | 828 | CLA  | O2A-CGA | 3.93  | 1.44        | 1.33     |
| 31  | A     | 824 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 31  | B     | 827 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 31  | 3     | 316 | CLA  | CHD-C4C | 3.93  | 1.48        | 1.39     |
| 31  | F     | 305 | CLA  | O2A-CGA | 3.92  | 1.45        | 1.33     |
| 31  | 7     | 309 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 31  | a     | 314 | CLA  | MG-NA   | -3.92 | 1.97        | 2.06     |
| 31  | 7     | 311 | CLA  | O2A-CGA | 3.92  | 1.44        | 1.33     |
| 31  | b     | 304 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 31  | 8     | 318 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 31  | 9     | 313 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 31  | A     | 845 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 31  | 3     | 310 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 36  | J     | 103 | LUT  | C12-C13 | 3.92  | 1.54        | 1.45     |
| 31  | 6     | 322 | CLA  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 32  | 5     | 322 | CHL  | C2C-C3C | 3.91  | 1.45        | 1.36     |
| 36  | 4     | 302 | LUT  | C35-C34 | 3.91  | 1.55        | 1.43     |
| 32  | 4     | 317 | CHL  | C2C-C3C | 3.91  | 1.45        | 1.36     |
| 31  | a     | 313 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 31  | 8     | 313 | CLA  | CHD-C4C | 3.91  | 1.48        | 1.39     |
| 31  | 8     | 315 | CLA  | MG-NC   | 3.91  | 2.15        | 2.06     |
| 31  | b     | 311 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 8     | 303 | LUT  | C8-C9   | 3.90  | 1.54        | 1.45     |
| 31  | b     | 305 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 31  | A     | 836 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 32  | 6     | 317 | CHL  | C2C-C3C | 3.90  | 1.45        | 1.36     |
| 31  | 2     | 310 | CLA  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 31  | 3     | 308 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 31  | 2     | 314 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 36  | 5     | 303 | LUT  | C8-C9   | 3.89  | 1.54        | 1.45     |
| 36  | 4     | 303 | LUT  | C12-C13 | 3.89  | 1.54        | 1.45     |
| 31  | G     | 204 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 32  | 3     | 315 | CHL  | MG-NC   | -3.89 | 1.97        | 2.06     |
| 31  | 8     | 312 | CLA  | CHD-C4C | 3.89  | 1.48        | 1.39     |
| 36  | 9     | 302 | LUT  | C35-C34 | 3.89  | 1.55        | 1.43     |
| 31  | A     | 832 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 31  | B     | 843 | CLA  | MG-ND   | -3.88 | 1.98        | 2.05     |
| 31  | B     | 821 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 31  | A     | 821 | CLA  | O2A-CGA | 3.88  | 1.44        | 1.33     |
| 31  | L     | 305 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 36  | a     | 303 | LUT  | C35-C34 | 3.88  | 1.55        | 1.43     |
| 31  | 3     | 317 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 31  | 9     | 311 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 31  | 7     | 312 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 31  | 4     | 306 | CLA  | CHD-C4C | 3.88  | 1.48        | 1.39     |
| 31  | A     | 851 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 31  | 7     | 312 | CLA  | MG-ND   | 3.87  | 2.13        | 2.05     |
| 31  | A     | 828 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 36  | b     | 301 | LUT  | C15-C14 | 3.87  | 1.55        | 1.43     |
| 31  | G     | 206 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 31  | 6     | 315 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 31  | 4     | 311 | CLA  | CHD-C4C | 3.87  | 1.48        | 1.39     |
| 32  | 9     | 322 | CHL  | C2C-C3C | 3.87  | 1.45        | 1.36     |
| 32  | 5     | 319 | CHL  | C2C-C3C | 3.87  | 1.45        | 1.36     |
| 36  | 3     | 304 | LUT  | C8-C9   | 3.86  | 1.54        | 1.45     |
| 32  | 5     | 322 | CHL  | CHD-C1D | 3.86  | 1.45        | 1.38     |
| 31  | H     | 902 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 31  | 5     | 308 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 31  | 9     | 316 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 31  | 3     | 319 | CLA  | CHD-C4C | 3.86  | 1.48        | 1.39     |
| 31  | 7     | 315 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 31  | B     | 820 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 31  | 6     | 314 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 32  | 6     | 309 | CHL  | C2C-C3C | 3.85  | 1.45        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 835 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 31  | B     | 823 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 31  | 5     | 321 | CLA  | CHD-C4C | 3.85  | 1.48        | 1.39     |
| 36  | 4     | 303 | LUT  | C11-C10 | 3.85  | 1.55        | 1.43     |
| 31  | a     | 319 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 36  | a     | 305 | LUT  | C31-C30 | 3.84  | 1.55        | 1.43     |
| 31  | A     | 842 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 31  | 3     | 309 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 31  | B     | 829 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 31  | 5     | 307 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 31  | A     | 829 | CLA  | CHC-C1C | 3.84  | 1.44        | 1.35     |
| 36  | 9     | 305 | LUT  | C32-C33 | 3.84  | 1.54        | 1.45     |
| 31  | B     | 848 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 31  | 2     | 305 | CLA  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 36  | 5     | 303 | LUT  | C35-C34 | 3.83  | 1.55        | 1.43     |
| 31  | 2     | 307 | CLA  | CHD-C4C | 3.83  | 1.48        | 1.39     |
| 31  | 4     | 320 | CLA  | MG-NA   | -3.83 | 1.97        | 2.06     |
| 36  | J     | 103 | LUT  | C15-C14 | 3.83  | 1.55        | 1.43     |
| 36  | b     | 301 | LUT  | C8-C9   | 3.83  | 1.54        | 1.45     |
| 31  | K     | 204 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 36  | 6     | 303 | LUT  | C8-C9   | 3.82  | 1.54        | 1.45     |
| 32  | b     | 309 | CHL  | C3B-C2B | 3.82  | 1.45        | 1.40     |
| 31  | A     | 848 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 31  | B     | 826 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 31  | 6     | 313 | CLA  | CHD-C4C | 3.82  | 1.48        | 1.39     |
| 32  | b     | 309 | CHL  | C2C-C3C | 3.82  | 1.45        | 1.36     |
| 31  | 2     | 312 | CLA  | OBD-CAD | 3.82  | 1.29        | 1.22     |
| 36  | 2     | 301 | LUT  | C35-C34 | 3.81  | 1.55        | 1.43     |
| 32  | 9     | 322 | CHL  | C3B-C2B | 3.81  | 1.45        | 1.40     |
| 31  | F     | 306 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 31  | A     | 842 | CLA  | O2A-CGA | 3.81  | 1.44        | 1.33     |
| 32  | 4     | 310 | CHL  | CHD-C1D | 3.81  | 1.45        | 1.38     |
| 36  | 4     | 303 | LUT  | C15-C14 | 3.81  | 1.55        | 1.43     |
| 31  | A     | 816 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 31  | B     | 819 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 31  | A     | 825 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 31  | B     | 824 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 31  | B     | 822 | CLA  | MG-ND   | 3.81  | 2.13        | 2.05     |
| 36  | 4     | 303 | LUT  | C28-C29 | 3.81  | 1.54        | 1.45     |
| 31  | 4     | 321 | CLA  | CHD-C4C | 3.81  | 1.47        | 1.39     |
| 32  | 5     | 317 | CHL  | C3B-C2B | 3.80  | 1.45        | 1.40     |
| 31  | A     | 817 | CLA  | MG-NC   | 3.80  | 2.15        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | A     | 852 | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 32  | 6     | 319 | CHL  | C2C-C3C | 3.80 | 1.44        | 1.36     |
| 32  | 7     | 319 | CHL  | C2C-C3C | 3.80 | 1.44        | 1.36     |
| 31  | B     | 825 | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 31  | B     | 844 | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 31  | B     | 849 | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 32  | A     | 831 | CHL  | C2C-C3C | 3.80 | 1.44        | 1.36     |
| 36  | 9     | 305 | LUT  | C8-C9   | 3.80 | 1.54        | 1.45     |
| 31  | A     | 818 | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 32  | 4     | 313 | CHL  | C2C-C3C | 3.80 | 1.44        | 1.36     |
| 32  | 5     | 319 | CHL  | CHD-C1D | 3.80 | 1.45        | 1.38     |
| 31  | A     | 821 | CLA  | CHD-C4C | 3.80 | 1.47        | 1.39     |
| 36  | 9     | 305 | LUT  | C15-C14 | 3.79 | 1.55        | 1.43     |
| 36  | 6     | 304 | LUT  | C12-C13 | 3.79 | 1.54        | 1.45     |
| 36  | 4     | 303 | LUT  | C31-C30 | 3.79 | 1.55        | 1.43     |
| 31  | A     | 829 | CLA  | MG-NA   | 3.79 | 2.15        | 2.06     |
| 36  | a     | 303 | LUT  | C31-C30 | 3.79 | 1.55        | 1.43     |
| 32  | 6     | 320 | CHL  | C2C-C3C | 3.79 | 1.44        | 1.36     |
| 32  | 7     | 324 | CHL  | C3B-C2B | 3.79 | 1.45        | 1.40     |
| 31  | 8     | 314 | CLA  | CHD-C4C | 3.79 | 1.47        | 1.39     |
| 32  | a     | 317 | CHL  | C2C-C3C | 3.78 | 1.44        | 1.36     |
| 31  | 2     | 311 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 32  | 7     | 319 | CHL  | C3B-C2B | 3.78 | 1.45        | 1.40     |
| 31  | b     | 302 | CLA  | CHD-C4C | 3.78 | 1.47        | 1.39     |
| 31  | 4     | 319 | CLA  | OBD-CAD | 3.78 | 1.29        | 1.22     |
| 31  | B     | 843 | CLA  | CHD-C4C | 3.78 | 1.47        | 1.39     |
| 31  | 3     | 307 | CLA  | CHD-C4C | 3.78 | 1.47        | 1.39     |
| 31  | 8     | 308 | CLA  | CHD-C4C | 3.78 | 1.47        | 1.39     |
| 31  | A     | 847 | CLA  | CHD-C4C | 3.78 | 1.47        | 1.39     |
| 36  | 4     | 302 | LUT  | C15-C14 | 3.78 | 1.55        | 1.43     |
| 32  | 6     | 318 | CHL  | CHD-C1D | 3.78 | 1.45        | 1.38     |
| 31  | A     | 856 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 32  | 5     | 322 | CHL  | C3B-C2B | 3.77 | 1.45        | 1.40     |
| 31  | 6     | 306 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 36  | 6     | 303 | LUT  | C15-C14 | 3.77 | 1.55        | 1.43     |
| 31  | B     | 842 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 31  | 7     | 322 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 31  | A     | 827 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 31  | A     | 833 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 31  | 8     | 321 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 31  | 6     | 310 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |
| 31  | 5     | 311 | CLA  | CHD-C4C | 3.77 | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 308 | CLA  | CHD-C4C | 3.77  | 1.47        | 1.39     |
| 36  | 8     | 303 | LUT  | C35-C34 | 3.76  | 1.55        | 1.43     |
| 31  | B     | 816 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 31  | 4     | 321 | CLA  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 32  | 5     | 317 | CHL  | C2C-C3C | 3.76  | 1.44        | 1.36     |
| 36  | 9     | 305 | LUT  | C31-C30 | 3.76  | 1.55        | 1.43     |
| 31  | A     | 817 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 31  | a     | 309 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 32  | 5     | 316 | CHL  | CHD-C1D | 3.76  | 1.45        | 1.38     |
| 36  | 6     | 304 | LUT  | C15-C14 | 3.76  | 1.55        | 1.43     |
| 36  | 9     | 305 | LUT  | C28-C29 | 3.76  | 1.54        | 1.45     |
| 31  | B     | 830 | CLA  | CHD-C4C | 3.76  | 1.47        | 1.39     |
| 36  | 4     | 302 | LUT  | C12-C13 | 3.75  | 1.54        | 1.45     |
| 31  | 9     | 317 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 31  | 4     | 309 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 31  | A     | 853 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 31  | A     | 830 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 30  | A     | 813 | CL0  | CHC-C1C | 3.75  | 1.44        | 1.35     |
| 31  | 7     | 313 | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 36  | L     | 304 | LUT  | C31-C30 | 3.75  | 1.55        | 1.43     |
| 31  | H     | 901 | CLA  | OBD-CAD | 3.75  | 1.28        | 1.22     |
| 35  | 7     | 303 | QTB  | C03-C02 | 3.74  | 1.40        | 1.35     |
| 31  | 5     | 323 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 31  | B     | 845 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 36  | 2     | 301 | LUT  | C31-C30 | 3.74  | 1.55        | 1.43     |
| 31  | a     | 312 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 36  | L     | 304 | LUT  | C12-C13 | 3.74  | 1.54        | 1.45     |
| 31  | O     | 204 | CLA  | OBD-CAD | 3.74  | 1.28        | 1.22     |
| 32  | 6     | 318 | CHL  | C2C-C3C | 3.74  | 1.44        | 1.36     |
| 31  | B     | 838 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 31  | 8     | 317 | CLA  | CHD-C4C | 3.74  | 1.47        | 1.39     |
| 31  | A     | 829 | CLA  | C3D-C4D | -3.74 | 1.35        | 1.44     |
| 36  | J     | 103 | LUT  | C31-C30 | 3.74  | 1.55        | 1.43     |
| 36  | 5     | 303 | LUT  | C15-C14 | 3.73  | 1.55        | 1.43     |
| 36  | 4     | 303 | LUT  | C32-C33 | 3.73  | 1.54        | 1.45     |
| 31  | 5     | 320 | CLA  | OBD-CAD | 3.73  | 1.28        | 1.22     |
| 36  | a     | 305 | LUT  | C11-C10 | 3.73  | 1.55        | 1.43     |
| 32  | 3     | 315 | CHL  | C2C-C3C | 3.73  | 1.44        | 1.36     |
| 31  | A     | 837 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 31  | 9     | 312 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 36  | 9     | 303 | LUT  | C15-C14 | 3.73  | 1.55        | 1.43     |
| 36  | 2     | 301 | LUT  | C28-C29 | 3.73  | 1.54        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | a     | 318 | CHL  | C2C-C3C | 3.73  | 1.44        | 1.36     |
| 36  | 6     | 303 | LUT  | C31-C30 | 3.73  | 1.55        | 1.43     |
| 36  | a     | 305 | LUT  | C26-C27 | 3.73  | 1.55        | 1.50     |
| 31  | 7     | 321 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 32  | 7     | 318 | CHL  | C3B-C2B | 3.73  | 1.45        | 1.40     |
| 31  | A     | 843 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 31  | B     | 833 | CLA  | CHD-C4C | 3.73  | 1.47        | 1.39     |
| 32  | a     | 320 | CHL  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 31  | A     | 838 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 32  | b     | 309 | CHL  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 32  | 4     | 313 | CHL  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 31  | 2     | 315 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 31  | 9     | 314 | CLA  | CHD-C4C | 3.72  | 1.47        | 1.39     |
| 36  | 4     | 302 | LUT  | C31-C30 | 3.72  | 1.55        | 1.43     |
| 32  | 6     | 319 | CHL  | CHD-C1D | 3.72  | 1.45        | 1.38     |
| 31  | 9     | 316 | CLA  | OBD-CAD | 3.72  | 1.28        | 1.22     |
| 36  | 7     | 305 | LUT  | C35-C34 | 3.71  | 1.55        | 1.43     |
| 36  | a     | 305 | LUT  | C15-C14 | 3.71  | 1.55        | 1.43     |
| 32  | 6     | 319 | CHL  | C3B-C2B | 3.71  | 1.45        | 1.40     |
| 31  | B     | 840 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 36  | 8     | 302 | LUT  | C15-C14 | 3.71  | 1.54        | 1.43     |
| 31  | B     | 836 | CLA  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 32  | 8     | 319 | CHL  | C3B-C2B | 3.71  | 1.45        | 1.40     |
| 35  | a     | 302 | QTB  | C03-C02 | 3.71  | 1.40        | 1.35     |
| 36  | b     | 301 | LUT  | C31-C30 | 3.71  | 1.54        | 1.43     |
| 32  | K     | 201 | CHL  | CHD-C4C | 3.71  | 1.47        | 1.39     |
| 32  | a     | 320 | CHL  | C2C-C3C | 3.71  | 1.44        | 1.36     |
| 36  | 3     | 305 | LUT  | C35-C34 | 3.70  | 1.54        | 1.43     |
| 31  | B     | 813 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 31  | 7     | 314 | CLA  | MG-ND   | -3.70 | 1.98        | 2.05     |
| 32  | 7     | 320 | CHL  | C3B-C2B | 3.70  | 1.45        | 1.40     |
| 31  | A     | 854 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 31  | J     | 105 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 36  | 9     | 303 | LUT  | C11-C10 | 3.70  | 1.54        | 1.43     |
| 32  | A     | 840 | CHL  | C2C-C3C | 3.70  | 1.44        | 1.36     |
| 31  | A     | 815 | CLA  | C1D-ND  | -3.70 | 1.33        | 1.37     |
| 36  | J     | 103 | LUT  | C11-C10 | 3.70  | 1.54        | 1.43     |
| 32  | 7     | 318 | CHL  | CHD-C1D | 3.70  | 1.45        | 1.38     |
| 31  | B     | 835 | CLA  | CHD-C4C | 3.70  | 1.47        | 1.39     |
| 32  | 4     | 317 | CHL  | C3B-C2B | 3.70  | 1.45        | 1.40     |
| 31  | 6     | 306 | CLA  | C4D-CHA | 3.69  | 1.51        | 1.38     |
| 32  | 7     | 320 | CHL  | C2C-C3C | 3.69  | 1.44        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | L     | 307 | CLA  | MG-NC   | -3.69 | 1.97        | 2.06     |
| 32  | 7     | 317 | CHL  | C3B-C2B | 3.69  | 1.45        | 1.40     |
| 32  | 8     | 316 | CHL  | C3B-C2B | 3.69  | 1.45        | 1.40     |
| 31  | 3     | 311 | CLA  | CHD-C4C | 3.69  | 1.47        | 1.39     |
| 36  | 5     | 304 | LUT  | C11-C10 | 3.68  | 1.54        | 1.43     |
| 31  | 4     | 314 | CLA  | OBD-CAD | 3.68  | 1.28        | 1.22     |
| 36  | b     | 301 | LUT  | C12-C13 | 3.68  | 1.53        | 1.45     |
| 36  | 7     | 305 | LUT  | C8-C9   | 3.68  | 1.53        | 1.45     |
| 36  | a     | 303 | LUT  | C15-C14 | 3.68  | 1.54        | 1.43     |
| 31  | A     | 826 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 32  | a     | 320 | CHL  | C3B-C2B | 3.68  | 1.45        | 1.40     |
| 31  | A     | 846 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 31  | B     | 831 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 36  | 3     | 304 | LUT  | C7-C6   | 3.68  | 1.58        | 1.45     |
| 31  | 8     | 307 | CLA  | CHD-C4C | 3.68  | 1.47        | 1.39     |
| 36  | 3     | 305 | LUT  | C31-C30 | 3.68  | 1.54        | 1.43     |
| 36  | 9     | 305 | LUT  | C11-C10 | 3.68  | 1.54        | 1.43     |
| 31  | 5     | 310 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 31  | F     | 305 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 36  | L     | 304 | LUT  | C32-C33 | 3.67  | 1.53        | 1.45     |
| 36  | 3     | 304 | LUT  | C35-C34 | 3.67  | 1.54        | 1.43     |
| 31  | A     | 841 | CLA  | CHD-C4C | 3.67  | 1.47        | 1.39     |
| 32  | 5     | 316 | CHL  | C2C-C3C | 3.67  | 1.44        | 1.36     |
| 31  | B     | 847 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 31  | b     | 303 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 31  | B     | 823 | CLA  | MG-ND   | 3.66  | 2.13        | 2.05     |
| 31  | 2     | 304 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 31  | A     | 820 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 36  | L     | 304 | LUT  | C15-C14 | 3.66  | 1.54        | 1.43     |
| 31  | 6     | 306 | CLA  | MG-ND   | 3.66  | 2.13        | 2.05     |
| 32  | 7     | 320 | CHL  | CHD-C1D | 3.66  | 1.45        | 1.38     |
| 31  | B     | 812 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 31  | 4     | 305 | CLA  | CHC-C1C | 3.66  | 1.44        | 1.35     |
| 31  | 5     | 313 | CLA  | CHD-C4C | 3.66  | 1.47        | 1.39     |
| 31  | 4     | 306 | CLA  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 36  | 4     | 302 | LUT  | C11-C10 | 3.66  | 1.54        | 1.43     |
| 32  | 6     | 321 | CHL  | CHD-C1D | 3.65  | 1.45        | 1.38     |
| 36  | J     | 103 | LUT  | C32-C33 | 3.65  | 1.53        | 1.45     |
| 32  | 4     | 317 | CHL  | CHD-C1D | 3.65  | 1.45        | 1.38     |
| 31  | 4     | 312 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 36  | 3     | 304 | LUT  | C31-C30 | 3.65  | 1.54        | 1.43     |
| 31  | 5     | 314 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | J     | 103 | LUT  | C28-C29 | 3.65  | 1.53        | 1.45     |
| 31  | 3     | 320 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 36  | 2     | 301 | LUT  | C15-C14 | 3.65  | 1.54        | 1.43     |
| 31  | B     | 843 | CLA  | OBD-CAD | 3.65  | 1.28        | 1.22     |
| 36  | 9     | 302 | LUT  | C31-C30 | 3.65  | 1.54        | 1.43     |
| 31  | A     | 844 | CLA  | CHD-C4C | 3.65  | 1.47        | 1.39     |
| 36  | F     | 304 | LUT  | C35-C34 | 3.64  | 1.54        | 1.43     |
| 36  | 5     | 304 | LUT  | C15-C14 | 3.64  | 1.54        | 1.43     |
| 31  | B     | 822 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 32  | 8     | 316 | CHL  | C2C-C3C | 3.64  | 1.44        | 1.36     |
| 31  | F     | 301 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 31  | 2     | 305 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 31  | 6     | 316 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 31  | H     | 903 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 36  | a     | 303 | LUT  | C8-C9   | 3.64  | 1.53        | 1.45     |
| 31  | L     | 307 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 31  | b     | 302 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 31  | B     | 818 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 36  | 5     | 303 | LUT  | C31-C30 | 3.64  | 1.54        | 1.43     |
| 31  | G     | 205 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 36  | 6     | 303 | LUT  | C28-C29 | 3.64  | 1.53        | 1.45     |
| 31  | A     | 857 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 31  | b     | 308 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 30  | A     | 813 | CL0  | C3B-C2B | 3.64  | 1.45        | 1.40     |
| 32  | 6     | 317 | CHL  | C3B-C2B | 3.64  | 1.45        | 1.40     |
| 31  | 2     | 308 | CLA  | CHD-C4C | 3.64  | 1.47        | 1.39     |
| 31  | 3     | 313 | CLA  | OBD-CAD | 3.64  | 1.28        | 1.22     |
| 36  | 9     | 305 | LUT  | C12-C13 | 3.64  | 1.53        | 1.45     |
| 31  | B     | 841 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 32  | 7     | 317 | CHL  | C2C-C3C | 3.63  | 1.44        | 1.36     |
| 36  | a     | 303 | LUT  | C12-C13 | 3.63  | 1.53        | 1.45     |
| 31  | L     | 306 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 31  | 3     | 318 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 31  | a     | 316 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 31  | B     | 846 | CLA  | C1D-ND  | -3.63 | 1.33        | 1.37     |
| 31  | K     | 206 | CLA  | OBD-CAD | 3.63  | 1.28        | 1.22     |
| 31  | B     | 811 | CLA  | CHD-C4C | 3.63  | 1.47        | 1.39     |
| 36  | a     | 303 | LUT  | C28-C29 | 3.63  | 1.53        | 1.45     |
| 32  | a     | 318 | CHL  | CHD-C1D | 3.62  | 1.45        | 1.38     |
| 36  | 6     | 303 | LUT  | C11-C10 | 3.62  | 1.54        | 1.43     |
| 32  | 6     | 320 | CHL  | C3B-C2B | 3.62  | 1.45        | 1.40     |
| 31  | B     | 820 | CLA  | MG-ND   | -3.62 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 850 | CLA  | CHD-C4C | 3.62  | 1.47        | 1.39     |
| 36  | 6     | 304 | LUT  | C32-C33 | 3.62  | 1.53        | 1.45     |
| 31  | 4     | 316 | CLA  | OBD-CAD | 3.62  | 1.28        | 1.22     |
| 30  | A     | 813 | CL0  | C3C-C2C | 3.62  | 1.44        | 1.36     |
| 31  | A     | 814 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 36  | 9     | 302 | LUT  | C8-C9   | 3.61  | 1.53        | 1.45     |
| 31  | B     | 832 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 36  | 3     | 305 | LUT  | C8-C9   | 3.61  | 1.53        | 1.45     |
| 36  | 6     | 303 | LUT  | C26-C27 | 3.61  | 1.55        | 1.50     |
| 36  | 6     | 304 | LUT  | C31-C30 | 3.61  | 1.54        | 1.43     |
| 31  | 9     | 315 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 32  | 9     | 320 | CHL  | C3B-C2B | 3.61  | 1.45        | 1.40     |
| 31  | A     | 818 | CLA  | C1D-ND  | -3.61 | 1.33        | 1.37     |
| 31  | 4     | 318 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 31  | 5     | 307 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 32  | a     | 317 | CHL  | CHD-C1D | 3.61  | 1.45        | 1.38     |
| 36  | 7     | 305 | LUT  | C31-C30 | 3.61  | 1.54        | 1.43     |
| 31  | 6     | 314 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 31  | A     | 815 | CLA  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 36  | b     | 301 | LUT  | C28-C29 | 3.61  | 1.53        | 1.45     |
| 31  | 2     | 313 | CLA  | OBD-CAD | 3.61  | 1.28        | 1.22     |
| 36  | 3     | 305 | LUT  | C32-C33 | 3.60  | 1.53        | 1.45     |
| 31  | b     | 310 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 31  | A     | 829 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 32  | 7     | 324 | CHL  | C2C-C3C | 3.60  | 1.44        | 1.36     |
| 31  | 2     | 309 | CLA  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 31  | A     | 850 | CLA  | CHD-C4C | 3.60  | 1.47        | 1.39     |
| 31  | 8     | 310 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 36  | b     | 301 | LUT  | C11-C10 | 3.59  | 1.54        | 1.43     |
| 31  | A     | 819 | CLA  | CHD-C4C | 3.59  | 1.47        | 1.39     |
| 31  | 6     | 312 | CLA  | OBD-CAD | 3.59  | 1.28        | 1.22     |
| 32  | 9     | 320 | CHL  | C2C-C3C | 3.59  | 1.44        | 1.36     |
| 36  | L     | 304 | LUT  | C26-C27 | 3.59  | 1.55        | 1.50     |
| 36  | a     | 303 | LUT  | C32-C33 | 3.59  | 1.53        | 1.45     |
| 36  | L     | 304 | LUT  | C11-C10 | 3.59  | 1.54        | 1.43     |
| 32  | 8     | 319 | CHL  | CHD-C1D | 3.59  | 1.45        | 1.38     |
| 42  | 4     | 304 | SQD  | O5-C1   | 3.59  | 1.51        | 1.41     |
| 31  | 5     | 312 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 32  | 4     | 310 | CHL  | C3B-C2B | 3.58  | 1.45        | 1.40     |
| 32  | A     | 839 | CHL  | C2C-C3C | 3.58  | 1.44        | 1.36     |
| 32  | 3     | 315 | CHL  | C3B-C2B | 3.58  | 1.45        | 1.40     |
| 31  | 7     | 314 | CLA  | MG-NA   | 3.58  | 2.14        | 2.06     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 812 | CLA  | C1D-ND  | -3.58 | 1.33        | 1.37     |
| 32  | 6     | 309 | CHL  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 32  | 4     | 310 | CHL  | CHD-C4C | 3.58  | 1.47        | 1.39     |
| 40  | 7     | 306 | XAT  | C10-C9  | 3.58  | 1.40        | 1.35     |
| 31  | b     | 304 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 31  | 5     | 323 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 32  | 6     | 317 | CHL  | CHD-C1D | 3.58  | 1.45        | 1.38     |
| 31  | 6     | 306 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 31  | O     | 202 | CLA  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 31  | b     | 311 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 31  | L     | 305 | CLA  | C1D-ND  | -3.57 | 1.33        | 1.37     |
| 31  | 4     | 320 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 32  | 6     | 309 | CHL  | C3B-C2B | 3.57  | 1.45        | 1.40     |
| 31  | 3     | 317 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 36  | 5     | 304 | LUT  | C31-C30 | 3.57  | 1.54        | 1.43     |
| 36  | b     | 301 | LUT  | C26-C27 | 3.57  | 1.55        | 1.50     |
| 31  | B     | 814 | CLA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 31  | 9     | 321 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 31  | 4     | 311 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 31  | 7     | 322 | CLA  | OBD-CAD | 3.57  | 1.28        | 1.22     |
| 32  | 7     | 319 | CHL  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 31  | 3     | 312 | CLA  | MG-ND   | -3.57 | 1.98        | 2.05     |
| 32  | A     | 839 | CHL  | C3B-C2B | 3.57  | 1.45        | 1.40     |
| 32  | A     | 831 | CHL  | CHD-C1D | 3.57  | 1.45        | 1.38     |
| 32  | 9     | 320 | CHL  | CHD-C1D | 3.56  | 1.45        | 1.38     |
| 31  | A     | 814 | CLA  | CHD-C4C | 3.56  | 1.47        | 1.39     |
| 32  | 5     | 319 | CHL  | C3B-C2B | 3.56  | 1.45        | 1.40     |
| 32  | 4     | 310 | CHL  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 35  | F     | 303 | QTB  | C03-C02 | 3.56  | 1.40        | 1.35     |
| 36  | 7     | 305 | LUT  | C15-C14 | 3.56  | 1.54        | 1.43     |
| 31  | 2     | 315 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 31  | A     | 826 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 31  | 2     | 307 | CLA  | OBD-CAD | 3.56  | 1.28        | 1.22     |
| 36  | 8     | 303 | LUT  | C15-C14 | 3.56  | 1.54        | 1.43     |
| 31  | 2     | 306 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 32  | 4     | 313 | CHL  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 31  | 4     | 316 | CLA  | CHD-C1D | 3.55  | 1.45        | 1.38     |
| 36  | 3     | 304 | LUT  | C15-C14 | 3.55  | 1.54        | 1.43     |
| 36  | 5     | 304 | LUT  | C12-C13 | 3.55  | 1.53        | 1.45     |
| 36  | 3     | 305 | LUT  | C15-C14 | 3.55  | 1.54        | 1.43     |
| 32  | 6     | 320 | CHL  | CHD-C1D | 3.55  | 1.45        | 1.38     |
| 32  | 5     | 316 | CHL  | C3D-C4D | -3.55 | 1.36        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 312 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 31  | K     | 204 | CLA  | C3D-C2D | 3.55  | 1.48        | 1.39     |
| 31  | 9     | 312 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 31  | b     | 306 | CLA  | OBD-CAD | 3.55  | 1.28        | 1.22     |
| 31  | 3     | 319 | CLA  | C1D-ND  | -3.54 | 1.33        | 1.37     |
| 31  | 2     | 314 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 31  | 5     | 315 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 31  | A     | 824 | CLA  | MG-ND   | -3.54 | 1.98        | 2.05     |
| 36  | 6     | 304 | LUT  | C11-C10 | 3.54  | 1.54        | 1.43     |
| 31  | 7     | 316 | CLA  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 31  | B     | 846 | CLA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 36  | a     | 305 | LUT  | C32-C33 | 3.53  | 1.53        | 1.45     |
| 31  | B     | 844 | CLA  | MG-ND   | 3.53  | 2.12        | 2.05     |
| 31  | 3     | 310 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 36  | L     | 304 | LUT  | C28-C29 | 3.53  | 1.53        | 1.45     |
| 31  | 8     | 313 | CLA  | MG-NC   | -3.53 | 1.97        | 2.06     |
| 32  | 7     | 317 | CHL  | CHD-C1D | 3.53  | 1.45        | 1.38     |
| 31  | 6     | 311 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 31  | B     | 835 | CLA  | C1D-ND  | -3.53 | 1.33        | 1.37     |
| 36  | 4     | 302 | LUT  | C23-C24 | 3.53  | 1.55        | 1.50     |
| 31  | A     | 844 | CLA  | MG-ND   | -3.53 | 1.98        | 2.05     |
| 32  | A     | 831 | CHL  | CHD-C4C | 3.53  | 1.47        | 1.39     |
| 36  | 7     | 305 | LUT  | C7-C6   | 3.53  | 1.57        | 1.45     |
| 31  | B     | 841 | CLA  | C1D-ND  | -3.53 | 1.33        | 1.37     |
| 31  | 6     | 322 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 31  | A     | 857 | CLA  | C1D-ND  | -3.53 | 1.33        | 1.37     |
| 31  | 6     | 310 | CLA  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 31  | a     | 312 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 31  | 7     | 315 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 36  | F     | 304 | LUT  | C23-C24 | 3.52  | 1.55        | 1.50     |
| 31  | 9     | 319 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 36  | 9     | 303 | LUT  | C32-C33 | 3.52  | 1.53        | 1.45     |
| 32  | 9     | 322 | CHL  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 32  | K     | 201 | CHL  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 31  | 8     | 318 | CLA  | MG-ND   | -3.52 | 1.98        | 2.05     |
| 36  | 5     | 303 | LUT  | C12-C13 | 3.52  | 1.53        | 1.45     |
| 31  | A     | 848 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 31  | 6     | 315 | CLA  | OBD-CAD | 3.52  | 1.28        | 1.22     |
| 32  | 5     | 322 | CHL  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 32  | 6     | 318 | CHL  | C3B-C2B | 3.52  | 1.45        | 1.40     |
| 31  | J     | 105 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 31  | 4     | 308 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 8     | 302 | LUT  | C31-C30 | 3.51  | 1.54        | 1.43     |
| 32  | 4     | 317 | CHL  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 36  | a     | 303 | LUT  | C26-C27 | 3.51  | 1.55        | 1.50     |
| 36  | 3     | 304 | LUT  | C11-C10 | 3.51  | 1.54        | 1.43     |
| 31  | 9     | 313 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 31  | 4     | 307 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 31  | 3     | 312 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 31  | 7     | 310 | CLA  | CHD-C4C | 3.51  | 1.47        | 1.39     |
| 36  | 9     | 303 | LUT  | C31-C30 | 3.51  | 1.54        | 1.43     |
| 42  | 4     | 304 | SQD  | O47-C45 | -3.51 | 1.37        | 1.46     |
| 31  | A     | 841 | CLA  | C1D-ND  | -3.51 | 1.33        | 1.37     |
| 32  | 7     | 324 | CHL  | CHD-C1D | 3.51  | 1.45        | 1.38     |
| 31  | b     | 307 | CLA  | OBD-CAD | 3.51  | 1.28        | 1.22     |
| 31  | 8     | 309 | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 31  | B     | 839 | CLA  | C1D-ND  | -3.50 | 1.33        | 1.37     |
| 31  | F     | 305 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 36  | b     | 301 | LUT  | C32-C33 | 3.50  | 1.53        | 1.45     |
| 31  | B     | 815 | CLA  | CHD-C4C | 3.50  | 1.47        | 1.39     |
| 36  | 4     | 302 | LUT  | C28-C29 | 3.50  | 1.53        | 1.45     |
| 36  | 6     | 303 | LUT  | C12-C13 | 3.50  | 1.53        | 1.45     |
| 31  | 2     | 310 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 31  | 8     | 309 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 36  | a     | 303 | LUT  | C23-C24 | 3.50  | 1.55        | 1.50     |
| 32  | 3     | 315 | CHL  | CHD-C1D | 3.50  | 1.45        | 1.38     |
| 31  | 9     | 314 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 36  | 9     | 302 | LUT  | C28-C29 | 3.50  | 1.53        | 1.45     |
| 31  | b     | 313 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 31  | 6     | 313 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 36  | 9     | 303 | LUT  | C28-C29 | 3.50  | 1.53        | 1.45     |
| 31  | 5     | 321 | CLA  | OBD-CAD | 3.50  | 1.28        | 1.22     |
| 36  | 9     | 302 | LUT  | C32-C33 | 3.50  | 1.53        | 1.45     |
| 31  | 2     | 311 | CLA  | C3D-C2D | 3.49  | 1.48        | 1.39     |
| 31  | 5     | 309 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 31  | 4     | 305 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 36  | 9     | 305 | LUT  | C26-C27 | 3.49  | 1.55        | 1.50     |
| 31  | 4     | 306 | CLA  | MG-ND   | -3.49 | 1.98        | 2.05     |
| 31  | 9     | 317 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 31  | K     | 205 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 32  | 4     | 310 | CHL  | C3D-C4D | -3.49 | 1.36        | 1.44     |
| 31  | a     | 315 | CLA  | OBD-CAD | 3.49  | 1.28        | 1.22     |
| 31  | 6     | 306 | CLA  | C3D-C4D | -3.49 | 1.36        | 1.44     |
| 32  | 5     | 317 | CHL  | CHD-C1D | 3.48  | 1.45        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 840 | CLA  | C1D-ND  | -3.48 | 1.33        | 1.37     |
| 31  | 5     | 313 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 40  | 7     | 306 | XAT  | C30-C29 | 3.48  | 1.40        | 1.35     |
| 31  | A     | 822 | CLA  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 36  | 4     | 302 | LUT  | C32-C33 | 3.48  | 1.53        | 1.45     |
| 31  | A     | 856 | CLA  | C1D-ND  | -3.48 | 1.33        | 1.37     |
| 36  | 6     | 304 | LUT  | C28-C29 | 3.48  | 1.53        | 1.45     |
| 32  | b     | 309 | CHL  | CHD-C4C | 3.48  | 1.47        | 1.39     |
| 31  | 7     | 312 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 31  | 8     | 307 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 31  | B     | 825 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 32  | 5     | 316 | CHL  | C3B-C2B | 3.48  | 1.45        | 1.40     |
| 31  | 8     | 312 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 31  | G     | 206 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 31  | A     | 825 | CLA  | OBD-CAD | 3.48  | 1.28        | 1.22     |
| 36  | F     | 304 | LUT  | C15-C14 | 3.48  | 1.54        | 1.43     |
| 31  | b     | 308 | CLA  | C3D-C2D | 3.47  | 1.48        | 1.39     |
| 31  | A     | 847 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 31  | 7     | 316 | CLA  | MG-ND   | 3.47  | 2.12        | 2.05     |
| 32  | 7     | 319 | CHL  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 31  | 5     | 318 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 36  | 5     | 303 | LUT  | C11-C10 | 3.47  | 1.54        | 1.43     |
| 31  | B     | 842 | CLA  | OBD-CAD | 3.47  | 1.28        | 1.22     |
| 36  | 8     | 303 | LUT  | C12-C13 | 3.46  | 1.53        | 1.45     |
| 36  | F     | 304 | LUT  | C31-C30 | 3.46  | 1.54        | 1.43     |
| 31  | 8     | 321 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 32  | 8     | 316 | CHL  | CHD-C1D | 3.46  | 1.45        | 1.38     |
| 36  | 2     | 301 | LUT  | C32-C33 | 3.46  | 1.53        | 1.45     |
| 32  | a     | 318 | CHL  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 31  | 9     | 321 | CLA  | MG-ND   | 3.46  | 2.12        | 2.05     |
| 31  | a     | 321 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 31  | 8     | 320 | CLA  | C3D-C2D | 3.46  | 1.48        | 1.39     |
| 32  | 6     | 319 | CHL  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 36  | 6     | 303 | LUT  | C32-C33 | 3.46  | 1.53        | 1.45     |
| 31  | a     | 310 | CLA  | CHD-C4C | 3.46  | 1.47        | 1.39     |
| 31  | 8     | 313 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 31  | 7     | 311 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 32  | 6     | 321 | CHL  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 31  | B     | 820 | CLA  | OBD-CAD | 3.46  | 1.28        | 1.22     |
| 36  | 3     | 304 | LUT  | C28-C29 | 3.46  | 1.53        | 1.45     |
| 36  | 8     | 303 | LUT  | C31-C30 | 3.46  | 1.54        | 1.43     |
| 31  | B     | 827 | CLA  | MG-ND   | -3.45 | 1.98        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 817 | CLA  | CHD-C4C | 3.45  | 1.47        | 1.39     |
| 36  | 8     | 302 | LUT  | C8-C9   | 3.45  | 1.53        | 1.45     |
| 36  | 4     | 302 | LUT  | C26-C27 | 3.45  | 1.55        | 1.50     |
| 31  | A     | 855 | CLA  | CHD-C4C | 3.45  | 1.47        | 1.39     |
| 31  | 3     | 309 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 32  | 4     | 313 | CHL  | C3B-C2B | 3.45  | 1.45        | 1.40     |
| 31  | 6     | 311 | CLA  | C3D-C2D | 3.45  | 1.48        | 1.39     |
| 31  | B     | 850 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 31  | 4     | 315 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 32  | a     | 317 | CHL  | C3B-C2B | 3.45  | 1.45        | 1.40     |
| 31  | B     | 811 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 31  | K     | 206 | CLA  | C3D-C2D | 3.45  | 1.48        | 1.39     |
| 36  | 9     | 302 | LUT  | C15-C14 | 3.45  | 1.54        | 1.43     |
| 31  | 3     | 314 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 31  | 8     | 320 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 36  | 3     | 304 | LUT  | C12-C13 | 3.45  | 1.53        | 1.45     |
| 31  | G     | 204 | CLA  | OBD-CAD | 3.45  | 1.28        | 1.22     |
| 31  | 2     | 304 | CLA  | MG-ND   | 3.44  | 2.12        | 2.05     |
| 32  | 5     | 319 | CHL  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 36  | F     | 304 | LUT  | C12-C13 | 3.44  | 1.53        | 1.45     |
| 36  | a     | 303 | LUT  | C11-C10 | 3.44  | 1.54        | 1.43     |
| 36  | 4     | 303 | LUT  | C7-C6   | 3.44  | 1.57        | 1.45     |
| 36  | 3     | 305 | LUT  | C28-C29 | 3.44  | 1.53        | 1.45     |
| 36  | 5     | 304 | LUT  | C32-C33 | 3.44  | 1.53        | 1.45     |
| 32  | 4     | 317 | CHL  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 31  | B     | 831 | CLA  | C1D-ND  | -3.44 | 1.33        | 1.37     |
| 32  | 7     | 318 | CHL  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 31  | 9     | 311 | CLA  | OBD-CAD | 3.44  | 1.28        | 1.22     |
| 31  | 2     | 306 | CLA  | C3D-C2D | 3.43  | 1.48        | 1.39     |
| 36  | 7     | 305 | LUT  | C28-C29 | 3.43  | 1.53        | 1.45     |
| 31  | 2     | 305 | CLA  | MG-ND   | -3.43 | 1.99        | 2.05     |
| 31  | 3     | 312 | CLA  | C3D-C2D | 3.43  | 1.48        | 1.39     |
| 31  | H     | 901 | CLA  | C3D-C2D | 3.43  | 1.48        | 1.39     |
| 31  | B     | 843 | CLA  | MG-NA   | 3.43  | 2.14        | 2.06     |
| 31  | B     | 821 | CLA  | OBD-CAD | 3.43  | 1.28        | 1.22     |
| 40  | 7     | 306 | XAT  | C14-C13 | 3.43  | 1.40        | 1.35     |
| 26  | 5     | 302 | BCR  | C30-C25 | -3.43 | 1.49        | 1.53     |
| 31  | B     | 811 | CLA  | C1D-ND  | -3.43 | 1.33        | 1.37     |
| 32  | 4     | 313 | CHL  | CHD-C4C | 3.43  | 1.47        | 1.39     |
| 31  | 2     | 308 | CLA  | MG-NA   | 3.43  | 2.14        | 2.06     |
| 31  | a     | 316 | CLA  | C3D-C2D | 3.43  | 1.48        | 1.39     |
| 31  | B     | 826 | CLA  | C1D-ND  | -3.43 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 3     | 315 | CHL  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 32  | 5     | 317 | CHL  | CHD-C4C | 3.42  | 1.47        | 1.39     |
| 31  | 2     | 315 | CLA  | C3D-C2D | 3.42  | 1.48        | 1.39     |
| 31  | A     | 820 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 31  | 8     | 317 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 32  | b     | 309 | CHL  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 31  | A     | 833 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 31  | 3     | 308 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 31  | A     | 834 | CLA  | C1D-ND  | -3.42 | 1.33        | 1.37     |
| 31  | K     | 204 | CLA  | C1D-ND  | -3.42 | 1.33        | 1.37     |
| 36  | 6     | 303 | LUT  | C23-C24 | 3.42  | 1.55        | 1.50     |
| 31  | 5     | 308 | CLA  | OBD-CAD | 3.42  | 1.28        | 1.22     |
| 36  | 5     | 304 | LUT  | C28-C29 | 3.41  | 1.53        | 1.45     |
| 31  | 3     | 316 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 31  | 6     | 307 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 31  | A     | 853 | CLA  | C1D-ND  | -3.41 | 1.33        | 1.37     |
| 31  | 4     | 311 | CLA  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 31  | L     | 306 | CLA  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 31  | a     | 309 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 31  | 4     | 319 | CLA  | C3D-C2D | 3.41  | 1.48        | 1.39     |
| 36  | L     | 304 | LUT  | C23-C24 | 3.41  | 1.55        | 1.50     |
| 31  | B     | 824 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 32  | 6     | 320 | CHL  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 31  | a     | 314 | CLA  | OBD-CAD | 3.41  | 1.28        | 1.22     |
| 32  | 3     | 315 | CHL  | C3D-C4D | -3.40 | 1.36        | 1.44     |
| 31  | b     | 303 | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 32  | 7     | 320 | CHL  | C3D-C4D | -3.40 | 1.36        | 1.44     |
| 36  | 8     | 302 | LUT  | C12-C13 | 3.40  | 1.53        | 1.45     |
| 31  | A     | 829 | CLA  | CHD-C4C | 3.40  | 1.47        | 1.39     |
| 31  | 5     | 307 | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 31  | A     | 817 | CLA  | C1D-ND  | -3.40 | 1.33        | 1.37     |
| 31  | 7     | 310 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 31  | O     | 203 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 31  | A     | 835 | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 32  | A     | 831 | CHL  | C3B-C2B | 3.40  | 1.45        | 1.40     |
| 31  | A     | 846 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 31  | 8     | 317 | CLA  | C1D-ND  | -3.40 | 1.33        | 1.37     |
| 31  | A     | 834 | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 31  | 2     | 313 | CLA  | C3D-C2D | 3.40  | 1.48        | 1.39     |
| 31  | A     | 844 | CLA  | OBD-CAD | 3.40  | 1.28        | 1.22     |
| 31  | a     | 319 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 36  | 2     | 301 | LUT  | C8-C9   | 3.39  | 1.53        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 813 | CLA  | C1D-ND  | -3.39 | 1.33        | 1.37     |
| 31  | J     | 105 | CLA  | C1D-ND  | -3.39 | 1.33        | 1.37     |
| 31  | A     | 829 | CLA  | CHD-C1D | 3.39  | 1.45        | 1.38     |
| 36  | 8     | 302 | LUT  | C32-C33 | 3.39  | 1.53        | 1.45     |
| 31  | 4     | 309 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 31  | 9     | 311 | CLA  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 36  | 3     | 305 | LUT  | C12-C13 | 3.39  | 1.53        | 1.45     |
| 32  | 6     | 321 | CHL  | CHD-C4C | 3.39  | 1.47        | 1.39     |
| 31  | 7     | 321 | CLA  | OBD-CAD | 3.39  | 1.28        | 1.22     |
| 31  | b     | 307 | CLA  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 31  | 6     | 314 | CLA  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 31  | 5     | 312 | CLA  | C3D-C2D | 3.39  | 1.48        | 1.39     |
| 31  | 8     | 310 | CLA  | C1D-ND  | -3.39 | 1.33        | 1.37     |
| 31  | B     | 827 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 36  | 3     | 304 | LUT  | C32-C33 | 3.38  | 1.53        | 1.45     |
| 31  | A     | 842 | CLA  | C1D-ND  | -3.38 | 1.33        | 1.37     |
| 31  | L     | 305 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 31  | 4     | 320 | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 31  | 3     | 318 | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 31  | b     | 311 | CLA  | C3D-C2D | 3.38  | 1.48        | 1.39     |
| 31  | A     | 854 | CLA  | OBD-CAD | 3.38  | 1.28        | 1.22     |
| 32  | 6     | 319 | CHL  | CHD-C4C | 3.38  | 1.46        | 1.39     |
| 32  | 6     | 317 | CHL  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 31  | 7     | 315 | CLA  | MG-NC   | -3.37 | 1.98        | 2.06     |
| 31  | a     | 315 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 31  | O     | 202 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 31  | 6     | 308 | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 32  | 5     | 322 | CHL  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 31  | B     | 812 | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 32  | a     | 318 | CHL  | C3D-C4D | -3.37 | 1.36        | 1.44     |
| 32  | 6     | 317 | CHL  | CHD-C4C | 3.37  | 1.46        | 1.39     |
| 31  | 5     | 308 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 31  | B     | 838 | CLA  | OBD-CAD | 3.37  | 1.28        | 1.22     |
| 31  | B     | 812 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 31  | 4     | 307 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 31  | 6     | 316 | CLA  | C1D-ND  | -3.37 | 1.33        | 1.37     |
| 32  | a     | 318 | CHL  | C1D-ND  | -3.37 | 1.33        | 1.37     |
| 31  | 3     | 313 | CLA  | C3D-C2D | 3.37  | 1.48        | 1.39     |
| 31  | H     | 903 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 31  | 5     | 318 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 31  | B     | 830 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 31  | 7     | 311 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 841 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 31  | 8     | 315 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 31  | 5     | 311 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 31  | B     | 847 | CLA  | C1D-ND  | -3.36 | 1.33        | 1.37     |
| 31  | 8     | 307 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 32  | 5     | 317 | CHL  | C3D-C4D | -3.36 | 1.36        | 1.44     |
| 36  | 5     | 303 | LUT  | C32-C33 | 3.36  | 1.53        | 1.45     |
| 31  | B     | 846 | CLA  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 32  | 9     | 322 | CHL  | C3D-C4D | -3.36 | 1.36        | 1.44     |
| 36  | 8     | 302 | LUT  | C28-C29 | 3.36  | 1.53        | 1.45     |
| 31  | 9     | 316 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 32  | 6     | 309 | CHL  | OBD-CAD | 3.36  | 1.28        | 1.22     |
| 31  | b     | 313 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 31  | B     | 843 | CLA  | C3D-C2D | 3.36  | 1.48        | 1.39     |
| 31  | 3     | 309 | CLA  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 32  | 6     | 320 | CHL  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 31  | 7     | 314 | CLA  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 31  | A     | 815 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 31  | a     | 322 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 31  | 7     | 314 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 32  | 8     | 319 | CHL  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 32  | 7     | 317 | CHL  | MG-NA   | 3.35  | 2.14        | 2.06     |
| 31  | A     | 828 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 31  | B     | 817 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 32  | a     | 320 | CHL  | C3D-C4D | -3.35 | 1.36        | 1.44     |
| 32  | 6     | 309 | CHL  | C3D-C4D | -3.35 | 1.36        | 1.44     |
| 31  | A     | 843 | CLA  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 31  | 8     | 321 | CLA  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 31  | 2     | 308 | CLA  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 32  | 5     | 317 | CHL  | OBD-CAD | 3.35  | 1.28        | 1.22     |
| 31  | F     | 305 | CLA  | C3D-C2D | 3.35  | 1.48        | 1.39     |
| 32  | a     | 317 | CHL  | C3D-C4D | -3.35 | 1.36        | 1.44     |
| 31  | B     | 827 | CLA  | C1D-ND  | -3.35 | 1.33        | 1.37     |
| 31  | A     | 846 | CLA  | C1D-ND  | -3.35 | 1.33        | 1.37     |
| 31  | B     | 820 | CLA  | C1D-ND  | -3.35 | 1.33        | 1.37     |
| 31  | B     | 825 | CLA  | C1D-ND  | -3.34 | 1.33        | 1.37     |
| 32  | 7     | 318 | CHL  | C3D-C4D | -3.34 | 1.36        | 1.44     |
| 36  | 7     | 305 | LUT  | C32-C33 | 3.34  | 1.53        | 1.45     |
| 32  | 8     | 319 | CHL  | CHD-C4C | 3.34  | 1.46        | 1.39     |
| 32  | 4     | 317 | CHL  | C3D-C4D | -3.34 | 1.36        | 1.44     |
| 31  | 2     | 314 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 36  | 9     | 302 | LUT  | C11-C10 | 3.34  | 1.53        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 312 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 31  | a     | 314 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 31  | O     | 203 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 31  | b     | 312 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 32  | 6     | 319 | CHL  | C3D-C4D | -3.34 | 1.36        | 1.44     |
| 31  | 3     | 319 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 31  | 4     | 314 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 31  | A     | 816 | CLA  | C3D-C2D | 3.34  | 1.48        | 1.39     |
| 31  | 5     | 310 | CLA  | OBD-CAD | 3.34  | 1.28        | 1.22     |
| 32  | 8     | 319 | CHL  | C3D-C4D | -3.33 | 1.36        | 1.44     |
| 31  | 3     | 320 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 31  | 7     | 316 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 31  | 4     | 318 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 31  | K     | 204 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 31  | G     | 205 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 32  | b     | 309 | CHL  | C3D-C4D | -3.33 | 1.36        | 1.44     |
| 31  | B     | 841 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 31  | 2     | 309 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 32  | 5     | 319 | CHL  | C3D-C4D | -3.33 | 1.36        | 1.44     |
| 31  | H     | 902 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 36  | F     | 304 | LUT  | C11-C10 | 3.33  | 1.53        | 1.43     |
| 31  | 2     | 312 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 31  | A     | 842 | CLA  | MG-ND   | -3.33 | 1.99        | 2.05     |
| 31  | 3     | 320 | CLA  | MG-ND   | -3.33 | 1.99        | 2.05     |
| 31  | L     | 305 | CLA  | C3D-C2D | 3.33  | 1.48        | 1.39     |
| 31  | A     | 849 | CLA  | OBD-CAD | 3.33  | 1.28        | 1.22     |
| 32  | 6     | 317 | CHL  | C3D-C4D | -3.33 | 1.36        | 1.44     |
| 31  | 2     | 306 | CLA  | MG-NC   | 3.32  | 2.14        | 2.06     |
| 31  | A     | 824 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 31  | 8     | 312 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 31  | 7     | 315 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 31  | a     | 311 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 31  | 6     | 310 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 32  | 6     | 318 | CHL  | CHD-C4C | 3.32  | 1.46        | 1.39     |
| 31  | 3     | 314 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 36  | 8     | 303 | LUT  | C26-C27 | 3.32  | 1.55        | 1.50     |
| 31  | A     | 845 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 31  | 8     | 308 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 31  | 2     | 304 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 31  | A     | 817 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 36  | 8     | 303 | LUT  | C32-C33 | 3.32  | 1.53        | 1.45     |
| 32  | 9     | 320 | CHL  | C3D-C4D | -3.32 | 1.36        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 2     | 310 | CLA  | C3D-C2D | 3.32  | 1.48        | 1.39     |
| 31  | B     | 828 | CLA  | OBD-CAD | 3.32  | 1.28        | 1.22     |
| 31  | 2     | 307 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 32  | 9     | 320 | CHL  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 26  | 2     | 302 | BCR  | C1-C6   | -3.31 | 1.49        | 1.53     |
| 31  | O     | 204 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | 5     | 323 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | 3     | 319 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 31  | 8     | 311 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 31  | A     | 816 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 31  | b     | 306 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | a     | 316 | CLA  | C1D-ND  | -3.31 | 1.33        | 1.37     |
| 31  | A     | 855 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 31  | 8     | 310 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 31  | 9     | 319 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | B     | 839 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | B     | 817 | CLA  | C1D-ND  | -3.31 | 1.33        | 1.37     |
| 31  | b     | 304 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | 5     | 309 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | b     | 305 | CLA  | C3D-C2D | 3.31  | 1.48        | 1.39     |
| 31  | 7     | 313 | CLA  | OBD-CAD | 3.31  | 1.28        | 1.22     |
| 36  | 6     | 304 | LUT  | C26-C27 | 3.31  | 1.55        | 1.50     |
| 31  | B     | 850 | CLA  | C1D-ND  | -3.31 | 1.33        | 1.37     |
| 36  | 9     | 303 | LUT  | C7-C6   | 3.30  | 1.56        | 1.45     |
| 32  | A     | 839 | CHL  | C3D-C4D | -3.30 | 1.36        | 1.44     |
| 31  | 3     | 316 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 32  | a     | 318 | CHL  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 32  | 5     | 322 | CHL  | C3D-C4D | -3.30 | 1.36        | 1.44     |
| 31  | A     | 853 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 31  | B     | 834 | CLA  | CHD-C4C | 3.30  | 1.46        | 1.39     |
| 31  | b     | 310 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 31  | 5     | 314 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 31  | A     | 824 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 36  | 7     | 305 | LUT  | C12-C13 | 3.30  | 1.53        | 1.45     |
| 31  | A     | 848 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 31  | 8     | 315 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 32  | 7     | 319 | CHL  | C1D-ND  | -3.30 | 1.33        | 1.37     |
| 31  | A     | 815 | CLA  | C3D-C2D | 3.30  | 1.48        | 1.39     |
| 31  | B     | 826 | CLA  | OBD-CAD | 3.30  | 1.28        | 1.22     |
| 31  | 3     | 314 | CLA  | C1D-ND  | -3.30 | 1.33        | 1.37     |
| 31  | A     | 837 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | a     | 311 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 315 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | A     | 823 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 31  | B     | 833 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 31  | 6     | 306 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 31  | B     | 831 | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 31  | 6     | 308 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | A     | 816 | CLA  | C1D-ND  | -3.29 | 1.33        | 1.37     |
| 31  | 7     | 312 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | a     | 319 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | 2     | 305 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | 3     | 317 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | 7     | 322 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | 5     | 311 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | A     | 849 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 32  | 8     | 316 | CHL  | C3D-C4D | -3.29 | 1.36        | 1.44     |
| 32  | a     | 320 | CHL  | CHD-C4C | 3.29  | 1.46        | 1.39     |
| 31  | B     | 816 | CLA  | OBD-CAD | 3.29  | 1.28        | 1.22     |
| 31  | 9     | 313 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 36  | 8     | 303 | LUT  | C11-C10 | 3.29  | 1.53        | 1.43     |
| 31  | L     | 307 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 31  | 4     | 306 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 32  | a     | 317 | CHL  | CHD-C4C | 3.29  | 1.46        | 1.39     |
| 31  | 8     | 313 | CLA  | C3D-C2D | 3.29  | 1.48        | 1.39     |
| 42  | 4     | 304 | SQD  | O47-C7  | 3.28  | 1.43        | 1.34     |
| 36  | 8     | 302 | LUT  | C11-C10 | 3.28  | 1.53        | 1.43     |
| 31  | A     | 837 | CLA  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 36  | 3     | 305 | LUT  | C11-C10 | 3.28  | 1.53        | 1.43     |
| 31  | B     | 816 | CLA  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 31  | B     | 842 | CLA  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 31  | 5     | 310 | CLA  | C3D-C2D | 3.28  | 1.48        | 1.39     |
| 31  | B     | 829 | CLA  | OBD-CAD | 3.28  | 1.28        | 1.22     |
| 31  | 3     | 310 | CLA  | C3D-C2D | 3.28  | 1.48        | 1.39     |
| 31  | 4     | 315 | CLA  | C3D-C2D | 3.28  | 1.48        | 1.39     |
| 31  | B     | 830 | CLA  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 31  | G     | 206 | CLA  | C1D-ND  | -3.28 | 1.33        | 1.37     |
| 31  | 8     | 310 | CLA  | C3D-C2D | 3.28  | 1.48        | 1.39     |
| 31  | 4     | 308 | CLA  | C3D-C2D | 3.28  | 1.48        | 1.39     |
| 32  | 6     | 318 | CHL  | C3D-C4D | -3.28 | 1.36        | 1.44     |
| 31  | B     | 835 | CLA  | MG-NC   | 3.27  | 2.14        | 2.06     |
| 31  | A     | 835 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 31  | 8     | 318 | CLA  | C1D-ND  | -3.27 | 1.33        | 1.37     |
| 39  | 7     | 301 | 3PH  | P-O11   | 3.27  | 1.70        | 1.60     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 856 | CLA  | C3D-C2D | 3.27  | 1.48        | 1.39     |
| 31  | 5     | 315 | CLA  | C3D-C2D | 3.27  | 1.48        | 1.39     |
| 31  | B     | 828 | CLA  | C3D-C2D | 3.27  | 1.48        | 1.39     |
| 31  | A     | 827 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 31  | B     | 840 | CLA  | OBD-CAD | 3.27  | 1.28        | 1.22     |
| 31  | B     | 836 | CLA  | C1D-ND  | -3.27 | 1.33        | 1.37     |
| 40  | 7     | 306 | XAT  | C34-C33 | 3.27  | 1.40        | 1.35     |
| 36  | 7     | 305 | LUT  | C11-C10 | 3.27  | 1.53        | 1.43     |
| 31  | A     | 826 | CLA  | C1D-ND  | -3.26 | 1.33        | 1.37     |
| 31  | A     | 832 | CLA  | C1D-ND  | -3.26 | 1.33        | 1.37     |
| 31  | A     | 826 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 31  | 9     | 318 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 31  | A     | 841 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 31  | A     | 857 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 32  | 7     | 324 | CHL  | C3D-C4D | -3.26 | 1.36        | 1.44     |
| 32  | 9     | 322 | CHL  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 31  | A     | 817 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 31  | 6     | 316 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 26  | 3     | 302 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 32  | 7     | 317 | CHL  | C3D-C4D | -3.26 | 1.36        | 1.44     |
| 31  | B     | 847 | CLA  | OBD-CAD | 3.26  | 1.28        | 1.22     |
| 31  | B     | 826 | CLA  | C3D-C2D | 3.26  | 1.48        | 1.39     |
| 31  | 9     | 318 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 31  | A     | 851 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 32  | 6     | 320 | CHL  | C3D-C4D | -3.25 | 1.36        | 1.44     |
| 31  | B     | 844 | CLA  | C1D-ND  | -3.25 | 1.33        | 1.37     |
| 32  | 4     | 313 | CHL  | C3D-C4D | -3.25 | 1.36        | 1.44     |
| 32  | 7     | 317 | CHL  | CHD-C4C | 3.25  | 1.46        | 1.39     |
| 31  | A     | 847 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | 5     | 313 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | B     | 813 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 32  | 5     | 319 | CHL  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 31  | 5     | 313 | CLA  | C4B-CHC | 3.25  | 1.50        | 1.41     |
| 32  | 7     | 324 | CHL  | CHD-C4C | 3.25  | 1.46        | 1.39     |
| 31  | K     | 205 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 32  | 7     | 319 | CHL  | C3D-C4D | -3.25 | 1.36        | 1.44     |
| 32  | 7     | 318 | CHL  | MG-NC   | -3.25 | 1.98        | 2.06     |
| 31  | A     | 845 | CLA  | C1D-ND  | -3.25 | 1.33        | 1.37     |
| 31  | F     | 301 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 31  | 4     | 321 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | 6     | 307 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | 6     | 322 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | G     | 206 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | A     | 823 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | 8     | 318 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 31  | B     | 825 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | A     | 836 | CLA  | OBD-CAD | 3.25  | 1.28        | 1.22     |
| 31  | B     | 845 | CLA  | C3D-C2D | 3.25  | 1.48        | 1.39     |
| 31  | 4     | 312 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 31  | 8     | 314 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 31  | B     | 836 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 31  | B     | 822 | CLA  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 32  | A     | 839 | CHL  | MG-NA   | 3.24  | 2.14        | 2.06     |
| 31  | B     | 820 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 31  | A     | 821 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 31  | a     | 322 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 32  | 7     | 317 | CHL  | OBD-CAD | 3.24  | 1.28        | 1.22     |
| 36  | 2     | 301 | LUT  | C11-C10 | 3.24  | 1.53        | 1.43     |
| 32  | 6     | 321 | CHL  | C3D-C4D | -3.24 | 1.36        | 1.44     |
| 31  | B     | 814 | CLA  | C1D-ND  | -3.24 | 1.33        | 1.37     |
| 31  | A     | 838 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 31  | A     | 853 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 31  | B     | 821 | CLA  | C3D-C2D | 3.24  | 1.48        | 1.39     |
| 32  | 7     | 320 | CHL  | CHD-C4C | 3.23  | 1.46        | 1.39     |
| 31  | 9     | 314 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 36  | 2     | 301 | LUT  | C12-C13 | 3.23  | 1.52        | 1.45     |
| 31  | B     | 837 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 32  | a     | 317 | CHL  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 31  | B     | 814 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 31  | a     | 321 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 31  | b     | 305 | CLA  | OBD-CAD | 3.23  | 1.28        | 1.22     |
| 31  | A     | 832 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 31  | B     | 838 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 31  | 7     | 309 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 31  | 3     | 308 | CLA  | C3D-C2D | 3.23  | 1.47        | 1.39     |
| 36  | 8     | 303 | LUT  | C28-C29 | 3.23  | 1.52        | 1.45     |
| 31  | 8     | 311 | CLA  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 31  | B     | 848 | CLA  | MG-NC   | 3.22  | 2.13        | 2.06     |
| 31  | B     | 823 | CLA  | C1D-ND  | -3.22 | 1.33        | 1.37     |
| 31  | A     | 857 | CLA  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 31  | A     | 828 | CLA  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 31  | B     | 847 | CLA  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 31  | 5     | 321 | CLA  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 31  | B     | 834 | CLA  | C1D-ND  | -3.22 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 832 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 31  | A     | 822 | CLA  | OBD-CAD | 3.22  | 1.28        | 1.22     |
| 31  | L     | 307 | CLA  | C4D-CHA | 3.22  | 1.49        | 1.38     |
| 31  | B     | 837 | CLA  | C1D-ND  | -3.22 | 1.33        | 1.37     |
| 31  | B     | 811 | CLA  | C3D-C2D | 3.22  | 1.47        | 1.39     |
| 31  | 4     | 316 | CLA  | C3D-C2D | 3.21  | 1.47        | 1.39     |
| 36  | 5     | 304 | LUT  | C7-C6   | 3.21  | 1.56        | 1.45     |
| 32  | 5     | 316 | CHL  | CHD-C4C | 3.21  | 1.46        | 1.39     |
| 31  | A     | 852 | CLA  | C3D-C2D | 3.21  | 1.47        | 1.39     |
| 31  | 3     | 307 | CLA  | C3D-C2D | 3.21  | 1.47        | 1.39     |
| 31  | A     | 828 | CLA  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 31  | 6     | 306 | CLA  | C1B-CHB | 3.21  | 1.49        | 1.41     |
| 31  | B     | 842 | CLA  | C3D-C2D | 3.21  | 1.47        | 1.39     |
| 31  | 8     | 317 | CLA  | MG-NC   | -3.21 | 1.98        | 2.06     |
| 31  | 9     | 312 | CLA  | C3D-C2D | 3.21  | 1.47        | 1.39     |
| 31  | 2     | 315 | CLA  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 31  | B     | 843 | CLA  | C1D-ND  | -3.21 | 1.33        | 1.37     |
| 32  | A     | 831 | CHL  | C3D-C4D | -3.21 | 1.36        | 1.44     |
| 31  | B     | 836 | CLA  | OBD-CAD | 3.21  | 1.28        | 1.22     |
| 31  | 9     | 317 | CLA  | C4D-CHA | 3.21  | 1.49        | 1.38     |
| 36  | 9     | 302 | LUT  | C12-C13 | 3.21  | 1.52        | 1.45     |
| 36  | F     | 304 | LUT  | C28-C29 | 3.21  | 1.52        | 1.45     |
| 31  | A     | 830 | CLA  | OBD-CAD | 3.21  | 1.28        | 1.22     |
| 32  | 6     | 318 | CHL  | OBD-CAD | 3.21  | 1.28        | 1.22     |
| 31  | A     | 825 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 31  | A     | 843 | CLA  | OBD-CAD | 3.20  | 1.28        | 1.22     |
| 31  | B     | 839 | CLA  | OBD-CAD | 3.20  | 1.28        | 1.22     |
| 31  | 4     | 309 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 31  | B     | 816 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 31  | 6     | 313 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 31  | A     | 830 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 36  | a     | 305 | LUT  | C7-C6   | 3.20  | 1.56        | 1.45     |
| 31  | 6     | 306 | CLA  | C4B-CHC | 3.20  | 1.49        | 1.41     |
| 31  | 5     | 312 | CLA  | C4D-CHA | 3.20  | 1.49        | 1.38     |
| 31  | B     | 827 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 31  | 7     | 321 | CLA  | C3D-C2D | 3.20  | 1.47        | 1.39     |
| 32  | A     | 840 | CHL  | C3D-C4D | -3.20 | 1.37        | 1.44     |
| 31  | 8     | 318 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 32  | 9     | 320 | CHL  | CHD-C4C | 3.19  | 1.46        | 1.39     |
| 26  | K     | 203 | BCR  | C30-C25 | -3.19 | 1.49        | 1.53     |
| 31  | A     | 822 | CLA  | C1D-ND  | -3.19 | 1.33        | 1.37     |
| 31  | A     | 843 | CLA  | C1D-ND  | -3.19 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 813 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 32  | 8     | 316 | CHL  | CHD-C4C | 3.19  | 1.46        | 1.39     |
| 31  | B     | 818 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 32  | A     | 840 | CHL  | CHD-C1D | 3.19  | 1.44        | 1.38     |
| 31  | 6     | 310 | CLA  | C4D-CHA | 3.19  | 1.49        | 1.38     |
| 31  | 8     | 308 | CLA  | OBD-CAD | 3.19  | 1.28        | 1.22     |
| 31  | A     | 825 | CLA  | C1D-ND  | -3.19 | 1.33        | 1.37     |
| 31  | A     | 827 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 31  | 9     | 321 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 31  | b     | 302 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 31  | A     | 818 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 31  | 7     | 309 | CLA  | OBD-CAD | 3.19  | 1.28        | 1.22     |
| 31  | B     | 822 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 31  | B     | 848 | CLA  | C3D-C2D | 3.19  | 1.47        | 1.39     |
| 32  | 8     | 316 | CHL  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 31  | 8     | 309 | CLA  | C3D-C2D | 3.18  | 1.47        | 1.39     |
| 31  | A     | 838 | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 31  | a     | 312 | CLA  | C3D-C2D | 3.18  | 1.47        | 1.39     |
| 31  | B     | 821 | CLA  | C1D-ND  | -3.18 | 1.33        | 1.37     |
| 31  | B     | 845 | CLA  | C1D-ND  | -3.18 | 1.33        | 1.37     |
| 31  | 4     | 318 | CLA  | C4D-CHA | 3.18  | 1.49        | 1.38     |
| 31  | A     | 854 | CLA  | C3D-C2D | 3.18  | 1.47        | 1.39     |
| 31  | 5     | 310 | CLA  | C4D-CHA | 3.18  | 1.49        | 1.38     |
| 31  | A     | 833 | CLA  | C3D-C2D | 3.18  | 1.47        | 1.39     |
| 31  | B     | 833 | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 31  | B     | 832 | CLA  | OBD-CAD | 3.18  | 1.28        | 1.22     |
| 31  | B     | 829 | CLA  | C3D-C2D | 3.18  | 1.47        | 1.39     |
| 31  | A     | 837 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 31  | a     | 310 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 31  | B     | 814 | CLA  | C3D-C2D | 3.17  | 1.47        | 1.39     |
| 31  | A     | 819 | CLA  | OBD-CAD | 3.17  | 1.27        | 1.22     |
| 31  | 7     | 316 | CLA  | C1D-ND  | -3.17 | 1.33        | 1.37     |
| 36  | F     | 304 | LUT  | C32-C33 | 3.17  | 1.52        | 1.45     |
| 31  | 8     | 317 | CLA  | C3D-C2D | 3.17  | 1.47        | 1.39     |
| 36  | J     | 103 | LUT  | C7-C6   | 3.17  | 1.56        | 1.45     |
| 31  | 5     | 313 | CLA  | C4D-CHA | 3.17  | 1.49        | 1.38     |
| 31  | 7     | 310 | CLA  | C3D-C2D | 3.17  | 1.47        | 1.39     |
| 31  | B     | 848 | CLA  | C1D-ND  | -3.17 | 1.33        | 1.37     |
| 31  | B     | 849 | CLA  | C3D-C2D | 3.17  | 1.47        | 1.39     |
| 31  | b     | 302 | CLA  | C4D-CHA | 3.17  | 1.49        | 1.38     |
| 31  | L     | 306 | CLA  | C1D-ND  | -3.17 | 1.33        | 1.37     |
| 32  | A     | 840 | CHL  | CHD-C4C | 3.17  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 821 | CLA  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 31  | a     | 313 | CLA  | C3D-C2D | 3.16  | 1.47        | 1.39     |
| 36  | 6     | 304 | LUT  | C7-C6   | 3.16  | 1.56        | 1.45     |
| 31  | B     | 818 | CLA  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 31  | b     | 313 | CLA  | C1D-ND  | -3.16 | 1.33        | 1.37     |
| 31  | B     | 840 | CLA  | C3D-C2D | 3.16  | 1.47        | 1.39     |
| 31  | B     | 823 | CLA  | C3D-C2D | 3.16  | 1.47        | 1.39     |
| 31  | B     | 850 | CLA  | C3D-C2D | 3.16  | 1.47        | 1.39     |
| 31  | 8     | 314 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 32  | 5     | 316 | CHL  | OBD-CAD | 3.15  | 1.27        | 1.22     |
| 31  | A     | 842 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 31  | 7     | 322 | CLA  | C1D-ND  | -3.15 | 1.33        | 1.37     |
| 31  | 8     | 309 | CLA  | C4D-CHA | 3.15  | 1.49        | 1.38     |
| 31  | 2     | 310 | CLA  | C4D-CHA | 3.15  | 1.49        | 1.38     |
| 31  | G     | 204 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 31  | 7     | 313 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 31  | 6     | 308 | CLA  | C4C-C3C | 3.15  | 1.50        | 1.45     |
| 31  | H     | 903 | CLA  | C1D-ND  | -3.15 | 1.33        | 1.37     |
| 31  | B     | 838 | CLA  | C1D-ND  | -3.15 | 1.33        | 1.37     |
| 31  | B     | 831 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 31  | 8     | 321 | CLA  | C1D-ND  | -3.15 | 1.33        | 1.37     |
| 31  | F     | 301 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 31  | A     | 819 | CLA  | C3D-C2D | 3.15  | 1.47        | 1.39     |
| 31  | K     | 205 | CLA  | MG-ND   | 3.15  | 2.12        | 2.05     |
| 36  | 8     | 303 | LUT  | C7-C6   | 3.15  | 1.56        | 1.45     |
| 31  | A     | 850 | CLA  | C1D-ND  | -3.14 | 1.33        | 1.37     |
| 31  | b     | 303 | CLA  | C4D-CHA | 3.14  | 1.49        | 1.38     |
| 31  | A     | 855 | CLA  | C1D-ND  | -3.14 | 1.33        | 1.37     |
| 32  | 7     | 324 | CHL  | OBD-CAD | 3.14  | 1.27        | 1.22     |
| 36  | 5     | 303 | LUT  | C28-C29 | 3.14  | 1.52        | 1.45     |
| 31  | A     | 822 | CLA  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 31  | B     | 828 | CLA  | C1D-ND  | -3.14 | 1.33        | 1.37     |
| 26  | A     | 805 | BCR  | C1-C6   | -3.14 | 1.49        | 1.53     |
| 36  | 4     | 302 | LUT  | C7-C6   | 3.14  | 1.56        | 1.45     |
| 32  | 7     | 320 | CHL  | OBD-CAD | 3.14  | 1.27        | 1.22     |
| 31  | F     | 306 | CLA  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 31  | a     | 310 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 31  | B     | 844 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 36  | L     | 304 | LUT  | C7-C6   | 3.13  | 1.56        | 1.45     |
| 31  | A     | 848 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | b     | 304 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | A     | 845 | CLA  | OBD-CAD | 3.13  | 1.27        | 1.22     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 829 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 31  | a     | 309 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 31  | 5     | 320 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 31  | B     | 835 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 31  | 8     | 313 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | 4     | 316 | CLA  | MG-ND   | 3.13  | 2.12        | 2.05     |
| 31  | J     | 105 | CLA  | C3D-C2D | 3.13  | 1.47        | 1.39     |
| 31  | b     | 313 | CLA  | C4C-C3C | 3.13  | 1.50        | 1.45     |
| 31  | A     | 838 | CLA  | C4D-CHA | 3.13  | 1.49        | 1.38     |
| 31  | 8     | 315 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | B     | 819 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | A     | 823 | CLA  | OBD-CAD | 3.13  | 1.27        | 1.22     |
| 31  | F     | 301 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | F     | 305 | CLA  | C1D-ND  | -3.13 | 1.33        | 1.37     |
| 31  | B     | 829 | CLA  | C4D-CHA | 3.12  | 1.49        | 1.38     |
| 31  | A     | 855 | CLA  | C3D-C2D | 3.12  | 1.47        | 1.39     |
| 32  | a     | 320 | CHL  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 31  | 8     | 320 | CLA  | C1D-ND  | -3.12 | 1.33        | 1.37     |
| 31  | A     | 830 | CLA  | C4D-CHA | 3.12  | 1.49        | 1.38     |
| 31  | a     | 311 | CLA  | C1D-ND  | -3.12 | 1.33        | 1.37     |
| 36  | 8     | 303 | LUT  | C23-C24 | 3.12  | 1.54        | 1.50     |
| 31  | A     | 818 | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 31  | B     | 845 | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 31  | 8     | 308 | CLA  | C1D-ND  | -3.12 | 1.33        | 1.37     |
| 31  | F     | 306 | CLA  | C4D-CHA | 3.12  | 1.49        | 1.38     |
| 26  | K     | 202 | BCR  | C1-C6   | -3.12 | 1.49        | 1.53     |
| 32  | 7     | 319 | CHL  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 31  | 9     | 317 | CLA  | C3D-C2D | 3.12  | 1.47        | 1.39     |
| 31  | B     | 835 | CLA  | OBD-CAD | 3.12  | 1.27        | 1.22     |
| 31  | A     | 835 | CLA  | C4D-CHA | 3.11  | 1.49        | 1.38     |
| 31  | a     | 309 | CLA  | C4D-CHA | 3.11  | 1.49        | 1.38     |
| 31  | 6     | 306 | CLA  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 36  | 4     | 303 | LUT  | C26-C27 | 3.11  | 1.54        | 1.50     |
| 31  | A     | 814 | CLA  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 32  | 7     | 318 | CHL  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 31  | B     | 824 | CLA  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 31  | A     | 844 | CLA  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 31  | 2     | 308 | CLA  | C3D-C2D | 3.11  | 1.47        | 1.39     |
| 32  | A     | 839 | CHL  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 31  | 7     | 310 | CLA  | C4D-CHA | 3.11  | 1.49        | 1.38     |
| 31  | 3     | 310 | CLA  | C1D-ND  | -3.11 | 1.34        | 1.37     |
| 36  | 5     | 303 | LUT  | C7-C6   | 3.10  | 1.56        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 307 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 31  | 3     | 316 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 36  | 2     | 301 | LUT  | C26-C27 | 3.10  | 1.54        | 1.50     |
| 31  | O     | 202 | CLA  | MG-ND   | 3.10  | 2.11        | 2.05     |
| 32  | a     | 317 | CHL  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 31  | a     | 321 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 31  | 9     | 315 | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 31  | 3     | 320 | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 31  | a     | 322 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 31  | 2     | 307 | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 26  | 6     | 302 | BCR  | C1-C6   | -3.10 | 1.49        | 1.53     |
| 31  | G     | 204 | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 31  | 3     | 313 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 31  | H     | 902 | CLA  | C3D-C2D | 3.10  | 1.47        | 1.39     |
| 31  | b     | 307 | CLA  | C4D-CHA | 3.10  | 1.49        | 1.38     |
| 31  | 3     | 308 | CLA  | C1D-ND  | -3.10 | 1.34        | 1.37     |
| 31  | B     | 822 | CLA  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 36  | b     | 301 | LUT  | C23-C24 | 3.09  | 1.54        | 1.50     |
| 31  | 9     | 321 | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 31  | A     | 836 | CLA  | C3D-C2D | 3.09  | 1.47        | 1.39     |
| 31  | B     | 824 | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 31  | a     | 319 | CLA  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 31  | O     | 203 | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 31  | B     | 815 | CLA  | C3D-C2D | 3.09  | 1.47        | 1.39     |
| 31  | 3     | 307 | CLA  | OBD-CAD | 3.09  | 1.27        | 1.22     |
| 32  | 3     | 315 | CHL  | OBD-CAD | 3.09  | 1.27        | 1.22     |
| 31  | 4     | 309 | CLA  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 31  | F     | 301 | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 31  | 8     | 311 | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 31  | b     | 312 | CLA  | C4D-CHA | 3.09  | 1.49        | 1.38     |
| 31  | 7     | 309 | CLA  | C1D-ND  | -3.09 | 1.34        | 1.37     |
| 31  | 9     | 311 | CLA  | C1D-ND  | -3.08 | 1.34        | 1.37     |
| 31  | H     | 901 | CLA  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 31  | O     | 204 | CLA  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 32  | A     | 831 | CHL  | C1D-ND  | -3.08 | 1.34        | 1.37     |
| 31  | 3     | 317 | CLA  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 30  | A     | 813 | CL0  | CHD-C1D | 3.08  | 1.44        | 1.38     |
| 31  | 2     | 306 | CLA  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 31  | 4     | 315 | CLA  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 31  | A     | 821 | CLA  | OBD-CAD | 3.08  | 1.27        | 1.22     |
| 31  | 4     | 308 | CLA  | C4D-CHA | 3.08  | 1.49        | 1.38     |
| 31  | 4     | 308 | CLA  | C1D-ND  | -3.08 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 848 | CLA  | OBD-CAD | 3.08  | 1.27        | 1.22     |
| 31  | A     | 849 | CLA  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 36  | a     | 303 | LUT  | C7-C6   | 3.07  | 1.56        | 1.45     |
| 31  | B     | 833 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 32  | 6     | 317 | CHL  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 32  | 5     | 319 | CHL  | MG-ND   | 3.07  | 2.11        | 2.05     |
| 26  | G     | 203 | BCR  | C30-C25 | -3.07 | 1.49        | 1.53     |
| 31  | 9     | 313 | CLA  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 31  | A     | 827 | CLA  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 26  | B     | 803 | BCR  | C1-C6   | -3.07 | 1.49        | 1.53     |
| 31  | A     | 844 | CLA  | C3D-C2D | 3.07  | 1.47        | 1.39     |
| 31  | A     | 836 | CLA  | MG-ND   | 3.07  | 2.11        | 2.05     |
| 31  | O     | 202 | CLA  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 31  | 9     | 319 | CLA  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 32  | A     | 831 | CHL  | OBD-CAD | 3.07  | 1.27        | 1.22     |
| 31  | A     | 854 | CLA  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 31  | 7     | 315 | CLA  | C4D-CHA | 3.07  | 1.49        | 1.38     |
| 31  | A     | 833 | CLA  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 31  | H     | 901 | CLA  | C1D-ND  | -3.07 | 1.34        | 1.37     |
| 31  | B     | 815 | CLA  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 31  | A     | 851 | CLA  | C1D-ND  | -3.06 | 1.34        | 1.37     |
| 31  | 5     | 308 | CLA  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 36  | 9     | 302 | LUT  | C26-C27 | 3.06  | 1.54        | 1.50     |
| 31  | 7     | 313 | CLA  | C1D-ND  | -3.06 | 1.34        | 1.37     |
| 31  | 6     | 314 | CLA  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 31  | A     | 820 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 31  | 5     | 311 | CLA  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 36  | F     | 304 | LUT  | C7-C6   | 3.06  | 1.56        | 1.45     |
| 31  | 2     | 315 | CLA  | MG-ND   | 3.06  | 2.11        | 2.05     |
| 32  | 8     | 316 | CHL  | C1D-ND  | -3.06 | 1.34        | 1.37     |
| 36  | 5     | 304 | LUT  | C26-C27 | 3.06  | 1.54        | 1.50     |
| 31  | B     | 846 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 31  | 6     | 312 | CLA  | C4D-CHA | 3.06  | 1.49        | 1.38     |
| 31  | A     | 829 | CLA  | C4B-NB  | 3.06  | 1.37        | 1.35     |
| 31  | B     | 817 | CLA  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 31  | 5     | 318 | CLA  | C1D-ND  | -3.06 | 1.34        | 1.37     |
| 31  | A     | 847 | CLA  | C1D-ND  | -3.05 | 1.34        | 1.37     |
| 31  | 4     | 312 | CLA  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 31  | b     | 310 | CLA  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 31  | 4     | 316 | CLA  | C1B-CHB | 3.05  | 1.49        | 1.41     |
| 32  | 4     | 310 | CHL  | C1D-ND  | -3.05 | 1.34        | 1.37     |
| 26  | A     | 804 | BCR  | C1-C6   | -3.05 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 823 | CLA  | OBD-CAD | 3.05  | 1.27        | 1.22     |
| 31  | 2     | 312 | CLA  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 31  | 6     | 313 | CLA  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 31  | 2     | 311 | CLA  | C1D-ND  | -3.05 | 1.34        | 1.37     |
| 31  | 6     | 308 | CLA  | C1D-ND  | -3.05 | 1.34        | 1.37     |
| 31  | A     | 824 | CLA  | C4D-CHA | 3.05  | 1.49        | 1.38     |
| 31  | 3     | 313 | CLA  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 31  | B     | 836 | CLA  | MG-ND   | 3.04  | 2.11        | 2.05     |
| 31  | 4     | 306 | CLA  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 31  | 8     | 307 | CLA  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 31  | a     | 310 | CLA  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 31  | 5     | 307 | CLA  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 31  | b     | 311 | CLA  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 31  | a     | 313 | CLA  | OBD-CAD | 3.04  | 1.27        | 1.22     |
| 31  | 7     | 321 | CLA  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 31  | A     | 851 | CLA  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 36  | 8     | 302 | LUT  | C23-C24 | 3.04  | 1.54        | 1.50     |
| 31  | A     | 835 | CLA  | C1D-ND  | -3.04 | 1.34        | 1.37     |
| 31  | 3     | 308 | CLA  | C4D-CHA | 3.04  | 1.49        | 1.38     |
| 32  | A     | 839 | CHL  | CHD-C4C | 3.03  | 1.46        | 1.39     |
| 31  | B     | 818 | CLA  | OBD-CAD | 3.03  | 1.27        | 1.22     |
| 31  | A     | 836 | CLA  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 31  | A     | 849 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | A     | 828 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 36  | 9     | 302 | LUT  | C7-C6   | 3.03  | 1.55        | 1.45     |
| 31  | 9     | 316 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | 3     | 309 | CLA  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 31  | 5     | 323 | CLA  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 31  | 5     | 314 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | A     | 819 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | 3     | 318 | CLA  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 32  | A     | 839 | CHL  | CHD-C1D | 3.03  | 1.44        | 1.38     |
| 31  | 2     | 314 | CLA  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 31  | 6     | 312 | CLA  | C1D-ND  | -3.03 | 1.34        | 1.37     |
| 31  | 4     | 314 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | 9     | 312 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | 7     | 316 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 31  | 6     | 308 | CLA  | C4D-CHA | 3.03  | 1.49        | 1.38     |
| 36  | a     | 305 | LUT  | C23-C24 | 3.02  | 1.54        | 1.50     |
| 31  | 2     | 309 | CLA  | C1D-ND  | -3.02 | 1.34        | 1.37     |
| 32  | 3     | 315 | CHL  | C1D-ND  | -3.02 | 1.34        | 1.37     |
| 31  | 8     | 315 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 815 | CLA  | C1D-ND  | -3.02 | 1.34        | 1.37     |
| 31  | 7     | 312 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 31  | H     | 902 | CLA  | C1D-ND  | -3.02 | 1.34        | 1.37     |
| 31  | B     | 838 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 31  | 4     | 321 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 31  | 4     | 311 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 31  | A     | 820 | CLA  | C1D-ND  | -3.02 | 1.34        | 1.37     |
| 31  | 2     | 309 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 31  | 8     | 312 | CLA  | C4D-CHA | 3.02  | 1.49        | 1.38     |
| 31  | B     | 816 | CLA  | MG-NA   | 3.01  | 2.13        | 2.06     |
| 31  | a     | 312 | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 31  | B     | 824 | CLA  | C1D-ND  | -3.01 | 1.34        | 1.37     |
| 31  | B     | 849 | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 36  | 9     | 305 | LUT  | C23-C24 | 3.01  | 1.54        | 1.50     |
| 31  | K     | 206 | CLA  | C1D-ND  | -3.01 | 1.34        | 1.37     |
| 31  | 9     | 312 | CLA  | C1D-ND  | -3.01 | 1.34        | 1.37     |
| 31  | A     | 846 | CLA  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 31  | B     | 849 | CLA  | C1D-ND  | -3.01 | 1.34        | 1.37     |
| 31  | B     | 819 | CLA  | MG-ND   | 3.01  | 2.11        | 2.05     |
| 31  | A     | 822 | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 31  | B     | 832 | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 31  | a     | 312 | CLA  | C1D-ND  | -3.01 | 1.34        | 1.37     |
| 31  | 6     | 322 | CLA  | C4D-CHA | 3.01  | 1.49        | 1.38     |
| 31  | 9     | 317 | CLA  | C4B-CHC | 3.01  | 1.49        | 1.41     |
| 31  | 7     | 311 | CLA  | C1D-ND  | -3.00 | 1.34        | 1.37     |
| 31  | A     | 852 | CLA  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 31  | B     | 845 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | a     | 319 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | F     | 306 | CLA  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 31  | 5     | 323 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 26  | 6     | 302 | BCR  | C30-C25 | -3.00 | 1.49        | 1.53     |
| 36  | 8     | 302 | LUT  | C7-C6   | 3.00  | 1.55        | 1.45     |
| 31  | 3     | 307 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | 2     | 304 | CLA  | C1D-ND  | -3.00 | 1.34        | 1.37     |
| 31  | a     | 311 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | 2     | 311 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | K     | 205 | CLA  | C1D-ND  | -3.00 | 1.34        | 1.37     |
| 31  | 2     | 305 | CLA  | C1D-ND  | -3.00 | 1.34        | 1.37     |
| 32  | A     | 839 | CHL  | OBD-CAD | 3.00  | 1.27        | 1.22     |
| 31  | A     | 841 | CLA  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 31  | 8     | 320 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | 3     | 312 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 30  | A     | 813 | CL0  | C3D-C2D | 3.00  | 1.47        | 1.39     |
| 31  | A     | 854 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | 8     | 307 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | A     | 837 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | G     | 205 | CLA  | C4D-CHA | 3.00  | 1.49        | 1.38     |
| 31  | 7     | 321 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 6     | 306 | CLA  | C1D-C2D | 2.99  | 1.51        | 1.45     |
| 31  | 8     | 308 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | F     | 305 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 6     | 315 | CLA  | C1D-ND  | -2.99 | 1.34        | 1.37     |
| 31  | 2     | 314 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 6     | 311 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | A     | 852 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 9     | 311 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | A     | 842 | CLA  | OBD-CAD | 2.99  | 1.27        | 1.22     |
| 31  | 3     | 320 | CLA  | C1D-ND  | -2.99 | 1.34        | 1.37     |
| 31  | K     | 205 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 4     | 319 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 3     | 309 | CLA  | C4D-CHA | 2.99  | 1.49        | 1.38     |
| 31  | 2     | 305 | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 31  | K     | 206 | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 31  | B     | 832 | CLA  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 36  | 2     | 301 | LUT  | C7-C6   | 2.98  | 1.55        | 1.45     |
| 31  | 7     | 314 | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 31  | 5     | 321 | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 31  | A     | 824 | CLA  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 32  | 6     | 309 | CHL  | MG-NC   | -2.98 | 1.99        | 2.06     |
| 31  | 9     | 315 | CLA  | C3D-C2D | 2.98  | 1.47        | 1.39     |
| 31  | 2     | 308 | CLA  | C4D-CHA | 2.98  | 1.49        | 1.38     |
| 31  | 7     | 314 | CLA  | C1D-ND  | -2.98 | 1.34        | 1.37     |
| 26  | 8     | 301 | BCR  | C30-C25 | -2.97 | 1.49        | 1.53     |
| 31  | A     | 842 | CLA  | C4D-CHA | 2.97  | 1.49        | 1.38     |
| 31  | A     | 833 | CLA  | C4D-CHA | 2.97  | 1.49        | 1.38     |
| 26  | G     | 203 | BCR  | C1-C6   | -2.97 | 1.49        | 1.53     |
| 31  | 3     | 312 | CLA  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 32  | 9     | 320 | CHL  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 31  | 7     | 313 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 31  | 2     | 304 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 32  | 5     | 317 | CHL  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 31  | A     | 847 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 32  | 7     | 317 | CHL  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 31  | B     | 822 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 845 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 31  | 5     | 320 | CLA  | C1D-ND  | -2.97 | 1.34        | 1.37     |
| 31  | b     | 306 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 31  | 5     | 315 | CLA  | C4D-CHA | 2.97  | 1.48        | 1.38     |
| 31  | 5     | 309 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | a     | 321 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | 9     | 318 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | L     | 306 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | H     | 902 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | B     | 832 | CLA  | C3D-C2D | 2.96  | 1.47        | 1.39     |
| 31  | 9     | 319 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 31  | 2     | 313 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 31  | B     | 836 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | A     | 843 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | A     | 852 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 31  | 6     | 315 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | H     | 903 | CLA  | C1B-CHB | 2.96  | 1.49        | 1.41     |
| 31  | a     | 310 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 31  | a     | 311 | CLA  | C1B-CHB | 2.96  | 1.49        | 1.41     |
| 31  | B     | 818 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | b     | 311 | CLA  | C4D-CHA | 2.96  | 1.48        | 1.38     |
| 31  | 8     | 311 | CLA  | C1D-ND  | -2.96 | 1.34        | 1.37     |
| 31  | B     | 819 | CLA  | C3D-C2D | 2.95  | 1.47        | 1.39     |
| 31  | 8     | 314 | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 31  | 2     | 315 | CLA  | MG-NA   | -2.95 | 1.99        | 2.06     |
| 31  | 3     | 316 | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 31  | 3     | 314 | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 31  | B     | 819 | CLA  | OBD-CAD | 2.95  | 1.27        | 1.22     |
| 36  | 9     | 305 | LUT  | C7-C6   | 2.95  | 1.55        | 1.45     |
| 31  | b     | 308 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 26  | L     | 303 | BCR  | C30-C25 | -2.95 | 1.49        | 1.53     |
| 31  | B     | 829 | CLA  | C1D-ND  | -2.95 | 1.34        | 1.37     |
| 36  | 3     | 305 | LUT  | C26-C27 | 2.95  | 1.54        | 1.50     |
| 31  | B     | 823 | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 31  | B     | 834 | CLA  | C4D-CHA | 2.95  | 1.48        | 1.38     |
| 31  | 4     | 312 | CLA  | MG-ND   | 2.95  | 2.11        | 2.05     |
| 27  | A     | 807 | LMT  | O3'-C3' | -2.95 | 1.36        | 1.43     |
| 33  | B     | 808 | DGD  | C3G-C2G | 2.94  | 1.59        | 1.50     |
| 31  | A     | 850 | CLA  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 26  | 3     | 303 | BCR  | C30-C25 | -2.94 | 1.49        | 1.53     |
| 31  | a     | 315 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 31  | 3     | 318 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 310 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 31  | 4     | 307 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 31  | 3     | 311 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 31  | 6     | 314 | CLA  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 31  | H     | 903 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 31  | 8     | 312 | CLA  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 32  | 5     | 322 | CHL  | MG-NC   | 2.94  | 2.13        | 2.06     |
| 31  | A     | 834 | CLA  | OBD-CAD | 2.94  | 1.27        | 1.22     |
| 31  | 5     | 314 | CLA  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 31  | 7     | 311 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 31  | 7     | 312 | CLA  | C1D-ND  | -2.94 | 1.34        | 1.37     |
| 31  | A     | 823 | CLA  | C4D-CHA | 2.94  | 1.48        | 1.38     |
| 32  | 7     | 318 | CHL  | OBD-CAD | 2.94  | 1.27        | 1.22     |
| 31  | 5     | 318 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | B     | 826 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 26  | I     | 801 | BCR  | C1-C6   | -2.93 | 1.49        | 1.53     |
| 31  | B     | 835 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | a     | 316 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | A     | 826 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | A     | 844 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | 2     | 313 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 32  | 4     | 313 | CHL  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | 8     | 311 | CLA  | MG-ND   | -2.93 | 2.00        | 2.05     |
| 31  | B     | 819 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | G     | 205 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | 6     | 312 | CLA  | MG-NC   | -2.93 | 1.99        | 2.06     |
| 31  | B     | 813 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | 7     | 310 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 32  | 8     | 319 | CHL  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | A     | 820 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | B     | 843 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | 9     | 314 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | a     | 309 | CLA  | MG-NC   | -2.93 | 1.99        | 2.06     |
| 31  | A     | 821 | CLA  | C4D-CHA | 2.93  | 1.48        | 1.38     |
| 31  | b     | 308 | CLA  | C4C-C3C | 2.93  | 1.50        | 1.45     |
| 31  | A     | 830 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | 4     | 307 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | a     | 315 | CLA  | C1D-ND  | -2.93 | 1.34        | 1.37     |
| 31  | 4     | 305 | CLA  | CHD-C1D | 2.93  | 1.44        | 1.38     |
| 31  | A     | 844 | CLA  | MG-NA   | 2.93  | 2.13        | 2.06     |
| 31  | b     | 313 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | 4     | 309 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | a     | 313 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | B     | 832 | CLA  | C1C-NC  | -2.92 | 1.33        | 1.37     |
| 42  | 4     | 304 | SQD  | C24-C23 | 2.92  | 1.59        | 1.50     |
| 31  | A     | 855 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | B     | 846 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | B     | 820 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | 5     | 307 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | 8     | 314 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 31  | 7     | 322 | CLA  | C1B-CHB | 2.92  | 1.49        | 1.41     |
| 31  | 9     | 318 | CLA  | C1B-CHB | 2.92  | 1.49        | 1.41     |
| 31  | A     | 838 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 32  | 6     | 321 | CHL  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 31  | O     | 204 | CLA  | C3A-C2A | -2.92 | 1.51        | 1.54     |
| 31  | O     | 202 | CLA  | C1B-CHB | 2.92  | 1.49        | 1.41     |
| 31  | 9     | 318 | CLA  | C4B-CHC | 2.92  | 1.49        | 1.41     |
| 31  | 5     | 307 | CLA  | MG-NC   | 2.92  | 2.13        | 2.06     |
| 31  | b     | 312 | CLA  | C4C-C3C | 2.92  | 1.50        | 1.45     |
| 31  | 9     | 314 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | 6     | 307 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | 4     | 314 | CLA  | C1D-ND  | -2.92 | 1.34        | 1.37     |
| 36  | 9     | 302 | LUT  | C23-C24 | 2.92  | 1.54        | 1.50     |
| 31  | B     | 842 | CLA  | C4D-CHA | 2.92  | 1.48        | 1.38     |
| 31  | 8     | 318 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | B     | 830 | CLA  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 31  | b     | 305 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | A     | 850 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | 4     | 320 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | 6     | 310 | CLA  | C1B-CHB | 2.91  | 1.49        | 1.41     |
| 31  | B     | 828 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | 9     | 316 | CLA  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 31  | 2     | 312 | CLA  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 31  | 2     | 306 | CLA  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 31  | B     | 850 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | b     | 306 | CLA  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 31  | 8     | 321 | CLA  | C4D-CHA | 2.91  | 1.48        | 1.38     |
| 31  | a     | 314 | CLA  | C1D-ND  | -2.91 | 1.34        | 1.37     |
| 31  | a     | 314 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 31  | 5     | 320 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 31  | 8     | 313 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 31  | 6     | 313 | CLA  | C1D-ND  | -2.90 | 1.34        | 1.37     |
| 31  | A     | 857 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 26  | G     | 201 | BCR  | C1-C6   | -2.90 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 821 | CLA  | C4D-CHA | 2.90  | 1.48        | 1.38     |
| 36  | 9     | 303 | LUT  | C26-C27 | 2.90  | 1.54        | 1.50     |
| 31  | 8     | 310 | CLA  | C4B-CHC | 2.90  | 1.49        | 1.41     |
| 31  | 4     | 319 | CLA  | C1B-CHB | 2.89  | 1.49        | 1.41     |
| 31  | O     | 203 | CLA  | MG-ND   | 2.89  | 2.11        | 2.05     |
| 32  | 6     | 320 | CHL  | C1D-ND  | -2.89 | 1.34        | 1.37     |
| 31  | 7     | 315 | CLA  | C1D-ND  | -2.89 | 1.34        | 1.37     |
| 31  | B     | 847 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 31  | 9     | 315 | CLA  | OBD-CAD | 2.89  | 1.27        | 1.22     |
| 31  | 2     | 315 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 31  | B     | 825 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 31  | 6     | 315 | CLA  | C1B-CHB | 2.89  | 1.49        | 1.41     |
| 36  | b     | 301 | LUT  | C7-C6   | 2.89  | 1.55        | 1.45     |
| 31  | b     | 308 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 31  | O     | 203 | CLA  | C4B-CHC | 2.89  | 1.49        | 1.41     |
| 31  | 6     | 311 | CLA  | C4C-C3C | 2.89  | 1.50        | 1.45     |
| 30  | A     | 813 | CL0  | OBD-CAD | 2.89  | 1.27        | 1.22     |
| 31  | B     | 845 | CLA  | C1C-NC  | -2.89 | 1.33        | 1.37     |
| 31  | 9     | 318 | CLA  | C1D-ND  | -2.89 | 1.34        | 1.37     |
| 31  | A     | 817 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 31  | 6     | 316 | CLA  | C1B-CHB | 2.89  | 1.49        | 1.41     |
| 31  | G     | 206 | CLA  | C4D-CHA | 2.89  | 1.48        | 1.38     |
| 31  | 3     | 311 | CLA  | OBD-CAD | 2.88  | 1.27        | 1.22     |
| 32  | a     | 320 | CHL  | C1D-ND  | -2.88 | 1.34        | 1.37     |
| 31  | 3     | 311 | CLA  | C3D-C2D | 2.88  | 1.47        | 1.39     |
| 31  | 6     | 314 | CLA  | C1B-CHB | 2.88  | 1.49        | 1.41     |
| 31  | A     | 848 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 31  | 6     | 307 | CLA  | C1D-ND  | -2.88 | 1.34        | 1.37     |
| 36  | F     | 304 | LUT  | C26-C27 | 2.88  | 1.54        | 1.50     |
| 31  | A     | 836 | CLA  | C4D-CHA | 2.88  | 1.48        | 1.38     |
| 31  | L     | 307 | CLA  | C4C-C3C | 2.88  | 1.50        | 1.45     |
| 31  | L     | 307 | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 31  | A     | 814 | CLA  | OBD-CAD | 2.87  | 1.27        | 1.22     |
| 31  | 3     | 311 | CLA  | C1D-ND  | -2.87 | 1.34        | 1.37     |
| 31  | 5     | 315 | CLA  | C1D-ND  | -2.87 | 1.34        | 1.37     |
| 31  | O     | 204 | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 31  | 8     | 309 | CLA  | C1C-NC  | -2.87 | 1.33        | 1.37     |
| 31  | B     | 848 | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 31  | a     | 322 | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 31  | A     | 819 | CLA  | C1D-ND  | -2.87 | 1.34        | 1.37     |
| 31  | 3     | 317 | CLA  | C1D-ND  | -2.87 | 1.34        | 1.37     |
| 31  | 5     | 309 | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 834 | CLA  | C3D-C2D | 2.87  | 1.47        | 1.39     |
| 36  | 5     | 303 | LUT  | C26-C27 | 2.87  | 1.54        | 1.50     |
| 26  | M     | 101 | BCR  | C1-C6   | -2.87 | 1.49        | 1.53     |
| 31  | b     | 304 | CLA  | C4D-CHA | 2.87  | 1.48        | 1.38     |
| 31  | A     | 857 | CLA  | C1B-CHB | 2.87  | 1.49        | 1.41     |
| 26  | 3     | 301 | BCR  | C30-C25 | -2.87 | 1.49        | 1.53     |
| 31  | 4     | 320 | CLA  | C1D-ND  | -2.87 | 1.34        | 1.37     |
| 31  | b     | 307 | CLA  | C1B-CHB | 2.86  | 1.49        | 1.41     |
| 31  | 4     | 319 | CLA  | C4B-CHC | 2.86  | 1.49        | 1.41     |
| 31  | F     | 306 | CLA  | C1D-ND  | -2.86 | 1.34        | 1.37     |
| 31  | 2     | 308 | CLA  | C1D-ND  | -2.86 | 1.34        | 1.37     |
| 36  | 6     | 303 | LUT  | C7-C6   | 2.86  | 1.55        | 1.45     |
| 31  | a     | 309 | CLA  | C1D-ND  | -2.86 | 1.34        | 1.37     |
| 31  | 7     | 309 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 31  | A     | 832 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 31  | J     | 105 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 30  | A     | 813 | CL0  | CHD-C4C | 2.86  | 1.45        | 1.39     |
| 31  | B     | 837 | CLA  | C4C-C3C | 2.86  | 1.50        | 1.45     |
| 31  | 4     | 321 | CLA  | C1D-ND  | -2.86 | 1.34        | 1.37     |
| 36  | 7     | 305 | LUT  | C26-C27 | 2.86  | 1.54        | 1.50     |
| 31  | B     | 811 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 31  | B     | 831 | CLA  | C4D-CHA | 2.86  | 1.48        | 1.38     |
| 31  | 5     | 320 | CLA  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 36  | J     | 103 | LUT  | C26-C27 | 2.85  | 1.54        | 1.50     |
| 31  | 7     | 310 | CLA  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 36  | 5     | 303 | LUT  | C23-C24 | 2.85  | 1.54        | 1.50     |
| 31  | 8     | 320 | CLA  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 26  | L     | 302 | BCR  | C1-C6   | -2.85 | 1.49        | 1.53     |
| 31  | 5     | 321 | CLA  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 31  | G     | 204 | CLA  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 31  | 4     | 319 | CLA  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 31  | 8     | 314 | CLA  | C1B-CHB | 2.85  | 1.48        | 1.41     |
| 31  | O     | 202 | CLA  | C4B-CHC | 2.85  | 1.48        | 1.41     |
| 31  | 8     | 317 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 36  | 8     | 303 | LUT  | C38-C25 | 2.85  | 1.55        | 1.50     |
| 31  | b     | 310 | CLA  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 31  | 9     | 317 | CLA  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 31  | A     | 827 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 32  | A     | 840 | CHL  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 32  | 4     | 317 | CHL  | C1D-ND  | -2.85 | 1.34        | 1.37     |
| 31  | 7     | 322 | CLA  | C4D-CHA | 2.85  | 1.48        | 1.38     |
| 31  | 5     | 320 | CLA  | C4B-CHC | 2.85  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 313 | CLA  | C4B-CHC | 2.85  | 1.48        | 1.41     |
| 31  | 4     | 320 | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 26  | G     | 201 | BCR  | C30-C25 | -2.84 | 1.49        | 1.53     |
| 36  | 3     | 305 | LUT  | C7-C6   | 2.84  | 1.55        | 1.45     |
| 31  | 6     | 316 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 31  | A     | 846 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 31  | B     | 827 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 31  | 7     | 311 | CLA  | C1B-CHB | 2.84  | 1.48        | 1.41     |
| 31  | B     | 831 | CLA  | C1C-NC  | -2.84 | 1.33        | 1.37     |
| 31  | 9     | 315 | CLA  | C1D-ND  | -2.84 | 1.34        | 1.37     |
| 31  | A     | 841 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 31  | 3     | 310 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 26  | A     | 803 | BCR  | C30-C25 | -2.84 | 1.49        | 1.53     |
| 31  | b     | 303 | CLA  | C4C-C3C | 2.84  | 1.49        | 1.45     |
| 31  | A     | 853 | CLA  | C4D-CHA | 2.84  | 1.48        | 1.38     |
| 31  | 3     | 308 | CLA  | C1B-CHB | 2.83  | 1.48        | 1.41     |
| 31  | B     | 814 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 31  | O     | 204 | CLA  | C1D-ND  | -2.83 | 1.34        | 1.37     |
| 31  | B     | 837 | CLA  | C1B-CHB | 2.83  | 1.48        | 1.41     |
| 31  | O     | 203 | CLA  | C1D-ND  | -2.83 | 1.34        | 1.37     |
| 31  | 3     | 310 | CLA  | MG-NA   | 2.83  | 2.13        | 2.06     |
| 31  | 2     | 313 | CLA  | C4C-C3C | 2.83  | 1.49        | 1.45     |
| 31  | 4     | 311 | CLA  | C1D-ND  | -2.83 | 1.34        | 1.37     |
| 32  | 6     | 309 | CHL  | C1D-ND  | -2.83 | 1.34        | 1.37     |
| 31  | B     | 844 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 26  | A     | 804 | BCR  | C30-C25 | -2.83 | 1.49        | 1.53     |
| 28  | A     | 811 | LHG  | O7-C5   | -2.83 | 1.39        | 1.46     |
| 31  | 3     | 320 | CLA  | C1B-CHB | 2.83  | 1.48        | 1.41     |
| 31  | K     | 204 | CLA  | C1B-CHB | 2.83  | 1.48        | 1.41     |
| 31  | B     | 833 | CLA  | C4D-CHA | 2.83  | 1.48        | 1.38     |
| 31  | L     | 306 | CLA  | MG-ND   | 2.82  | 2.11        | 2.05     |
| 31  | B     | 839 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 31  | A     | 856 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 31  | 5     | 309 | CLA  | MG-NC   | 2.82  | 2.13        | 2.06     |
| 31  | A     | 820 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | B     | 816 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | A     | 834 | CLA  | C4D-CHA | 2.82  | 1.48        | 1.38     |
| 31  | 9     | 321 | CLA  | C1D-ND  | -2.82 | 1.34        | 1.37     |
| 31  | 5     | 311 | CLA  | C1D-ND  | -2.82 | 1.34        | 1.37     |
| 31  | b     | 311 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | A     | 843 | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |
| 31  | A     | 855 | CLA  | C1C-NC  | -2.82 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 855 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | a     | 309 | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 31  | 2     | 315 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | A     | 856 | CLA  | OBD-CAD | 2.82  | 1.27        | 1.22     |
| 36  | 2     | 301 | LUT  | C18-C5  | 2.82  | 1.55        | 1.50     |
| 31  | 8     | 307 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | 5     | 313 | CLA  | C4B-NB  | 2.82  | 1.37        | 1.35     |
| 31  | b     | 303 | CLA  | C4D-ND  | 2.82  | 1.41        | 1.37     |
| 31  | 5     | 313 | CLA  | C1B-CHB | 2.82  | 1.48        | 1.41     |
| 31  | b     | 307 | CLA  | C1D-ND  | -2.82 | 1.34        | 1.37     |
| 31  | B     | 850 | CLA  | C4B-CHC | 2.82  | 1.48        | 1.41     |
| 31  | b     | 306 | CLA  | C4B-CHC | 2.81  | 1.48        | 1.41     |
| 31  | 6     | 315 | CLA  | C4B-CHC | 2.81  | 1.48        | 1.41     |
| 31  | B     | 834 | CLA  | OBD-CAD | 2.81  | 1.27        | 1.22     |
| 31  | B     | 837 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 31  | A     | 825 | CLA  | C4D-CHA | 2.81  | 1.48        | 1.38     |
| 31  | A     | 850 | CLA  | OBD-CAD | 2.81  | 1.27        | 1.22     |
| 31  | a     | 312 | CLA  | C1B-CHB | 2.81  | 1.48        | 1.41     |
| 31  | b     | 308 | CLA  | C4B-CHC | 2.81  | 1.48        | 1.41     |
| 32  | 6     | 318 | CHL  | C1D-ND  | -2.81 | 1.34        | 1.37     |
| 31  | 8     | 312 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | A     | 838 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | 9     | 317 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | 2     | 308 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | G     | 205 | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 31  | 2     | 310 | CLA  | C1D-ND  | -2.80 | 1.34        | 1.37     |
| 31  | B     | 837 | CLA  | C3D-C2D | 2.80  | 1.46        | 1.39     |
| 31  | L     | 307 | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 31  | B     | 812 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 31  | 4     | 307 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | 9     | 317 | CLA  | C1D-C2D | 2.80  | 1.50        | 1.45     |
| 31  | B     | 816 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 31  | b     | 312 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | B     | 830 | CLA  | C4D-CHA | 2.80  | 1.48        | 1.38     |
| 31  | 7     | 310 | CLA  | C1C-NC  | -2.80 | 1.33        | 1.37     |
| 31  | 9     | 317 | CLA  | C4C-C3C | 2.80  | 1.49        | 1.45     |
| 31  | 2     | 311 | CLA  | C4B-CHC | 2.80  | 1.48        | 1.41     |
| 31  | a     | 314 | CLA  | C1B-CHB | 2.80  | 1.48        | 1.41     |
| 31  | 4     | 306 | CLA  | C4B-CHC | 2.79  | 1.48        | 1.41     |
| 31  | 5     | 310 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 32  | 5     | 319 | CHL  | C1D-ND  | -2.79 | 1.34        | 1.37     |
| 36  | 7     | 305 | LUT  | C18-C5  | 2.79  | 1.55        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | a     | 319 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | 9     | 314 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | B     | 822 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | B     | 835 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | 4     | 312 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | A     | 816 | CLA  | C4D-CHA | 2.79  | 1.48        | 1.38     |
| 31  | 7     | 314 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | b     | 303 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | 5     | 323 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 31  | 6     | 311 | CLA  | C1B-CHB | 2.79  | 1.48        | 1.41     |
| 32  | 7     | 324 | CHL  | MG-NA   | 2.79  | 2.12        | 2.06     |
| 31  | B     | 822 | CLA  | C1C-NC  | -2.79 | 1.33        | 1.37     |
| 31  | 5     | 310 | CLA  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 31  | K     | 204 | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 31  | 5     | 309 | CLA  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 31  | 5     | 312 | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 36  | 9     | 302 | LUT  | C18-C5  | 2.78  | 1.55        | 1.50     |
| 31  | 2     | 310 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | 6     | 313 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | 2     | 307 | CLA  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 32  | 6     | 319 | CHL  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 32  | K     | 201 | CHL  | C1D-C2D | 2.78  | 1.50        | 1.45     |
| 31  | B     | 847 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | B     | 829 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 32  | 5     | 322 | CHL  | C1D-ND  | -2.78 | 1.34        | 1.37     |
| 31  | O     | 204 | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 31  | 2     | 304 | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 31  | H     | 902 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | A     | 841 | CLA  | C1C-NC  | -2.78 | 1.33        | 1.37     |
| 31  | 4     | 318 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | B     | 840 | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 31  | 2     | 308 | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 31  | 5     | 308 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | 2     | 305 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 31  | 4     | 315 | CLA  | C4B-CHC | 2.78  | 1.48        | 1.41     |
| 36  | a     | 303 | LUT  | C18-C5  | 2.78  | 1.55        | 1.50     |
| 31  | 3     | 319 | CLA  | C4D-CHA | 2.78  | 1.48        | 1.38     |
| 31  | 2     | 306 | CLA  | C1B-CHB | 2.78  | 1.48        | 1.41     |
| 36  | 4     | 303 | LUT  | C23-C24 | 2.78  | 1.54        | 1.50     |
| 31  | B     | 817 | CLA  | C4D-CHA | 2.77  | 1.48        | 1.38     |
| 31  | 4     | 311 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 31  | A     | 825 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 311 | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 31  | 5     | 309 | CLA  | C4C-C3C | 2.77  | 1.49        | 1.45     |
| 31  | A     | 836 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 36  | J     | 103 | LUT  | C18-C5  | 2.77  | 1.55        | 1.50     |
| 31  | b     | 302 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 31  | A     | 851 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 31  | 9     | 313 | CLA  | C1D-ND  | -2.77 | 1.34        | 1.37     |
| 31  | B     | 823 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 31  | 5     | 314 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 31  | 9     | 319 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 31  | 4     | 320 | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 31  | 9     | 313 | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 31  | B     | 835 | CLA  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 31  | 2     | 312 | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 32  | 7     | 320 | CHL  | C1D-ND  | -2.77 | 1.34        | 1.37     |
| 31  | 9     | 313 | CLA  | C1B-CHB | 2.77  | 1.48        | 1.41     |
| 32  | b     | 309 | CHL  | C1D-ND  | -2.77 | 1.34        | 1.37     |
| 31  | 3     | 320 | CLA  | C4B-CHC | 2.77  | 1.48        | 1.41     |
| 31  | L     | 305 | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 31  | 7     | 310 | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 31  | 2     | 304 | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 31  | B     | 825 | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 31  | A     | 851 | CLA  | OBD-CAD | 2.76  | 1.27        | 1.22     |
| 31  | b     | 304 | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 31  | B     | 824 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 31  | J     | 105 | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 31  | 3     | 313 | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 31  | b     | 310 | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 31  | A     | 838 | CLA  | C1C-NC  | -2.76 | 1.33        | 1.37     |
| 31  | H     | 903 | CLA  | C4C-C3C | 2.76  | 1.49        | 1.45     |
| 31  | 2     | 310 | CLA  | C4B-CHC | 2.76  | 1.48        | 1.41     |
| 31  | G     | 204 | CLA  | C4C-C3C | 2.76  | 1.49        | 1.45     |
| 31  | L     | 305 | CLA  | C4D-CHA | 2.76  | 1.48        | 1.38     |
| 31  | A     | 829 | CLA  | C1B-NB  | -2.76 | 1.32        | 1.35     |
| 31  | 2     | 314 | CLA  | C1B-CHB | 2.76  | 1.48        | 1.41     |
| 31  | 3     | 320 | CLA  | MG-NC   | -2.75 | 1.99        | 2.06     |
| 31  | A     | 846 | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 31  | 5     | 312 | CLA  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 31  | 6     | 311 | CLA  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 27  | A     | 808 | LMT  | O3'-C3' | -2.75 | 1.36        | 1.43     |
| 27  | 9     | 306 | LMT  | O3'-C3' | -2.75 | 1.36        | 1.43     |
| 31  | 8     | 309 | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 3     | 305 | LUT  | C23-C24 | 2.75  | 1.54        | 1.50     |
| 31  | 4     | 306 | CLA  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 31  | b     | 304 | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 31  | b     | 311 | CLA  | C4B-CHC | 2.75  | 1.48        | 1.41     |
| 31  | H     | 901 | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 31  | 9     | 317 | CLA  | C4B-NB  | 2.75  | 1.37        | 1.35     |
| 31  | a     | 313 | CLA  | MG-ND   | -2.75 | 2.00        | 2.05     |
| 31  | F     | 306 | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 31  | 8     | 309 | CLA  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 31  | 4     | 312 | CLA  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 31  | 6     | 310 | CLA  | C1D-ND  | -2.75 | 1.34        | 1.37     |
| 31  | O     | 203 | CLA  | C1B-CHB | 2.75  | 1.48        | 1.41     |
| 31  | 4     | 312 | CLA  | C4B-CHC | 2.75  | 1.48        | 1.41     |
| 31  | 5     | 321 | CLA  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 31  | 8     | 313 | CLA  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 31  | A     | 814 | CLA  | C4D-CHA | 2.74  | 1.48        | 1.38     |
| 31  | G     | 205 | CLA  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 31  | 6     | 308 | CLA  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 31  | O     | 204 | CLA  | C4C-C3C | 2.74  | 1.49        | 1.45     |
| 31  | B     | 814 | CLA  | C1C-NC  | -2.74 | 1.33        | 1.37     |
| 31  | B     | 826 | CLA  | C1B-CHB | 2.74  | 1.48        | 1.41     |
| 31  | 5     | 308 | CLA  | C4B-CHC | 2.74  | 1.48        | 1.41     |
| 32  | K     | 201 | CHL  | C3D-C2D | 2.74  | 1.46        | 1.39     |
| 31  | B     | 844 | CLA  | OBD-CAD | 2.73  | 1.27        | 1.22     |
| 31  | 5     | 312 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 4     | 311 | CLA  | C4D-ND  | 2.73  | 1.41        | 1.37     |
| 31  | 3     | 313 | CLA  | C4C-C3C | 2.73  | 1.49        | 1.45     |
| 31  | 8     | 309 | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 31  | 9     | 312 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 8     | 314 | CLA  | C1C-NC  | -2.73 | 1.33        | 1.37     |
| 31  | a     | 309 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 4     | 305 | CLA  | C3D-C2D | 2.73  | 1.46        | 1.39     |
| 26  | L     | 301 | BCR  | C1-C6   | -2.73 | 1.50        | 1.53     |
| 31  | A     | 837 | CLA  | C1C-NC  | -2.73 | 1.33        | 1.37     |
| 31  | 8     | 308 | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 31  | B     | 822 | CLA  | C4C-C3C | 2.73  | 1.49        | 1.45     |
| 31  | 8     | 314 | CLA  | C4C-C3C | 2.73  | 1.49        | 1.45     |
| 31  | B     | 834 | CLA  | C1C-NC  | -2.73 | 1.33        | 1.37     |
| 31  | A     | 835 | CLA  | C4C-C3C | 2.73  | 1.49        | 1.45     |
| 31  | A     | 826 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | A     | 818 | CLA  | C4D-CHA | 2.73  | 1.48        | 1.38     |
| 31  | 3     | 307 | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 307 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 8     | 321 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 5     | 315 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 4     | 315 | CLA  | C1D-ND  | -2.73 | 1.34        | 1.37     |
| 31  | A     | 848 | CLA  | C1C-NC  | -2.73 | 1.33        | 1.37     |
| 31  | 7     | 315 | CLA  | C1B-CHB | 2.73  | 1.48        | 1.41     |
| 31  | 6     | 316 | CLA  | C4B-CHC | 2.73  | 1.48        | 1.41     |
| 31  | 4     | 318 | CLA  | C4C-C3C | 2.72  | 1.49        | 1.45     |
| 31  | A     | 825 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 31  | 5     | 310 | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 36  | J     | 103 | LUT  | C23-C24 | 2.72  | 1.54        | 1.50     |
| 31  | b     | 306 | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 31  | 5     | 314 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 36  | 9     | 305 | LUT  | C38-C25 | 2.72  | 1.55        | 1.50     |
| 31  | A     | 814 | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 31  | A     | 851 | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 31  | b     | 308 | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 31  | 4     | 314 | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 31  | 2     | 309 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 31  | 6     | 307 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 31  | B     | 815 | CLA  | C1C-NC  | -2.72 | 1.33        | 1.37     |
| 31  | b     | 305 | CLA  | C1D-ND  | -2.72 | 1.34        | 1.37     |
| 31  | 4     | 307 | CLA  | C4C-C3C | 2.72  | 1.49        | 1.45     |
| 31  | b     | 307 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 31  | 2     | 306 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 31  | B     | 818 | CLA  | C1B-CHB | 2.72  | 1.48        | 1.41     |
| 31  | a     | 312 | CLA  | C4B-CHC | 2.72  | 1.48        | 1.41     |
| 31  | 5     | 321 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 31  | 3     | 310 | CLA  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 31  | 3     | 312 | CLA  | C4C-C3C | 2.71  | 1.49        | 1.45     |
| 31  | 3     | 318 | CLA  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 31  | 5     | 308 | CLA  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 31  | B     | 813 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 31  | 6     | 312 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 31  | O     | 202 | CLA  | C1D-ND  | -2.71 | 1.34        | 1.37     |
| 31  | L     | 305 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 31  | a     | 322 | CLA  | C4C-C3C | 2.71  | 1.49        | 1.45     |
| 31  | 9     | 318 | CLA  | C4C-C3C | 2.71  | 1.49        | 1.45     |
| 31  | 9     | 316 | CLA  | C1B-CHB | 2.71  | 1.48        | 1.41     |
| 31  | A     | 814 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 31  | H     | 902 | CLA  | C4B-CHC | 2.71  | 1.48        | 1.41     |
| 31  | 4     | 321 | CLA  | C1B-CHB | 2.71  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 317 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 31  | 2     | 311 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 31  | 2     | 312 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 32  | 9     | 322 | CHL  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 31  | 6     | 310 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 31  | A     | 830 | CLA  | C1C-NC  | -2.70 | 1.33        | 1.37     |
| 31  | B     | 833 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 31  | b     | 310 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 31  | A     | 816 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 31  | 3     | 313 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 31  | H     | 901 | CLA  | MG-ND   | -2.70 | 2.00        | 2.05     |
| 32  | 7     | 324 | CHL  | C1D-ND  | -2.70 | 1.34        | 1.37     |
| 31  | B     | 831 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 31  | 7     | 312 | CLA  | C1B-CHB | 2.70  | 1.48        | 1.41     |
| 31  | 2     | 307 | CLA  | C4B-CHC | 2.70  | 1.48        | 1.41     |
| 26  | B     | 806 | BCR  | C1-C6   | -2.70 | 1.50        | 1.53     |
| 31  | B     | 849 | CLA  | OBD-CAD | 2.69  | 1.27        | 1.22     |
| 31  | 7     | 321 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 31  | 9     | 315 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 31  | A     | 857 | CLA  | C1C-NC  | -2.69 | 1.33        | 1.37     |
| 31  | 3     | 312 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 31  | 7     | 309 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 31  | 2     | 309 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 31  | A     | 833 | CLA  | C4C-C3C | 2.69  | 1.49        | 1.45     |
| 31  | 4     | 314 | CLA  | C4C-C3C | 2.69  | 1.49        | 1.45     |
| 36  | F     | 304 | LUT  | C18-C5  | 2.69  | 1.55        | 1.50     |
| 31  | K     | 205 | CLA  | C1B-CHB | 2.69  | 1.48        | 1.41     |
| 31  | 7     | 316 | CLA  | C4B-CHC | 2.69  | 1.48        | 1.41     |
| 36  | 3     | 304 | LUT  | C23-C24 | 2.69  | 1.54        | 1.50     |
| 31  | A     | 835 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 31  | A     | 843 | CLA  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 31  | A     | 845 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 9     | 321 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | b     | 305 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 2     | 313 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 6     | 307 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | a     | 313 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 7     | 313 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | B     | 828 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 8     | 310 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 6     | 322 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 7     | 309 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 3     | 309 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 31  | L     | 306 | CLA  | C1B-CHB | 2.68  | 1.48        | 1.41     |
| 31  | 2     | 305 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 31  | 4     | 321 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 31  | 8     | 307 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 36  | a     | 305 | LUT  | C18-C5  | 2.68  | 1.55        | 1.50     |
| 31  | 5     | 318 | CLA  | C4C-C3C | 2.68  | 1.49        | 1.45     |
| 31  | A     | 853 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 31  | a     | 313 | CLA  | C1D-ND  | -2.68 | 1.34        | 1.37     |
| 31  | 7     | 311 | CLA  | C4B-CHC | 2.68  | 1.48        | 1.41     |
| 31  | A     | 814 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 31  | B     | 816 | CLA  | C1C-NC  | -2.68 | 1.33        | 1.37     |
| 31  | 6     | 322 | CLA  | C1D-ND  | -2.68 | 1.34        | 1.37     |
| 31  | B     | 841 | CLA  | C4D-CHA | 2.67  | 1.47        | 1.38     |
| 31  | 4     | 314 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | 6     | 322 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | K     | 205 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 31  | b     | 312 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | 9     | 321 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | a     | 315 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | 6     | 311 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | B     | 840 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | 3     | 314 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | F     | 301 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | B     | 848 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | 4     | 309 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | b     | 307 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 31  | a     | 321 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | a     | 314 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | 8     | 313 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | a     | 311 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 31  | K     | 206 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | B     | 820 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | 3     | 317 | CLA  | C1B-CHB | 2.67  | 1.48        | 1.41     |
| 31  | 4     | 312 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 31  | 9     | 319 | CLA  | C4C-C3C | 2.67  | 1.49        | 1.45     |
| 31  | 6     | 313 | CLA  | MG-ND   | -2.67 | 2.00        | 2.05     |
| 31  | A     | 823 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | 5     | 309 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 27  | 5     | 301 | LMT  | O2'-C2' | -2.67 | 1.36        | 1.43     |
| 31  | 3     | 308 | CLA  | C4B-CHC | 2.67  | 1.48        | 1.41     |
| 31  | 3     | 319 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 824 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 31  | 8     | 308 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 31  | B     | 825 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 31  | A     | 816 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 31  | 4     | 308 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 31  | B     | 835 | CLA  | MG-ND   | 2.66  | 2.11        | 2.05     |
| 31  | O     | 202 | CLA  | C4C-C3C | 2.66  | 1.49        | 1.44     |
| 31  | B     | 820 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 31  | 2     | 313 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 31  | A     | 815 | CLA  | C4D-CHA | 2.66  | 1.47        | 1.38     |
| 31  | A     | 837 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 31  | 4     | 306 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 31  | 6     | 312 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 26  | O     | 201 | BCR  | C1-C6   | -2.66 | 1.50        | 1.53     |
| 31  | 8     | 312 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 31  | b     | 302 | CLA  | C1D-ND  | -2.66 | 1.34        | 1.37     |
| 31  | H     | 901 | CLA  | C4C-C3C | 2.66  | 1.49        | 1.45     |
| 31  | 3     | 311 | CLA  | C1B-CHB | 2.66  | 1.48        | 1.41     |
| 31  | 6     | 313 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 26  | B     | 802 | BCR  | C1-C6   | -2.66 | 1.50        | 1.53     |
| 31  | 5     | 313 | CLA  | C1C-NC  | -2.66 | 1.33        | 1.37     |
| 31  | B     | 840 | CLA  | C4B-CHC | 2.66  | 1.48        | 1.41     |
| 31  | B     | 825 | CLA  | MG-ND   | 2.65  | 2.11        | 2.05     |
| 31  | 2     | 311 | CLA  | C4C-C3C | 2.65  | 1.49        | 1.45     |
| 31  | 5     | 315 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 31  | B     | 830 | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 31  | a     | 310 | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 31  | A     | 833 | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 31  | B     | 832 | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 31  | a     | 322 | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 31  | b     | 305 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 31  | 8     | 314 | CLA  | MG-NC   | 2.65  | 2.12        | 2.06     |
| 31  | B     | 837 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 31  | 4     | 318 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 31  | 4     | 315 | CLA  | C1B-CHB | 2.65  | 1.48        | 1.41     |
| 31  | 7     | 315 | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 31  | B     | 817 | CLA  | C1C-NC  | -2.65 | 1.33        | 1.37     |
| 26  | F     | 302 | BCR  | C1-C6   | -2.65 | 1.50        | 1.53     |
| 31  | a     | 315 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 31  | A     | 855 | CLA  | C4B-CHC | 2.65  | 1.48        | 1.41     |
| 31  | a     | 310 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | 8     | 315 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 27  | 5     | 301 | LMT  | O3'-C3' | -2.64 | 1.36        | 1.43     |
| 31  | A     | 835 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | b     | 313 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | 8     | 311 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | A     | 822 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | 4     | 305 | CLA  | MG-NC   | 2.64  | 2.12        | 2.06     |
| 31  | 7     | 314 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.44     |
| 31  | a     | 312 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | 5     | 313 | CLA  | C1D-ND  | -2.64 | 1.34        | 1.37     |
| 31  | 3     | 309 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | B     | 846 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | A     | 847 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | 7     | 316 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | B     | 846 | CLA  | C1B-CHB | 2.64  | 1.48        | 1.41     |
| 31  | K     | 204 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 31  | 2     | 314 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 31  | B     | 843 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 31  | A     | 836 | CLA  | C4B-CHC | 2.64  | 1.48        | 1.41     |
| 31  | B     | 838 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | 3     | 317 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 31  | B     | 830 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | F     | 305 | CLA  | C4C-C3C | 2.64  | 1.49        | 1.45     |
| 36  | 5     | 304 | LUT  | C23-C24 | 2.64  | 1.53        | 1.50     |
| 31  | B     | 836 | CLA  | C1C-NC  | -2.64 | 1.33        | 1.37     |
| 31  | A     | 843 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | 9     | 314 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 26  | K     | 203 | BCR  | C1-C6   | -2.63 | 1.50        | 1.53     |
| 31  | b     | 303 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 31  | A     | 850 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | 3     | 316 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 31  | A     | 830 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | b     | 312 | CLA  | C1D-ND  | -2.63 | 1.34        | 1.37     |
| 31  | B     | 823 | CLA  | C1C-NC  | -2.63 | 1.33        | 1.37     |
| 31  | B     | 838 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 31  | 9     | 315 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | A     | 823 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | 5     | 321 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 31  | 5     | 318 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | 3     | 319 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | 3     | 320 | CLA  | C4D-ND  | 2.63  | 1.41        | 1.37     |
| 31  | 9     | 321 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 31  | O     | 203 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | F     | 303 | QTB  | C09-C02 | -2.63 | 1.40        | 1.45     |
| 31  | 2     | 309 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 32  | 5     | 316 | CHL  | C1D-ND  | -2.63 | 1.34        | 1.37     |
| 31  | A     | 851 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 31  | 7     | 314 | CLA  | C4B-CHC | 2.63  | 1.48        | 1.41     |
| 31  | b     | 307 | CLA  | C4D-ND  | 2.63  | 1.41        | 1.37     |
| 31  | b     | 306 | CLA  | C4C-C3C | 2.63  | 1.49        | 1.45     |
| 31  | B     | 821 | CLA  | C1B-CHB | 2.63  | 1.48        | 1.41     |
| 31  | 9     | 319 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 26  | M     | 101 | BCR  | C30-C25 | -2.62 | 1.50        | 1.53     |
| 31  | 7     | 312 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | 4     | 308 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | 5     | 313 | CLA  | MG-ND   | 2.62  | 2.11        | 2.05     |
| 38  | a     | 304 | AXT  | C4-C5   | -2.62 | 1.47        | 1.51     |
| 31  | 2     | 314 | CLA  | MG-NC   | 2.62  | 2.12        | 2.06     |
| 26  | B     | 805 | BCR  | C1-C6   | -2.62 | 1.50        | 1.53     |
| 31  | 6     | 314 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | 5     | 311 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | B     | 838 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | 3     | 314 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | b     | 302 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | A     | 828 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | A     | 815 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 31  | B     | 848 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | a     | 311 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | A     | 845 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 26  | B     | 803 | BCR  | C30-C25 | -2.62 | 1.50        | 1.53     |
| 31  | B     | 824 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | B     | 835 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | 5     | 307 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | 5     | 307 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 36  | 2     | 301 | LUT  | C23-C24 | 2.62  | 1.53        | 1.50     |
| 31  | B     | 815 | CLA  | OBD-CAD | 2.62  | 1.27        | 1.22     |
| 31  | H     | 901 | CLA  | C4B-CHC | 2.62  | 1.48        | 1.41     |
| 31  | B     | 815 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | J     | 105 | CLA  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 31  | A     | 853 | CLA  | C1B-CHB | 2.62  | 1.48        | 1.41     |
| 31  | A     | 832 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 31  | A     | 856 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 31  | B     | 831 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | B     | 842 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | 4     | 311 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 317 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 31  | 5     | 323 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | A     | 830 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 27  | A     | 807 | LMT  | O2'-C2' | -2.61 | 1.36        | 1.43     |
| 31  | L     | 305 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 31  | A     | 832 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 31  | a     | 319 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | H     | 903 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | 2     | 307 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 31  | 3     | 316 | CLA  | C1C-NC  | -2.61 | 1.33        | 1.37     |
| 31  | A     | 817 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | A     | 852 | CLA  | C1B-CHB | 2.61  | 1.48        | 1.41     |
| 31  | 2     | 306 | CLA  | C4C-C3C | 2.61  | 1.49        | 1.45     |
| 36  | a     | 305 | LUT  | C38-C25 | 2.61  | 1.55        | 1.50     |
| 31  | 2     | 315 | CLA  | C4B-CHC | 2.61  | 1.48        | 1.41     |
| 31  | L     | 307 | CLA  | C1D-ND  | -2.60 | 1.34        | 1.37     |
| 31  | 9     | 311 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 31  | B     | 837 | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 31  | A     | 821 | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 31  | 9     | 316 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 31  | B     | 821 | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 31  | a     | 322 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 31  | B     | 846 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 31  | 8     | 315 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 36  | 5     | 303 | LUT  | C18-C5  | 2.60  | 1.55        | 1.50     |
| 36  | 8     | 302 | LUT  | C18-C5  | 2.60  | 1.55        | 1.50     |
| 31  | 4     | 319 | CLA  | MG-ND   | 2.60  | 2.10        | 2.05     |
| 31  | 9     | 312 | CLA  | C4B-CHC | 2.60  | 1.48        | 1.41     |
| 31  | A     | 827 | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 31  | a     | 319 | CLA  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 32  | b     | 309 | CHL  | MG-ND   | -2.60 | 2.00        | 2.05     |
| 31  | B     | 827 | CLA  | C1B-CHB | 2.60  | 1.48        | 1.41     |
| 31  | F     | 301 | CLA  | C4C-C3C | 2.60  | 1.49        | 1.45     |
| 26  | 5     | 302 | BCR  | C1-C6   | -2.59 | 1.50        | 1.53     |
| 31  | A     | 844 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 31  | 8     | 308 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 31  | 5     | 321 | CLA  | C4D-ND  | 2.59  | 1.41        | 1.37     |
| 31  | F     | 305 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 31  | 8     | 318 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 31  | A     | 842 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 31  | L     | 306 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 31  | B     | 821 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 319 | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 31  | A     | 822 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 31  | 2     | 314 | CLA  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 31  | G     | 204 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 31  | a     | 310 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 31  | B     | 850 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 40  | 7     | 306 | XAT  | C8-C9   | -2.59 | 1.40        | 1.45     |
| 31  | B     | 819 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 31  | B     | 829 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 31  | 8     | 320 | CLA  | C1C-NC  | -2.59 | 1.33        | 1.37     |
| 31  | 3     | 316 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 31  | 6     | 314 | CLA  | MG-ND   | 2.59  | 2.10        | 2.05     |
| 31  | a     | 316 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 31  | B     | 845 | CLA  | C1B-CHB | 2.59  | 1.48        | 1.41     |
| 32  | 4     | 310 | CHL  | C4C-C3C | 2.59  | 1.49        | 1.45     |
| 31  | B     | 826 | CLA  | C4B-CHC | 2.59  | 1.48        | 1.41     |
| 31  | L     | 307 | CLA  | C4D-ND  | 2.59  | 1.41        | 1.37     |
| 31  | B     | 839 | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 31  | B     | 843 | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 36  | 8     | 302 | LUT  | C26-C27 | 2.58  | 1.54        | 1.50     |
| 31  | 7     | 321 | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |
| 31  | G     | 204 | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |
| 31  | A     | 849 | CLA  | C4C-C3C | 2.58  | 1.49        | 1.45     |
| 31  | A     | 852 | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |
| 31  | 7     | 314 | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 31  | A     | 819 | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |
| 31  | 4     | 307 | CLA  | C4B-CHC | 2.58  | 1.48        | 1.41     |
| 31  | A     | 854 | CLA  | C1B-CHB | 2.58  | 1.48        | 1.41     |
| 31  | A     | 835 | CLA  | C1C-NC  | -2.58 | 1.34        | 1.37     |
| 31  | 5     | 308 | CLA  | C4D-ND  | 2.58  | 1.41        | 1.37     |
| 31  | A     | 849 | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 31  | A     | 819 | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 31  | 5     | 312 | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 31  | b     | 302 | CLA  | C4D-ND  | 2.57  | 1.41        | 1.37     |
| 31  | 7     | 315 | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 31  | a     | 319 | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 36  | a     | 305 | LUT  | C1-C6   | 2.57  | 1.57        | 1.53     |
| 31  | O     | 204 | CLA  | C4D-ND  | 2.57  | 1.41        | 1.37     |
| 31  | B     | 844 | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 36  | 7     | 305 | LUT  | C23-C24 | 2.57  | 1.53        | 1.50     |
| 31  | B     | 844 | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 36  | 9     | 303 | LUT  | C23-C24 | 2.57  | 1.53        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 841 | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 31  | A     | 829 | CLA  | MG-ND   | 2.57  | 2.10        | 2.05     |
| 31  | 7     | 322 | CLA  | MG-NA   | 2.57  | 2.12        | 2.06     |
| 31  | F     | 301 | CLA  | C1C-NC  | -2.57 | 1.34        | 1.37     |
| 31  | 7     | 313 | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 26  | B     | 804 | BCR  | C30-C25 | -2.57 | 1.50        | 1.53     |
| 31  | 5     | 310 | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 27  | 9     | 306 | LMT  | O2'-C2' | -2.57 | 1.36        | 1.43     |
| 31  | A     | 837 | CLA  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 32  | A     | 840 | CHL  | OBD-CAD | 2.57  | 1.26        | 1.22     |
| 31  | G     | 206 | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 31  | 9     | 311 | CLA  | C1B-CHB | 2.57  | 1.48        | 1.41     |
| 31  | F     | 306 | CLA  | C4C-C3C | 2.57  | 1.49        | 1.45     |
| 31  | b     | 312 | CLA  | C4D-ND  | 2.57  | 1.41        | 1.37     |
| 36  | L     | 304 | LUT  | C18-C5  | 2.56  | 1.55        | 1.50     |
| 26  | B     | 804 | BCR  | C1-C6   | -2.56 | 1.50        | 1.53     |
| 31  | 5     | 313 | CLA  | C1D-C2D | 2.56  | 1.50        | 1.45     |
| 26  | B     | 806 | BCR  | C30-C25 | -2.56 | 1.50        | 1.53     |
| 31  | 7     | 313 | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 31  | A     | 841 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 31  | B     | 818 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 31  | a     | 309 | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 31  | B     | 828 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 31  | H     | 902 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 31  | A     | 845 | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 31  | B     | 813 | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 31  | 7     | 322 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 36  | 3     | 304 | LUT  | C26-C27 | 2.56  | 1.54        | 1.50     |
| 31  | 2     | 307 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 40  | 7     | 306 | XAT  | C32-C33 | -2.56 | 1.40        | 1.45     |
| 31  | A     | 816 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 31  | A     | 838 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 31  | b     | 311 | CLA  | C4C-C3C | 2.56  | 1.49        | 1.45     |
| 31  | 2     | 307 | CLA  | C1C-NC  | -2.56 | 1.34        | 1.37     |
| 31  | a     | 316 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 26  | A     | 806 | BCR  | C30-C25 | -2.56 | 1.50        | 1.53     |
| 26  | 3     | 303 | BCR  | C1-C6   | -2.56 | 1.50        | 1.53     |
| 31  | B     | 850 | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 31  | J     | 105 | CLA  | C4B-CHC | 2.56  | 1.48        | 1.41     |
| 36  | 4     | 302 | LUT  | C18-C5  | 2.56  | 1.55        | 1.50     |
| 31  | G     | 204 | CLA  | C1B-CHB | 2.56  | 1.48        | 1.41     |
| 26  | 3     | 301 | BCR  | C1-C6   | -2.55 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 814 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 31  | B     | 815 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 31  | A     | 824 | CLA  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 31  | 3     | 307 | CLA  | MG-NC   | 2.55  | 2.12        | 2.06     |
| 31  | A     | 824 | CLA  | C4C-C3C | 2.55  | 1.49        | 1.45     |
| 31  | B     | 825 | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 31  | 7     | 321 | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 31  | B     | 849 | CLA  | C4C-C3C | 2.55  | 1.49        | 1.45     |
| 31  | B     | 849 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 31  | 3     | 311 | CLA  | C1C-NC  | -2.55 | 1.34        | 1.37     |
| 31  | 3     | 318 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 40  | 7     | 306 | XAT  | C28-C29 | -2.55 | 1.40        | 1.45     |
| 31  | B     | 817 | CLA  | C1B-CHB | 2.55  | 1.48        | 1.41     |
| 31  | B     | 841 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 31  | B     | 833 | CLA  | C4B-CHC | 2.55  | 1.48        | 1.41     |
| 32  | a     | 320 | CHL  | MG-ND   | 2.54  | 2.10        | 2.05     |
| 31  | a     | 313 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 31  | 5     | 318 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 31  | 5     | 311 | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 31  | A     | 827 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 40  | 7     | 306 | XAT  | C12-C13 | -2.54 | 1.40        | 1.45     |
| 31  | F     | 305 | CLA  | C1C-NC  | -2.54 | 1.34        | 1.37     |
| 31  | A     | 849 | CLA  | C1B-CHB | 2.54  | 1.48        | 1.41     |
| 31  | K     | 205 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 31  | 3     | 312 | CLA  | C4B-CHC | 2.54  | 1.48        | 1.41     |
| 31  | 6     | 311 | CLA  | MG-NC   | -2.53 | 2.00        | 2.06     |
| 31  | B     | 812 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 31  | B     | 842 | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 31  | B     | 822 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 32  | 6     | 309 | CHL  | MG-ND   | -2.53 | 2.00        | 2.05     |
| 31  | 4     | 305 | CLA  | C4D-ND  | 2.53  | 1.41        | 1.37     |
| 31  | 8     | 320 | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 31  | 6     | 314 | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 31  | B     | 823 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 31  | A     | 836 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 31  | 9     | 314 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 36  | 5     | 304 | LUT  | C18-C5  | 2.53  | 1.55        | 1.50     |
| 31  | 8     | 314 | CLA  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 31  | 2     | 310 | CLA  | C4D-ND  | 2.53  | 1.41        | 1.37     |
| 31  | A     | 854 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 31  | B     | 844 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 31  | B     | 818 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 833 | CLA  | C1C-NC  | -2.53 | 1.34        | 1.37     |
| 31  | 8     | 315 | CLA  | C1B-CHB | 2.53  | 1.48        | 1.41     |
| 31  | G     | 206 | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 31  | a     | 314 | CLA  | C4C-C3C | 2.53  | 1.49        | 1.45     |
| 36  | b     | 301 | LUT  | C38-C25 | 2.53  | 1.55        | 1.50     |
| 35  | 7     | 303 | QTB  | C09-C02 | -2.52 | 1.40        | 1.45     |
| 31  | A     | 841 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 31  | 6     | 308 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 31  | A     | 852 | CLA  | C1C-NC  | -2.52 | 1.34        | 1.37     |
| 31  | a     | 321 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 31  | 4     | 315 | CLA  | C4C-C3C | 2.52  | 1.49        | 1.45     |
| 31  | 9     | 316 | CLA  | C1C-NC  | -2.52 | 1.34        | 1.37     |
| 26  | B     | 802 | BCR  | C30-C25 | -2.52 | 1.50        | 1.53     |
| 31  | b     | 310 | CLA  | C4C-C3C | 2.52  | 1.49        | 1.45     |
| 31  | 8     | 320 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 31  | A     | 819 | CLA  | C1B-CHB | 2.52  | 1.48        | 1.41     |
| 31  | 5     | 311 | CLA  | C4B-CHC | 2.52  | 1.48        | 1.41     |
| 31  | A     | 828 | CLA  | C4B-CHC | 2.51  | 1.48        | 1.41     |
| 31  | A     | 823 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 31  | b     | 302 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 36  | 7     | 305 | LUT  | C1-C6   | 2.51  | 1.57        | 1.53     |
| 31  | 5     | 312 | CLA  | C4D-ND  | 2.51  | 1.41        | 1.37     |
| 31  | B     | 826 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 31  | 2     | 304 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 31  | K     | 206 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 26  | L     | 303 | BCR  | C1-C6   | -2.51 | 1.50        | 1.53     |
| 31  | 7     | 310 | CLA  | C4D-ND  | 2.51  | 1.41        | 1.37     |
| 31  | 3     | 318 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 31  | A     | 846 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 31  | 4     | 308 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 31  | A     | 830 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 31  | B     | 841 | CLA  | C1C-NC  | -2.51 | 1.34        | 1.37     |
| 32  | 5     | 322 | CHL  | C3D-C2D | 2.51  | 1.46        | 1.39     |
| 31  | B     | 830 | CLA  | C4B-CHC | 2.51  | 1.48        | 1.41     |
| 31  | 9     | 313 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 31  | B     | 835 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 31  | 6     | 310 | CLA  | C4C-C3C | 2.51  | 1.49        | 1.45     |
| 31  | 5     | 315 | CLA  | C4C-C3C | 2.50  | 1.49        | 1.45     |
| 31  | F     | 306 | CLA  | C4B-CHC | 2.50  | 1.48        | 1.41     |
| 31  | 9     | 315 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 31  | A     | 823 | CLA  | C4C-C3C | 2.50  | 1.49        | 1.45     |
| 31  | 4     | 316 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 6     | 307 | CLA  | C4C-C3C | 2.50  | 1.49        | 1.45     |
| 31  | 4     | 305 | CLA  | CHD-C4C | 2.50  | 1.44        | 1.39     |
| 31  | 3     | 310 | CLA  | C4B-CHC | 2.50  | 1.47        | 1.41     |
| 32  | 4     | 310 | CHL  | MG-NC   | -2.50 | 2.00        | 2.06     |
| 31  | B     | 844 | CLA  | C4C-C3C | 2.50  | 1.49        | 1.45     |
| 26  | 2     | 302 | BCR  | C30-C25 | -2.50 | 1.50        | 1.53     |
| 31  | B     | 842 | CLA  | C1C-NC  | -2.50 | 1.34        | 1.37     |
| 27  | 5     | 301 | LMT  | O3B-C3B | -2.50 | 1.37        | 1.43     |
| 37  | G     | 202 | LMG  | C4-C5   | 2.50  | 1.58        | 1.53     |
| 31  | A     | 844 | CLA  | C1B-CHB | 2.50  | 1.47        | 1.41     |
| 36  | 9     | 303 | LUT  | C38-C25 | 2.50  | 1.55        | 1.50     |
| 31  | A     | 825 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 31  | A     | 834 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 31  | 4     | 308 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 31  | 2     | 310 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 31  | A     | 821 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 31  | 8     | 311 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 31  | G     | 206 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 26  | A     | 806 | BCR  | C1-C6   | -2.49 | 1.50        | 1.53     |
| 31  | 3     | 309 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 31  | 6     | 313 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 26  | 8     | 301 | BCR  | C1-C6   | -2.49 | 1.50        | 1.53     |
| 31  | B     | 849 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 31  | B     | 849 | CLA  | C1B-CHB | 2.49  | 1.47        | 1.41     |
| 31  | 6     | 311 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 31  | K     | 206 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 31  | 2     | 308 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 31  | 4     | 320 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 31  | 5     | 310 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 31  | 5     | 320 | CLA  | C4C-C3C | 2.49  | 1.49        | 1.45     |
| 31  | A     | 833 | CLA  | C4B-CHC | 2.49  | 1.47        | 1.41     |
| 36  | 7     | 305 | LUT  | C38-C25 | 2.49  | 1.55        | 1.50     |
| 31  | 8     | 313 | CLA  | C1C-NC  | -2.49 | 1.34        | 1.37     |
| 31  | 5     | 321 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 31  | A     | 842 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 31  | A     | 853 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 32  | 9     | 322 | CHL  | C3D-C2D | 2.48  | 1.45        | 1.39     |
| 31  | 8     | 318 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 27  | A     | 807 | LMT  | O2B-C2B | -2.48 | 1.37        | 1.43     |
| 31  | 5     | 315 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 31  | 6     | 307 | CLA  | C4D-ND  | 2.48  | 1.41        | 1.37     |
| 31  | 9     | 316 | CLA  | C4C-C3C | 2.48  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 9     | 316 | CLA  | MG-ND   | 2.48  | 2.10        | 2.05     |
| 31  | 5     | 307 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 26  | 7     | 304 | BCR  | C30-C25 | -2.48 | 1.50        | 1.53     |
| 31  | A     | 815 | CLA  | C1B-CHB | 2.48  | 1.47        | 1.41     |
| 27  | 9     | 306 | LMT  | O3B-C3B | -2.48 | 1.37        | 1.43     |
| 26  | 7     | 304 | BCR  | C1-C6   | -2.48 | 1.50        | 1.53     |
| 31  | L     | 305 | CLA  | C1C-NC  | -2.48 | 1.34        | 1.37     |
| 31  | A     | 846 | CLA  | C4B-CHC | 2.48  | 1.47        | 1.41     |
| 26  | A     | 805 | BCR  | C30-C25 | -2.48 | 1.50        | 1.53     |
| 31  | A     | 854 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 31  | 2     | 310 | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 31  | A     | 834 | CLA  | C4C-C3C | 2.47  | 1.49        | 1.45     |
| 31  | B     | 827 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 26  | A     | 803 | BCR  | C1-C6   | -2.47 | 1.50        | 1.53     |
| 31  | A     | 828 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 31  | 4     | 312 | CLA  | C4D-ND  | 2.47  | 1.41        | 1.37     |
| 32  | a     | 318 | CHL  | C3D-C2D | 2.47  | 1.45        | 1.39     |
| 31  | B     | 821 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 31  | A     | 822 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 31  | F     | 306 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 31  | A     | 843 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 31  | B     | 843 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 31  | A     | 842 | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 31  | A     | 848 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 31  | B     | 836 | CLA  | C1B-CHB | 2.47  | 1.47        | 1.41     |
| 31  | 6     | 322 | CLA  | C4D-ND  | 2.47  | 1.41        | 1.37     |
| 31  | O     | 203 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 31  | A     | 826 | CLA  | C4B-CHC | 2.47  | 1.47        | 1.41     |
| 31  | A     | 849 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 31  | 3     | 312 | CLA  | C1C-NC  | -2.47 | 1.34        | 1.37     |
| 32  | 6     | 309 | CHL  | C3D-C2D | 2.47  | 1.45        | 1.39     |
| 31  | A     | 847 | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 36  | 6     | 304 | LUT  | C23-C24 | 2.46  | 1.53        | 1.50     |
| 31  | 9     | 317 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 31  | A     | 820 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 31  | A     | 848 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 31  | B     | 847 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 31  | 2     | 312 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 31  | 2     | 313 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 31  | A     | 826 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 31  | B     | 834 | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 31  | b     | 308 | CLA  | C4D-ND  | 2.46  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 4     | 319 | CLA  | C4D-ND  | 2.46  | 1.41        | 1.37     |
| 31  | A     | 856 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 31  | 4     | 309 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 31  | B     | 834 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 31  | 7     | 312 | CLA  | C4C-C3C | 2.46  | 1.49        | 1.45     |
| 31  | B     | 814 | CLA  | C1B-CHB | 2.46  | 1.47        | 1.41     |
| 31  | A     | 850 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 36  | 4     | 302 | LUT  | C38-C25 | 2.46  | 1.55        | 1.50     |
| 31  | 8     | 312 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 31  | 9     | 311 | CLA  | C1C-NC  | -2.46 | 1.34        | 1.37     |
| 36  | 6     | 304 | LUT  | C38-C25 | 2.46  | 1.55        | 1.50     |
| 31  | B     | 845 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 31  | B     | 839 | CLA  | C4B-CHC | 2.46  | 1.47        | 1.41     |
| 31  | B     | 847 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | B     | 811 | CLA  | C1B-CHB | 2.45  | 1.47        | 1.41     |
| 31  | 3     | 307 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | B     | 850 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 31  | B     | 819 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | 2     | 305 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 31  | 3     | 311 | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 31  | B     | 814 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 31  | 4     | 315 | CLA  | C4D-ND  | 2.45  | 1.41        | 1.37     |
| 31  | 6     | 311 | CLA  | C4D-ND  | 2.45  | 1.41        | 1.37     |
| 31  | 9     | 318 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | 4     | 311 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | A     | 818 | CLA  | C4B-CHC | 2.45  | 1.47        | 1.41     |
| 31  | A     | 832 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 31  | B     | 836 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 31  | 7     | 322 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | L     | 307 | CLA  | C1C-NC  | -2.45 | 1.34        | 1.37     |
| 31  | b     | 303 | CLA  | C1D-ND  | -2.45 | 1.34        | 1.37     |
| 31  | 4     | 306 | CLA  | C4C-C3C | 2.45  | 1.49        | 1.45     |
| 31  | 8     | 311 | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 31  | 3     | 318 | CLA  | C4D-ND  | 2.44  | 1.41        | 1.37     |
| 31  | 9     | 321 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 31  | B     | 829 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 36  | 3     | 305 | LUT  | C38-C25 | 2.44  | 1.55        | 1.50     |
| 32  | A     | 831 | CHL  | MG-NA   | 2.44  | 2.12        | 2.06     |
| 31  | B     | 816 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 26  | O     | 201 | BCR  | C30-C25 | -2.44 | 1.50        | 1.53     |
| 36  | 5     | 304 | LUT  | C38-C25 | 2.44  | 1.55        | 1.50     |
| 31  | 3     | 320 | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 321 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 31  | 4     | 315 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 31  | A     | 833 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 31  | 8     | 307 | CLA  | C1C-NC  | -2.44 | 1.34        | 1.37     |
| 31  | A     | 834 | CLA  | C1B-CHB | 2.44  | 1.47        | 1.41     |
| 31  | 6     | 310 | CLA  | C4D-ND  | 2.44  | 1.41        | 1.37     |
| 31  | A     | 817 | CLA  | C1B-CHB | 2.44  | 1.47        | 1.41     |
| 31  | 8     | 308 | CLA  | MG-NC   | 2.44  | 2.12        | 2.06     |
| 31  | 4     | 309 | CLA  | C4B-CHC | 2.44  | 1.47        | 1.41     |
| 31  | B     | 831 | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 31  | a     | 313 | CLA  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 31  | 4     | 306 | CLA  | MG-NC   | 2.43  | 2.12        | 2.06     |
| 31  | B     | 812 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 32  | 5     | 319 | CHL  | C3D-C2D | 2.43  | 1.45        | 1.39     |
| 31  | 4     | 318 | CLA  | C4D-ND  | 2.43  | 1.41        | 1.37     |
| 31  | B     | 824 | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 31  | 9     | 312 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 36  | 9     | 305 | LUT  | C18-C5  | 2.43  | 1.54        | 1.50     |
| 31  | 3     | 308 | CLA  | C4D-ND  | 2.43  | 1.41        | 1.37     |
| 31  | A     | 854 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 31  | B     | 828 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 36  | 6     | 304 | LUT  | C18-C5  | 2.43  | 1.54        | 1.50     |
| 31  | 5     | 323 | CLA  | C4D-ND  | 2.43  | 1.41        | 1.37     |
| 31  | 8     | 318 | CLA  | C4B-CHC | 2.43  | 1.47        | 1.41     |
| 31  | B     | 823 | CLA  | C4C-C3C | 2.43  | 1.49        | 1.45     |
| 31  | A     | 850 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 27  | 9     | 306 | LMT  | O2B-C2B | -2.43 | 1.37        | 1.43     |
| 31  | 3     | 317 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 31  | A     | 834 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 31  | A     | 856 | CLA  | C1C-NC  | -2.43 | 1.34        | 1.37     |
| 31  | F     | 305 | CLA  | C4B-CHC | 2.42  | 1.47        | 1.41     |
| 31  | A     | 824 | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 31  | 7     | 315 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | 5     | 310 | CLA  | C4D-ND  | 2.42  | 1.41        | 1.37     |
| 36  | b     | 301 | LUT  | C18-C5  | 2.42  | 1.54        | 1.50     |
| 31  | A     | 836 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | a     | 316 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | 4     | 321 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | A     | 821 | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 31  | 3     | 309 | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 31  | 4     | 318 | CLA  | C1D-ND  | -2.42 | 1.34        | 1.37     |
| 31  | G     | 205 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 3     | 304 | LUT  | C18-C5  | 2.42  | 1.54        | 1.50     |
| 31  | 2     | 305 | CLA  | C4D-ND  | 2.42  | 1.41        | 1.37     |
| 32  | 4     | 317 | CHL  | C3D-C2D | 2.42  | 1.45        | 1.39     |
| 31  | A     | 841 | CLA  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 31  | 7     | 322 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | F     | 301 | CLA  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 27  | A     | 808 | LMT  | O2B-C2B | -2.42 | 1.37        | 1.43     |
| 31  | 8     | 321 | CLA  | C1C-NC  | -2.42 | 1.34        | 1.37     |
| 31  | B     | 816 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | a     | 321 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | 5     | 308 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 31  | A     | 830 | CLA  | C4D-ND  | 2.42  | 1.41        | 1.37     |
| 31  | 6     | 315 | CLA  | C4C-C3C | 2.42  | 1.49        | 1.45     |
| 32  | a     | 317 | CHL  | C3D-C2D | 2.42  | 1.45        | 1.39     |
| 31  | A     | 852 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | 6     | 306 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | 4     | 307 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | 8     | 309 | CLA  | C4D-ND  | 2.41  | 1.41        | 1.37     |
| 31  | 3     | 308 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | 7     | 316 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | 8     | 311 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | 6     | 310 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | 5     | 308 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | 8     | 318 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | A     | 818 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | B     | 830 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | a     | 310 | CLA  | C4D-ND  | 2.41  | 1.41        | 1.37     |
| 31  | K     | 206 | CLA  | C4D-ND  | 2.41  | 1.41        | 1.37     |
| 31  | 6     | 313 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | A     | 857 | CLA  | C4B-CHC | 2.41  | 1.47        | 1.41     |
| 31  | B     | 811 | CLA  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | a     | 309 | CLA  | C4D-ND  | 2.41  | 1.41        | 1.37     |
| 32  | 9     | 322 | CHL  | C4C-C3C | 2.41  | 1.49        | 1.45     |
| 31  | 2     | 314 | CLA  | C1C-NC  | -2.41 | 1.34        | 1.37     |
| 31  | B     | 812 | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 31  | O     | 202 | CLA  | C4D-ND  | 2.40  | 1.41        | 1.37     |
| 31  | 5     | 311 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 26  | F     | 302 | BCR  | C30-C25 | -2.40 | 1.50        | 1.53     |
| 31  | B     | 819 | CLA  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 31  | b     | 303 | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 31  | 7     | 309 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 31  | B     | 846 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | a     | 315 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 31  | 3     | 311 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 31  | H     | 903 | CLA  | C4D-ND  | 2.40  | 1.40        | 1.37     |
| 31  | 5     | 318 | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 32  | 6     | 321 | CHL  | C3D-C2D | 2.40  | 1.45        | 1.39     |
| 31  | A     | 846 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 31  | A     | 848 | CLA  | C1B-CHB | 2.40  | 1.47        | 1.41     |
| 31  | 3     | 314 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 31  | B     | 840 | CLA  | C1C-NC  | -2.40 | 1.34        | 1.37     |
| 31  | a     | 310 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 31  | 5     | 313 | CLA  | C4C-C3C | 2.40  | 1.49        | 1.45     |
| 32  | 7     | 319 | CHL  | C3D-C2D | 2.40  | 1.45        | 1.39     |
| 31  | a     | 314 | CLA  | C1C-NC  | -2.39 | 1.34        | 1.37     |
| 32  | K     | 201 | CHL  | C1D-ND  | -2.39 | 1.34        | 1.37     |
| 31  | B     | 824 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | A     | 838 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 31  | B     | 848 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | b     | 311 | CLA  | C1C-NC  | -2.39 | 1.34        | 1.37     |
| 31  | 3     | 308 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | 3     | 311 | CLA  | C4D-ND  | 2.39  | 1.40        | 1.37     |
| 31  | A     | 818 | CLA  | C1C-NC  | -2.39 | 1.34        | 1.37     |
| 31  | A     | 844 | CLA  | C4B-CHC | 2.39  | 1.47        | 1.41     |
| 31  | b     | 305 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | 2     | 315 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | A     | 818 | CLA  | C1B-CHB | 2.39  | 1.47        | 1.41     |
| 32  | b     | 309 | CHL  | C3D-C2D | 2.39  | 1.45        | 1.39     |
| 31  | 8     | 312 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | 6     | 322 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | B     | 813 | CLA  | C1C-NC  | -2.39 | 1.34        | 1.37     |
| 27  | 5     | 301 | LMT  | O4'-C4B | -2.39 | 1.37        | 1.43     |
| 31  | L     | 306 | CLA  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 31  | K     | 204 | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 31  | a     | 313 | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 32  | 9     | 320 | CHL  | C3D-C2D | 2.38  | 1.45        | 1.39     |
| 32  | 6     | 317 | CHL  | C3D-C2D | 2.38  | 1.45        | 1.39     |
| 31  | A     | 837 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 31  | 4     | 314 | CLA  | C4D-ND  | 2.38  | 1.40        | 1.37     |
| 31  | G     | 206 | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 31  | 5     | 307 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 31  | 6     | 316 | CLA  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 26  | B     | 805 | BCR  | C30-C25 | -2.38 | 1.50        | 1.53     |
| 31  | B     | 831 | CLA  | MG-ND   | 2.38  | 2.10        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | B     | 811 | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 31  | O     | 202 | CLA  | C1C-NC  | -2.38 | 1.34        | 1.37     |
| 32  | A     | 831 | CHL  | C4C-C3C | 2.38  | 1.49        | 1.45     |
| 27  | A     | 808 | LMT  | O4'-C4B | -2.37 | 1.37        | 1.43     |
| 31  | 5     | 309 | CLA  | C4D-ND  | 2.37  | 1.40        | 1.37     |
| 31  | b     | 306 | CLA  | C4D-ND  | 2.37  | 1.40        | 1.37     |
| 31  | 8     | 317 | CLA  | C4B-CHC | 2.37  | 1.47        | 1.41     |
| 31  | 7     | 311 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 31  | 5     | 323 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 31  | b     | 304 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 36  | 8     | 303 | LUT  | C18-C5  | 2.37  | 1.54        | 1.50     |
| 31  | K     | 205 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 31  | 3     | 314 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 31  | K     | 206 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 31  | 7     | 321 | CLA  | MG-NC   | -2.37 | 2.00        | 2.06     |
| 31  | 6     | 313 | CLA  | C4D-ND  | 2.37  | 1.40        | 1.37     |
| 31  | A     | 820 | CLA  | C1C-NC  | -2.37 | 1.34        | 1.37     |
| 31  | 9     | 311 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 31  | 6     | 314 | CLA  | C4D-ND  | 2.37  | 1.40        | 1.37     |
| 31  | A     | 816 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 31  | A     | 827 | CLA  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 31  | 8     | 308 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 32  | 4     | 313 | CHL  | C3D-C2D | 2.36  | 1.45        | 1.39     |
| 32  | 6     | 319 | CHL  | C3D-C2D | 2.36  | 1.45        | 1.39     |
| 31  | 2     | 315 | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 31  | 4     | 319 | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 31  | H     | 901 | CLA  | C4D-ND  | 2.36  | 1.40        | 1.37     |
| 32  | 7     | 318 | CHL  | C3D-C2D | 2.36  | 1.45        | 1.39     |
| 31  | 5     | 320 | CLA  | C4D-ND  | 2.36  | 1.40        | 1.37     |
| 31  | 3     | 307 | CLA  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 32  | 6     | 320 | CHL  | C3D-C2D | 2.36  | 1.45        | 1.39     |
| 32  | 4     | 317 | CHL  | MG-NA   | -2.36 | 2.00        | 2.06     |
| 31  | A     | 815 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 31  | B     | 811 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 36  | L     | 304 | LUT  | C38-C25 | 2.36  | 1.55        | 1.50     |
| 31  | H     | 903 | CLA  | C1C-NC  | -2.36 | 1.34        | 1.37     |
| 31  | A     | 832 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 31  | 2     | 314 | CLA  | C4D-ND  | 2.36  | 1.40        | 1.37     |
| 31  | B     | 838 | CLA  | C4B-CHC | 2.36  | 1.47        | 1.41     |
| 31  | 4     | 306 | CLA  | C4D-ND  | 2.36  | 1.40        | 1.37     |
| 31  | B     | 840 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 31  | G     | 205 | CLA  | C1C-NC  | -2.35 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 820 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 31  | B     | 839 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 28  | 7     | 307 | LHG  | O7-C5   | -2.35 | 1.40        | 1.46     |
| 32  | 6     | 318 | CHL  | C3D-C2D | 2.35  | 1.45        | 1.39     |
| 31  | H     | 901 | CLA  | C1C-NC  | -2.35 | 1.34        | 1.37     |
| 26  | L     | 302 | BCR  | C30-C25 | -2.35 | 1.50        | 1.53     |
| 31  | 5     | 315 | CLA  | C4D-ND  | 2.35  | 1.40        | 1.37     |
| 31  | 5     | 323 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 31  | A     | 827 | CLA  | C1C-NC  | -2.35 | 1.34        | 1.37     |
| 30  | A     | 813 | CL0  | C1D-C2D | 2.35  | 1.50        | 1.45     |
| 31  | 5     | 314 | CLA  | C4C-C3C | 2.35  | 1.49        | 1.45     |
| 32  | 5     | 317 | CHL  | C3D-C2D | 2.35  | 1.45        | 1.39     |
| 31  | 9     | 313 | CLA  | C1C-NC  | -2.34 | 1.34        | 1.37     |
| 31  | A     | 814 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 31  | B     | 825 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 31  | 4     | 309 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 31  | 9     | 312 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 31  | A     | 851 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 36  | 6     | 303 | LUT  | C18-C5  | 2.34  | 1.54        | 1.50     |
| 31  | B     | 827 | CLA  | C4B-CHC | 2.34  | 1.47        | 1.41     |
| 32  | 7     | 319 | CHL  | C3A-C2A | -2.34 | 1.47        | 1.54     |
| 31  | 2     | 307 | CLA  | C4D-ND  | 2.34  | 1.40        | 1.37     |
| 31  | 5     | 312 | CLA  | C1C-NC  | -2.34 | 1.34        | 1.37     |
| 32  | 6     | 309 | CHL  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 31  | a     | 309 | CLA  | C4C-C3C | 2.34  | 1.49        | 1.45     |
| 31  | 5     | 309 | CLA  | C1C-NC  | -2.34 | 1.34        | 1.37     |
| 31  | b     | 312 | CLA  | C1C-NC  | -2.34 | 1.34        | 1.37     |
| 31  | 7     | 312 | CLA  | C1C-NC  | -2.34 | 1.34        | 1.37     |
| 27  | A     | 807 | LMT  | O3B-C3B | -2.33 | 1.37        | 1.43     |
| 31  | A     | 817 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 31  | B     | 833 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 31  | A     | 818 | CLA  | C1B-NB  | -2.33 | 1.33        | 1.35     |
| 31  | 7     | 310 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.44     |
| 31  | 2     | 311 | CLA  | C4D-ND  | 2.33  | 1.40        | 1.37     |
| 31  | 9     | 314 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 31  | 9     | 321 | CLA  | C4D-ND  | 2.33  | 1.40        | 1.37     |
| 31  | 4     | 307 | CLA  | C4D-ND  | 2.33  | 1.40        | 1.37     |
| 36  | 3     | 305 | LUT  | C18-C5  | 2.33  | 1.54        | 1.50     |
| 31  | 8     | 309 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 32  | 3     | 315 | CHL  | C3D-C2D | 2.33  | 1.45        | 1.39     |
| 36  | J     | 103 | LUT  | C4-C5   | 2.33  | 1.54        | 1.51     |
| 31  | 6     | 312 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | O     | 203 | CLA  | C4D-ND  | 2.33  | 1.40        | 1.37     |
| 31  | A     | 849 | CLA  | MG-NC   | 2.33  | 2.11        | 2.06     |
| 31  | 3     | 310 | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 35  | 9     | 304 | QTB  | C09-C02 | -2.33 | 1.40        | 1.45     |
| 31  | A     | 842 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 31  | A     | 844 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 31  | A     | 822 | CLA  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 31  | A     | 826 | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 31  | a     | 322 | CLA  | C4D-ND  | 2.33  | 1.40        | 1.37     |
| 35  | a     | 302 | QTB  | C09-C02 | -2.33 | 1.40        | 1.45     |
| 31  | a     | 322 | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 31  | 6     | 307 | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 31  | a     | 311 | CLA  | C1C-NC  | -2.33 | 1.34        | 1.37     |
| 27  | A     | 808 | LMT  | O3B-C3B | -2.32 | 1.37        | 1.43     |
| 31  | 8     | 307 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 31  | B     | 817 | CLA  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 28  | A     | 810 | LHG  | P-O6    | 2.32  | 1.68        | 1.59     |
| 31  | 7     | 311 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 31  | b     | 313 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 31  | b     | 306 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 31  | 4     | 321 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 31  | 7     | 316 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 32  | a     | 320 | CHL  | C3D-C2D | 2.32  | 1.45        | 1.39     |
| 31  | B     | 842 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 31  | a     | 315 | CLA  | C1C-NC  | -2.32 | 1.34        | 1.37     |
| 31  | 9     | 315 | CLA  | C4D-ND  | 2.32  | 1.40        | 1.37     |
| 31  | B     | 829 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 36  | F     | 304 | LUT  | C38-C25 | 2.32  | 1.54        | 1.50     |
| 31  | B     | 841 | CLA  | MG-ND   | 2.32  | 2.10        | 2.05     |
| 31  | A     | 853 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 31  | J     | 105 | CLA  | C4C-C3C | 2.32  | 1.49        | 1.45     |
| 31  | A     | 847 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 31  | 2     | 305 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 31  | A     | 815 | CLA  | C4C-C3C | 2.31  | 1.49        | 1.45     |
| 31  | 6     | 314 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 31  | B     | 843 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 31  | B     | 847 | CLA  | C4B-CHC | 2.31  | 1.47        | 1.41     |
| 31  | B     | 833 | CLA  | MG-ND   | 2.31  | 2.10        | 2.05     |
| 31  | 6     | 315 | CLA  | C4D-ND  | 2.31  | 1.40        | 1.37     |
| 31  | 8     | 310 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 36  | 6     | 303 | LUT  | C38-C25 | 2.31  | 1.54        | 1.50     |
| 31  | 2     | 306 | CLA  | C4D-ND  | 2.31  | 1.40        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | A     | 817 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 31  | b     | 302 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 31  | 4     | 320 | CLA  | C4D-ND  | 2.31  | 1.40        | 1.37     |
| 31  | B     | 820 | CLA  | C1C-NC  | -2.31 | 1.34        | 1.37     |
| 31  | 6     | 312 | CLA  | C4D-ND  | 2.30  | 1.40        | 1.37     |
| 31  | A     | 820 | CLA  | MG-ND   | 2.30  | 2.10        | 2.05     |
| 31  | J     | 105 | CLA  | C4D-ND  | 2.30  | 1.40        | 1.37     |
| 31  | G     | 205 | CLA  | C4D-ND  | 2.30  | 1.40        | 1.37     |
| 27  | A     | 808 | LMT  | O2'-C2' | -2.30 | 1.37        | 1.43     |
| 31  | 3     | 316 | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 27  | 5     | 301 | LMT  | O2B-C2B | -2.30 | 1.37        | 1.43     |
| 31  | 7     | 309 | CLA  | C1C-NC  | -2.30 | 1.34        | 1.37     |
| 31  | B     | 845 | CLA  | C4C-C3C | 2.30  | 1.49        | 1.45     |
| 31  | A     | 815 | CLA  | MG-ND   | 2.30  | 2.10        | 2.05     |
| 32  | 7     | 317 | CHL  | C3D-C2D | 2.30  | 1.45        | 1.39     |
| 36  | 3     | 304 | LUT  | C1-C6   | 2.30  | 1.56        | 1.53     |
| 37  | J     | 104 | LMG  | C1-C2   | 2.30  | 1.59        | 1.52     |
| 31  | B     | 819 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 31  | b     | 313 | CLA  | C4D-ND  | 2.29  | 1.40        | 1.37     |
| 31  | a     | 312 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 31  | B     | 836 | CLA  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 31  | A     | 856 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 31  | 4     | 306 | CLA  | C1C-NC  | -2.29 | 1.34        | 1.37     |
| 31  | 9     | 318 | CLA  | C4D-ND  | 2.29  | 1.40        | 1.37     |
| 32  | 8     | 319 | CHL  | C3D-C2D | 2.29  | 1.45        | 1.39     |
| 31  | 8     | 312 | CLA  | C4D-ND  | 2.29  | 1.40        | 1.37     |
| 31  | b     | 308 | CLA  | C1C-NC  | -2.29 | 1.34        | 1.37     |
| 31  | A     | 847 | CLA  | C4C-C3C | 2.29  | 1.49        | 1.45     |
| 31  | B     | 832 | CLA  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 31  | 6     | 306 | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 31  | 4     | 312 | CLA  | C1C-NC  | -2.28 | 1.34        | 1.37     |
| 31  | G     | 204 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 32  | 5     | 316 | CHL  | C3A-C2A | -2.28 | 1.48        | 1.54     |
| 31  | 4     | 305 | CLA  | C4C-C3C | 2.28  | 1.49        | 1.45     |
| 31  | H     | 902 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 31  | 3     | 307 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 31  | B     | 832 | CLA  | C4C-C3C | 2.28  | 1.49        | 1.45     |
| 31  | 4     | 321 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 31  | 8     | 317 | CLA  | C1C-NC  | -2.28 | 1.34        | 1.37     |
| 31  | 4     | 319 | CLA  | C1C-C2C | 2.28  | 1.49        | 1.44     |
| 31  | A     | 845 | CLA  | C4C-C3C | 2.28  | 1.49        | 1.45     |
| 36  | L     | 304 | LUT  | C4-C5   | 2.28  | 1.54        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 5     | 318 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 31  | A     | 835 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 31  | 2     | 312 | CLA  | C4D-ND  | 2.28  | 1.40        | 1.37     |
| 31  | B     | 812 | CLA  | C1B-CHB | 2.28  | 1.47        | 1.41     |
| 31  | 5     | 314 | CLA  | C4D-ND  | 2.27  | 1.40        | 1.37     |
| 36  | 4     | 303 | LUT  | C38-C25 | 2.27  | 1.54        | 1.50     |
| 31  | B     | 826 | CLA  | C4C-C3C | 2.27  | 1.49        | 1.45     |
| 31  | 5     | 307 | CLA  | C4D-ND  | 2.27  | 1.40        | 1.37     |
| 36  | 8     | 302 | LUT  | C38-C25 | 2.27  | 1.54        | 1.50     |
| 32  | a     | 320 | CHL  | MG-NA   | 2.27  | 2.11        | 2.06     |
| 32  | 4     | 317 | CHL  | C4C-C3C | 2.27  | 1.49        | 1.45     |
| 31  | 6     | 322 | CLA  | C1C-NC  | -2.27 | 1.34        | 1.37     |
| 31  | A     | 850 | CLA  | C4C-C3C | 2.27  | 1.48        | 1.45     |
| 31  | 9     | 313 | CLA  | C4D-ND  | 2.27  | 1.40        | 1.37     |
| 31  | 4     | 308 | CLA  | C4D-ND  | 2.26  | 1.40        | 1.37     |
| 32  | 7     | 324 | CHL  | C3D-C2D | 2.26  | 1.45        | 1.39     |
| 36  | 8     | 303 | LUT  | C4-C5   | 2.26  | 1.54        | 1.51     |
| 31  | 4     | 316 | CLA  | C4D-ND  | 2.26  | 1.40        | 1.37     |
| 31  | b     | 305 | CLA  | C4D-ND  | 2.26  | 1.40        | 1.37     |
| 26  | J     | 102 | BCR  | C30-C25 | -2.26 | 1.50        | 1.53     |
| 31  | K     | 204 | CLA  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 31  | 3     | 318 | CLA  | C1C-NC  | -2.26 | 1.34        | 1.37     |
| 32  | b     | 309 | CHL  | C4C-C3C | 2.26  | 1.48        | 1.45     |
| 32  | 8     | 316 | CHL  | C3D-C2D | 2.26  | 1.45        | 1.39     |
| 32  | 6     | 318 | CHL  | C3A-C2A | -2.26 | 1.48        | 1.54     |
| 32  | 5     | 319 | CHL  | C4C-C3C | 2.25  | 1.48        | 1.45     |
| 31  | 3     | 312 | CLA  | C4D-ND  | 2.25  | 1.40        | 1.37     |
| 31  | 6     | 312 | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 31  | H     | 902 | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 31  | 9     | 311 | CLA  | C4D-ND  | 2.25  | 1.40        | 1.37     |
| 32  | 5     | 316 | CHL  | C3D-C2D | 2.25  | 1.45        | 1.39     |
| 31  | 4     | 318 | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 36  | 3     | 304 | LUT  | C38-C25 | 2.25  | 1.54        | 1.50     |
| 31  | a     | 316 | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 31  | O     | 204 | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 31  | 6     | 315 | CLA  | C1C-NC  | -2.25 | 1.34        | 1.37     |
| 31  | 8     | 308 | CLA  | C4D-ND  | 2.24  | 1.40        | 1.37     |
| 31  | 8     | 313 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 31  | 9     | 319 | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 31  | A     | 828 | CLA  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 31  | b     | 304 | CLA  | C1C-NC  | -2.24 | 1.34        | 1.37     |
| 31  | 2     | 312 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | A     | 831 | CHL  | C3D-C2D | 2.23  | 1.45        | 1.39     |
| 26  | J     | 102 | BCR  | C1-C6   | -2.23 | 1.50        | 1.53     |
| 31  | 3     | 319 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 31  | 6     | 316 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 31  | A     | 825 | CLA  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 31  | 3     | 316 | CLA  | C4D-ND  | 2.23  | 1.40        | 1.37     |
| 31  | 9     | 319 | CLA  | C4D-ND  | 2.23  | 1.40        | 1.37     |
| 31  | b     | 305 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 28  | 6     | 305 | LHG  | O7-C5   | -2.23 | 1.41        | 1.46     |
| 31  | 4     | 320 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 31  | 5     | 314 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 31  | 8     | 315 | CLA  | C4D-ND  | 2.23  | 1.40        | 1.37     |
| 31  | 8     | 315 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 32  | K     | 201 | CHL  | MG-NA   | -2.23 | 2.01        | 2.06     |
| 31  | 2     | 306 | CLA  | C1C-NC  | -2.23 | 1.34        | 1.37     |
| 32  | 5     | 322 | CHL  | C4C-C3C | 2.23  | 1.48        | 1.45     |
| 31  | A     | 821 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 31  | B     | 813 | CLA  | C1C-C2C | 2.22  | 1.48        | 1.44     |
| 31  | b     | 307 | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 31  | A     | 857 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 32  | 6     | 317 | CHL  | MG-ND   | 2.22  | 2.10        | 2.05     |
| 31  | 3     | 310 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 31  | 2     | 308 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 31  | b     | 302 | CLA  | MG-ND   | -2.22 | 2.01        | 2.05     |
| 31  | a     | 321 | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 32  | 4     | 313 | CHL  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 31  | B     | 848 | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 31  | 6     | 308 | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 31  | A     | 855 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 31  | B     | 839 | CLA  | C1C-NC  | -2.22 | 1.34        | 1.37     |
| 31  | b     | 310 | CLA  | C4D-ND  | 2.22  | 1.40        | 1.37     |
| 31  | a     | 312 | CLA  | C4D-ND  | 2.22  | 1.40        | 1.37     |
| 31  | A     | 819 | CLA  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 33  | 7     | 308 | DGD  | O2G-C2G | -2.21 | 1.41        | 1.46     |
| 31  | a     | 319 | CLA  | C4D-ND  | 2.21  | 1.40        | 1.37     |
| 31  | 3     | 308 | CLA  | C1C-C2C | 2.21  | 1.48        | 1.44     |
| 31  | 3     | 320 | CLA  | C1C-NC  | -2.21 | 1.34        | 1.37     |
| 32  | 9     | 320 | CHL  | C3A-C2A | -2.21 | 1.48        | 1.54     |
| 32  | 6     | 319 | CHL  | C3A-C2A | -2.21 | 1.48        | 1.54     |
| 31  | 3     | 313 | CLA  | C4D-ND  | 2.21  | 1.40        | 1.37     |
| 31  | 7     | 315 | CLA  | C4D-ND  | 2.21  | 1.40        | 1.37     |
| 31  | L     | 306 | CLA  | C1C-NC  | -2.21 | 1.34        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 36  | 9     | 302 | LUT  | C38-C25 | 2.21  | 1.54        | 1.50     |
| 31  | a     | 314 | CLA  | C4D-ND  | 2.21  | 1.40        | 1.37     |
| 36  | 5     | 303 | LUT  | C38-C25 | 2.21  | 1.54        | 1.50     |
| 32  | 7     | 320 | CHL  | C3D-C2D | 2.21  | 1.45        | 1.39     |
| 31  | 8     | 320 | CLA  | C4D-ND  | 2.20  | 1.40        | 1.37     |
| 26  | 3     | 302 | BCR  | C30-C25 | -2.20 | 1.50        | 1.53     |
| 32  | 4     | 310 | CHL  | C3D-C2D | 2.20  | 1.45        | 1.39     |
| 31  | 8     | 310 | CLA  | C1C-C2C | 2.20  | 1.48        | 1.44     |
| 32  | 6     | 319 | CHL  | C4C-C3C | 2.20  | 1.48        | 1.45     |
| 31  | 3     | 311 | CLA  | C3D-C4D | -2.20 | 1.39        | 1.44     |
| 36  | J     | 103 | LUT  | C38-C25 | 2.20  | 1.54        | 1.50     |
| 31  | B     | 830 | CLA  | C4D-ND  | 2.20  | 1.40        | 1.37     |
| 31  | 5     | 314 | CLA  | MG-NC   | 2.20  | 2.11        | 2.06     |
| 31  | 2     | 304 | CLA  | C1C-NC  | -2.20 | 1.34        | 1.37     |
| 31  | 4     | 316 | CLA  | C1C-NC  | -2.20 | 1.34        | 1.37     |
| 31  | 7     | 322 | CLA  | C4D-ND  | 2.20  | 1.40        | 1.37     |
| 31  | B     | 850 | CLA  | MG-ND   | 2.19  | 2.10        | 2.05     |
| 31  | B     | 820 | CLA  | C4C-C3C | 2.19  | 1.48        | 1.45     |
| 31  | B     | 818 | CLA  | C4B-CHC | 2.19  | 1.47        | 1.41     |
| 31  | B     | 829 | CLA  | C4D-ND  | 2.19  | 1.40        | 1.37     |
| 31  | B     | 832 | CLA  | C4D-ND  | 2.19  | 1.40        | 1.37     |
| 31  | B     | 840 | CLA  | MG-ND   | 2.19  | 2.10        | 2.05     |
| 36  | 9     | 302 | LUT  | C1-C6   | 2.19  | 1.56        | 1.53     |
| 31  | B     | 824 | CLA  | C4D-ND  | 2.19  | 1.40        | 1.37     |
| 31  | O     | 203 | CLA  | C1C-C2C | 2.19  | 1.48        | 1.44     |
| 31  | 9     | 318 | CLA  | C1C-C2C | 2.19  | 1.48        | 1.44     |
| 31  | a     | 315 | CLA  | C4D-ND  | 2.19  | 1.40        | 1.37     |
| 31  | 5     | 320 | CLA  | C1C-C2C | 2.19  | 1.48        | 1.44     |
| 36  | 2     | 301 | LUT  | C38-C25 | 2.19  | 1.54        | 1.50     |
| 27  | 9     | 306 | LMT  | O1'-C1' | -2.18 | 1.36        | 1.40     |
| 31  | b     | 304 | CLA  | C4D-ND  | 2.18  | 1.40        | 1.37     |
| 32  | 6     | 317 | CHL  | C3A-C2A | -2.18 | 1.48        | 1.54     |
| 31  | 7     | 313 | CLA  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 26  | K     | 202 | BCR  | C30-C25 | -2.18 | 1.50        | 1.53     |
| 31  | a     | 322 | CLA  | MG-ND   | -2.18 | 2.01        | 2.05     |
| 28  | B     | 807 | LHG  | O7-C5   | -2.18 | 1.41        | 1.46     |
| 31  | 3     | 313 | CLA  | C1C-NC  | -2.18 | 1.34        | 1.37     |
| 31  | B     | 813 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 31  | b     | 311 | CLA  | C4D-ND  | 2.17  | 1.40        | 1.37     |
| 31  | A     | 820 | CLA  | C1C-C2C | 2.17  | 1.48        | 1.44     |
| 31  | A     | 814 | CLA  | MG-NC   | 2.17  | 2.11        | 2.06     |
| 42  | 4     | 304 | SQD  | O9-S    | 2.17  | 1.51        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 8     | 307 | CLA  | C4D-ND  | 2.17  | 1.40        | 1.37     |
| 31  | B     | 815 | CLA  | C4C-C3C | 2.17  | 1.48        | 1.45     |
| 31  | 9     | 312 | CLA  | C4D-ND  | 2.17  | 1.40        | 1.37     |
| 31  | 2     | 309 | CLA  | C4D-ND  | 2.17  | 1.40        | 1.37     |
| 31  | B     | 838 | CLA  | C4D-ND  | 2.17  | 1.40        | 1.37     |
| 36  | 9     | 303 | LUT  | C18-C5  | 2.16  | 1.54        | 1.50     |
| 31  | 4     | 305 | CLA  | C1D-C2D | 2.16  | 1.49        | 1.45     |
| 31  | 9     | 315 | CLA  | C3D-C4D | -2.16 | 1.39        | 1.44     |
| 31  | b     | 306 | CLA  | C1C-C2C | 2.16  | 1.48        | 1.44     |
| 36  | a     | 303 | LUT  | C38-C25 | 2.16  | 1.54        | 1.50     |
| 31  | A     | 849 | CLA  | C4D-ND  | 2.16  | 1.40        | 1.37     |
| 32  | A     | 840 | CHL  | C3D-C2D | 2.16  | 1.45        | 1.39     |
| 31  | 2     | 308 | CLA  | C1C-C2C | 2.15  | 1.48        | 1.44     |
| 33  | 7     | 308 | DGD  | O1G-C1G | -2.15 | 1.40        | 1.45     |
| 31  | 6     | 306 | CLA  | C1C-NC  | -2.15 | 1.34        | 1.37     |
| 31  | A     | 825 | CLA  | MG-ND   | -2.14 | 2.01        | 2.05     |
| 31  | 5     | 312 | CLA  | C1C-C2C | 2.14  | 1.48        | 1.44     |
| 31  | A     | 830 | CLA  | MG-ND   | -2.14 | 2.01        | 2.05     |
| 31  | 5     | 320 | CLA  | C1C-NC  | -2.14 | 1.34        | 1.37     |
| 31  | A     | 828 | CLA  | C4D-ND  | 2.14  | 1.40        | 1.37     |
| 31  | 9     | 314 | CLA  | C4D-ND  | 2.14  | 1.40        | 1.37     |
| 32  | 4     | 317 | CHL  | C1B-CHB | 2.14  | 1.46        | 1.41     |
| 28  | 8     | 304 | LHG  | O7-C5   | -2.14 | 1.41        | 1.46     |
| 32  | 6     | 318 | CHL  | C4C-C3C | 2.14  | 1.48        | 1.45     |
| 32  | 3     | 315 | CHL  | C3A-C2A | -2.14 | 1.48        | 1.54     |
| 32  | 4     | 313 | CHL  | C3A-C2A | -2.13 | 1.48        | 1.54     |
| 31  | F     | 306 | CLA  | C4D-ND  | 2.13  | 1.40        | 1.37     |
| 36  | F     | 304 | LUT  | C4-C5   | 2.13  | 1.54        | 1.51     |
| 27  | A     | 807 | LMT  | O1'-C1' | -2.13 | 1.36        | 1.40     |
| 31  | 8     | 313 | CLA  | C4D-ND  | 2.13  | 1.40        | 1.37     |
| 31  | 7     | 313 | CLA  | C4D-ND  | 2.13  | 1.40        | 1.37     |
| 32  | 6     | 309 | CHL  | C3A-C2A | -2.13 | 1.48        | 1.54     |
| 32  | A     | 839 | CHL  | C3A-C2A | -2.13 | 1.48        | 1.54     |
| 31  | 8     | 315 | CLA  | MG-ND   | -2.13 | 2.01        | 2.05     |
| 28  | A     | 809 | LHG  | P-O6    | 2.13  | 1.67        | 1.59     |
| 31  | 4     | 306 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 31  | B     | 837 | CLA  | C3D-C4D | -2.12 | 1.39        | 1.44     |
| 32  | 8     | 319 | CHL  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 31  | A     | 834 | CLA  | MG-NC   | 2.12  | 2.11        | 2.06     |
| 31  | 9     | 313 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |
| 32  | b     | 309 | CHL  | C3A-C2A | -2.12 | 1.48        | 1.54     |
| 31  | B     | 820 | CLA  | C1C-C2C | 2.12  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 321 | CLA  | C4D-ND  | 2.12  | 1.40        | 1.37     |
| 31  | 3     | 317 | CLA  | C4D-ND  | 2.12  | 1.40        | 1.37     |
| 32  | 8     | 316 | CHL  | C3A-C2A | -2.12 | 1.48        | 1.54     |
| 31  | 2     | 311 | CLA  | C1C-NC  | -2.12 | 1.34        | 1.37     |
| 31  | 8     | 320 | CLA  | MG-ND   | -2.12 | 2.01        | 2.05     |
| 31  | A     | 845 | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 31  | a     | 311 | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 31  | 4     | 312 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 31  | A     | 838 | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 31  | 7     | 309 | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 31  | B     | 825 | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 32  | 6     | 320 | CHL  | C3A-C2A | -2.11 | 1.48        | 1.54     |
| 32  | A     | 840 | CHL  | C3A-C2A | -2.11 | 1.48        | 1.54     |
| 31  | 4     | 309 | CLA  | MG-ND   | -2.11 | 2.01        | 2.05     |
| 31  | 5     | 314 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 36  | 4     | 303 | LUT  | C18-C5  | 2.11  | 1.54        | 1.50     |
| 31  | L     | 306 | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 28  | a     | 306 | LHG  | O7-C5   | -2.11 | 1.41        | 1.46     |
| 32  | a     | 317 | CHL  | C3A-C2A | -2.11 | 1.48        | 1.54     |
| 32  | a     | 320 | CHL  | C3A-C2A | -2.11 | 1.48        | 1.54     |
| 31  | 7     | 316 | CLA  | C4D-ND  | 2.11  | 1.40        | 1.37     |
| 31  | b     | 311 | CLA  | C1C-C2C | 2.11  | 1.48        | 1.44     |
| 31  | A     | 829 | CLA  | C1B-CHB | 2.11  | 1.46        | 1.41     |
| 31  | 3     | 309 | CLA  | C4D-ND  | 2.10  | 1.40        | 1.37     |
| 31  | A     | 836 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 31  | A     | 854 | CLA  | C4D-ND  | 2.10  | 1.40        | 1.37     |
| 30  | A     | 813 | CL0  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 31  | 8     | 307 | CLA  | MG-NC   | 2.10  | 2.11        | 2.06     |
| 31  | 2     | 308 | CLA  | C4D-ND  | 2.10  | 1.40        | 1.37     |
| 31  | A     | 825 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 31  | B     | 838 | CLA  | MG-ND   | -2.10 | 2.01        | 2.05     |
| 31  | 2     | 312 | CLA  | C1C-C2C | 2.10  | 1.48        | 1.44     |
| 31  | B     | 830 | CLA  | C3D-C4D | -2.10 | 1.39        | 1.44     |
| 31  | B     | 827 | CLA  | C4C-C3C | 2.10  | 1.48        | 1.45     |
| 31  | 4     | 311 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 32  | a     | 318 | CHL  | C3A-C2A | -2.09 | 1.48        | 1.54     |
| 37  | J     | 101 | LMG  | C7-C8   | 2.09  | 1.57        | 1.50     |
| 32  | 9     | 322 | CHL  | C3A-C2A | -2.09 | 1.48        | 1.54     |
| 31  | 9     | 315 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 31  | B     | 834 | CLA  | MG-NC   | -2.09 | 2.01        | 2.06     |
| 31  | 5     | 311 | CLA  | C4D-ND  | 2.09  | 1.40        | 1.37     |
| 31  | 6     | 315 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | G     | 205 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 31  | a     | 313 | CLA  | C4D-ND  | 2.09  | 1.40        | 1.37     |
| 31  | 2     | 311 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 31  | 7     | 314 | CLA  | C4D-ND  | 2.09  | 1.40        | 1.37     |
| 31  | 7     | 321 | CLA  | C4C-C3C | 2.09  | 1.48        | 1.45     |
| 31  | 8     | 307 | CLA  | C1C-C2C | 2.09  | 1.48        | 1.44     |
| 31  | 2     | 304 | CLA  | C1C-C2C | 2.08  | 1.48        | 1.44     |
| 31  | a     | 316 | CLA  | C4D-ND  | 2.08  | 1.40        | 1.37     |
| 31  | 9     | 316 | CLA  | C4D-ND  | 2.08  | 1.40        | 1.37     |
| 31  | 2     | 304 | CLA  | C4D-ND  | 2.08  | 1.40        | 1.37     |
| 31  | B     | 843 | CLA  | C4D-ND  | 2.08  | 1.40        | 1.37     |
| 27  | 9     | 306 | LMT  | O4'-C4B | -2.08 | 1.38        | 1.43     |
| 42  | 4     | 304 | SQD  | O7-S    | 2.08  | 1.51        | 1.45     |
| 31  | 2     | 313 | CLA  | C4D-ND  | 2.08  | 1.40        | 1.37     |
| 31  | 4     | 314 | CLA  | C1C-NC  | -2.08 | 1.34        | 1.37     |
| 33  | 7     | 308 | DGD  | O3G-C3G | -2.07 | 1.40        | 1.43     |
| 31  | 7     | 309 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 31  | 2     | 309 | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 31  | A     | 850 | CLA  | C3D-C4D | -2.07 | 1.39        | 1.44     |
| 31  | 6     | 308 | CLA  | C4D-ND  | 2.07  | 1.40        | 1.37     |
| 31  | 4     | 320 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 31  | b     | 305 | CLA  | C1C-C2C | 2.07  | 1.48        | 1.44     |
| 32  | 8     | 319 | CHL  | C3A-C2A | -2.07 | 1.48        | 1.54     |
| 31  | A     | 836 | CLA  | C4D-ND  | 2.07  | 1.40        | 1.37     |
| 31  | F     | 301 | CLA  | C4D-ND  | 2.07  | 1.40        | 1.37     |
| 32  | 6     | 321 | CHL  | C4C-C3C | 2.07  | 1.48        | 1.45     |
| 32  | 7     | 320 | CHL  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 31  | 7     | 311 | CLA  | C4D-ND  | 2.07  | 1.40        | 1.37     |
| 32  | a     | 320 | CHL  | C1B-CHB | 2.07  | 1.46        | 1.41     |
| 31  | b     | 310 | CLA  | C1C-NC  | -2.07 | 1.34        | 1.37     |
| 27  | A     | 807 | LMT  | O4'-C4B | -2.07 | 1.38        | 1.43     |
| 32  | 5     | 319 | CHL  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 32  | 6     | 317 | CHL  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 32  | 5     | 319 | CHL  | C3A-C2A | -2.06 | 1.48        | 1.54     |
| 31  | B     | 834 | CLA  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 32  | 8     | 319 | CHL  | C1B-CHB | 2.06  | 1.46        | 1.41     |
| 32  | 5     | 317 | CHL  | C3A-C2A | -2.06 | 1.48        | 1.54     |
| 31  | 7     | 312 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 31  | O     | 202 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 31  | B     | 828 | CLA  | C1C-NC  | -2.06 | 1.34        | 1.37     |
| 31  | b     | 307 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 31  | 4     | 316 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | 7     | 317 | CHL  | C3A-C2A | -2.06 | 1.48        | 1.54     |
| 31  | A     | 819 | CLA  | C1C-C2C | 2.06  | 1.48        | 1.44     |
| 32  | a     | 317 | CHL  | C4C-C3C | 2.06  | 1.48        | 1.45     |
| 31  | 3     | 309 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 31  | B     | 846 | CLA  | C4D-ND  | 2.05  | 1.40        | 1.37     |
| 31  | 3     | 313 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 31  | 8     | 314 | CLA  | C4D-ND  | 2.05  | 1.40        | 1.37     |
| 32  | 9     | 322 | CHL  | MG-NC   | -2.05 | 2.01        | 2.06     |
| 31  | 2     | 310 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 32  | 5     | 322 | CHL  | C3A-C2A | -2.05 | 1.48        | 1.54     |
| 32  | 6     | 321 | CHL  | C3A-C2A | -2.05 | 1.48        | 1.54     |
| 37  | J     | 101 | LMG  | O2-C2   | -2.05 | 1.38        | 1.43     |
| 31  | 4     | 305 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 26  | 2     | 302 | BCR  | C33-C5  | -2.05 | 1.47        | 1.50     |
| 31  | H     | 902 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 31  | 6     | 310 | CLA  | C1C-C2C | 2.05  | 1.48        | 1.44     |
| 31  | A     | 844 | CLA  | C4D-ND  | 2.05  | 1.40        | 1.37     |
| 37  | J     | 101 | LMG  | C4-C5   | 2.05  | 1.57        | 1.53     |
| 33  | B     | 808 | DGD  | O1G-C1G | -2.05 | 1.40        | 1.45     |
| 28  | A     | 809 | LHG  | O7-C5   | -2.05 | 1.41        | 1.46     |
| 31  | 5     | 320 | CLA  | C3D-C4D | -2.05 | 1.39        | 1.44     |
| 31  | 9     | 317 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 31  | A     | 846 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 31  | 5     | 313 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 31  | B     | 817 | CLA  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 32  | A     | 831 | CHL  | C4B-CHC | 2.04  | 1.46        | 1.41     |
| 31  | 6     | 316 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 31  | 2     | 315 | CLA  | C4D-ND  | 2.04  | 1.40        | 1.37     |
| 31  | O     | 204 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 31  | K     | 204 | CLA  | C1C-C2C | 2.04  | 1.48        | 1.44     |
| 31  | 2     | 306 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 33  | 7     | 308 | DGD  | O4D-C4D | -2.03 | 1.38        | 1.43     |
| 31  | 5     | 310 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 31  | 4     | 309 | CLA  | C4D-ND  | 2.03  | 1.40        | 1.37     |
| 31  | a     | 312 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 31  | 3     | 320 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 31  | a     | 309 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 32  | 4     | 313 | CHL  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 35  | F     | 303 | QTB  | C17-C11 | 2.03  | 1.57        | 1.55     |
| 32  | 4     | 310 | CHL  | C3A-C2A | -2.03 | 1.48        | 1.54     |
| 32  | 7     | 319 | CHL  | C4C-C3C | 2.03  | 1.48        | 1.45     |
| 31  | b     | 308 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | 7     | 316 | CLA  | C1C-C2C | 2.03  | 1.48        | 1.44     |
| 31  | 6     | 313 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 31  | A     | 819 | CLA  | C4D-ND  | 2.02  | 1.40        | 1.37     |
| 31  | 3     | 307 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 32  | 8     | 316 | CHL  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 32  | b     | 309 | CHL  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 31  | 3     | 319 | CLA  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 32  | K     | 201 | CHL  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 32  | 7     | 317 | CHL  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 31  | B     | 819 | CLA  | C3D-C4D | -2.02 | 1.39        | 1.44     |
| 31  | B     | 840 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 32  | 5     | 317 | CHL  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 31  | 8     | 313 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 32  | 7     | 318 | CHL  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 32  | 6     | 321 | CHL  | C4B-CHC | 2.02  | 1.46        | 1.41     |
| 31  | B     | 820 | CLA  | C4D-ND  | 2.02  | 1.40        | 1.37     |
| 32  | 7     | 320 | CHL  | C4C-C3C | 2.02  | 1.48        | 1.45     |
| 31  | b     | 304 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 32  | 7     | 324 | CHL  | C3A-C2A | -2.02 | 1.48        | 1.54     |
| 32  | 5     | 322 | CHL  | C1B-CHB | 2.02  | 1.46        | 1.41     |
| 31  | 8     | 308 | CLA  | C1C-C2C | 2.02  | 1.48        | 1.44     |
| 31  | B     | 831 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 31  | A     | 833 | CLA  | C4D-ND  | 2.01  | 1.40        | 1.37     |
| 31  | 7     | 313 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 31  | 7     | 312 | CLA  | C4D-ND  | 2.01  | 1.40        | 1.37     |
| 32  | K     | 201 | CHL  | C4B-CHC | 2.01  | 1.46        | 1.41     |
| 31  | 5     | 321 | CLA  | C1C-C2C | 2.01  | 1.48        | 1.44     |
| 31  | 3     | 314 | CLA  | C4D-ND  | 2.01  | 1.40        | 1.37     |
| 26  | 3     | 303 | BCR  | C33-C5  | -2.00 | 1.47        | 1.50     |
| 32  | 6     | 309 | CHL  | C1B-CHB | 2.00  | 1.46        | 1.41     |
| 31  | 5     | 315 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |
| 31  | B     | 838 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 31  | a     | 313 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 31  | F     | 305 | CLA  | C4D-ND  | 2.00  | 1.40        | 1.37     |
| 31  | B     | 839 | CLA  | C3D-C4D | -2.00 | 1.39        | 1.44     |
| 31  | K     | 205 | CLA  | C4D-ND  | 2.00  | 1.40        | 1.37     |
| 31  | 4     | 315 | CLA  | C1C-C2C | 2.00  | 1.48        | 1.44     |

All (6253) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 31  | 5     | 315 | CLA  | C4-C3-C5 | -19.91 | 81.78       | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 31  | 5     | 315 | CLA  | C5-C3-C2    | 19.18  | 159.93      | 121.12   |
| 31  | 5     | 315 | CLA  | C4-C3-C2    | -17.67 | 78.34       | 123.68   |
| 36  | 7     | 305 | LUT  | C15-C14-C13 | -17.12 | 102.87      | 127.31   |
| 36  | 2     | 301 | LUT  | C15-C14-C13 | -16.15 | 104.26      | 127.31   |
| 36  | 9     | 305 | LUT  | C15-C35-C34 | 15.60  | 155.43      | 123.47   |
| 31  | 4     | 305 | CLA  | C1D-ND-C4D  | -15.43 | 95.37       | 106.33   |
| 36  | 8     | 302 | LUT  | C15-C14-C13 | -15.21 | 105.60      | 127.31   |
| 36  | 8     | 303 | LUT  | C15-C14-C13 | -14.81 | 106.18      | 127.31   |
| 36  | J     | 103 | LUT  | C15-C35-C34 | 14.38  | 152.93      | 123.47   |
| 36  | 3     | 305 | LUT  | C15-C14-C13 | -14.36 | 106.82      | 127.31   |
| 36  | 9     | 302 | LUT  | C15-C35-C34 | 14.18  | 152.52      | 123.47   |
| 36  | 3     | 304 | LUT  | C15-C14-C13 | -14.11 | 107.17      | 127.31   |
| 36  | 8     | 303 | LUT  | C18-C5-C6   | -14.05 | 108.75      | 124.53   |
| 31  | 4     | 305 | CLA  | C4A-NA-C1A  | -13.88 | 100.47      | 106.71   |
| 36  | 9     | 303 | LUT  | C15-C14-C13 | -13.87 | 107.52      | 127.31   |
| 36  | a     | 305 | LUT  | C15-C35-C34 | 13.74  | 151.62      | 123.47   |
| 36  | b     | 301 | LUT  | C15-C35-C34 | 13.65  | 151.43      | 123.47   |
| 36  | 3     | 305 | LUT  | C18-C5-C6   | -13.35 | 109.54      | 124.53   |
| 31  | A     | 829 | CLA  | CHD-C1D-ND  | -13.34 | 112.20      | 124.45   |
| 36  | 4     | 302 | LUT  | C15-C35-C34 | 13.26  | 150.64      | 123.47   |
| 36  | L     | 304 | LUT  | C15-C35-C34 | 13.07  | 150.25      | 123.47   |
| 36  | a     | 305 | LUT  | C19-C9-C10  | -12.96 | 104.77      | 122.92   |
| 36  | F     | 304 | LUT  | C15-C35-C34 | 12.83  | 149.75      | 123.47   |
| 36  | F     | 304 | LUT  | C18-C5-C6   | -12.68 | 110.28      | 124.53   |
| 36  | 6     | 303 | LUT  | C18-C5-C6   | -12.67 | 110.30      | 124.53   |
| 36  | 3     | 305 | LUT  | C11-C10-C9  | -12.53 | 109.43      | 127.31   |
| 36  | 5     | 304 | LUT  | C15-C35-C34 | 12.46  | 148.99      | 123.47   |
| 36  | 6     | 303 | LUT  | C15-C35-C34 | 12.36  | 148.80      | 123.47   |
| 36  | 5     | 303 | LUT  | C15-C35-C34 | 12.36  | 148.79      | 123.47   |
| 36  | 9     | 303 | LUT  | C18-C5-C6   | -12.35 | 110.66      | 124.53   |
| 36  | 6     | 304 | LUT  | C15-C35-C34 | 12.30  | 148.67      | 123.47   |
| 36  | a     | 303 | LUT  | C15-C14-C13 | -12.28 | 109.79      | 127.31   |
| 36  | F     | 304 | LUT  | C11-C10-C9  | -12.23 | 109.86      | 127.31   |
| 36  | 5     | 303 | LUT  | C15-C14-C13 | -12.13 | 110.00      | 127.31   |
| 36  | 9     | 305 | LUT  | C35-C34-C33 | -12.12 | 110.01      | 127.31   |
| 36  | 4     | 302 | LUT  | C31-C30-C29 | -12.11 | 110.02      | 127.31   |
| 36  | 3     | 304 | LUT  | C31-C30-C29 | -12.11 | 110.03      | 127.31   |
| 36  | 4     | 303 | LUT  | C18-C5-C6   | -12.11 | 110.93      | 124.53   |
| 36  | 3     | 304 | LUT  | C11-C10-C9  | -12.05 | 110.11      | 127.31   |
| 36  | J     | 103 | LUT  | C31-C30-C29 | -12.01 | 110.17      | 127.31   |
| 31  | A     | 829 | CLA  | C4A-NA-C1A  | 11.99  | 112.10      | 106.71   |
| 36  | 8     | 303 | LUT  | C31-C30-C29 | -11.86 | 110.39      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 36  | 9     | 305 | LUT  | C15-C14-C13 | -11.85 | 110.41      | 127.31   |
| 31  | 4     | 316 | CLA  | CHD-C1D-ND  | -11.84 | 113.57      | 124.45   |
| 36  | 9     | 302 | LUT  | C11-C10-C9  | -11.81 | 110.45      | 127.31   |
| 36  | F     | 304 | LUT  | C31-C30-C29 | -11.73 | 110.57      | 127.31   |
| 36  | 4     | 303 | LUT  | C15-C35-C34 | 11.73  | 147.50      | 123.47   |
| 36  | 4     | 302 | LUT  | C15-C14-C13 | -11.65 | 110.68      | 127.31   |
| 31  | A     | 838 | CLA  | C4A-NA-C1A  | 11.54  | 111.89      | 106.71   |
| 36  | 2     | 301 | LUT  | C11-C10-C9  | -11.51 | 110.89      | 127.31   |
| 36  | a     | 303 | LUT  | C11-C10-C9  | -11.47 | 110.94      | 127.31   |
| 36  | a     | 303 | LUT  | C15-C35-C34 | 11.44  | 146.92      | 123.47   |
| 36  | b     | 301 | LUT  | C11-C10-C9  | -11.43 | 110.99      | 127.31   |
| 36  | J     | 103 | LUT  | C11-C10-C9  | -11.43 | 111.00      | 127.31   |
| 36  | 3     | 304 | LUT  | C15-C35-C34 | 11.40  | 146.84      | 123.47   |
| 36  | a     | 305 | LUT  | C11-C12-C13 | 11.40  | 158.43      | 126.42   |
| 36  | J     | 103 | LUT  | C15-C14-C13 | -11.36 | 111.09      | 127.31   |
| 36  | 2     | 301 | LUT  | C31-C30-C29 | -11.29 | 111.19      | 127.31   |
| 36  | b     | 301 | LUT  | C18-C5-C6   | -11.26 | 111.89      | 124.53   |
| 36  | 8     | 302 | LUT  | C15-C35-C34 | 11.18  | 146.38      | 123.47   |
| 30  | A     | 813 | CL0  | C1D-ND-C4D  | -11.16 | 98.40       | 106.33   |
| 36  | 8     | 302 | LUT  | C11-C10-C9  | -11.15 | 111.39      | 127.31   |
| 36  | L     | 304 | LUT  | C18-C5-C6   | -11.09 | 112.08      | 124.53   |
| 36  | 5     | 303 | LUT  | C31-C30-C29 | -11.09 | 111.49      | 127.31   |
| 36  | 8     | 302 | LUT  | C31-C30-C29 | -11.06 | 111.53      | 127.31   |
| 36  | 4     | 303 | LUT  | C15-C14-C13 | -11.06 | 111.53      | 127.31   |
| 36  | 9     | 305 | LUT  | C18-C5-C6   | -11.05 | 112.12      | 124.53   |
| 36  | L     | 304 | LUT  | C31-C30-C29 | -11.05 | 111.54      | 127.31   |
| 36  | 6     | 303 | LUT  | C15-C14-C13 | -11.05 | 111.54      | 127.31   |
| 36  | 9     | 303 | LUT  | C31-C30-C29 | -11.05 | 111.55      | 127.31   |
| 36  | 7     | 305 | LUT  | C11-C10-C9  | -11.01 | 111.59      | 127.31   |
| 36  | 7     | 305 | LUT  | C15-C35-C34 | 11.00  | 146.02      | 123.47   |
| 36  | 8     | 303 | LUT  | C15-C35-C34 | 10.99  | 145.99      | 123.47   |
| 36  | 5     | 304 | LUT  | C18-C5-C6   | -10.97 | 112.21      | 124.53   |
| 36  | 3     | 305 | LUT  | C31-C30-C29 | -10.97 | 111.66      | 127.31   |
| 36  | 4     | 302 | LUT  | C18-C5-C6   | -10.91 | 112.28      | 124.53   |
| 36  | 9     | 302 | LUT  | C18-C5-C6   | -10.85 | 112.35      | 124.53   |
| 36  | 5     | 304 | LUT  | C31-C30-C29 | -10.84 | 111.84      | 127.31   |
| 31  | B     | 832 | CLA  | C4A-NA-C1A  | 10.84  | 111.58      | 106.71   |
| 36  | J     | 103 | LUT  | C18-C5-C6   | -10.77 | 112.43      | 124.53   |
| 36  | 5     | 303 | LUT  | C18-C5-C6   | -10.74 | 112.47      | 124.53   |
| 36  | F     | 304 | LUT  | C11-C12-C13 | 10.73  | 156.55      | 126.42   |
| 36  | L     | 304 | LUT  | C15-C14-C13 | -10.72 | 112.01      | 127.31   |
| 36  | a     | 303 | LUT  | C31-C32-C33 | 10.64  | 156.30      | 126.42   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 36  | 4     | 302 | LUT  | C11-C10-C9  | -10.61 | 112.17      | 127.31   |
| 31  | 4     | 305 | CLA  | C2C-C1C-NC  | 10.58  | 119.89      | 109.97   |
| 36  | 5     | 303 | LUT  | C11-C10-C9  | -10.58 | 112.22      | 127.31   |
| 36  | 8     | 302 | LUT  | C18-C5-C6   | -10.58 | 112.65      | 124.53   |
| 36  | 3     | 305 | LUT  | C15-C35-C34 | 10.57  | 145.12      | 123.47   |
| 31  | A     | 833 | CLA  | C4A-NA-C1A  | 10.53  | 111.44      | 106.71   |
| 31  | A     | 841 | CLA  | C4A-NA-C1A  | 10.51  | 111.43      | 106.71   |
| 36  | 4     | 303 | LUT  | C11-C10-C9  | -10.49 | 112.34      | 127.31   |
| 36  | 9     | 302 | LUT  | C15-C14-C13 | -10.48 | 112.35      | 127.31   |
| 36  | 7     | 305 | LUT  | C31-C30-C29 | -10.45 | 112.39      | 127.31   |
| 36  | 6     | 304 | LUT  | C18-C5-C6   | -10.45 | 112.79      | 124.53   |
| 31  | B     | 847 | CLA  | C4A-NA-C1A  | 10.38  | 111.37      | 106.71   |
| 31  | A     | 852 | CLA  | C4A-NA-C1A  | 10.37  | 111.37      | 106.71   |
| 36  | 9     | 305 | LUT  | C31-C32-C33 | 10.37  | 155.56      | 126.42   |
| 36  | 5     | 303 | LUT  | C35-C34-C33 | -10.35 | 112.53      | 127.31   |
| 31  | A     | 855 | CLA  | C4A-NA-C1A  | 10.34  | 111.35      | 106.71   |
| 36  | 4     | 303 | LUT  | C11-C12-C13 | 10.34  | 155.45      | 126.42   |
| 36  | b     | 301 | LUT  | C31-C30-C29 | -10.33 | 112.57      | 127.31   |
| 36  | a     | 305 | LUT  | C18-C5-C6   | -10.33 | 112.93      | 124.53   |
| 36  | 6     | 304 | LUT  | C31-C30-C29 | -10.29 | 112.63      | 127.31   |
| 36  | 9     | 302 | LUT  | C39-C29-C30 | -10.27 | 108.54      | 122.92   |
| 36  | 6     | 303 | LUT  | C11-C12-C13 | 10.26  | 155.25      | 126.42   |
| 36  | 4     | 302 | LUT  | C35-C34-C33 | -10.25 | 112.68      | 127.31   |
| 36  | 2     | 301 | LUT  | C15-C35-C34 | 10.24  | 144.46      | 123.47   |
| 36  | L     | 304 | LUT  | C11-C12-C13 | 10.24  | 155.18      | 126.42   |
| 31  | 5     | 313 | CLA  | C4A-NA-C1A  | 10.22  | 111.30      | 106.71   |
| 36  | 5     | 304 | LUT  | C11-C10-C9  | -10.18 | 112.78      | 127.31   |
| 31  | A     | 822 | CLA  | C4A-NA-C1A  | 10.17  | 111.28      | 106.71   |
| 36  | 2     | 301 | LUT  | C18-C5-C6   | -10.15 | 113.13      | 124.53   |
| 31  | B     | 829 | CLA  | C4A-NA-C1A  | 10.14  | 111.27      | 106.71   |
| 36  | L     | 304 | LUT  | C19-C9-C10  | -10.14 | 108.72      | 122.92   |
| 36  | a     | 305 | LUT  | C15-C14-C13 | -10.11 | 112.88      | 127.31   |
| 36  | J     | 103 | LUT  | C11-C12-C13 | 10.09  | 154.77      | 126.42   |
| 36  | 6     | 304 | LUT  | C15-C14-C13 | -10.08 | 112.92      | 127.31   |
| 36  | F     | 304 | LUT  | C19-C9-C10  | -10.00 | 108.92      | 122.92   |
| 31  | B     | 826 | CLA  | C4A-NA-C1A  | 9.97   | 111.19      | 106.71   |
| 36  | 9     | 303 | LUT  | C15-C35-C34 | 9.97   | 143.89      | 123.47   |
| 36  | 9     | 305 | LUT  | C20-C13-C14 | -9.96  | 108.97      | 122.92   |
| 36  | 9     | 305 | LUT  | C31-C30-C29 | -9.91  | 113.16      | 127.31   |
| 36  | a     | 305 | LUT  | C31-C30-C29 | -9.90  | 113.18      | 127.31   |
| 36  | 9     | 302 | LUT  | C31-C30-C29 | -9.89  | 113.19      | 127.31   |
| 31  | A     | 826 | CLA  | C4A-NA-C1A  | 9.87   | 111.14      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 4     | 303 | LUT  | C31-C30-C29 | -9.86 | 113.23      | 127.31   |
| 31  | 8     | 309 | CLA  | C4A-NA-C1A  | 9.83  | 111.13      | 106.71   |
| 36  | L     | 304 | LUT  | C40-C33-C34 | -9.83 | 109.15      | 122.92   |
| 31  | 3     | 317 | CLA  | C4A-NA-C1A  | 9.83  | 111.13      | 106.71   |
| 31  | A     | 851 | CLA  | C4A-NA-C1A  | 9.83  | 111.12      | 106.71   |
| 31  | b     | 303 | CLA  | C4A-NA-C1A  | 9.80  | 111.11      | 106.71   |
| 36  | a     | 303 | LUT  | C18-C5-C6   | -9.80 | 113.53      | 124.53   |
| 36  | 6     | 303 | LUT  | C31-C30-C29 | -9.79 | 113.34      | 127.31   |
| 36  | 9     | 303 | LUT  | C11-C10-C9  | -9.78 | 113.35      | 127.31   |
| 31  | B     | 845 | CLA  | C4A-NA-C1A  | 9.76  | 111.09      | 106.71   |
| 36  | 5     | 304 | LUT  | C11-C12-C13 | 9.72  | 153.72      | 126.42   |
| 31  | A     | 856 | CLA  | C4A-NA-C1A  | 9.68  | 111.06      | 106.71   |
| 31  | a     | 319 | CLA  | C4A-NA-C1A  | 9.66  | 111.05      | 106.71   |
| 31  | B     | 840 | CLA  | C4A-NA-C1A  | 9.64  | 111.04      | 106.71   |
| 31  | A     | 857 | CLA  | C4A-NA-C1A  | 9.64  | 111.04      | 106.71   |
| 36  | L     | 304 | LUT  | C35-C34-C33 | -9.63 | 113.57      | 127.31   |
| 31  | 6     | 306 | CLA  | C4A-NA-C1A  | 9.63  | 111.03      | 106.71   |
| 36  | L     | 304 | LUT  | C20-C13-C14 | -9.61 | 109.46      | 122.92   |
| 31  | 9     | 317 | CLA  | C4A-NA-C1A  | 9.61  | 111.03      | 106.71   |
| 31  | F     | 306 | CLA  | C4A-NA-C1A  | 9.59  | 111.02      | 106.71   |
| 31  | L     | 307 | CLA  | C4A-NA-C1A  | 9.58  | 111.02      | 106.71   |
| 36  | 3     | 304 | LUT  | C31-C32-C33 | 9.58  | 153.34      | 126.42   |
| 31  | A     | 814 | CLA  | C4A-NA-C1A  | 9.58  | 111.01      | 106.71   |
| 31  | B     | 823 | CLA  | C4A-NA-C1A  | 9.57  | 111.01      | 106.71   |
| 31  | 8     | 307 | CLA  | C4A-NA-C1A  | 9.52  | 110.99      | 106.71   |
| 36  | J     | 103 | LUT  | C39-C29-C30 | -9.51 | 109.60      | 122.92   |
| 36  | b     | 301 | LUT  | C40-C33-C34 | -9.51 | 109.61      | 122.92   |
| 36  | a     | 305 | LUT  | C31-C32-C33 | 9.50  | 153.11      | 126.42   |
| 31  | A     | 830 | CLA  | C4A-NA-C1A  | 9.50  | 110.97      | 106.71   |
| 31  | 3     | 308 | CLA  | C4A-NA-C1A  | 9.49  | 110.97      | 106.71   |
| 31  | 7     | 311 | CLA  | C4A-NA-C1A  | 9.46  | 110.96      | 106.71   |
| 31  | A     | 820 | CLA  | C4A-NA-C1A  | 9.44  | 110.95      | 106.71   |
| 36  | 8     | 303 | LUT  | C11-C10-C9  | -9.42 | 113.87      | 127.31   |
| 36  | 4     | 302 | LUT  | C39-C29-C30 | -9.42 | 109.73      | 122.92   |
| 31  | 3     | 320 | CLA  | C4A-NA-C1A  | 9.41  | 110.94      | 106.71   |
| 31  | 9     | 313 | CLA  | C4A-NA-C1A  | 9.40  | 110.93      | 106.71   |
| 31  | A     | 827 | CLA  | C4A-NA-C1A  | 9.38  | 110.92      | 106.71   |
| 36  | 5     | 303 | LUT  | C40-C33-C34 | -9.37 | 109.80      | 122.92   |
| 36  | b     | 301 | LUT  | C19-C9-C10  | -9.37 | 109.80      | 122.92   |
| 36  | 4     | 302 | LUT  | C31-C32-C33 | 9.37  | 152.73      | 126.42   |
| 36  | L     | 304 | LUT  | C11-C10-C9  | -9.36 | 113.95      | 127.31   |
| 30  | A     | 813 | CL0  | C2C-C1C-NC  | 9.36  | 118.74      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | J     | 105 | CLA  | C4A-NA-C1A  | 9.36  | 110.91      | 106.71   |
| 31  | b     | 302 | CLA  | C4A-NA-C1A  | 9.36  | 110.91      | 106.71   |
| 31  | A     | 825 | CLA  | C4A-NA-C1A  | 9.35  | 110.91      | 106.71   |
| 31  | F     | 301 | CLA  | C4A-NA-C1A  | 9.34  | 110.91      | 106.71   |
| 31  | B     | 824 | CLA  | C4A-NA-C1A  | 9.34  | 110.91      | 106.71   |
| 31  | b     | 307 | CLA  | C4A-NA-C1A  | 9.34  | 110.91      | 106.71   |
| 31  | 4     | 314 | CLA  | C4A-NA-C1A  | 9.33  | 110.90      | 106.71   |
| 31  | 6     | 310 | CLA  | C4A-NA-C1A  | 9.33  | 110.90      | 106.71   |
| 36  | a     | 305 | LUT  | C20-C13-C14 | -9.31 | 109.88      | 122.92   |
| 31  | 7     | 321 | CLA  | C4A-NA-C1A  | 9.31  | 110.89      | 106.71   |
| 36  | 6     | 303 | LUT  | C40-C33-C34 | -9.29 | 109.90      | 122.92   |
| 36  | J     | 103 | LUT  | C19-C9-C10  | -9.29 | 109.91      | 122.92   |
| 31  | B     | 825 | CLA  | C4A-NA-C1A  | 9.28  | 110.88      | 106.71   |
| 36  | 9     | 305 | LUT  | C40-C33-C34 | -9.28 | 109.92      | 122.92   |
| 36  | a     | 305 | LUT  | C39-C29-C30 | -9.25 | 109.96      | 122.92   |
| 31  | B     | 811 | CLA  | C4A-NA-C1A  | 9.25  | 110.86      | 106.71   |
| 31  | 4     | 316 | CLA  | C4A-NA-C1A  | 9.25  | 110.86      | 106.71   |
| 31  | 6     | 313 | CLA  | C4A-NA-C1A  | 9.24  | 110.86      | 106.71   |
| 36  | F     | 304 | LUT  | C35-C34-C33 | -9.23 | 114.14      | 127.31   |
| 36  | 6     | 303 | LUT  | C31-C32-C33 | 9.20  | 152.27      | 126.42   |
| 36  | 9     | 305 | LUT  | C19-C9-C10  | -9.19 | 110.05      | 122.92   |
| 36  | L     | 304 | LUT  | C31-C32-C33 | 9.18  | 152.21      | 126.42   |
| 31  | 3     | 313 | CLA  | C4A-NA-C1A  | 9.18  | 110.83      | 106.71   |
| 36  | 3     | 305 | LUT  | C31-C32-C33 | 9.16  | 152.14      | 126.42   |
| 31  | A     | 842 | CLA  | C4A-NA-C1A  | 9.16  | 110.82      | 106.71   |
| 31  | 5     | 321 | CLA  | C4A-NA-C1A  | 9.15  | 110.82      | 106.71   |
| 36  | 4     | 303 | LUT  | C19-C9-C10  | -9.15 | 110.11      | 122.92   |
| 36  | 9     | 305 | LUT  | C39-C29-C30 | -9.15 | 110.11      | 122.92   |
| 36  | 8     | 302 | LUT  | C40-C33-C34 | -9.14 | 110.12      | 122.92   |
| 36  | 7     | 305 | LUT  | C31-C32-C33 | 9.13  | 152.06      | 126.42   |
| 36  | 5     | 303 | LUT  | C39-C29-C30 | -9.12 | 110.14      | 122.92   |
| 31  | B     | 816 | CLA  | C4A-NA-C1A  | 9.12  | 110.81      | 106.71   |
| 36  | J     | 103 | LUT  | C20-C13-C14 | -9.10 | 110.17      | 122.92   |
| 31  | 8     | 312 | CLA  | C4A-NA-C1A  | 9.10  | 110.80      | 106.71   |
| 36  | 9     | 305 | LUT  | C11-C12-C13 | 9.08  | 151.92      | 126.42   |
| 36  | 9     | 302 | LUT  | C35-C34-C33 | -9.08 | 114.36      | 127.31   |
| 31  | B     | 835 | CLA  | C4A-NA-C1A  | 9.05  | 110.77      | 106.71   |
| 31  | 5     | 312 | CLA  | C4A-NA-C1A  | 9.04  | 110.77      | 106.71   |
| 31  | 5     | 323 | CLA  | C4A-NA-C1A  | 9.04  | 110.77      | 106.71   |
| 31  | 6     | 315 | CLA  | C4A-NA-C1A  | 9.04  | 110.77      | 106.71   |
| 31  | 9     | 316 | CLA  | C4A-NA-C1A  | 9.03  | 110.76      | 106.71   |
| 36  | F     | 304 | LUT  | C15-C14-C13 | -9.02 | 114.43      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | J     | 103 | LUT  | C40-C33-C34 | -9.02 | 110.29      | 122.92   |
| 31  | 7     | 316 | CLA  | C4A-NA-C1A  | 9.02  | 110.76      | 106.71   |
| 31  | B     | 846 | CLA  | C4A-NA-C1A  | 9.01  | 110.75      | 106.71   |
| 31  | 2     | 310 | CLA  | C4A-NA-C1A  | 9.01  | 110.75      | 106.71   |
| 31  | O     | 204 | CLA  | C4A-NA-C1A  | 9.00  | 110.75      | 106.71   |
| 36  | 2     | 301 | LUT  | C40-C33-C34 | -9.00 | 110.31      | 122.92   |
| 31  | A     | 854 | CLA  | C4A-NA-C1A  | 9.00  | 110.75      | 106.71   |
| 36  | 6     | 303 | LUT  | C11-C10-C9  | -8.98 | 114.49      | 127.31   |
| 31  | A     | 828 | CLA  | C4A-NA-C1A  | 8.98  | 110.74      | 106.71   |
| 31  | A     | 837 | CLA  | C4A-NA-C1A  | 8.97  | 110.74      | 106.71   |
| 31  | A     | 821 | CLA  | C4A-NA-C1A  | 8.97  | 110.74      | 106.71   |
| 36  | 6     | 304 | LUT  | C11-C12-C13 | 8.96  | 151.60      | 126.42   |
| 31  | B     | 818 | CLA  | C4A-NA-C1A  | 8.96  | 110.74      | 106.71   |
| 31  | a     | 311 | CLA  | C4A-NA-C1A  | 8.96  | 110.73      | 106.71   |
| 36  | 9     | 302 | LUT  | C31-C32-C33 | 8.94  | 151.54      | 126.42   |
| 31  | 2     | 312 | CLA  | C4A-NA-C1A  | 8.94  | 110.73      | 106.71   |
| 31  | 9     | 312 | CLA  | C4A-NA-C1A  | 8.94  | 110.72      | 106.71   |
| 36  | a     | 303 | LUT  | C39-C29-C30 | -8.94 | 110.41      | 122.92   |
| 31  | A     | 835 | CLA  | C4A-NA-C1A  | 8.93  | 110.72      | 106.71   |
| 31  | A     | 843 | CLA  | C4A-NA-C1A  | 8.93  | 110.72      | 106.71   |
| 31  | A     | 850 | CLA  | C4A-NA-C1A  | 8.93  | 110.72      | 106.71   |
| 31  | 5     | 309 | CLA  | C4A-NA-C1A  | 8.93  | 110.72      | 106.71   |
| 36  | 8     | 303 | LUT  | C38-C25-C24 | -8.93 | 104.46      | 123.56   |
| 31  | L     | 305 | CLA  | C4A-NA-C1A  | 8.93  | 110.72      | 106.71   |
| 31  | 2     | 315 | CLA  | C4A-NA-C1A  | 8.93  | 110.72      | 106.71   |
| 36  | 9     | 305 | LUT  | C11-C10-C9  | -8.92 | 114.58      | 127.31   |
| 36  | 5     | 303 | LUT  | C31-C32-C33 | 8.92  | 151.48      | 126.42   |
| 31  | A     | 853 | CLA  | C4A-NA-C1A  | 8.92  | 110.72      | 106.71   |
| 31  | B     | 843 | CLA  | C4A-NA-C1A  | 8.92  | 110.72      | 106.71   |
| 36  | 2     | 301 | LUT  | C31-C32-C33 | 8.91  | 151.45      | 126.42   |
| 36  | b     | 301 | LUT  | C31-C32-C33 | 8.91  | 151.45      | 126.42   |
| 36  | 6     | 303 | LUT  | C39-C29-C30 | -8.91 | 110.44      | 122.92   |
| 31  | B     | 822 | CLA  | C4A-NA-C1A  | 8.90  | 110.71      | 106.71   |
| 36  | 5     | 304 | LUT  | C40-C33-C34 | -8.90 | 110.45      | 122.92   |
| 31  | 6     | 308 | CLA  | C4A-NA-C1A  | 8.89  | 110.70      | 106.71   |
| 36  | 4     | 302 | LUT  | C40-C33-C34 | -8.89 | 110.47      | 122.92   |
| 36  | 6     | 303 | LUT  | C19-C9-C10  | -8.89 | 110.47      | 122.92   |
| 36  | 9     | 303 | LUT  | C1-C6-C5    | -8.89 | 110.09      | 122.61   |
| 31  | 4     | 318 | CLA  | C4A-NA-C1A  | 8.89  | 110.70      | 106.71   |
| 36  | L     | 304 | LUT  | C39-C29-C30 | -8.88 | 110.48      | 122.92   |
| 36  | 5     | 304 | LUT  | C15-C14-C13 | -8.88 | 114.63      | 127.31   |
| 36  | 2     | 301 | LUT  | C20-C13-C14 | -8.87 | 110.50      | 122.92   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 3     | 304 | LUT  | C40-C33-C34 | -8.85 | 110.52      | 122.92   |
| 31  | A     | 845 | CLA  | C4A-NA-C1A  | 8.84  | 110.68      | 106.71   |
| 31  | A     | 846 | CLA  | C4A-NA-C1A  | 8.83  | 110.67      | 106.71   |
| 31  | 7     | 310 | CLA  | C4A-NA-C1A  | 8.82  | 110.67      | 106.71   |
| 36  | F     | 304 | LUT  | C20-C13-C14 | -8.80 | 110.59      | 122.92   |
| 31  | 8     | 310 | CLA  | C4A-NA-C1A  | 8.80  | 110.66      | 106.71   |
| 36  | a     | 303 | LUT  | C31-C30-C29 | -8.76 | 114.81      | 127.31   |
| 31  | A     | 817 | CLA  | C4A-NA-C1A  | 8.75  | 110.64      | 106.71   |
| 36  | F     | 304 | LUT  | C40-C33-C34 | -8.75 | 110.66      | 122.92   |
| 36  | 8     | 302 | LUT  | C31-C32-C33 | 8.75  | 150.99      | 126.42   |
| 31  | a     | 310 | CLA  | C4A-NA-C1A  | 8.75  | 110.64      | 106.71   |
| 36  | 9     | 302 | LUT  | C20-C13-C14 | -8.74 | 110.67      | 122.92   |
| 36  | b     | 301 | LUT  | C35-C34-C33 | -8.74 | 114.83      | 127.31   |
| 36  | 3     | 304 | LUT  | C39-C29-C30 | -8.74 | 110.68      | 122.92   |
| 31  | 2     | 305 | CLA  | C4A-NA-C1A  | 8.74  | 110.64      | 106.71   |
| 31  | B     | 842 | CLA  | C4A-NA-C1A  | 8.74  | 110.63      | 106.71   |
| 36  | b     | 301 | LUT  | C15-C14-C13 | -8.72 | 114.87      | 127.31   |
| 31  | b     | 312 | CLA  | C4A-NA-C1A  | 8.71  | 110.62      | 106.71   |
| 36  | 2     | 301 | LUT  | C32-C33-C34 | -8.71 | 105.57      | 118.94   |
| 31  | F     | 305 | CLA  | C4A-NA-C1A  | 8.71  | 110.62      | 106.71   |
| 36  | a     | 305 | LUT  | C40-C33-C34 | -8.71 | 110.73      | 122.92   |
| 31  | 5     | 308 | CLA  | C4A-NA-C1A  | 8.70  | 110.62      | 106.71   |
| 31  | H     | 901 | CLA  | C4A-NA-C1A  | 8.69  | 110.61      | 106.71   |
| 31  | 5     | 320 | CLA  | C4A-NA-C1A  | 8.69  | 110.61      | 106.71   |
| 31  | 2     | 311 | CLA  | C4A-NA-C1A  | 8.68  | 110.61      | 106.71   |
| 31  | 6     | 311 | CLA  | C4A-NA-C1A  | 8.68  | 110.61      | 106.71   |
| 36  | 2     | 301 | LUT  | C39-C29-C30 | -8.68 | 110.77      | 122.92   |
| 31  | A     | 818 | CLA  | C4A-NA-C1A  | 8.67  | 110.61      | 106.71   |
| 31  | a     | 312 | CLA  | C4A-NA-C1A  | 8.65  | 110.60      | 106.71   |
| 36  | 9     | 302 | LUT  | C11-C12-C13 | 8.64  | 150.70      | 126.42   |
| 31  | A     | 819 | CLA  | C4A-NA-C1A  | 8.64  | 110.59      | 106.71   |
| 31  | B     | 813 | CLA  | C4A-NA-C1A  | 8.63  | 110.59      | 106.71   |
| 31  | A     | 824 | CLA  | C4A-NA-C1A  | 8.63  | 110.58      | 106.71   |
| 36  | 9     | 303 | LUT  | C19-C9-C10  | -8.63 | 110.84      | 122.92   |
| 36  | 9     | 303 | LUT  | C11-C12-C13 | 8.61  | 150.59      | 126.42   |
| 32  | A     | 839 | CHL  | O2D-CGD-O1D | -8.60 | 107.02      | 123.84   |
| 36  | 5     | 304 | LUT  | C19-C9-C10  | -8.60 | 110.88      | 122.92   |
| 31  | A     | 836 | CLA  | C4A-NA-C1A  | 8.59  | 110.57      | 106.71   |
| 31  | a     | 315 | CLA  | C4A-NA-C1A  | 8.59  | 110.57      | 106.71   |
| 31  | 9     | 318 | CLA  | C4A-NA-C1A  | 8.58  | 110.56      | 106.71   |
| 36  | F     | 304 | LUT  | C31-C32-C33 | 8.58  | 150.51      | 126.42   |
| 31  | 9     | 321 | CLA  | C4A-NA-C1A  | 8.55  | 110.55      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | K     | 206 | CLA  | C4A-NA-C1A  | 8.55  | 110.55      | 106.71   |
| 36  | b     | 301 | LUT  | C39-C29-C30 | -8.55 | 110.95      | 122.92   |
| 36  | 5     | 304 | LUT  | C31-C32-C33 | 8.54  | 150.42      | 126.42   |
| 31  | 3     | 312 | CLA  | C4A-NA-C1A  | 8.54  | 110.55      | 106.71   |
| 31  | 6     | 314 | CLA  | C4A-NA-C1A  | 8.52  | 110.54      | 106.71   |
| 31  | B     | 838 | CLA  | C4A-NA-C1A  | 8.52  | 110.54      | 106.71   |
| 36  | 4     | 302 | LUT  | C19-C9-C10  | -8.51 | 111.00      | 122.92   |
| 36  | 4     | 302 | LUT  | C20-C13-C14 | -8.51 | 111.00      | 122.92   |
| 31  | B     | 812 | CLA  | C4A-NA-C1A  | 8.49  | 110.52      | 106.71   |
| 36  | 6     | 303 | LUT  | C20-C13-C14 | -8.49 | 111.04      | 122.92   |
| 31  | K     | 205 | CLA  | C4A-NA-C1A  | 8.47  | 110.51      | 106.71   |
| 31  | 7     | 314 | CLA  | C4A-NA-C1A  | 8.46  | 110.51      | 106.71   |
| 31  | 5     | 314 | CLA  | C4A-NA-C1A  | 8.46  | 110.51      | 106.71   |
| 31  | B     | 850 | CLA  | C4A-NA-C1A  | 8.45  | 110.51      | 106.71   |
| 31  | G     | 204 | CLA  | C4A-NA-C1A  | 8.43  | 110.49      | 106.71   |
| 36  | F     | 304 | LUT  | C12-C13-C14 | -8.42 | 106.01      | 118.94   |
| 31  | B     | 819 | CLA  | C4A-NA-C1A  | 8.42  | 110.49      | 106.71   |
| 31  | B     | 814 | CLA  | C4A-NA-C1A  | 8.41  | 110.49      | 106.71   |
| 36  | 8     | 302 | LUT  | C39-C29-C30 | -8.40 | 111.16      | 122.92   |
| 31  | G     | 205 | CLA  | C4A-NA-C1A  | 8.37  | 110.47      | 106.71   |
| 31  | 7     | 322 | CLA  | C4A-NA-C1A  | 8.37  | 110.47      | 106.71   |
| 31  | B     | 815 | CLA  | C4A-NA-C1A  | 8.36  | 110.46      | 106.71   |
| 36  | 3     | 304 | LUT  | C35-C34-C33 | -8.36 | 115.38      | 127.31   |
| 31  | 4     | 311 | CLA  | C4A-NA-C1A  | 8.35  | 110.46      | 106.71   |
| 36  | 3     | 304 | LUT  | C32-C33-C34 | -8.35 | 106.12      | 118.94   |
| 31  | 4     | 319 | CLA  | C4A-NA-C1A  | 8.35  | 110.46      | 106.71   |
| 36  | 5     | 303 | LUT  | C20-C13-C14 | -8.35 | 111.22      | 122.92   |
| 31  | 3     | 309 | CLA  | C4A-NA-C1A  | 8.34  | 110.45      | 106.71   |
| 31  | 2     | 314 | CLA  | C4A-NA-C1A  | 8.34  | 110.45      | 106.71   |
| 36  | 7     | 305 | LUT  | C35-C34-C33 | -8.33 | 115.42      | 127.31   |
| 31  | A     | 849 | CLA  | C4A-NA-C1A  | 8.32  | 110.45      | 106.71   |
| 36  | b     | 301 | LUT  | C11-C12-C13 | 8.32  | 149.78      | 126.42   |
| 31  | 3     | 310 | CLA  | C4A-NA-C1A  | 8.31  | 110.44      | 106.71   |
| 31  | B     | 820 | CLA  | C4A-NA-C1A  | 8.31  | 110.44      | 106.71   |
| 31  | B     | 844 | CLA  | C4A-NA-C1A  | 8.30  | 110.44      | 106.71   |
| 31  | H     | 902 | CLA  | C4A-NA-C1A  | 8.29  | 110.43      | 106.71   |
| 31  | B     | 848 | CLA  | C4A-NA-C1A  | 8.28  | 110.43      | 106.71   |
| 31  | 8     | 313 | CLA  | C4A-NA-C1A  | 8.28  | 110.43      | 106.71   |
| 31  | 8     | 317 | CLA  | C4A-NA-C1A  | 8.28  | 110.43      | 106.71   |
| 31  | A     | 844 | CLA  | C4A-NA-C1A  | 8.27  | 110.43      | 106.71   |
| 31  | 8     | 311 | CLA  | C4A-NA-C1A  | 8.27  | 110.42      | 106.71   |
| 31  | 9     | 319 | CLA  | C4A-NA-C1A  | 8.27  | 110.42      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 312 | CLA  | C4A-NA-C1A  | 8.27  | 110.42      | 106.71   |
| 31  | B     | 828 | CLA  | C4A-NA-C1A  | 8.26  | 110.42      | 106.71   |
| 31  | H     | 903 | CLA  | C4A-NA-C1A  | 8.26  | 110.42      | 106.71   |
| 31  | 7     | 312 | CLA  | C4A-NA-C1A  | 8.26  | 110.42      | 106.71   |
| 31  | 7     | 315 | CLA  | C4A-NA-C1A  | 8.25  | 110.42      | 106.71   |
| 36  | 6     | 304 | LUT  | C19-C9-C10  | -8.25 | 111.36      | 122.92   |
| 36  | 9     | 302 | LUT  | C40-C33-C34 | -8.24 | 111.39      | 122.92   |
| 36  | 3     | 304 | LUT  | C20-C13-C14 | -8.23 | 111.39      | 122.92   |
| 36  | 5     | 303 | LUT  | C11-C12-C13 | 8.23  | 149.53      | 126.42   |
| 36  | 7     | 305 | LUT  | C39-C29-C30 | -8.22 | 111.40      | 122.92   |
| 31  | 4     | 308 | CLA  | C4A-NA-C1A  | 8.22  | 110.40      | 106.71   |
| 36  | 6     | 304 | LUT  | C38-C25-C24 | -8.22 | 105.97      | 123.56   |
| 36  | F     | 304 | LUT  | C32-C33-C34 | -8.22 | 106.33      | 118.94   |
| 31  | B     | 817 | CLA  | C4A-NA-C1A  | 8.22  | 110.40      | 106.71   |
| 36  | 4     | 302 | LUT  | C11-C12-C13 | 8.21  | 149.49      | 126.42   |
| 31  | B     | 836 | CLA  | C4A-NA-C1A  | 8.21  | 110.40      | 106.71   |
| 31  | B     | 849 | CLA  | C4A-NA-C1A  | 8.20  | 110.39      | 106.71   |
| 36  | 4     | 303 | LUT  | C1-C6-C5    | -8.20 | 111.07      | 122.61   |
| 32  | K     | 201 | CHL  | CMD-C2D-C1D | 8.19  | 139.14      | 124.71   |
| 36  | a     | 305 | LUT  | C35-C34-C33 | -8.18 | 115.63      | 127.31   |
| 36  | 4     | 303 | LUT  | C39-C29-C30 | -8.18 | 111.46      | 122.92   |
| 36  | 7     | 305 | LUT  | C20-C13-C14 | -8.18 | 111.46      | 122.92   |
| 31  | a     | 314 | CLA  | C4A-NA-C1A  | 8.18  | 110.38      | 106.71   |
| 36  | 3     | 305 | LUT  | C39-C29-C30 | -8.18 | 111.47      | 122.92   |
| 36  | 7     | 305 | LUT  | C40-C33-C34 | -8.18 | 111.47      | 122.92   |
| 31  | A     | 847 | CLA  | C4A-NA-C1A  | 8.16  | 110.37      | 106.71   |
| 36  | 6     | 304 | LUT  | C31-C32-C33 | 8.15  | 149.32      | 126.42   |
| 31  | b     | 311 | CLA  | C4A-NA-C1A  | 8.15  | 110.37      | 106.71   |
| 36  | a     | 303 | LUT  | C40-C33-C34 | -8.14 | 111.51      | 122.92   |
| 31  | 2     | 308 | CLA  | C4A-NA-C1A  | 8.14  | 110.36      | 106.71   |
| 31  | 6     | 316 | CLA  | C4A-NA-C1A  | 8.13  | 110.36      | 106.71   |
| 36  | 9     | 303 | LUT  | C20-C13-C14 | -8.10 | 111.58      | 122.92   |
| 36  | 5     | 304 | LUT  | C35-C34-C33 | -8.10 | 115.75      | 127.31   |
| 36  | 3     | 305 | LUT  | C32-C33-C34 | -8.09 | 106.53      | 118.94   |
| 31  | O     | 203 | CLA  | C4A-NA-C1A  | 8.08  | 110.34      | 106.71   |
| 36  | 6     | 304 | LUT  | C20-C13-C14 | -8.08 | 111.60      | 122.92   |
| 31  | B     | 821 | CLA  | C4A-NA-C1A  | 8.08  | 110.34      | 106.71   |
| 36  | 5     | 304 | LUT  | C38-C25-C24 | -8.07 | 106.29      | 123.56   |
| 36  | 4     | 303 | LUT  | C31-C32-C33 | 8.06  | 149.07      | 126.42   |
| 31  | 5     | 310 | CLA  | C4A-NA-C1A  | 8.06  | 110.33      | 106.71   |
| 31  | A     | 815 | CLA  | C4A-NA-C1A  | 8.04  | 110.32      | 106.71   |
| 31  | a     | 313 | CLA  | C4A-NA-C1A  | 8.02  | 110.31      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 8     | 303 | LUT  | C31-C32-C33 | 8.02  | 148.94      | 126.42   |
| 31  | 2     | 307 | CLA  | C4A-NA-C1A  | 8.01  | 110.31      | 106.71   |
| 36  | J     | 103 | LUT  | C31-C32-C33 | 8.01  | 148.90      | 126.42   |
| 31  | A     | 823 | CLA  | C4A-NA-C1A  | 8.00  | 110.30      | 106.71   |
| 31  | 8     | 321 | CLA  | C4A-NA-C1A  | 8.00  | 110.30      | 106.71   |
| 31  | 9     | 314 | CLA  | C4A-NA-C1A  | 7.99  | 110.30      | 106.71   |
| 31  | 4     | 305 | CLA  | CMD-C2D-C1D | 7.99  | 138.80      | 124.71   |
| 36  | 2     | 301 | LUT  | C8-C9-C10   | -7.99 | 106.68      | 118.94   |
| 36  | 5     | 303 | LUT  | C19-C9-C10  | -7.99 | 111.73      | 122.92   |
| 31  | B     | 834 | CLA  | C4A-NA-C1A  | 7.98  | 110.30      | 106.71   |
| 31  | 4     | 307 | CLA  | C4A-NA-C1A  | 7.98  | 110.29      | 106.71   |
| 31  | A     | 816 | CLA  | C4A-NA-C1A  | 7.97  | 110.29      | 106.71   |
| 31  | B     | 839 | CLA  | C4A-NA-C1A  | 7.97  | 110.29      | 106.71   |
| 31  | 5     | 315 | CLA  | C4A-NA-C1A  | 7.96  | 110.29      | 106.71   |
| 31  | 7     | 313 | CLA  | C4A-NA-C1A  | 7.95  | 110.28      | 106.71   |
| 32  | A     | 839 | CHL  | O1D-CGD-CBD | -7.95 | 108.22      | 124.48   |
| 31  | A     | 832 | CLA  | C4A-NA-C1A  | 7.94  | 110.27      | 106.71   |
| 31  | B     | 830 | CLA  | C4A-NA-C1A  | 7.93  | 110.27      | 106.71   |
| 31  | B     | 833 | CLA  | C4A-NA-C1A  | 7.92  | 110.27      | 106.71   |
| 36  | 3     | 305 | LUT  | C20-C13-C14 | -7.91 | 111.85      | 122.92   |
| 36  | b     | 301 | LUT  | C38-C25-C24 | -7.89 | 106.68      | 123.56   |
| 36  | 9     | 302 | LUT  | C38-C25-C24 | -7.89 | 106.68      | 123.56   |
| 36  | 6     | 304 | LUT  | C8-C9-C10   | -7.89 | 106.83      | 118.94   |
| 31  | b     | 310 | CLA  | C4A-NA-C1A  | 7.89  | 110.25      | 106.71   |
| 36  | 5     | 304 | LUT  | C39-C29-C30 | -7.86 | 111.91      | 122.92   |
| 36  | a     | 303 | LUT  | C20-C13-C14 | -7.85 | 111.92      | 122.92   |
| 36  | 3     | 305 | LUT  | C40-C33-C34 | -7.85 | 111.92      | 122.92   |
| 36  | 2     | 301 | LUT  | C19-C9-C10  | -7.85 | 111.92      | 122.92   |
| 32  | K     | 201 | CHL  | C2C-C3C-C4C | -7.84 | 100.90      | 106.49   |
| 31  | 8     | 315 | CLA  | C4A-NA-C1A  | 7.83  | 110.23      | 106.71   |
| 31  | 8     | 314 | CLA  | C4A-NA-C1A  | 7.82  | 110.22      | 106.71   |
| 31  | a     | 321 | CLA  | C4A-NA-C1A  | 7.82  | 110.22      | 106.71   |
| 36  | 8     | 302 | LUT  | C19-C9-C10  | -7.81 | 111.98      | 122.92   |
| 36  | 4     | 303 | LUT  | C20-C13-C14 | -7.80 | 111.99      | 122.92   |
| 31  | 8     | 318 | CLA  | C4A-NA-C1A  | 7.80  | 110.21      | 106.71   |
| 31  | B     | 837 | CLA  | C4A-NA-C1A  | 7.79  | 110.21      | 106.71   |
| 36  | 3     | 304 | LUT  | C19-C9-C10  | -7.76 | 112.05      | 122.92   |
| 36  | F     | 304 | LUT  | C39-C29-C30 | -7.76 | 112.05      | 122.92   |
| 31  | 2     | 309 | CLA  | C4A-NA-C1A  | 7.75  | 110.19      | 106.71   |
| 36  | 6     | 304 | LUT  | C11-C10-C9  | -7.73 | 116.28      | 127.31   |
| 31  | 4     | 305 | CLA  | C3C-C4C-NC  | 7.70  | 119.21      | 110.57   |
| 36  | 2     | 301 | LUT  | C38-C25-C24 | -7.70 | 107.09      | 123.56   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 4     | 303 | LUT  | C40-C33-C34 | -7.70 | 112.14      | 122.92   |
| 31  | K     | 204 | CLA  | C4A-NA-C1A  | 7.69  | 110.16      | 106.71   |
| 32  | 7     | 319 | CHL  | O2D-CGD-CBD | 7.69  | 124.93      | 111.27   |
| 36  | 6     | 303 | LUT  | C1-C6-C5    | -7.69 | 111.79      | 122.61   |
| 36  | 7     | 305 | LUT  | C11-C12-C13 | 7.68  | 147.99      | 126.42   |
| 31  | 3     | 311 | CLA  | C4A-NA-C1A  | 7.67  | 110.15      | 106.71   |
| 36  | 3     | 305 | LUT  | C38-C25-C24 | -7.66 | 107.18      | 123.56   |
| 31  | A     | 829 | CLA  | CMD-C2D-C1D | 7.64  | 138.18      | 124.71   |
| 36  | 2     | 301 | LUT  | C20-C13-C12 | -7.64 | 106.04      | 118.08   |
| 31  | 9     | 315 | CLA  | C4A-NA-C1A  | 7.63  | 110.14      | 106.71   |
| 31  | a     | 309 | CLA  | C4A-NA-C1A  | 7.63  | 110.14      | 106.71   |
| 31  | L     | 306 | CLA  | C4A-NA-C1A  | 7.62  | 110.13      | 106.71   |
| 36  | 3     | 305 | LUT  | C19-C9-C10  | -7.62 | 112.25      | 122.92   |
| 31  | 4     | 320 | CLA  | C4A-NA-C1A  | 7.62  | 110.13      | 106.71   |
| 36  | 6     | 303 | LUT  | C32-C33-C34 | -7.60 | 107.28      | 118.94   |
| 36  | a     | 303 | LUT  | C19-C9-C10  | -7.58 | 112.31      | 122.92   |
| 36  | 7     | 305 | LUT  | C38-C25-C24 | -7.58 | 107.35      | 123.56   |
| 31  | 4     | 309 | CLA  | C4A-NA-C1A  | 7.58  | 110.11      | 106.71   |
| 31  | 3     | 316 | CLA  | C4A-NA-C1A  | 7.57  | 110.11      | 106.71   |
| 36  | b     | 301 | LUT  | C40-C33-C32 | -7.57 | 106.15      | 118.08   |
| 31  | b     | 308 | CLA  | C4A-NA-C1A  | 7.57  | 110.11      | 106.71   |
| 36  | 8     | 303 | LUT  | C19-C9-C10  | -7.55 | 112.35      | 122.92   |
| 36  | a     | 303 | LUT  | C38-C25-C24 | -7.55 | 107.41      | 123.56   |
| 32  | A     | 831 | CHL  | O2D-CGD-O1D | -7.55 | 109.09      | 123.84   |
| 36  | 8     | 303 | LUT  | C20-C13-C14 | -7.54 | 112.36      | 122.92   |
| 36  | 8     | 303 | LUT  | C40-C33-C34 | -7.52 | 112.39      | 122.92   |
| 36  | a     | 303 | LUT  | C32-C33-C34 | -7.52 | 107.40      | 118.94   |
| 31  | 4     | 321 | CLA  | C4A-NA-C1A  | 7.51  | 110.08      | 106.71   |
| 31  | 6     | 306 | CLA  | CMD-C2D-C1D | 7.51  | 137.94      | 124.71   |
| 36  | a     | 305 | LUT  | C11-C10-C9  | -7.50 | 116.60      | 127.31   |
| 31  | O     | 202 | CLA  | C4A-NA-C1A  | 7.49  | 110.08      | 106.71   |
| 31  | B     | 831 | CLA  | C4A-NA-C1A  | 7.48  | 110.07      | 106.71   |
| 36  | 9     | 303 | LUT  | C38-C25-C24 | -7.47 | 107.58      | 123.56   |
| 36  | a     | 303 | LUT  | C8-C9-C10   | -7.47 | 107.48      | 118.94   |
| 36  | 5     | 303 | LUT  | C38-C25-C24 | -7.45 | 107.63      | 123.56   |
| 31  | B     | 827 | CLA  | C4A-NA-C1A  | 7.44  | 110.05      | 106.71   |
| 31  | 5     | 311 | CLA  | C4A-NA-C1A  | 7.44  | 110.05      | 106.71   |
| 31  | 8     | 308 | CLA  | C4A-NA-C1A  | 7.43  | 110.05      | 106.71   |
| 36  | 8     | 302 | LUT  | C8-C9-C10   | -7.43 | 107.54      | 118.94   |
| 36  | b     | 301 | LUT  | C20-C13-C14 | -7.43 | 112.52      | 122.92   |
| 31  | b     | 306 | CLA  | C4A-NA-C1A  | 7.42  | 110.04      | 106.71   |
| 31  | 2     | 313 | CLA  | C4A-NA-C1A  | 7.42  | 110.04      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 8     | 302 | LUT  | C35-C34-C33 | -7.42 | 116.71      | 127.31   |
| 36  | 4     | 303 | LUT  | C38-C25-C24 | -7.42 | 107.69      | 123.56   |
| 36  | 9     | 302 | LUT  | C19-C9-C10  | -7.40 | 112.56      | 122.92   |
| 36  | 5     | 304 | LUT  | C20-C13-C14 | -7.39 | 112.56      | 122.92   |
| 31  | 6     | 322 | CLA  | C4A-NA-C1A  | 7.39  | 110.03      | 106.71   |
| 36  | 3     | 304 | LUT  | C11-C12-C13 | 7.39  | 147.17      | 126.42   |
| 36  | 7     | 305 | LUT  | C32-C33-C34 | -7.37 | 107.62      | 118.94   |
| 31  | G     | 206 | CLA  | C4A-NA-C1A  | 7.36  | 110.01      | 106.71   |
| 32  | 3     | 315 | CHL  | O2D-CGD-O1D | -7.34 | 109.49      | 123.84   |
| 36  | 6     | 304 | LUT  | C40-C33-C34 | -7.34 | 112.64      | 122.92   |
| 32  | 6     | 319 | CHL  | O2D-CGD-CBD | 7.32  | 124.28      | 111.27   |
| 31  | b     | 304 | CLA  | C4A-NA-C1A  | 7.32  | 110.00      | 106.71   |
| 31  | 6     | 306 | CLA  | CHD-C1D-ND  | -7.29 | 117.76      | 124.45   |
| 36  | 8     | 302 | LUT  | C20-C13-C14 | -7.27 | 112.74      | 122.92   |
| 31  | a     | 322 | CLA  | C4A-NA-C1A  | 7.26  | 109.97      | 106.71   |
| 31  | 3     | 318 | CLA  | C4A-NA-C1A  | 7.26  | 109.97      | 106.71   |
| 36  | 6     | 304 | LUT  | C39-C29-C30 | -7.26 | 112.76      | 122.92   |
| 31  | 3     | 307 | CLA  | C4A-NA-C1A  | 7.24  | 109.96      | 106.71   |
| 36  | 6     | 303 | LUT  | C35-C34-C33 | -7.24 | 116.98      | 127.31   |
| 31  | 6     | 312 | CLA  | C4A-NA-C1A  | 7.22  | 109.95      | 106.71   |
| 31  | 4     | 315 | CLA  | C4A-NA-C1A  | 7.21  | 109.95      | 106.71   |
| 36  | 8     | 302 | LUT  | C11-C12-C13 | 7.17  | 146.56      | 126.42   |
| 36  | a     | 303 | LUT  | C11-C12-C13 | 7.16  | 146.54      | 126.42   |
| 36  | 5     | 303 | LUT  | C20-C13-C12 | -7.16 | 106.79      | 118.08   |
| 36  | 6     | 304 | LUT  | C35-C34-C33 | -7.15 | 117.11      | 127.31   |
| 31  | B     | 841 | CLA  | C4A-NA-C1A  | 7.15  | 109.92      | 106.71   |
| 36  | F     | 304 | LUT  | C35-C15-C14 | -7.15 | 108.84      | 123.47   |
| 36  | b     | 301 | LUT  | C20-C13-C12 | -7.14 | 106.83      | 118.08   |
| 32  | A     | 831 | CHL  | O1D-CGD-CBD | -7.14 | 109.87      | 124.48   |
| 31  | 4     | 306 | CLA  | C4A-NA-C1A  | 7.11  | 109.90      | 106.71   |
| 36  | 8     | 303 | LUT  | C40-C33-C32 | -7.11 | 106.88      | 118.08   |
| 36  | 6     | 303 | LUT  | C20-C13-C12 | -7.10 | 106.89      | 118.08   |
| 31  | 9     | 317 | CLA  | CMD-C2D-C1D | 7.09  | 137.22      | 124.71   |
| 31  | 2     | 304 | CLA  | C4A-NA-C1A  | 7.09  | 109.89      | 106.71   |
| 36  | 8     | 302 | LUT  | C20-C13-C12 | -7.09 | 106.91      | 118.08   |
| 32  | A     | 839 | CHL  | C4A-NA-C1A  | 7.09  | 109.89      | 106.71   |
| 36  | 9     | 303 | LUT  | C40-C33-C34 | -7.06 | 113.03      | 122.92   |
| 36  | 9     | 303 | LUT  | C39-C29-C30 | -7.06 | 113.03      | 122.92   |
| 36  | 8     | 303 | LUT  | C39-C29-C30 | -7.06 | 113.03      | 122.92   |
| 31  | 8     | 320 | CLA  | C4A-NA-C1A  | 7.05  | 109.88      | 106.71   |
| 32  | 7     | 319 | CHL  | O2D-CGD-O1D | -7.03 | 110.09      | 123.84   |
| 32  | 7     | 324 | CHL  | C4A-NA-C1A  | 7.00  | 109.85      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 8     | 303 | LUT  | C20-C13-C12 | -6.99 | 107.07      | 118.08   |
| 31  | A     | 848 | CLA  | C4A-NA-C1A  | 6.99  | 109.85      | 106.71   |
| 36  | 6     | 303 | LUT  | C38-C25-C24 | -6.98 | 108.62      | 123.56   |
| 32  | 7     | 320 | CHL  | C4A-NA-C1A  | 6.97  | 109.84      | 106.71   |
| 36  | 7     | 305 | LUT  | C39-C29-C28 | -6.96 | 107.12      | 118.08   |
| 36  | 7     | 305 | LUT  | C19-C9-C10  | -6.94 | 113.21      | 122.92   |
| 36  | a     | 303 | LUT  | C35-C34-C33 | -6.93 | 117.42      | 127.31   |
| 32  | 7     | 319 | CHL  | O1D-CGD-CBD | -6.92 | 110.33      | 124.48   |
| 36  | 3     | 304 | LUT  | C38-C25-C24 | -6.92 | 108.77      | 123.56   |
| 36  | 7     | 305 | LUT  | C20-C13-C12 | -6.91 | 107.19      | 118.08   |
| 36  | 3     | 305 | LUT  | C8-C9-C10   | -6.90 | 108.35      | 118.94   |
| 36  | 9     | 302 | LUT  | C32-C33-C34 | -6.89 | 108.37      | 118.94   |
| 31  | 3     | 314 | CLA  | C4A-NA-C1A  | 6.89  | 109.80      | 106.71   |
| 31  | 7     | 309 | CLA  | C4A-NA-C1A  | 6.84  | 109.78      | 106.71   |
| 36  | 6     | 304 | LUT  | C20-C13-C12 | -6.83 | 107.31      | 118.08   |
| 32  | a     | 320 | CHL  | O2D-CGD-CBD | 6.83  | 123.40      | 111.27   |
| 36  | J     | 103 | LUT  | C40-C33-C32 | -6.81 | 107.35      | 118.08   |
| 36  | a     | 305 | LUT  | C32-C33-C34 | -6.81 | 108.50      | 118.94   |
| 36  | 9     | 303 | LUT  | C31-C32-C33 | 6.79  | 145.49      | 126.42   |
| 36  | L     | 304 | LUT  | C38-C25-C24 | -6.78 | 109.05      | 123.56   |
| 31  | 5     | 310 | CLA  | O2D-CGD-CBD | 6.78  | 123.31      | 111.27   |
| 36  | J     | 103 | LUT  | C38-C25-C24 | -6.76 | 109.09      | 123.56   |
| 36  | 4     | 302 | LUT  | C38-C25-C24 | -6.74 | 109.14      | 123.56   |
| 36  | 8     | 303 | LUT  | C11-C12-C13 | 6.72  | 145.30      | 126.42   |
| 36  | 9     | 303 | LUT  | C39-C29-C28 | -6.71 | 107.50      | 118.08   |
| 36  | 3     | 304 | LUT  | C18-C5-C6   | -6.71 | 116.99      | 124.53   |
| 36  | 3     | 305 | LUT  | C1-C6-C5    | -6.71 | 113.16      | 122.61   |
| 32  | 7     | 318 | CHL  | O2D-CGD-CBD | 6.69  | 123.16      | 111.27   |
| 32  | 6     | 318 | CHL  | O2D-CGD-CBD | 6.69  | 123.15      | 111.27   |
| 36  | 9     | 302 | LUT  | C8-C9-C10   | -6.69 | 108.68      | 118.94   |
| 36  | 3     | 305 | LUT  | C11-C12-C13 | 6.68  | 145.18      | 126.42   |
| 36  | 8     | 302 | LUT  | C32-C33-C34 | -6.68 | 108.69      | 118.94   |
| 36  | 9     | 305 | LUT  | C38-C25-C24 | -6.68 | 109.28      | 123.56   |
| 36  | 9     | 303 | LUT  | C40-C33-C32 | -6.67 | 107.58      | 118.08   |
| 36  | 3     | 304 | LUT  | C7-C8-C9    | -6.66 | 116.17      | 126.23   |
| 31  | 9     | 319 | CLA  | O2D-CGD-CBD | 6.66  | 123.10      | 111.27   |
| 36  | J     | 103 | LUT  | C35-C34-C33 | -6.65 | 117.82      | 127.31   |
| 36  | 8     | 303 | LUT  | C35-C34-C33 | -6.64 | 117.83      | 127.31   |
| 31  | 6     | 307 | CLA  | C4A-NA-C1A  | 6.64  | 109.69      | 106.71   |
| 36  | a     | 303 | LUT  | C20-C13-C12 | -6.63 | 107.63      | 118.08   |
| 36  | 8     | 303 | LUT  | C8-C9-C10   | -6.63 | 108.77      | 118.94   |
| 36  | 9     | 305 | LUT  | C8-C9-C10   | -6.58 | 108.84      | 118.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 8     | 319 | CHL  | O2D-CGD-CBD | 6.57  | 122.94      | 111.27   |
| 32  | 9     | 322 | CHL  | C4A-NA-C1A  | 6.56  | 109.65      | 106.71   |
| 36  | 2     | 301 | LUT  | C11-C12-C13 | 6.54  | 144.79      | 126.42   |
| 36  | 3     | 305 | LUT  | C20-C13-C12 | -6.52 | 107.81      | 118.08   |
| 36  | 4     | 303 | LUT  | C40-C33-C32 | -6.51 | 107.81      | 118.08   |
| 36  | 3     | 305 | LUT  | C35-C34-C33 | -6.51 | 118.02      | 127.31   |
| 36  | 8     | 302 | LUT  | C38-C25-C24 | -6.51 | 109.64      | 123.56   |
| 36  | 9     | 302 | LUT  | C39-C29-C28 | -6.51 | 107.83      | 118.08   |
| 30  | A     | 813 | CL0  | C3C-C4C-NC  | 6.50  | 117.86      | 110.57   |
| 31  | 5     | 313 | CLA  | CMD-C2D-C1D | 6.47  | 136.12      | 124.71   |
| 36  | 8     | 302 | LUT  | C40-C33-C32 | -6.46 | 107.90      | 118.08   |
| 36  | 7     | 305 | LUT  | C8-C9-C10   | -6.45 | 109.04      | 118.94   |
| 36  | 7     | 305 | LUT  | C18-C5-C6   | -6.45 | 117.29      | 124.53   |
| 31  | A     | 816 | CLA  | O2D-CGD-CBD | 6.44  | 122.72      | 111.27   |
| 32  | K     | 201 | CHL  | CHD-C1D-ND  | -6.44 | 118.54      | 124.45   |
| 36  | 5     | 303 | LUT  | C28-C29-C30 | -6.41 | 109.10      | 118.94   |
| 30  | A     | 813 | CL0  | CMD-C2D-C1D | 6.41  | 136.01      | 124.71   |
| 36  | 5     | 304 | LUT  | C40-C33-C32 | -6.40 | 108.00      | 118.08   |
| 36  | 3     | 305 | LUT  | C39-C29-C28 | -6.39 | 108.01      | 118.08   |
| 36  | a     | 305 | LUT  | C28-C29-C30 | -6.39 | 109.14      | 118.94   |
| 36  | 4     | 303 | LUT  | C35-C34-C33 | -6.38 | 118.20      | 127.31   |
| 36  | 4     | 303 | LUT  | C39-C29-C28 | -6.38 | 108.02      | 118.08   |
| 31  | A     | 834 | CLA  | C4A-NA-C1A  | 6.38  | 109.57      | 106.71   |
| 36  | 3     | 304 | LUT  | C20-C13-C12 | -6.38 | 108.03      | 118.08   |
| 36  | J     | 103 | LUT  | C20-C13-C12 | -6.36 | 108.05      | 118.08   |
| 36  | F     | 304 | LUT  | C39-C29-C28 | -6.36 | 108.06      | 118.08   |
| 32  | 8     | 319 | CHL  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 36  | 6     | 303 | LUT  | C28-C29-C30 | -6.36 | 109.19      | 118.94   |
| 32  | 4     | 317 | CHL  | C4A-NA-C1A  | 6.35  | 109.56      | 106.71   |
| 36  | 8     | 302 | LUT  | C39-C29-C28 | -6.34 | 108.08      | 118.08   |
| 36  | b     | 301 | LUT  | C8-C9-C10   | -6.31 | 109.26      | 118.94   |
| 36  | 9     | 305 | LUT  | C19-C9-C8   | -6.29 | 108.17      | 118.08   |
| 36  | J     | 103 | LUT  | C39-C29-C28 | -6.28 | 108.18      | 118.08   |
| 36  | 5     | 303 | LUT  | C8-C9-C10   | -6.27 | 109.32      | 118.94   |
| 36  | 9     | 302 | LUT  | C12-C13-C14 | -6.27 | 109.33      | 118.94   |
| 31  | L     | 306 | CLA  | O2D-CGD-CBD | 6.24  | 122.35      | 111.27   |
| 36  | 5     | 303 | LUT  | C39-C29-C28 | -6.23 | 108.26      | 118.08   |
| 36  | 7     | 305 | LUT  | C7-C8-C9    | -6.23 | 116.82      | 126.23   |
| 31  | 5     | 307 | CLA  | O2D-CGD-CBD | 6.23  | 122.34      | 111.27   |
| 32  | 5     | 316 | CHL  | O2D-CGD-CBD | 6.23  | 122.34      | 111.27   |
| 32  | A     | 831 | CHL  | C4A-NA-C1A  | 6.23  | 109.50      | 106.71   |
| 32  | 5     | 319 | CHL  | C4A-NA-C1A  | 6.23  | 109.50      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 314 | CLA  | C4D-CHA-C1A | -6.20 | 113.70      | 121.25   |
| 36  | a     | 305 | LUT  | C38-C25-C24 | -6.20 | 110.30      | 123.56   |
| 31  | A     | 847 | CLA  | O2D-CGD-CBD | 6.19  | 122.28      | 111.27   |
| 31  | 3     | 319 | CLA  | C4A-NA-C1A  | 6.19  | 109.49      | 106.71   |
| 36  | L     | 304 | LUT  | C12-C13-C14 | -6.19 | 109.45      | 118.94   |
| 36  | 6     | 304 | LUT  | C39-C29-C28 | -6.18 | 108.34      | 118.08   |
| 31  | b     | 313 | CLA  | C4A-NA-C1A  | 6.17  | 109.48      | 106.71   |
| 36  | a     | 303 | LUT  | C39-C29-C28 | -6.16 | 108.36      | 118.08   |
| 36  | 9     | 303 | LUT  | C19-C9-C8   | -6.16 | 108.37      | 118.08   |
| 31  | 3     | 313 | CLA  | O2D-CGD-CBD | 6.15  | 122.19      | 111.27   |
| 36  | b     | 301 | LUT  | C28-C29-C30 | -6.15 | 109.51      | 118.94   |
| 36  | F     | 304 | LUT  | C38-C25-C24 | -6.13 | 110.44      | 123.56   |
| 36  | J     | 103 | LUT  | C32-C33-C34 | -6.13 | 109.53      | 118.94   |
| 31  | 4     | 305 | CLA  | C3B-C4B-NB  | 6.13  | 117.13      | 109.21   |
| 36  | F     | 304 | LUT  | C28-C29-C30 | -6.11 | 109.57      | 118.94   |
| 36  | 5     | 304 | LUT  | C20-C13-C12 | -6.08 | 108.49      | 118.08   |
| 36  | 9     | 305 | LUT  | C20-C13-C12 | -6.08 | 108.49      | 118.08   |
| 36  | 9     | 302 | LUT  | C20-C13-C12 | -6.08 | 108.50      | 118.08   |
| 36  | 5     | 304 | LUT  | C8-C9-C10   | -6.07 | 109.62      | 118.94   |
| 32  | 7     | 317 | CHL  | C4A-NA-C1A  | 6.07  | 109.43      | 106.71   |
| 36  | 5     | 304 | LUT  | C39-C29-C28 | -6.06 | 108.54      | 118.08   |
| 36  | 2     | 301 | LUT  | C35-C34-C33 | -6.06 | 118.67      | 127.31   |
| 31  | 2     | 308 | CLA  | O2D-CGD-CBD | 6.05  | 122.02      | 111.27   |
| 31  | B     | 834 | CLA  | C2D-C1D-ND  | 6.05  | 114.56      | 110.10   |
| 36  | 6     | 304 | LUT  | C40-C33-C32 | -6.04 | 108.56      | 118.08   |
| 36  | a     | 305 | LUT  | C40-C33-C32 | -6.04 | 108.56      | 118.08   |
| 31  | 5     | 318 | CLA  | C4A-NA-C1A  | 6.02  | 109.41      | 106.71   |
| 31  | 9     | 311 | CLA  | O2D-CGD-CBD | 5.98  | 121.90      | 111.27   |
| 31  | 2     | 306 | CLA  | C4A-NA-C1A  | 5.98  | 109.39      | 106.71   |
| 36  | L     | 304 | LUT  | C32-C33-C34 | -5.98 | 109.77      | 118.94   |
| 36  | a     | 305 | LUT  | C12-C13-C14 | -5.96 | 109.80      | 118.94   |
| 32  | A     | 831 | CHL  | O2D-CGD-CBD | 5.96  | 121.85      | 111.27   |
| 36  | 3     | 304 | LUT  | C39-C29-C28 | -5.95 | 108.70      | 118.08   |
| 31  | b     | 305 | CLA  | C4A-NA-C1A  | 5.95  | 109.38      | 106.71   |
| 31  | a     | 311 | CLA  | O2D-CGD-CBD | 5.95  | 121.84      | 111.27   |
| 32  | 3     | 315 | CHL  | C4A-NA-C1A  | 5.94  | 109.38      | 106.71   |
| 36  | 4     | 302 | LUT  | C20-C13-C12 | -5.94 | 108.72      | 118.08   |
| 31  | 7     | 314 | CLA  | O2D-CGD-CBD | 5.94  | 121.82      | 111.27   |
| 36  | 6     | 304 | LUT  | C32-C33-C34 | -5.94 | 109.83      | 118.94   |
| 36  | 8     | 303 | LUT  | C1-C6-C5    | -5.92 | 114.28      | 122.61   |
| 31  | 8     | 317 | CLA  | CHD-C1D-ND  | -5.92 | 119.02      | 124.45   |
| 32  | 8     | 316 | CHL  | C4A-NA-C1A  | 5.91  | 109.36      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 828 | CLA  | O2D-CGD-CBD | 5.91  | 121.77      | 111.27   |
| 31  | 3     | 320 | CLA  | O2D-CGD-CBD | 5.91  | 121.77      | 111.27   |
| 36  | 4     | 302 | LUT  | C8-C9-C10   | -5.87 | 109.94      | 118.94   |
| 31  | 4     | 316 | CLA  | C2D-C1D-ND  | -5.87 | 105.78      | 110.10   |
| 32  | 5     | 316 | CHL  | O2D-CGD-O1D | -5.85 | 112.39      | 123.84   |
| 31  | L     | 305 | CLA  | C2D-C1D-ND  | 5.84  | 114.41      | 110.10   |
| 32  | 5     | 319 | CHL  | O2D-CGD-CBD | 5.84  | 121.64      | 111.27   |
| 36  | J     | 103 | LUT  | C19-C9-C8   | -5.83 | 108.90      | 118.08   |
| 31  | 6     | 313 | CLA  | O2D-CGD-CBD | 5.82  | 121.62      | 111.27   |
| 36  | 8     | 303 | LUT  | C28-C29-C30 | -5.82 | 110.00      | 118.94   |
| 31  | O     | 203 | CLA  | O2D-CGD-CBD | 5.80  | 121.57      | 111.27   |
| 36  | L     | 304 | LUT  | C39-C29-C28 | -5.80 | 108.95      | 118.08   |
| 31  | A     | 824 | CLA  | O2D-CGD-CBD | 5.79  | 121.56      | 111.27   |
| 32  | 5     | 322 | CHL  | C4A-NA-C1A  | 5.79  | 109.31      | 106.71   |
| 36  | a     | 303 | LUT  | C28-C29-C30 | -5.79 | 110.06      | 118.94   |
| 36  | 6     | 303 | LUT  | C8-C9-C10   | -5.78 | 110.06      | 118.94   |
| 31  | A     | 815 | CLA  | C2D-C1D-ND  | 5.78  | 114.37      | 110.10   |
| 32  | b     | 309 | CHL  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 31  | 6     | 307 | CLA  | O2D-CGD-CBD | 5.76  | 121.50      | 111.27   |
| 31  | 4     | 305 | CLA  | C3D-C4D-ND  | 5.76  | 119.55      | 110.24   |
| 32  | 5     | 317 | CHL  | C4A-NA-C1A  | 5.76  | 109.30      | 106.71   |
| 31  | b     | 311 | CLA  | O2D-CGD-CBD | 5.76  | 121.50      | 111.27   |
| 31  | 3     | 309 | CLA  | O2D-CGD-CBD | 5.75  | 121.49      | 111.27   |
| 31  | A     | 829 | CLA  | C1C-C2C-C3C | -5.74 | 100.92      | 106.96   |
| 32  | a     | 320 | CHL  | C4A-NA-C1A  | 5.74  | 109.29      | 106.71   |
| 32  | 4     | 313 | CHL  | C4A-NA-C1A  | 5.74  | 109.29      | 106.71   |
| 32  | 3     | 315 | CHL  | O2D-CGD-CBD | 5.74  | 121.46      | 111.27   |
| 31  | B     | 837 | CLA  | O2D-CGD-CBD | 5.72  | 121.43      | 111.27   |
| 36  | 5     | 303 | LUT  | C32-C33-C34 | -5.70 | 110.19      | 118.94   |
| 36  | 5     | 304 | LUT  | C28-C29-C30 | -5.70 | 110.19      | 118.94   |
| 36  | 2     | 301 | LUT  | C40-C33-C32 | -5.69 | 109.11      | 118.08   |
| 31  | 4     | 305 | CLA  | CHD-C4C-C3C | -5.69 | 116.47      | 124.84   |
| 36  | 4     | 302 | LUT  | C32-C33-C34 | -5.69 | 110.21      | 118.94   |
| 31  | 3     | 318 | CLA  | O2D-CGD-CBD | 5.69  | 121.37      | 111.27   |
| 32  | 9     | 322 | CHL  | O2D-CGD-CBD | 5.68  | 121.36      | 111.27   |
| 31  | B     | 845 | CLA  | C2C-C1C-NC  | 5.67  | 115.28      | 109.97   |
| 32  | A     | 839 | CHL  | O2D-CGD-CBD | 5.67  | 121.34      | 111.27   |
| 31  | 4     | 305 | CLA  | C2D-C1D-ND  | 5.65  | 114.27      | 110.10   |
| 31  | A     | 843 | CLA  | O2D-CGD-CBD | 5.65  | 121.31      | 111.27   |
| 31  | b     | 303 | CLA  | O2D-CGD-CBD | 5.65  | 121.31      | 111.27   |
| 31  | 4     | 305 | CLA  | O2D-CGD-CBD | 5.65  | 121.30      | 111.27   |
| 36  | 8     | 303 | LUT  | C32-C33-C34 | -5.64 | 110.29      | 118.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 819 | CLA  | O2D-CGD-CBD | 5.63  | 121.26      | 111.27   |
| 32  | K     | 201 | CHL  | O2D-CGD-CBD | 5.62  | 121.26      | 111.27   |
| 31  | A     | 838 | CLA  | O2D-CGD-CBD | 5.62  | 121.26      | 111.27   |
| 32  | 7     | 318 | CHL  | C4A-NA-C1A  | 5.61  | 109.23      | 106.71   |
| 36  | 8     | 303 | LUT  | C39-C29-C28 | -5.61 | 109.24      | 118.08   |
| 32  | 4     | 310 | CHL  | O2D-CGD-O1D | -5.60 | 112.88      | 123.84   |
| 31  | 5     | 321 | CLA  | C4D-CHA-C1A | -5.59 | 114.45      | 121.25   |
| 32  | 6     | 309 | CHL  | C4A-NA-C1A  | 5.59  | 109.22      | 106.71   |
| 30  | A     | 813 | CL0  | CHD-C4C-C3C | -5.58 | 116.63      | 124.84   |
| 31  | a     | 315 | CLA  | O2D-CGD-O1D | -5.58 | 112.92      | 123.84   |
| 36  | F     | 304 | LUT  | C7-C8-C9    | -5.58 | 117.80      | 126.23   |
| 31  | a     | 316 | CLA  | C4A-NA-C1A  | 5.57  | 109.21      | 106.71   |
| 36  | 8     | 302 | LUT  | C28-C29-C30 | -5.57 | 110.39      | 118.94   |
| 36  | 6     | 303 | LUT  | C40-C33-C32 | -5.57 | 109.31      | 118.08   |
| 36  | 2     | 301 | LUT  | C19-C9-C8   | -5.57 | 109.31      | 118.08   |
| 30  | A     | 813 | CL0  | C3B-C4B-NB  | 5.56  | 116.40      | 109.21   |
| 31  | B     | 818 | CLA  | C2C-C1C-NC  | 5.56  | 115.18      | 109.97   |
| 31  | F     | 305 | CLA  | O2D-CGD-CBD | 5.56  | 121.14      | 111.27   |
| 31  | 3     | 317 | CLA  | O2D-CGD-CBD | 5.56  | 121.14      | 111.27   |
| 32  | 6     | 321 | CHL  | C4A-NA-C1A  | 5.55  | 109.20      | 106.71   |
| 36  | 3     | 305 | LUT  | C4-C5-C6    | -5.55 | 108.48      | 120.85   |
| 31  | 3     | 319 | CLA  | CHD-C1D-ND  | -5.55 | 119.36      | 124.45   |
| 32  | a     | 317 | CHL  | C4A-NA-C1A  | 5.55  | 109.20      | 106.71   |
| 32  | 6     | 321 | CHL  | O2D-CGD-CBD | 5.54  | 121.11      | 111.27   |
| 32  | 7     | 319 | CHL  | C4A-NA-C1A  | 5.54  | 109.19      | 106.71   |
| 30  | A     | 813 | CL0  | C3D-C4D-ND  | 5.52  | 119.17      | 110.24   |
| 31  | 2     | 306 | CLA  | O2D-CGD-CBD | 5.52  | 121.08      | 111.27   |
| 36  | 6     | 304 | LUT  | C28-C29-C30 | -5.50 | 110.50      | 118.94   |
| 36  | F     | 304 | LUT  | C40-C33-C32 | -5.50 | 109.41      | 118.08   |
| 32  | 6     | 319 | CHL  | C4A-NA-C1A  | 5.50  | 109.18      | 106.71   |
| 36  | 4     | 303 | LUT  | C32-C33-C34 | -5.48 | 110.53      | 118.94   |
| 31  | a     | 319 | CLA  | O2D-CGD-CBD | 5.48  | 121.01      | 111.27   |
| 30  | A     | 813 | CL0  | C1C-C2C-C3C | -5.48 | 101.20      | 106.96   |
| 31  | B     | 816 | CLA  | O2D-CGD-CBD | 5.47  | 120.98      | 111.27   |
| 36  | 2     | 301 | LUT  | C39-C29-C28 | -5.46 | 109.47      | 118.08   |
| 31  | 4     | 316 | CLA  | CMD-C2D-C1D | 5.46  | 134.33      | 124.71   |
| 31  | 7     | 310 | CLA  | C1C-C2C-C3C | -5.46 | 102.07      | 107.07   |
| 32  | 4     | 310 | CHL  | O2D-CGD-CBD | 5.45  | 120.96      | 111.27   |
| 30  | A     | 813 | CL0  | C2D-C1D-ND  | 5.44  | 114.12      | 110.10   |
| 36  | 9     | 303 | LUT  | C4-C5-C6    | -5.44 | 108.72      | 120.85   |
| 31  | B     | 827 | CLA  | CHD-C1D-ND  | -5.44 | 119.45      | 124.45   |
| 36  | 9     | 305 | LUT  | C28-C29-C30 | -5.44 | 110.59      | 118.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 316 | CLA  | O2D-CGD-CBD | 5.44  | 120.93      | 111.27   |
| 36  | 9     | 303 | LUT  | C35-C34-C33 | -5.44 | 119.55      | 127.31   |
| 31  | a     | 322 | CLA  | O2D-CGD-CBD | 5.44  | 120.93      | 111.27   |
| 31  | B     | 848 | CLA  | CHD-C1D-ND  | -5.43 | 119.47      | 124.45   |
| 32  | 8     | 316 | CHL  | O2D-CGD-CBD | 5.42  | 120.91      | 111.27   |
| 36  | b     | 301 | LUT  | C19-C9-C8   | -5.42 | 109.53      | 118.08   |
| 31  | 5     | 315 | CLA  | O2D-CGD-CBD | 5.42  | 120.90      | 111.27   |
| 31  | a     | 321 | CLA  | CHD-C1D-ND  | -5.42 | 119.47      | 124.45   |
| 31  | 5     | 307 | CLA  | C4A-NA-C1A  | 5.42  | 109.14      | 106.71   |
| 31  | 4     | 305 | CLA  | C4D-CHA-C1A | -5.41 | 114.66      | 121.25   |
| 31  | 9     | 311 | CLA  | C4A-NA-C1A  | 5.41  | 109.14      | 106.71   |
| 31  | A     | 856 | CLA  | CHD-C1D-ND  | -5.41 | 119.48      | 124.45   |
| 31  | 8     | 312 | CLA  | O2D-CGD-CBD | 5.40  | 120.86      | 111.27   |
| 36  | 9     | 303 | LUT  | C32-C33-C34 | -5.40 | 110.66      | 118.94   |
| 31  | B     | 843 | CLA  | C2C-C1C-NC  | 5.40  | 115.03      | 109.97   |
| 31  | B     | 819 | CLA  | C2C-C1C-NC  | 5.40  | 115.03      | 109.97   |
| 31  | 6     | 314 | CLA  | O2D-CGD-CBD | 5.39  | 120.85      | 111.27   |
| 31  | 7     | 315 | CLA  | O2D-CGD-CBD | 5.39  | 120.84      | 111.27   |
| 31  | B     | 832 | CLA  | C2C-C1C-NC  | 5.38  | 115.01      | 109.97   |
| 36  | 4     | 302 | LUT  | C39-C29-C28 | -5.37 | 109.62      | 118.08   |
| 36  | L     | 304 | LUT  | C28-C29-C30 | -5.37 | 110.71      | 118.94   |
| 32  | 5     | 317 | CHL  | O2D-CGD-O1D | -5.36 | 113.35      | 123.84   |
| 36  | 5     | 303 | LUT  | C40-C33-C32 | -5.36 | 109.63      | 118.08   |
| 31  | 5     | 309 | CLA  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 31  | b     | 312 | CLA  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 31  | a     | 316 | CLA  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 31  | 8     | 318 | CLA  | O2D-CGD-CBD | 5.36  | 120.79      | 111.27   |
| 32  | K     | 201 | CHL  | C3C-C4C-NC  | 5.36  | 116.58      | 110.57   |
| 36  | 4     | 302 | LUT  | C40-C33-C32 | -5.35 | 109.65      | 118.08   |
| 31  | A     | 847 | CLA  | CHD-C1D-ND  | -5.35 | 119.54      | 124.45   |
| 31  | 3     | 310 | CLA  | CHD-C1D-ND  | -5.34 | 119.55      | 124.45   |
| 36  | 7     | 305 | LUT  | C28-C29-C30 | -5.34 | 110.75      | 118.94   |
| 31  | 6     | 311 | CLA  | O2D-CGD-CBD | 5.34  | 120.75      | 111.27   |
| 31  | G     | 206 | CLA  | CHD-C1D-ND  | -5.34 | 119.55      | 124.45   |
| 31  | A     | 833 | CLA  | C2C-C1C-NC  | 5.32  | 114.96      | 109.97   |
| 31  | 4     | 319 | CLA  | O2D-CGD-CBD | 5.32  | 120.72      | 111.27   |
| 31  | F     | 301 | CLA  | O2D-CGD-CBD | 5.32  | 120.71      | 111.27   |
| 30  | A     | 813 | CL0  | O2D-CGD-CBD | 5.31  | 120.71      | 111.27   |
| 36  | 9     | 302 | LUT  | C40-C33-C32 | -5.31 | 109.71      | 118.08   |
| 31  | H     | 901 | CLA  | O2D-CGD-CBD | 5.31  | 120.70      | 111.27   |
| 31  | 5     | 321 | CLA  | O2D-CGD-CBD | 5.30  | 120.69      | 111.27   |
| 32  | 7     | 320 | CHL  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 6     | 303 | LUT  | C19-C9-C8   | -5.29 | 109.74      | 118.08   |
| 31  | B     | 832 | CLA  | O2D-CGD-CBD | 5.29  | 120.67      | 111.27   |
| 31  | 8     | 310 | CLA  | CHD-C4C-C3C | -5.29 | 117.06      | 124.84   |
| 32  | 4     | 313 | CHL  | O2D-CGD-CBD | 5.29  | 120.66      | 111.27   |
| 31  | 7     | 314 | CLA  | C1C-C2C-C3C | -5.28 | 102.23      | 107.07   |
| 36  | L     | 304 | LUT  | C40-C33-C32 | -5.27 | 109.77      | 118.08   |
| 31  | 8     | 317 | CLA  | CHD-C4C-C3C | -5.27 | 117.09      | 124.84   |
| 31  | B     | 847 | CLA  | O2D-CGD-CBD | 5.27  | 120.63      | 111.27   |
| 31  | B     | 845 | CLA  | C1C-C2C-C3C | -5.27 | 101.42      | 106.96   |
| 32  | a     | 318 | CHL  | O2D-CGD-CBD | 5.26  | 120.61      | 111.27   |
| 32  | 5     | 316 | CHL  | C4A-NA-C1A  | 5.25  | 109.07      | 106.71   |
| 31  | B     | 841 | CLA  | C2D-C1D-ND  | 5.25  | 113.97      | 110.10   |
| 31  | 5     | 313 | CLA  | O2D-CGD-CBD | 5.24  | 120.58      | 111.27   |
| 31  | B     | 819 | CLA  | C1C-C2C-C3C | -5.24 | 101.45      | 106.96   |
| 36  | F     | 304 | LUT  | C8-C9-C10   | -5.24 | 110.90      | 118.94   |
| 31  | B     | 841 | CLA  | CHD-C4C-C3C | -5.23 | 117.15      | 124.84   |
| 36  | b     | 301 | LUT  | C39-C29-C28 | -5.23 | 109.83      | 118.08   |
| 31  | a     | 316 | CLA  | CHD-C1D-ND  | -5.23 | 119.65      | 124.45   |
| 35  | 9     | 304 | QTB  | C01-C02-C03 | -5.22 | 115.61      | 122.92   |
| 36  | 4     | 303 | LUT  | C20-C13-C12 | -5.22 | 109.86      | 118.08   |
| 31  | L     | 305 | CLA  | CHD-C1D-ND  | -5.22 | 119.66      | 124.45   |
| 31  | B     | 847 | CLA  | C2C-C1C-NC  | 5.22  | 114.86      | 109.97   |
| 31  | A     | 842 | CLA  | O2D-CGD-CBD | 5.21  | 120.52      | 111.27   |
| 31  | 7     | 310 | CLA  | O2D-CGD-CBD | 5.21  | 120.52      | 111.27   |
| 31  | A     | 851 | CLA  | O2D-CGD-CBD | 5.21  | 120.52      | 111.27   |
| 31  | 7     | 322 | CLA  | O2D-CGD-CBD | 5.20  | 120.52      | 111.27   |
| 31  | B     | 827 | CLA  | C1C-C2C-C3C | -5.20 | 101.49      | 106.96   |
| 36  | 9     | 305 | LUT  | C39-C29-C28 | -5.20 | 109.89      | 118.08   |
| 31  | b     | 307 | CLA  | O2D-CGD-O1D | -5.20 | 113.67      | 123.84   |
| 36  | 7     | 305 | LUT  | C17-C1-C6   | 5.20  | 118.73      | 110.30   |
| 31  | 8     | 321 | CLA  | O2D-CGD-CBD | 5.19  | 120.50      | 111.27   |
| 31  | K     | 205 | CLA  | CHD-C1D-ND  | -5.19 | 119.68      | 124.45   |
| 31  | 9     | 317 | CLA  | CHD-C1D-ND  | -5.19 | 119.68      | 124.45   |
| 31  | B     | 812 | CLA  | C2D-C1D-ND  | 5.19  | 113.93      | 110.10   |
| 31  | B     | 817 | CLA  | O2D-CGD-CBD | 5.19  | 120.48      | 111.27   |
| 36  | 9     | 303 | LUT  | C7-C8-C9    | -5.18 | 118.40      | 126.23   |
| 36  | 6     | 303 | LUT  | C39-C29-C28 | -5.18 | 109.92      | 118.08   |
| 31  | B     | 819 | CLA  | CHD-C1D-ND  | -5.17 | 119.70      | 124.45   |
| 31  | 6     | 322 | CLA  | O2D-CGD-CBD | 5.17  | 120.45      | 111.27   |
| 32  | 4     | 317 | CHL  | O2D-CGD-CBD | 5.17  | 120.45      | 111.27   |
| 31  | a     | 321 | CLA  | O2D-CGD-CBD | 5.17  | 120.45      | 111.27   |
| 31  | 2     | 304 | CLA  | O2D-CGD-CBD | 5.16  | 120.44      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 811 | CLA  | O2D-CGD-CBD | 5.16  | 120.44      | 111.27   |
| 32  | b     | 309 | CHL  | O2D-CGD-CBD | 5.16  | 120.43      | 111.27   |
| 31  | A     | 835 | CLA  | O2D-CGD-CBD | 5.15  | 120.43      | 111.27   |
| 31  | K     | 204 | CLA  | O2D-CGD-CBD | 5.15  | 120.42      | 111.27   |
| 31  | 9     | 318 | CLA  | O2D-CGD-CBD | 5.15  | 120.41      | 111.27   |
| 31  | b     | 302 | CLA  | O2D-CGD-CBD | 5.14  | 120.40      | 111.27   |
| 31  | O     | 202 | CLA  | C1C-C2C-C3C | -5.13 | 102.37      | 107.07   |
| 36  | 3     | 304 | LUT  | C19-C9-C8   | -5.13 | 110.00      | 118.08   |
| 36  | 4     | 302 | LUT  | C28-C29-C30 | -5.12 | 111.08      | 118.94   |
| 31  | 8     | 310 | CLA  | C2D-C1D-ND  | 5.12  | 113.88      | 110.10   |
| 31  | 4     | 320 | CLA  | O2D-CGD-CBD | 5.12  | 120.37      | 111.27   |
| 36  | b     | 301 | LUT  | C7-C6-C5    | -5.11 | 109.08      | 121.46   |
| 31  | B     | 811 | CLA  | C4D-CHA-C1A | -5.10 | 115.04      | 121.25   |
| 31  | 6     | 310 | CLA  | O2D-CGD-CBD | 5.09  | 120.32      | 111.27   |
| 31  | b     | 310 | CLA  | CHD-C1D-ND  | -5.09 | 119.77      | 124.45   |
| 31  | 4     | 307 | CLA  | O2D-CGD-CBD | 5.09  | 120.31      | 111.27   |
| 30  | A     | 813 | CL0  | CHD-C1D-ND  | -5.09 | 119.78      | 124.45   |
| 31  | A     | 855 | CLA  | C2D-C1D-ND  | 5.08  | 113.85      | 110.10   |
| 31  | 6     | 308 | CLA  | O2D-CGD-CBD | 5.08  | 120.30      | 111.27   |
| 31  | B     | 841 | CLA  | CHD-C1D-ND  | -5.07 | 119.79      | 124.45   |
| 31  | A     | 847 | CLA  | C2C-C1C-NC  | 5.07  | 114.72      | 109.97   |
| 31  | B     | 833 | CLA  | CHD-C1D-ND  | -5.07 | 119.80      | 124.45   |
| 36  | 3     | 305 | LUT  | C40-C33-C32 | -5.07 | 110.09      | 118.08   |
| 31  | b     | 304 | CLA  | O2D-CGD-CBD | 5.07  | 120.28      | 111.27   |
| 31  | B     | 829 | CLA  | C2C-C1C-NC  | 5.07  | 114.72      | 109.97   |
| 31  | 7     | 311 | CLA  | O2D-CGD-CBD | 5.07  | 120.27      | 111.27   |
| 31  | b     | 306 | CLA  | O2D-CGD-CBD | 5.06  | 120.27      | 111.27   |
| 32  | 7     | 318 | CHL  | O2D-CGD-O1D | -5.06 | 113.94      | 123.84   |
| 31  | a     | 312 | CLA  | O2D-CGD-CBD | 5.06  | 120.26      | 111.27   |
| 31  | A     | 845 | CLA  | O2D-CGD-CBD | 5.05  | 120.25      | 111.27   |
| 31  | 8     | 317 | CLA  | C2D-C1D-ND  | 5.05  | 113.83      | 110.10   |
| 31  | J     | 105 | CLA  | O2D-CGD-CBD | 5.05  | 120.24      | 111.27   |
| 31  | a     | 314 | CLA  | O2D-CGD-CBD | 5.05  | 120.24      | 111.27   |
| 31  | 5     | 323 | CLA  | O2D-CGD-CBD | 5.05  | 120.23      | 111.27   |
| 31  | B     | 848 | CLA  | O2D-CGD-CBD | 5.04  | 120.23      | 111.27   |
| 31  | B     | 850 | CLA  | C2D-C1D-ND  | 5.04  | 113.82      | 110.10   |
| 31  | A     | 823 | CLA  | O2D-CGD-CBD | 5.04  | 120.23      | 111.27   |
| 31  | a     | 314 | CLA  | O2D-CGD-O1D | -5.04 | 113.98      | 123.84   |
| 31  | 6     | 316 | CLA  | CHD-C1D-ND  | -5.04 | 119.83      | 124.45   |
| 31  | L     | 307 | CLA  | O2D-CGD-CBD | 5.04  | 120.22      | 111.27   |
| 31  | B     | 827 | CLA  | C2C-C1C-NC  | 5.04  | 114.69      | 109.97   |
| 31  | A     | 817 | CLA  | C2D-C1D-ND  | 5.03  | 113.81      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | F     | 304 | LUT  | C1-C6-C5    | -5.03 | 115.53      | 122.61   |
| 31  | 4     | 309 | CLA  | C2D-C1D-ND  | 5.03  | 113.81      | 110.10   |
| 36  | 9     | 302 | LUT  | C35-C15-C14 | -5.03 | 113.17      | 123.47   |
| 31  | 9     | 315 | CLA  | O2D-CGD-CBD | 5.02  | 120.19      | 111.27   |
| 31  | B     | 829 | CLA  | C1C-C2C-C3C | -5.02 | 101.68      | 106.96   |
| 32  | 7     | 319 | CHL  | CHD-C1D-ND  | -5.02 | 119.84      | 124.45   |
| 31  | B     | 831 | CLA  | O2D-CGD-CBD | 5.02  | 120.18      | 111.27   |
| 36  | 3     | 304 | LUT  | C1-C6-C5    | -5.02 | 115.55      | 122.61   |
| 31  | A     | 841 | CLA  | C2D-C1D-ND  | 5.01  | 113.80      | 110.10   |
| 31  | B     | 832 | CLA  | C1C-C2C-C3C | -5.01 | 101.69      | 106.96   |
| 31  | 8     | 321 | CLA  | CHD-C1D-ND  | -5.01 | 119.85      | 124.45   |
| 31  | A     | 836 | CLA  | O2D-CGD-CBD | 5.01  | 120.17      | 111.27   |
| 31  | A     | 844 | CLA  | C2C-C1C-NC  | 5.01  | 114.66      | 109.97   |
| 31  | 7     | 315 | CLA  | C2C-C1C-NC  | 5.00  | 114.66      | 109.97   |
| 31  | b     | 311 | CLA  | CHD-C1D-ND  | -5.00 | 119.86      | 124.45   |
| 31  | 3     | 319 | CLA  | C2D-C1D-ND  | 5.00  | 113.79      | 110.10   |
| 31  | 3     | 319 | CLA  | CHD-C4C-C3C | -5.00 | 117.50      | 124.84   |
| 31  | 2     | 313 | CLA  | O2D-CGD-CBD | 4.99  | 120.14      | 111.27   |
| 36  | 9     | 303 | LUT  | C28-C29-C30 | -4.99 | 111.28      | 118.94   |
| 31  | A     | 841 | CLA  | CHD-C1D-ND  | -4.99 | 119.87      | 124.45   |
| 31  | A     | 825 | CLA  | O2D-CGD-CBD | 4.99  | 120.13      | 111.27   |
| 31  | B     | 817 | CLA  | C2C-C1C-NC  | 4.98  | 114.64      | 109.97   |
| 31  | 2     | 309 | CLA  | CHD-C1D-ND  | -4.98 | 119.88      | 124.45   |
| 31  | 4     | 305 | CLA  | CAC-C3C-C4C | 4.98  | 131.27      | 124.81   |
| 31  | B     | 821 | CLA  | CHD-C1D-ND  | -4.97 | 119.88      | 124.45   |
| 31  | A     | 846 | CLA  | C2D-C1D-ND  | 4.97  | 113.77      | 110.10   |
| 31  | a     | 309 | CLA  | O1D-CGD-CBD | -4.97 | 114.31      | 124.48   |
| 31  | A     | 854 | CLA  | O2D-CGD-CBD | 4.97  | 120.10      | 111.27   |
| 31  | B     | 848 | CLA  | C2D-C1D-ND  | 4.97  | 113.76      | 110.10   |
| 36  | 5     | 304 | LUT  | C12-C13-C14 | -4.97 | 111.32      | 118.94   |
| 31  | 3     | 308 | CLA  | O2D-CGD-CBD | 4.97  | 120.09      | 111.27   |
| 32  | 6     | 309 | CHL  | O2D-CGD-CBD | 4.97  | 120.09      | 111.27   |
| 31  | B     | 814 | CLA  | C2D-C1D-ND  | 4.96  | 113.76      | 110.10   |
| 31  | 8     | 307 | CLA  | O2D-CGD-CBD | 4.96  | 120.09      | 111.27   |
| 36  | 7     | 305 | LUT  | C40-C33-C32 | -4.96 | 110.26      | 118.08   |
| 31  | A     | 843 | CLA  | C2C-C1C-NC  | 4.96  | 114.62      | 109.97   |
| 31  | B     | 839 | CLA  | CHD-C1D-ND  | -4.96 | 119.90      | 124.45   |
| 31  | B     | 816 | CLA  | C2D-C1D-ND  | 4.96  | 113.76      | 110.10   |
| 31  | B     | 835 | CLA  | O2D-CGD-CBD | 4.95  | 120.07      | 111.27   |
| 31  | 2     | 306 | CLA  | CHD-C1D-ND  | -4.95 | 119.90      | 124.45   |
| 31  | 9     | 321 | CLA  | C2C-C1C-NC  | 4.95  | 114.61      | 109.97   |
| 31  | 3     | 319 | CLA  | O2D-CGD-CBD | 4.95  | 120.06      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 843 | CLA  | C1C-C2C-C3C | -4.94 | 101.76      | 106.96   |
| 31  | L     | 306 | CLA  | CHD-C1D-ND  | -4.94 | 119.91      | 124.45   |
| 31  | G     | 204 | CLA  | O2D-CGD-CBD | 4.94  | 120.05      | 111.27   |
| 32  | 5     | 322 | CHL  | C1C-C2C-C3C | -4.94 | 103.19      | 107.11   |
| 31  | 3     | 316 | CLA  | O2D-CGD-CBD | 4.94  | 120.05      | 111.27   |
| 35  | a     | 302 | QTB  | C01-C02-C03 | -4.94 | 116.01      | 122.92   |
| 31  | 5     | 314 | CLA  | O2D-CGD-CBD | 4.94  | 120.04      | 111.27   |
| 31  | a     | 319 | CLA  | C2C-C1C-NC  | 4.94  | 114.60      | 109.97   |
| 31  | b     | 304 | CLA  | CHD-C1D-ND  | -4.94 | 119.92      | 124.45   |
| 31  | A     | 822 | CLA  | C2D-C1D-ND  | 4.93  | 113.74      | 110.10   |
| 31  | 5     | 318 | CLA  | CHD-C1D-ND  | -4.93 | 119.92      | 124.45   |
| 31  | B     | 815 | CLA  | C2D-C1D-ND  | 4.93  | 113.73      | 110.10   |
| 31  | A     | 817 | CLA  | CHD-C1D-ND  | -4.93 | 119.93      | 124.45   |
| 36  | L     | 304 | LUT  | C20-C13-C12 | -4.92 | 110.32      | 118.08   |
| 36  | 9     | 303 | LUT  | C20-C13-C12 | -4.92 | 110.32      | 118.08   |
| 31  | 2     | 315 | CLA  | O2D-CGD-CBD | 4.92  | 120.01      | 111.27   |
| 31  | F     | 305 | CLA  | C2C-C1C-NC  | 4.92  | 114.58      | 109.97   |
| 31  | 2     | 314 | CLA  | O2D-CGD-CBD | 4.92  | 120.00      | 111.27   |
| 31  | A     | 814 | CLA  | C2D-C1D-ND  | 4.91  | 113.73      | 110.10   |
| 36  | 4     | 302 | LUT  | C19-C9-C8   | -4.91 | 110.33      | 118.08   |
| 32  | 3     | 315 | CHL  | O1D-CGD-CBD | -4.91 | 114.43      | 124.48   |
| 31  | 9     | 315 | CLA  | C1C-C2C-C3C | -4.91 | 101.79      | 106.96   |
| 31  | 2     | 305 | CLA  | O2D-CGD-CBD | 4.91  | 120.00      | 111.27   |
| 31  | 7     | 316 | CLA  | O2D-CGD-O1D | -4.91 | 114.23      | 123.84   |
| 31  | 4     | 309 | CLA  | CHD-C1D-ND  | -4.91 | 119.94      | 124.45   |
| 31  | A     | 854 | CLA  | C2D-C1D-ND  | 4.91  | 113.72      | 110.10   |
| 31  | B     | 828 | CLA  | CHD-C1D-ND  | -4.90 | 119.95      | 124.45   |
| 31  | 8     | 311 | CLA  | O2D-CGD-CBD | 4.90  | 119.98      | 111.27   |
| 31  | a     | 321 | CLA  | C2C-C1C-NC  | 4.90  | 114.56      | 109.97   |
| 36  | L     | 304 | LUT  | C19-C9-C8   | -4.90 | 110.36      | 118.08   |
| 32  | 6     | 320 | CHL  | O2D-CGD-CBD | 4.90  | 119.97      | 111.27   |
| 32  | 7     | 317 | CHL  | C1-C2-C3    | -4.90 | 117.57      | 126.04   |
| 36  | 9     | 302 | LUT  | C28-C29-C30 | -4.90 | 111.43      | 118.94   |
| 31  | A     | 847 | CLA  | C1C-C2C-C3C | -4.90 | 101.81      | 106.96   |
| 31  | 8     | 310 | CLA  | O2D-CGD-CBD | 4.89  | 119.97      | 111.27   |
| 31  | 7     | 310 | CLA  | C2C-C1C-NC  | 4.89  | 114.56      | 109.97   |
| 31  | 8     | 320 | CLA  | O2D-CGD-CBD | 4.89  | 119.95      | 111.27   |
| 31  | K     | 206 | CLA  | C2C-C1C-NC  | 4.89  | 114.55      | 109.97   |
| 31  | 9     | 316 | CLA  | C2C-C1C-NC  | 4.89  | 114.55      | 109.97   |
| 31  | A     | 833 | CLA  | C1C-C2C-C3C | -4.88 | 101.82      | 106.96   |
| 31  | A     | 829 | CLA  | C3D-C2D-C1D | -4.88 | 99.17       | 105.83   |
| 32  | 5     | 317 | CHL  | O2D-CGD-CBD | 4.88  | 119.94      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 840 | CLA  | CHD-C1D-ND  | -4.88 | 119.97      | 124.45   |
| 32  | 6     | 318 | CHL  | C4A-NA-C1A  | 4.88  | 108.90      | 106.71   |
| 31  | 3     | 314 | CLA  | CHD-C1D-ND  | -4.88 | 119.97      | 124.45   |
| 31  | B     | 831 | CLA  | C2D-C1D-ND  | 4.88  | 113.70      | 110.10   |
| 31  | H     | 902 | CLA  | O2D-CGD-CBD | 4.88  | 119.94      | 111.27   |
| 31  | 3     | 310 | CLA  | CHD-C4C-C3C | -4.88 | 117.67      | 124.84   |
| 31  | b     | 302 | CLA  | C2C-C1C-NC  | 4.88  | 114.54      | 109.97   |
| 31  | 6     | 313 | CLA  | C2C-C1C-NC  | 4.88  | 114.54      | 109.97   |
| 31  | 3     | 311 | CLA  | C2C-C1C-NC  | 4.87  | 114.54      | 109.97   |
| 31  | 2     | 312 | CLA  | CHD-C1D-ND  | -4.87 | 119.97      | 124.45   |
| 31  | B     | 844 | CLA  | CHD-C1D-ND  | -4.87 | 119.98      | 124.45   |
| 31  | B     | 823 | CLA  | C2C-C1C-NC  | 4.87  | 114.53      | 109.97   |
| 36  | a     | 305 | LUT  | C19-C9-C8   | -4.87 | 110.40      | 118.08   |
| 31  | 8     | 317 | CLA  | C2C-C1C-NC  | 4.87  | 114.53      | 109.97   |
| 31  | B     | 848 | CLA  | CHD-C4C-C3C | -4.87 | 117.69      | 124.84   |
| 32  | 4     | 317 | CHL  | C1C-C2C-C3C | -4.87 | 103.25      | 107.11   |
| 31  | A     | 848 | CLA  | C2C-C1C-NC  | 4.86  | 114.53      | 109.97   |
| 32  | 3     | 315 | CHL  | C1-C2-C3    | -4.86 | 117.63      | 126.04   |
| 31  | B     | 818 | CLA  | C1C-C2C-C3C | -4.86 | 101.84      | 106.96   |
| 31  | A     | 850 | CLA  | C2D-C1D-ND  | 4.86  | 113.69      | 110.10   |
| 31  | 2     | 308 | CLA  | C2D-C1D-ND  | 4.86  | 113.69      | 110.10   |
| 31  | a     | 310 | CLA  | C2D-C1D-ND  | 4.86  | 113.69      | 110.10   |
| 31  | A     | 856 | CLA  | C2D-C1D-ND  | 4.86  | 113.68      | 110.10   |
| 31  | 4     | 308 | CLA  | C2C-C1C-NC  | 4.86  | 114.52      | 109.97   |
| 31  | B     | 846 | CLA  | O2D-CGD-CBD | 4.86  | 119.90      | 111.27   |
| 31  | B     | 817 | CLA  | CHD-C4C-C3C | -4.86 | 117.70      | 124.84   |
| 31  | 5     | 323 | CLA  | C2D-C1D-ND  | 4.86  | 113.68      | 110.10   |
| 31  | a     | 321 | CLA  | C1C-C2C-C3C | -4.85 | 101.86      | 106.96   |
| 31  | 9     | 315 | CLA  | C2C-C1C-NC  | 4.85  | 114.52      | 109.97   |
| 31  | 2     | 309 | CLA  | O2D-CGD-CBD | 4.85  | 119.88      | 111.27   |
| 31  | A     | 821 | CLA  | CHD-C1D-ND  | -4.85 | 120.00      | 124.45   |
| 31  | 4     | 311 | CLA  | O2D-CGD-CBD | 4.84  | 119.87      | 111.27   |
| 31  | B     | 836 | CLA  | C2C-C1C-NC  | 4.84  | 114.51      | 109.97   |
| 31  | A     | 816 | CLA  | C2C-C1C-NC  | 4.84  | 114.50      | 109.97   |
| 31  | 3     | 310 | CLA  | C2C-C1C-NC  | 4.84  | 114.50      | 109.97   |
| 31  | 2     | 315 | CLA  | C2D-C1D-ND  | 4.83  | 113.66      | 110.10   |
| 31  | 6     | 315 | CLA  | C2D-C1D-ND  | 4.83  | 113.66      | 110.10   |
| 31  | 4     | 320 | CLA  | C4D-CHA-C1A | -4.83 | 115.38      | 121.25   |
| 32  | a     | 318 | CHL  | C4A-NA-C1A  | 4.82  | 108.88      | 106.71   |
| 36  | 4     | 303 | LUT  | C19-C9-C8   | -4.82 | 110.48      | 118.08   |
| 36  | 4     | 303 | LUT  | C8-C9-C10   | -4.82 | 111.54      | 118.94   |
| 31  | 5     | 315 | CLA  | C1C-C2C-C3C | -4.82 | 101.89      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 308 | CLA  | O2D-CGD-CBD | 4.82  | 119.83      | 111.27   |
| 31  | 2     | 307 | CLA  | O2D-CGD-CBD | 4.81  | 119.82      | 111.27   |
| 31  | 3     | 318 | CLA  | C2C-C1C-NC  | 4.81  | 114.48      | 109.97   |
| 36  | 3     | 304 | LUT  | C8-C9-C10   | -4.81 | 111.55      | 118.94   |
| 31  | B     | 847 | CLA  | C2D-C1D-ND  | 4.81  | 113.65      | 110.10   |
| 31  | 8     | 321 | CLA  | CHD-C4C-C3C | -4.81 | 117.77      | 124.84   |
| 31  | 5     | 311 | CLA  | C2C-C1C-NC  | 4.81  | 114.47      | 109.97   |
| 32  | 6     | 320 | CHL  | C1C-C2C-C3C | -4.80 | 103.30      | 107.11   |
| 31  | a     | 310 | CLA  | C2C-C1C-NC  | 4.80  | 114.47      | 109.97   |
| 31  | O     | 204 | CLA  | O2D-CGD-CBD | 4.80  | 119.81      | 111.27   |
| 31  | 8     | 317 | CLA  | O2D-CGD-CBD | 4.80  | 119.80      | 111.27   |
| 31  | A     | 838 | CLA  | C2C-C1C-NC  | 4.80  | 114.47      | 109.97   |
| 31  | 3     | 307 | CLA  | O1D-CGD-CBD | -4.80 | 114.67      | 124.48   |
| 31  | B     | 849 | CLA  | C2D-C1D-ND  | 4.80  | 113.64      | 110.10   |
| 31  | 3     | 310 | CLA  | C1C-C2C-C3C | -4.80 | 101.91      | 106.96   |
| 31  | b     | 312 | CLA  | C2C-C1C-NC  | 4.80  | 114.47      | 109.97   |
| 31  | 4     | 321 | CLA  | O2D-CGD-CBD | 4.79  | 119.79      | 111.27   |
| 31  | A     | 848 | CLA  | C1C-C2C-C3C | -4.79 | 101.92      | 106.96   |
| 31  | B     | 838 | CLA  | O2D-CGD-CBD | 4.79  | 119.78      | 111.27   |
| 32  | 5     | 319 | CHL  | C1C-C2C-C3C | -4.79 | 103.31      | 107.11   |
| 31  | 5     | 323 | CLA  | C2C-C1C-NC  | 4.79  | 114.46      | 109.97   |
| 31  | 4     | 309 | CLA  | C2C-C1C-NC  | 4.79  | 114.46      | 109.97   |
| 31  | 3     | 312 | CLA  | O2D-CGD-CBD | 4.79  | 119.78      | 111.27   |
| 32  | 7     | 324 | CHL  | O2D-CGD-CBD | 4.79  | 119.77      | 111.27   |
| 31  | 6     | 312 | CLA  | O2D-CGD-O1D | -4.78 | 114.48      | 123.84   |
| 32  | A     | 840 | CHL  | C4A-NA-C1A  | 4.78  | 108.86      | 106.71   |
| 31  | 8     | 318 | CLA  | CHD-C1D-ND  | -4.78 | 120.06      | 124.45   |
| 31  | B     | 818 | CLA  | C2D-C1D-ND  | 4.78  | 113.63      | 110.10   |
| 36  | 9     | 305 | LUT  | C32-C33-C34 | -4.78 | 111.61      | 118.94   |
| 36  | 3     | 304 | LUT  | C28-C29-C30 | -4.78 | 111.61      | 118.94   |
| 31  | B     | 823 | CLA  | C1C-C2C-C3C | -4.78 | 101.93      | 106.96   |
| 31  | K     | 204 | CLA  | C1C-C2C-C3C | -4.78 | 101.93      | 106.96   |
| 31  | a     | 319 | CLA  | C1C-C2C-C3C | -4.78 | 101.93      | 106.96   |
| 31  | B     | 838 | CLA  | C2C-C1C-NC  | 4.77  | 114.44      | 109.97   |
| 31  | a     | 309 | CLA  | C2D-C1D-ND  | 4.77  | 113.62      | 110.10   |
| 31  | A     | 853 | CLA  | C2D-C1D-ND  | 4.77  | 113.62      | 110.10   |
| 36  | 7     | 305 | LUT  | C19-C9-C8   | -4.77 | 110.57      | 118.08   |
| 31  | A     | 814 | CLA  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 31  | A     | 832 | CLA  | CHD-C1D-ND  | -4.76 | 120.08      | 124.45   |
| 33  | 7     | 308 | DGD  | O3G-C3G-C2G | -4.76 | 99.41       | 110.90   |
| 31  | b     | 310 | CLA  | O2D-CGD-CBD | 4.76  | 119.73      | 111.27   |
| 31  | B     | 822 | CLA  | O2D-CGD-O1D | -4.76 | 114.53      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 834 | CLA  | CHD-C1D-ND  | -4.76 | 120.08      | 124.45   |
| 31  | B     | 845 | CLA  | C2D-C1D-ND  | 4.76  | 113.61      | 110.10   |
| 31  | 8     | 309 | CLA  | C2C-C1C-NC  | 4.76  | 114.43      | 109.97   |
| 31  | 4     | 320 | CLA  | C2C-C1C-NC  | 4.76  | 114.43      | 109.97   |
| 31  | a     | 309 | CLA  | O2D-CGD-CBD | 4.76  | 119.72      | 111.27   |
| 31  | 4     | 320 | CLA  | CHD-C1D-ND  | -4.76 | 120.08      | 124.45   |
| 31  | a     | 311 | CLA  | C1C-C2C-C3C | -4.75 | 101.96      | 106.96   |
| 31  | 9     | 314 | CLA  | O2D-CGD-CBD | 4.75  | 119.72      | 111.27   |
| 36  | a     | 305 | LUT  | C8-C9-C10   | -4.75 | 111.65      | 118.94   |
| 31  | a     | 315 | CLA  | O1D-CGD-CBD | -4.75 | 114.76      | 124.48   |
| 36  | 4     | 303 | LUT  | C18-C5-C4   | -4.75 | 105.55      | 114.36   |
| 31  | 5     | 313 | CLA  | CHD-C1D-ND  | -4.75 | 120.09      | 124.45   |
| 31  | b     | 303 | CLA  | C2C-C1C-NC  | 4.75  | 114.42      | 109.97   |
| 31  | 4     | 321 | CLA  | C2C-C1C-NC  | 4.75  | 114.42      | 109.97   |
| 36  | 9     | 305 | LUT  | C7-C6-C5    | -4.74 | 109.97      | 121.46   |
| 36  | 2     | 301 | LUT  | C28-C29-C30 | -4.74 | 111.67      | 118.94   |
| 31  | B     | 814 | CLA  | O2D-CGD-O1D | -4.74 | 114.57      | 123.84   |
| 31  | A     | 842 | CLA  | CHD-C1D-ND  | -4.74 | 120.10      | 124.45   |
| 31  | 6     | 313 | CLA  | C1C-C2C-C3C | -4.74 | 101.97      | 106.96   |
| 31  | 2     | 315 | CLA  | C2C-C1C-NC  | 4.74  | 114.41      | 109.97   |
| 31  | B     | 816 | CLA  | C1C-C2C-C3C | -4.73 | 101.98      | 106.96   |
| 31  | 4     | 306 | CLA  | O2D-CGD-CBD | 4.73  | 119.68      | 111.27   |
| 32  | 9     | 320 | CHL  | C4A-NA-C1A  | 4.73  | 108.83      | 106.71   |
| 31  | 4     | 305 | CLA  | C1B-CHB-C4A | -4.73 | 120.75      | 130.12   |
| 31  | B     | 826 | CLA  | C1C-C2C-C3C | -4.73 | 101.98      | 106.96   |
| 31  | 8     | 314 | CLA  | C2C-C1C-NC  | 4.73  | 114.41      | 109.97   |
| 32  | 6     | 320 | CHL  | C4A-NA-C1A  | 4.73  | 108.83      | 106.71   |
| 31  | 4     | 312 | CLA  | O2D-CGD-CBD | 4.73  | 119.67      | 111.27   |
| 31  | B     | 829 | CLA  | C2D-C1D-ND  | 4.73  | 113.59      | 110.10   |
| 42  | 4     | 304 | SQD  | O9-S-C6     | 4.73  | 112.56      | 106.94   |
| 31  | A     | 850 | CLA  | C1C-C2C-C3C | -4.73 | 101.99      | 106.96   |
| 31  | 8     | 320 | CLA  | C2C-C1C-NC  | 4.73  | 114.40      | 109.97   |
| 31  | 9     | 311 | CLA  | C1C-C2C-C3C | -4.73 | 101.99      | 106.96   |
| 31  | H     | 903 | CLA  | C2C-C1C-NC  | 4.73  | 114.40      | 109.97   |
| 31  | 8     | 309 | CLA  | C2D-C1D-ND  | 4.73  | 113.59      | 110.10   |
| 31  | B     | 842 | CLA  | CHD-C1D-ND  | -4.73 | 120.11      | 124.45   |
| 31  | b     | 305 | CLA  | CHD-C1D-ND  | -4.72 | 120.11      | 124.45   |
| 31  | 3     | 320 | CLA  | C1C-C2C-C3C | -4.72 | 101.99      | 106.96   |
| 31  | b     | 313 | CLA  | CAC-C3C-C4C | 4.72  | 130.94      | 124.81   |
| 31  | 3     | 314 | CLA  | C2C-C1C-NC  | 4.72  | 114.40      | 109.97   |
| 31  | A     | 823 | CLA  | CHD-C1D-ND  | -4.72 | 120.11      | 124.45   |
| 31  | 2     | 313 | CLA  | C2C-C1C-NC  | 4.72  | 114.39      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 816 | CLA  | C2C-C1C-NC  | 4.72  | 114.39      | 109.97   |
| 31  | 4     | 320 | CLA  | C1C-C2C-C3C | -4.72 | 102.00      | 106.96   |
| 31  | 3     | 311 | CLA  | O2D-CGD-CBD | 4.72  | 119.65      | 111.27   |
| 31  | A     | 820 | CLA  | C2D-C1D-ND  | 4.72  | 113.58      | 110.10   |
| 31  | A     | 837 | CLA  | CHD-C1D-ND  | -4.71 | 120.12      | 124.45   |
| 31  | J     | 105 | CLA  | C2C-C1C-NC  | 4.71  | 114.39      | 109.97   |
| 31  | B     | 834 | CLA  | CHD-C4C-C3C | -4.71 | 117.91      | 124.84   |
| 31  | 2     | 308 | CLA  | CHD-C4C-C3C | -4.71 | 117.92      | 124.84   |
| 31  | 5     | 312 | CLA  | O2D-CGD-O1D | -4.71 | 114.63      | 123.84   |
| 31  | A     | 837 | CLA  | O2D-CGD-CBD | 4.71  | 119.64      | 111.27   |
| 31  | A     | 836 | CLA  | CHD-C1D-ND  | -4.71 | 120.13      | 124.45   |
| 31  | 3     | 312 | CLA  | C2C-C1C-NC  | 4.71  | 114.38      | 109.97   |
| 31  | a     | 311 | CLA  | C2C-C1C-NC  | 4.71  | 114.38      | 109.97   |
| 31  | 9     | 312 | CLA  | CHD-C4C-C3C | -4.71 | 117.92      | 124.84   |
| 36  | 8     | 303 | LUT  | C18-C5-C4   | -4.71 | 105.64      | 114.36   |
| 31  | a     | 312 | CLA  | C2D-C1D-ND  | 4.71  | 113.57      | 110.10   |
| 31  | 3     | 310 | CLA  | C2D-C1D-ND  | 4.71  | 113.57      | 110.10   |
| 31  | a     | 311 | CLA  | C4D-CHA-C1A | -4.70 | 115.53      | 121.25   |
| 31  | B     | 849 | CLA  | CHD-C1D-ND  | -4.70 | 120.13      | 124.45   |
| 31  | A     | 857 | CLA  | C2D-C1D-ND  | 4.70  | 113.57      | 110.10   |
| 36  | 8     | 302 | LUT  | C8-C7-C6    | -4.70 | 114.00      | 127.20   |
| 31  | 3     | 307 | CLA  | C2D-C1D-ND  | 4.70  | 113.57      | 110.10   |
| 31  | 5     | 315 | CLA  | C2C-C1C-NC  | 4.70  | 114.37      | 109.97   |
| 31  | 5     | 318 | CLA  | C2C-C1C-NC  | 4.70  | 114.37      | 109.97   |
| 31  | A     | 821 | CLA  | C2D-C1D-ND  | 4.70  | 113.57      | 110.10   |
| 31  | A     | 822 | CLA  | CHD-C4C-C3C | -4.70 | 117.94      | 124.84   |
| 32  | 6     | 317 | CHL  | C4A-NA-C1A  | 4.70  | 108.82      | 106.71   |
| 31  | 7     | 313 | CLA  | C2D-C1D-ND  | 4.70  | 113.56      | 110.10   |
| 31  | 3     | 310 | CLA  | C4D-CHA-C1A | -4.69 | 115.54      | 121.25   |
| 31  | A     | 834 | CLA  | C2C-C1C-NC  | 4.69  | 114.37      | 109.97   |
| 31  | 7     | 309 | CLA  | CHD-C1D-ND  | -4.69 | 120.14      | 124.45   |
| 31  | A     | 815 | CLA  | O2D-CGD-CBD | 4.69  | 119.61      | 111.27   |
| 31  | 6     | 314 | CLA  | C2C-C1C-NC  | 4.69  | 114.37      | 109.97   |
| 31  | 8     | 308 | CLA  | C2D-C1D-ND  | 4.69  | 113.56      | 110.10   |
| 31  | 3     | 314 | CLA  | C1C-C2C-C3C | -4.69 | 102.03      | 106.96   |
| 31  | 3     | 309 | CLA  | CHD-C1D-ND  | -4.69 | 120.15      | 124.45   |
| 31  | b     | 308 | CLA  | O2D-CGD-CBD | 4.68  | 119.59      | 111.27   |
| 31  | B     | 817 | CLA  | C2D-C1D-ND  | 4.68  | 113.55      | 110.10   |
| 32  | 7     | 318 | CHL  | C1C-C2C-C3C | -4.68 | 103.40      | 107.11   |
| 31  | 4     | 316 | CLA  | O2D-CGD-CBD | 4.68  | 119.58      | 111.27   |
| 31  | 6     | 306 | CLA  | O2D-CGD-CBD | 4.67  | 119.58      | 111.27   |
| 31  | A     | 821 | CLA  | CHD-C4C-C3C | -4.67 | 117.97      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 315 | CLA  | C1C-C2C-C3C | -4.67 | 102.04      | 106.96   |
| 31  | 6     | 307 | CLA  | C1C-C2C-C3C | -4.67 | 102.04      | 106.96   |
| 31  | 2     | 307 | CLA  | C2C-C1C-NC  | 4.67  | 114.35      | 109.97   |
| 31  | 9     | 314 | CLA  | C2D-C1D-ND  | 4.67  | 113.55      | 110.10   |
| 31  | B     | 821 | CLA  | C2C-C1C-NC  | 4.67  | 114.34      | 109.97   |
| 31  | B     | 833 | CLA  | C2D-C1D-ND  | 4.67  | 113.54      | 110.10   |
| 31  | B     | 813 | CLA  | CHD-C1D-ND  | -4.66 | 120.17      | 124.45   |
| 31  | 9     | 321 | CLA  | C1C-C2C-C3C | -4.66 | 102.05      | 106.96   |
| 31  | 8     | 313 | CLA  | C2D-C1D-ND  | 4.66  | 113.54      | 110.10   |
| 31  | B     | 830 | CLA  | C4D-CHA-C1A | -4.66 | 115.57      | 121.25   |
| 31  | A     | 832 | CLA  | C2C-C1C-NC  | 4.66  | 114.34      | 109.97   |
| 31  | 2     | 312 | CLA  | O2D-CGD-O1D | -4.66 | 114.72      | 123.84   |
| 31  | 2     | 311 | CLA  | O2D-CGD-CBD | 4.66  | 119.55      | 111.27   |
| 31  | B     | 825 | CLA  | O2D-CGD-CBD | 4.66  | 119.55      | 111.27   |
| 31  | B     | 826 | CLA  | CHD-C4C-C3C | -4.66 | 117.99      | 124.84   |
| 31  | F     | 306 | CLA  | C2C-C1C-NC  | 4.66  | 114.34      | 109.97   |
| 31  | 4     | 305 | CLA  | C1C-C2C-C3C | -4.66 | 102.06      | 106.96   |
| 31  | b     | 307 | CLA  | C2C-C1C-NC  | 4.66  | 114.33      | 109.97   |
| 31  | B     | 813 | CLA  | O2D-CGD-O1D | -4.66 | 114.73      | 123.84   |
| 31  | 8     | 314 | CLA  | C2D-C1D-ND  | 4.66  | 113.53      | 110.10   |
| 31  | 8     | 311 | CLA  | CHD-C1D-ND  | -4.66 | 120.18      | 124.45   |
| 31  | A     | 853 | CLA  | C2C-C1C-NC  | 4.65  | 114.33      | 109.97   |
| 31  | B     | 826 | CLA  | C2C-C1C-NC  | 4.65  | 114.33      | 109.97   |
| 31  | 5     | 320 | CLA  | C4D-CHA-C1A | -4.65 | 115.59      | 121.25   |
| 31  | b     | 313 | CLA  | O2D-CGD-CBD | 4.65  | 119.53      | 111.27   |
| 31  | B     | 847 | CLA  | C1C-C2C-C3C | -4.65 | 102.07      | 106.96   |
| 31  | B     | 817 | CLA  | C4D-CHA-C1A | -4.65 | 115.59      | 121.25   |
| 31  | K     | 206 | CLA  | C1C-C2C-C3C | -4.65 | 102.07      | 106.96   |
| 31  | 7     | 312 | CLA  | O2D-CGD-CBD | 4.64  | 119.52      | 111.27   |
| 32  | A     | 839 | CHL  | CHD-C4C-C3C | -4.64 | 118.01      | 124.84   |
| 31  | 3     | 317 | CLA  | C2C-C1C-NC  | 4.64  | 114.32      | 109.97   |
| 31  | B     | 840 | CLA  | C2D-C1D-ND  | 4.64  | 113.53      | 110.10   |
| 31  | 7     | 321 | CLA  | C2D-C1D-ND  | 4.64  | 113.53      | 110.10   |
| 31  | B     | 813 | CLA  | CHD-C4C-C3C | -4.64 | 118.02      | 124.84   |
| 31  | 5     | 308 | CLA  | O2D-CGD-CBD | 4.64  | 119.51      | 111.27   |
| 31  | 4     | 315 | CLA  | O2D-CGD-CBD | 4.64  | 119.51      | 111.27   |
| 31  | 9     | 311 | CLA  | C2C-C1C-NC  | 4.64  | 114.32      | 109.97   |
| 31  | a     | 313 | CLA  | CHD-C1D-ND  | -4.64 | 120.19      | 124.45   |
| 31  | 5     | 311 | CLA  | C1C-C2C-C3C | -4.64 | 102.08      | 106.96   |
| 31  | A     | 850 | CLA  | C2C-C1C-NC  | 4.63  | 114.31      | 109.97   |
| 31  | J     | 105 | CLA  | CHD-C4C-C3C | -4.63 | 118.03      | 124.84   |
| 31  | 7     | 314 | CLA  | C2C-C1C-NC  | 4.63  | 114.31      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 840 | CLA  | O2D-CGD-CBD | 4.63  | 119.50      | 111.27   |
| 31  | A     | 825 | CLA  | CHD-C4C-C3C | -4.63 | 118.04      | 124.84   |
| 31  | G     | 206 | CLA  | C2D-C1D-ND  | 4.63  | 113.52      | 110.10   |
| 31  | A     | 845 | CLA  | C2C-C1C-NC  | 4.63  | 114.31      | 109.97   |
| 31  | 9     | 319 | CLA  | C2C-C1C-NC  | 4.63  | 114.31      | 109.97   |
| 31  | 4     | 307 | CLA  | C2C-C1C-NC  | 4.63  | 114.31      | 109.97   |
| 31  | 5     | 309 | CLA  | C2C-C1C-NC  | 4.63  | 114.31      | 109.97   |
| 31  | A     | 819 | CLA  | C2D-C1D-ND  | 4.63  | 113.51      | 110.10   |
| 31  | 2     | 310 | CLA  | O2D-CGD-CBD | 4.63  | 119.49      | 111.27   |
| 32  | 8     | 319 | CHL  | C1C-C2C-C3C | -4.63 | 103.44      | 107.11   |
| 31  | B     | 812 | CLA  | CAC-C3C-C4C | 4.62  | 130.81      | 124.81   |
| 31  | A     | 844 | CLA  | C1C-C2C-C3C | -4.62 | 102.09      | 106.96   |
| 30  | A     | 813 | CL0  | C3D-C2D-C1D | -4.62 | 99.52       | 105.83   |
| 31  | 2     | 314 | CLA  | C2C-C1C-NC  | 4.62  | 114.30      | 109.97   |
| 36  | a     | 305 | LUT  | C35-C15-C14 | -4.62 | 114.00      | 123.47   |
| 36  | 9     | 303 | LUT  | C7-C6-C5    | -4.62 | 110.27      | 121.46   |
| 31  | 2     | 307 | CLA  | O2D-CGD-O1D | -4.62 | 114.80      | 123.84   |
| 31  | K     | 204 | CLA  | C2C-C1C-NC  | 4.62  | 114.30      | 109.97   |
| 31  | A     | 827 | CLA  | C2C-C1C-NC  | 4.62  | 114.30      | 109.97   |
| 31  | 9     | 312 | CLA  | C2D-C1D-ND  | 4.62  | 113.51      | 110.10   |
| 31  | 5     | 318 | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 31  | 3     | 318 | CLA  | C1C-C2C-C3C | -4.62 | 102.10      | 106.96   |
| 31  | A     | 855 | CLA  | CHD-C4C-C3C | -4.62 | 118.06      | 124.84   |
| 36  | a     | 305 | LUT  | C7-C6-C5    | -4.62 | 110.28      | 121.46   |
| 31  | 6     | 307 | CLA  | CHD-C1D-ND  | -4.61 | 120.21      | 124.45   |
| 31  | 8     | 313 | CLA  | O2D-CGD-O1D | -4.61 | 114.82      | 123.84   |
| 31  | 8     | 309 | CLA  | O2D-CGD-CBD | 4.61  | 119.46      | 111.27   |
| 31  | 5     | 307 | CLA  | C2D-C1D-ND  | 4.61  | 113.50      | 110.10   |
| 31  | A     | 818 | CLA  | C4D-CHA-C1A | -4.61 | 115.64      | 121.25   |
| 31  | 3     | 313 | CLA  | CHD-C1D-ND  | -4.61 | 120.22      | 124.45   |
| 32  | a     | 318 | CHL  | CHD-C4C-C3C | -4.61 | 118.06      | 124.84   |
| 31  | 3     | 311 | CLA  | C1C-C2C-C3C | -4.61 | 102.11      | 106.96   |
| 31  | 8     | 321 | CLA  | C2D-C1D-ND  | 4.61  | 113.50      | 110.10   |
| 31  | B     | 821 | CLA  | C1C-C2C-C3C | -4.61 | 102.11      | 106.96   |
| 31  | 5     | 311 | CLA  | O2D-CGD-CBD | 4.61  | 119.46      | 111.27   |
| 32  | 3     | 315 | CHL  | C1C-C2C-C3C | -4.61 | 103.46      | 107.11   |
| 31  | B     | 842 | CLA  | C2D-C1D-ND  | 4.61  | 113.50      | 110.10   |
| 31  | 6     | 311 | CLA  | C2C-C1C-NC  | 4.60  | 114.29      | 109.97   |
| 31  | 6     | 307 | CLA  | C2C-C1C-NC  | 4.60  | 114.28      | 109.97   |
| 31  | A     | 857 | CLA  | CHD-C4C-C3C | -4.60 | 118.07      | 124.84   |
| 36  | 5     | 304 | LUT  | C18-C5-C4   | -4.60 | 105.83      | 114.36   |
| 31  | b     | 302 | CLA  | C2D-C1D-ND  | 4.60  | 113.50      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | a     | 320 | CHL  | C1C-C2C-C3C | -4.60 | 103.46      | 107.11   |
| 31  | 9     | 317 | CLA  | O2D-CGD-CBD | 4.60  | 119.44      | 111.27   |
| 31  | a     | 312 | CLA  | CHD-C4C-C3C | -4.60 | 118.08      | 124.84   |
| 31  | A     | 845 | CLA  | C1C-C2C-C3C | -4.60 | 102.12      | 106.96   |
| 31  | 4     | 321 | CLA  | C1C-C2C-C3C | -4.60 | 102.12      | 106.96   |
| 31  | 8     | 311 | CLA  | C1C-C2C-C3C | -4.60 | 102.12      | 106.96   |
| 31  | b     | 303 | CLA  | C4D-CHA-C1A | -4.60 | 115.65      | 121.25   |
| 31  | 7     | 310 | CLA  | C2D-C1D-ND  | 4.60  | 113.49      | 110.10   |
| 31  | 9     | 318 | CLA  | C2D-C1D-ND  | 4.59  | 113.49      | 110.10   |
| 31  | 8     | 313 | CLA  | CHD-C1D-ND  | -4.59 | 120.23      | 124.45   |
| 31  | 6     | 310 | CLA  | C2C-C1C-NC  | 4.59  | 114.27      | 109.97   |
| 31  | 3     | 308 | CLA  | CHD-C4C-C3C | -4.59 | 118.09      | 124.84   |
| 31  | A     | 827 | CLA  | C2D-C1D-ND  | 4.59  | 113.49      | 110.10   |
| 31  | 8     | 318 | CLA  | C2C-C1C-NC  | 4.59  | 114.27      | 109.97   |
| 31  | 5     | 309 | CLA  | C1C-C2C-C3C | -4.59 | 102.13      | 106.96   |
| 31  | A     | 853 | CLA  | CHD-C1D-ND  | -4.59 | 120.24      | 124.45   |
| 31  | 4     | 308 | CLA  | C1C-C2C-C3C | -4.59 | 102.13      | 106.96   |
| 31  | A     | 832 | CLA  | C1C-C2C-C3C | -4.59 | 102.14      | 106.96   |
| 31  | a     | 322 | CLA  | C2C-C1C-NC  | 4.59  | 114.27      | 109.97   |
| 31  | 4     | 306 | CLA  | CHD-C1D-ND  | -4.59 | 120.24      | 124.45   |
| 31  | A     | 825 | CLA  | C2D-C1D-ND  | 4.59  | 113.48      | 110.10   |
| 31  | 6     | 308 | CLA  | CAC-C3C-C4C | 4.59  | 130.76      | 124.81   |
| 31  | 5     | 314 | CLA  | C1C-C2C-C3C | -4.58 | 102.14      | 106.96   |
| 31  | 5     | 323 | CLA  | C1C-C2C-C3C | -4.58 | 102.14      | 106.96   |
| 31  | B     | 824 | CLA  | O2D-CGD-CBD | 4.58  | 119.41      | 111.27   |
| 31  | A     | 834 | CLA  | O2D-CGD-O1D | -4.58 | 114.88      | 123.84   |
| 32  | 9     | 322 | CHL  | C1C-C2C-C3C | -4.58 | 103.48      | 107.11   |
| 32  | 6     | 317 | CHL  | O2D-CGD-CBD | 4.58  | 119.41      | 111.27   |
| 31  | B     | 813 | CLA  | C2D-C1D-ND  | 4.58  | 113.48      | 110.10   |
| 31  | b     | 305 | CLA  | O2D-CGD-CBD | 4.58  | 119.41      | 111.27   |
| 32  | 6     | 321 | CHL  | C1C-C2C-C3C | -4.58 | 103.48      | 107.11   |
| 31  | F     | 305 | CLA  | C1C-C2C-C3C | -4.58 | 102.14      | 106.96   |
| 31  | 8     | 311 | CLA  | C2C-C1C-NC  | 4.58  | 114.26      | 109.97   |
| 31  | 2     | 305 | CLA  | C2C-C1C-NC  | 4.58  | 114.26      | 109.97   |
| 36  | 8     | 303 | LUT  | C7-C8-C9    | -4.58 | 119.32      | 126.23   |
| 31  | A     | 830 | CLA  | O2D-CGD-O1D | -4.58 | 114.89      | 123.84   |
| 31  | B     | 813 | CLA  | O2D-CGD-CBD | 4.57  | 119.40      | 111.27   |
| 31  | A     | 833 | CLA  | O2D-CGD-O1D | -4.57 | 114.89      | 123.84   |
| 31  | b     | 306 | CLA  | C2C-C1C-NC  | 4.57  | 114.26      | 109.97   |
| 31  | 3     | 312 | CLA  | C1C-C2C-C3C | -4.57 | 102.15      | 106.96   |
| 31  | K     | 205 | CLA  | O2D-CGD-CBD | 4.57  | 119.39      | 111.27   |
| 31  | A     | 835 | CLA  | C2D-C1D-ND  | 4.57  | 113.47      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | L     | 304 | LUT  | C35-C15-C14 | -4.57 | 114.11      | 123.47   |
| 31  | 8     | 320 | CLA  | C1C-C2C-C3C | -4.57 | 102.15      | 106.96   |
| 31  | 3     | 320 | CLA  | C2C-C1C-NC  | 4.57  | 114.25      | 109.97   |
| 31  | A     | 838 | CLA  | C1C-C2C-C3C | -4.57 | 102.16      | 106.96   |
| 31  | 8     | 318 | CLA  | C2D-C1D-ND  | 4.56  | 113.47      | 110.10   |
| 36  | b     | 301 | LUT  | C12-C13-C14 | -4.56 | 111.94      | 118.94   |
| 31  | 9     | 316 | CLA  | C1C-C2C-C3C | -4.56 | 102.16      | 106.96   |
| 31  | a     | 315 | CLA  | C2C-C1C-NC  | 4.56  | 114.25      | 109.97   |
| 31  | 4     | 307 | CLA  | CHD-C1D-ND  | -4.56 | 120.26      | 124.45   |
| 36  | 8     | 303 | LUT  | C19-C9-C8   | -4.56 | 110.89      | 118.08   |
| 32  | 9     | 320 | CHL  | O2D-CGD-CBD | 4.56  | 119.37      | 111.27   |
| 31  | a     | 315 | CLA  | CHD-C1D-ND  | -4.56 | 120.27      | 124.45   |
| 31  | O     | 202 | CLA  | CHD-C1D-ND  | -4.56 | 120.27      | 124.45   |
| 31  | K     | 205 | CLA  | C2C-C1C-NC  | 4.55  | 114.24      | 109.97   |
| 31  | a     | 322 | CLA  | CHD-C1D-ND  | -4.55 | 120.27      | 124.45   |
| 31  | A     | 846 | CLA  | O2D-CGD-CBD | 4.55  | 119.36      | 111.27   |
| 31  | 7     | 313 | CLA  | C1C-C2C-C3C | -4.55 | 102.17      | 106.96   |
| 32  | 7     | 319 | CHL  | CGD-CBD-CAD | 4.55  | 125.48      | 110.73   |
| 31  | B     | 812 | CLA  | CHD-C1D-ND  | -4.55 | 120.27      | 124.45   |
| 31  | 8     | 307 | CLA  | C1C-C2C-C3C | -4.55 | 102.17      | 106.96   |
| 31  | 3     | 314 | CLA  | O2D-CGD-O1D | -4.55 | 114.94      | 123.84   |
| 31  | b     | 303 | CLA  | C1C-C2C-C3C | -4.55 | 102.17      | 106.96   |
| 31  | 9     | 317 | CLA  | C2C-C1C-NC  | 4.55  | 114.23      | 109.97   |
| 31  | 5     | 308 | CLA  | C2C-C1C-NC  | 4.55  | 114.23      | 109.97   |
| 31  | 5     | 310 | CLA  | C2C-C1C-NC  | 4.55  | 114.23      | 109.97   |
| 31  | A     | 816 | CLA  | C4D-CHA-C1A | -4.55 | 115.71      | 121.25   |
| 31  | 6     | 322 | CLA  | CHD-C1D-ND  | -4.55 | 120.28      | 124.45   |
| 31  | L     | 306 | CLA  | C2C-C1C-NC  | 4.55  | 114.23      | 109.97   |
| 31  | 4     | 319 | CLA  | C2C-C1C-NC  | 4.55  | 114.23      | 109.97   |
| 31  | 4     | 308 | CLA  | C2D-C1D-ND  | 4.54  | 113.45      | 110.10   |
| 31  | A     | 855 | CLA  | O2D-CGD-CBD | 4.54  | 119.34      | 111.27   |
| 31  | H     | 903 | CLA  | O2D-CGD-O1D | -4.54 | 114.95      | 123.84   |
| 31  | A     | 834 | CLA  | CHD-C4C-C3C | -4.54 | 118.16      | 124.84   |
| 32  | a     | 317 | CHL  | C1C-C2C-C3C | -4.54 | 103.51      | 107.11   |
| 31  | 5     | 311 | CLA  | C2D-C1D-ND  | 4.54  | 113.45      | 110.10   |
| 31  | A     | 821 | CLA  | O2D-CGD-CBD | 4.54  | 119.33      | 111.27   |
| 31  | A     | 819 | CLA  | C1C-C2C-C3C | -4.54 | 102.18      | 106.96   |
| 31  | 8     | 307 | CLA  | C2C-C1C-NC  | 4.54  | 114.22      | 109.97   |
| 31  | A     | 845 | CLA  | C2D-C1D-ND  | 4.54  | 113.45      | 110.10   |
| 31  | K     | 204 | CLA  | C4D-CHA-C1A | -4.54 | 115.73      | 121.25   |
| 31  | b     | 307 | CLA  | C1C-C2C-C3C | -4.54 | 102.19      | 106.96   |
| 32  | b     | 309 | CHL  | C1C-C2C-C3C | -4.54 | 103.51      | 107.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 312 | CLA  | C2C-C1C-NC  | 4.53  | 114.22      | 109.97   |
| 32  | 4     | 313 | CHL  | C1C-C2C-C3C | -4.53 | 103.52      | 107.11   |
| 31  | A     | 828 | CLA  | C2D-C1D-ND  | 4.53  | 113.44      | 110.10   |
| 31  | A     | 842 | CLA  | C2D-C1D-ND  | 4.53  | 113.44      | 110.10   |
| 31  | A     | 836 | CLA  | C1C-C2C-C3C | -4.53 | 102.19      | 106.96   |
| 31  | B     | 825 | CLA  | C2D-C1D-ND  | 4.53  | 113.44      | 110.10   |
| 31  | 8     | 321 | CLA  | C2C-C1C-NC  | 4.53  | 114.22      | 109.97   |
| 31  | L     | 307 | CLA  | C2C-C1C-NC  | 4.53  | 114.22      | 109.97   |
| 31  | A     | 833 | CLA  | C2D-C1D-ND  | 4.53  | 113.44      | 110.10   |
| 31  | K     | 204 | CLA  | C2D-C1D-ND  | 4.53  | 113.44      | 110.10   |
| 31  | b     | 302 | CLA  | C1C-C2C-C3C | -4.52 | 102.20      | 106.96   |
| 32  | 4     | 310 | CHL  | C1C-C2C-C3C | -4.52 | 103.53      | 107.11   |
| 31  | 7     | 311 | CLA  | C1C-C2C-C3C | -4.52 | 102.20      | 106.96   |
| 31  | 6     | 322 | CLA  | C1C-C2C-C3C | -4.52 | 102.20      | 106.96   |
| 31  | 6     | 315 | CLA  | O2D-CGD-CBD | 4.52  | 119.30      | 111.27   |
| 31  | A     | 820 | CLA  | CHD-C4C-C3C | -4.52 | 118.20      | 124.84   |
| 31  | B     | 826 | CLA  | C2D-C1D-ND  | 4.52  | 113.43      | 110.10   |
| 31  | 5     | 314 | CLA  | CHD-C4C-C3C | -4.52 | 118.20      | 124.84   |
| 31  | B     | 836 | CLA  | C2D-C1D-ND  | 4.52  | 113.43      | 110.10   |
| 31  | A     | 845 | CLA  | CHD-C1D-ND  | -4.52 | 120.30      | 124.45   |
| 31  | 4     | 319 | CLA  | CHD-C1D-ND  | -4.52 | 120.30      | 124.45   |
| 31  | b     | 306 | CLA  | C1C-C2C-C3C | -4.52 | 102.21      | 106.96   |
| 31  | H     | 903 | CLA  | O2D-CGD-CBD | 4.51  | 119.29      | 111.27   |
| 31  | 9     | 311 | CLA  | CHD-C1D-ND  | -4.51 | 120.31      | 124.45   |
| 31  | 4     | 312 | CLA  | C1C-C2C-C3C | -4.51 | 102.21      | 106.96   |
| 31  | 9     | 312 | CLA  | CHD-C1D-ND  | -4.51 | 120.31      | 124.45   |
| 31  | b     | 312 | CLA  | C1C-C2C-C3C | -4.51 | 102.21      | 106.96   |
| 31  | 5     | 320 | CLA  | CHD-C1D-ND  | -4.51 | 120.31      | 124.45   |
| 31  | A     | 852 | CLA  | C2D-C1D-ND  | 4.51  | 113.43      | 110.10   |
| 31  | B     | 827 | CLA  | O2D-CGD-CBD | 4.51  | 119.28      | 111.27   |
| 31  | a     | 313 | CLA  | C4D-CHA-C1A | -4.51 | 115.76      | 121.25   |
| 36  | 6     | 304 | LUT  | C19-C9-C8   | -4.51 | 110.97      | 118.08   |
| 31  | 8     | 315 | CLA  | CHD-C1D-ND  | -4.51 | 120.31      | 124.45   |
| 31  | 2     | 312 | CLA  | O2D-CGD-CBD | 4.51  | 119.28      | 111.27   |
| 31  | H     | 903 | CLA  | C1C-C2C-C3C | -4.51 | 102.22      | 106.96   |
| 32  | 8     | 316 | CHL  | O2D-CGD-O1D | -4.51 | 115.03      | 123.84   |
| 32  | K     | 201 | CHL  | C3D-C2D-C1D | -4.50 | 99.68       | 105.83   |
| 32  | a     | 318 | CHL  | O1D-CGD-CBD | -4.50 | 115.28      | 124.48   |
| 31  | 7     | 313 | CLA  | C2C-C1C-NC  | 4.50  | 114.19      | 109.97   |
| 31  | 4     | 309 | CLA  | C1C-C2C-C3C | -4.50 | 102.23      | 106.96   |
| 31  | 3     | 316 | CLA  | CHD-C1D-ND  | -4.50 | 120.32      | 124.45   |
| 31  | 6     | 316 | CLA  | CHD-C4C-C3C | -4.50 | 118.23      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 821 | CLA  | C2C-C1C-NC  | 4.50  | 114.19      | 109.97   |
| 31  | 6     | 322 | CLA  | C2C-C1C-NC  | 4.50  | 114.19      | 109.97   |
| 31  | 8     | 307 | CLA  | C2D-C1D-ND  | 4.50  | 113.42      | 110.10   |
| 31  | 5     | 311 | CLA  | CHD-C1D-ND  | -4.50 | 120.32      | 124.45   |
| 31  | A     | 849 | CLA  | C2C-C1C-NC  | 4.49  | 114.18      | 109.97   |
| 31  | L     | 306 | CLA  | C1C-C2C-C3C | -4.49 | 102.23      | 106.96   |
| 31  | J     | 105 | CLA  | C1C-C2C-C3C | -4.49 | 102.23      | 106.96   |
| 31  | B     | 839 | CLA  | O2D-CGD-O1D | -4.49 | 115.06      | 123.84   |
| 31  | 5     | 318 | CLA  | O2D-CGD-O1D | -4.49 | 115.06      | 123.84   |
| 31  | A     | 826 | CLA  | C2D-C1D-ND  | 4.49  | 113.41      | 110.10   |
| 31  | B     | 824 | CLA  | C2C-C1C-NC  | 4.49  | 114.18      | 109.97   |
| 31  | A     | 827 | CLA  | C1C-C2C-C3C | -4.49 | 102.24      | 106.96   |
| 32  | 7     | 320 | CHL  | C1C-C2C-C3C | -4.49 | 103.55      | 107.11   |
| 32  | 6     | 317 | CHL  | C1C-C2C-C3C | -4.49 | 103.55      | 107.11   |
| 31  | 7     | 321 | CLA  | C1C-C2C-C3C | -4.49 | 102.24      | 106.96   |
| 31  | B     | 811 | CLA  | C2D-C1D-ND  | 4.49  | 113.41      | 110.10   |
| 36  | 3     | 304 | LUT  | C17-C1-C6   | 4.49  | 117.58      | 110.30   |
| 31  | 8     | 314 | CLA  | O2D-CGD-O1D | -4.48 | 115.07      | 123.84   |
| 31  | a     | 310 | CLA  | O2D-CGD-CBD | 4.48  | 119.24      | 111.27   |
| 31  | 4     | 308 | CLA  | O2D-CGD-O1D | -4.48 | 115.07      | 123.84   |
| 31  | 8     | 312 | CLA  | C2C-C1C-NC  | 4.48  | 114.17      | 109.97   |
| 31  | 5     | 307 | CLA  | CHD-C1D-ND  | -4.48 | 120.33      | 124.45   |
| 31  | 6     | 316 | CLA  | C2D-C1D-ND  | 4.48  | 113.41      | 110.10   |
| 36  | 3     | 305 | LUT  | C28-C29-C30 | -4.48 | 112.07      | 118.94   |
| 31  | A     | 843 | CLA  | C1C-C2C-C3C | -4.48 | 102.25      | 106.96   |
| 31  | a     | 315 | CLA  | C1C-C2C-C3C | -4.48 | 102.25      | 106.96   |
| 31  | a     | 322 | CLA  | C1C-C2C-C3C | -4.48 | 102.25      | 106.96   |
| 31  | A     | 846 | CLA  | CHD-C4C-C3C | -4.48 | 118.26      | 124.84   |
| 31  | G     | 206 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | 5     | 321 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | B     | 815 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | B     | 837 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | 5     | 314 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | 4     | 314 | CLA  | C1C-C2C-C3C | -4.47 | 102.26      | 106.96   |
| 31  | A     | 820 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | A     | 854 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | K     | 206 | CLA  | O2D-CGD-CBD | 4.47  | 119.21      | 111.27   |
| 31  | b     | 307 | CLA  | O2D-CGD-CBD | 4.47  | 119.21      | 111.27   |
| 31  | B     | 835 | CLA  | C2D-C1D-ND  | 4.47  | 113.40      | 110.10   |
| 31  | H     | 902 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | G     | 205 | CLA  | O2D-CGD-O1D | -4.47 | 115.10      | 123.84   |
| 31  | a     | 314 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 322 | CLA  | C2C-C1C-NC  | 4.47  | 114.16      | 109.97   |
| 31  | A     | 846 | CLA  | C1C-C2C-C3C | -4.47 | 102.26      | 106.96   |
| 31  | 2     | 313 | CLA  | CHD-C1D-ND  | -4.47 | 120.35      | 124.45   |
| 31  | 3     | 309 | CLA  | C2D-C1D-ND  | 4.46  | 113.39      | 110.10   |
| 31  | 9     | 313 | CLA  | C4D-CHA-C1A | -4.46 | 115.82      | 121.25   |
| 31  | 6     | 312 | CLA  | CHD-C1D-ND  | -4.46 | 120.35      | 124.45   |
| 31  | H     | 903 | CLA  | C4D-CHA-C1A | -4.46 | 115.82      | 121.25   |
| 31  | b     | 310 | CLA  | C2C-C1C-NC  | 4.46  | 114.15      | 109.97   |
| 36  | a     | 303 | LUT  | C40-C33-C32 | -4.46 | 111.05      | 118.08   |
| 31  | B     | 820 | CLA  | C1C-C2C-C3C | -4.46 | 102.27      | 106.96   |
| 31  | 8     | 315 | CLA  | C2C-C1C-NC  | 4.46  | 114.15      | 109.97   |
| 31  | B     | 831 | CLA  | C4D-CHA-C1A | -4.46 | 115.82      | 121.25   |
| 31  | B     | 842 | CLA  | C2C-C1C-NC  | 4.46  | 114.15      | 109.97   |
| 31  | 4     | 312 | CLA  | C2C-C1C-NC  | 4.46  | 114.15      | 109.97   |
| 31  | A     | 851 | CLA  | C1C-C2C-C3C | -4.46 | 102.27      | 106.96   |
| 31  | B     | 827 | CLA  | C2D-C1D-ND  | 4.46  | 113.39      | 110.10   |
| 31  | b     | 306 | CLA  | C4D-CHA-C1A | -4.46 | 115.82      | 121.25   |
| 31  | A     | 857 | CLA  | C2C-C1C-NC  | 4.46  | 114.15      | 109.97   |
| 31  | A     | 820 | CLA  | C1C-C2C-C3C | -4.46 | 102.27      | 106.96   |
| 31  | 2     | 310 | CLA  | C1C-C2C-C3C | -4.46 | 102.27      | 106.96   |
| 31  | 4     | 305 | CLA  | C3D-C2D-C1D | -4.46 | 99.75       | 105.83   |
| 31  | B     | 816 | CLA  | CHD-C1D-ND  | -4.45 | 120.36      | 124.45   |
| 31  | B     | 820 | CLA  | C2D-C1D-ND  | 4.45  | 113.39      | 110.10   |
| 31  | B     | 813 | CLA  | C1C-C2C-C3C | -4.45 | 102.27      | 106.96   |
| 31  | G     | 205 | CLA  | CHD-C4C-C3C | -4.45 | 118.29      | 124.84   |
| 31  | B     | 829 | CLA  | CHD-C1D-ND  | -4.45 | 120.36      | 124.45   |
| 31  | B     | 846 | CLA  | C2C-C1C-NC  | 4.45  | 114.14      | 109.97   |
| 31  | A     | 830 | CLA  | C2D-C1D-ND  | 4.45  | 113.39      | 110.10   |
| 31  | B     | 820 | CLA  | CHD-C4C-C3C | -4.45 | 118.30      | 124.84   |
| 31  | 9     | 315 | CLA  | C2D-C1D-ND  | 4.45  | 113.38      | 110.10   |
| 31  | A     | 841 | CLA  | C2C-C1C-NC  | 4.45  | 114.14      | 109.97   |
| 31  | B     | 844 | CLA  | C2D-C1D-ND  | 4.45  | 113.38      | 110.10   |
| 31  | B     | 847 | CLA  | CHD-C4C-C3C | -4.45 | 118.30      | 124.84   |
| 31  | b     | 305 | CLA  | C1C-C2C-C3C | -4.45 | 102.28      | 106.96   |
| 31  | B     | 824 | CLA  | O2D-CGD-O1D | -4.45 | 115.15      | 123.84   |
| 31  | B     | 836 | CLA  | O2D-CGD-CBD | 4.44  | 119.17      | 111.27   |
| 31  | 8     | 313 | CLA  | CHD-C4C-C3C | -4.44 | 118.31      | 124.84   |
| 31  | 4     | 314 | CLA  | C2C-C1C-NC  | 4.44  | 114.14      | 109.97   |
| 31  | 2     | 313 | CLA  | C1C-C2C-C3C | -4.44 | 102.28      | 106.96   |
| 31  | 9     | 321 | CLA  | CHD-C1D-ND  | -4.44 | 120.37      | 124.45   |
| 36  | 4     | 303 | LUT  | C28-C29-C30 | -4.44 | 112.13      | 118.94   |
| 31  | B     | 817 | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 321 | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |
| 31  | B     | 812 | CLA  | O2D-CGD-CBD | 4.44  | 119.16      | 111.27   |
| 31  | J     | 105 | CLA  | C2D-C1D-ND  | 4.44  | 113.38      | 110.10   |
| 31  | b     | 311 | CLA  | C2C-C1C-NC  | 4.44  | 114.13      | 109.97   |
| 31  | a     | 313 | CLA  | O2D-CGD-CBD | 4.44  | 119.15      | 111.27   |
| 31  | 8     | 315 | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |
| 31  | 7     | 321 | CLA  | C2C-C1C-NC  | 4.44  | 114.13      | 109.97   |
| 31  | G     | 205 | CLA  | C1C-C2C-C3C | -4.44 | 102.29      | 106.96   |
| 31  | G     | 204 | CLA  | C2C-C1C-NC  | 4.44  | 114.13      | 109.97   |
| 31  | B     | 831 | CLA  | C1C-C2C-C3C | -4.43 | 102.29      | 106.96   |
| 31  | 9     | 317 | CLA  | C1C-C2C-C3C | -4.43 | 102.29      | 106.96   |
| 32  | 8     | 316 | CHL  | CHD-C4C-C3C | -4.43 | 118.32      | 124.84   |
| 31  | 6     | 312 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 31  | B     | 832 | CLA  | O2D-CGD-O1D | -4.43 | 115.17      | 123.84   |
| 31  | 5     | 308 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 31  | 7     | 321 | CLA  | O2D-CGD-CBD | 4.43  | 119.14      | 111.27   |
| 31  | F     | 306 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 31  | 2     | 314 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 31  | 4     | 319 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 31  | 4     | 307 | CLA  | C1C-C2C-C3C | -4.43 | 102.30      | 106.96   |
| 31  | b     | 304 | CLA  | C2D-C1D-ND  | 4.43  | 113.37      | 110.10   |
| 31  | a     | 313 | CLA  | C2C-C1C-NC  | 4.43  | 114.12      | 109.97   |
| 31  | 9     | 313 | CLA  | C2D-C1D-ND  | 4.43  | 113.37      | 110.10   |
| 31  | F     | 301 | CLA  | C2C-C1C-NC  | 4.43  | 114.12      | 109.97   |
| 31  | B     | 828 | CLA  | CHD-C4C-C3C | -4.43 | 118.33      | 124.84   |
| 36  | L     | 304 | LUT  | C8-C9-C10   | -4.43 | 112.15      | 118.94   |
| 31  | A     | 818 | CLA  | CHD-C1D-ND  | -4.43 | 120.39      | 124.45   |
| 31  | 9     | 314 | CLA  | CHD-C4C-C3C | -4.43 | 118.33      | 124.84   |
| 32  | 7     | 320 | CHL  | O2D-CGD-O1D | -4.43 | 115.19      | 123.84   |
| 31  | 6     | 308 | CLA  | C2D-C1D-ND  | 4.43  | 113.36      | 110.10   |
| 31  | b     | 304 | CLA  | CHD-C4C-C3C | -4.42 | 118.34      | 124.84   |
| 31  | 2     | 307 | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 31  | A     | 853 | CLA  | CHD-C4C-C3C | -4.42 | 118.34      | 124.84   |
| 31  | B     | 820 | CLA  | CHD-C1D-ND  | -4.42 | 120.39      | 124.45   |
| 31  | 3     | 313 | CLA  | C4D-CHA-C1A | -4.42 | 115.87      | 121.25   |
| 31  | 2     | 305 | CLA  | C4D-CHA-C1A | -4.42 | 115.87      | 121.25   |
| 31  | A     | 847 | CLA  | C2D-C1D-ND  | 4.42  | 113.36      | 110.10   |
| 31  | b     | 310 | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 31  | 6     | 314 | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 36  | 4     | 303 | LUT  | C4-C5-C6    | -4.42 | 111.00      | 120.85   |
| 31  | A     | 849 | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |
| 31  | a     | 314 | CLA  | C1C-C2C-C3C | -4.42 | 102.31      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 815 | CLA  | C4D-CHA-C1A | -4.42 | 115.87      | 121.25   |
| 31  | 3     | 311 | CLA  | C4D-CHA-C1A | -4.42 | 115.87      | 121.25   |
| 31  | A     | 844 | CLA  | O2D-CGD-O1D | -4.42 | 115.20      | 123.84   |
| 31  | 4     | 305 | CLA  | C1D-CHD-C4C | -4.42 | 116.53      | 126.06   |
| 31  | B     | 811 | CLA  | CHD-C4C-C3C | -4.41 | 118.35      | 124.84   |
| 31  | F     | 306 | CLA  | C2D-C1D-ND  | 4.41  | 113.36      | 110.10   |
| 36  | 9     | 305 | LUT  | C40-C33-C32 | -4.41 | 111.12      | 118.08   |
| 31  | 3     | 313 | CLA  | C1C-C2C-C3C | -4.41 | 102.32      | 106.96   |
| 31  | B     | 831 | CLA  | C2C-C1C-NC  | 4.41  | 114.11      | 109.97   |
| 31  | 7     | 309 | CLA  | C2D-C1D-ND  | 4.41  | 113.36      | 110.10   |
| 31  | b     | 313 | CLA  | C2D-C1D-ND  | 4.41  | 113.36      | 110.10   |
| 31  | 4     | 306 | CLA  | C2C-C1C-NC  | 4.41  | 114.10      | 109.97   |
| 31  | 7     | 312 | CLA  | CHD-C4C-C3C | -4.41 | 118.36      | 124.84   |
| 31  | 4     | 305 | CLA  | C6-C5-C3    | -4.41 | 107.41      | 114.62   |
| 31  | 6     | 315 | CLA  | C1C-C2C-C3C | -4.41 | 102.32      | 106.96   |
| 31  | H     | 902 | CLA  | C1C-C2C-C3C | -4.41 | 102.32      | 106.96   |
| 31  | a     | 313 | CLA  | C1C-C2C-C3C | -4.41 | 102.32      | 106.96   |
| 31  | A     | 817 | CLA  | CHD-C4C-C3C | -4.41 | 118.36      | 124.84   |
| 31  | A     | 816 | CLA  | C1C-C2C-C3C | -4.41 | 102.33      | 106.96   |
| 31  | A     | 837 | CLA  | C2D-C1D-ND  | 4.40  | 113.35      | 110.10   |
| 31  | 4     | 306 | CLA  | C1C-C2C-C3C | -4.40 | 102.33      | 106.96   |
| 31  | B     | 814 | CLA  | O2D-CGD-CBD | 4.40  | 119.09      | 111.27   |
| 31  | 5     | 312 | CLA  | C2C-C1C-NC  | 4.40  | 114.10      | 109.97   |
| 31  | 2     | 310 | CLA  | C2C-C1C-NC  | 4.40  | 114.10      | 109.97   |
| 31  | 7     | 309 | CLA  | O2D-CGD-CBD | 4.40  | 119.09      | 111.27   |
| 31  | H     | 901 | CLA  | C2C-C1C-NC  | 4.40  | 114.09      | 109.97   |
| 36  | 6     | 303 | LUT  | C4-C5-C6    | -4.40 | 111.04      | 120.85   |
| 31  | B     | 843 | CLA  | O2D-CGD-O1D | -4.40 | 115.24      | 123.84   |
| 31  | 3     | 308 | CLA  | C1C-C2C-C3C | -4.40 | 102.33      | 106.96   |
| 31  | 8     | 312 | CLA  | C1C-C2C-C3C | -4.40 | 102.33      | 106.96   |
| 32  | a     | 318 | CHL  | CHD-C1D-ND  | -4.40 | 120.41      | 124.45   |
| 31  | 9     | 314 | CLA  | C2C-C1C-NC  | 4.40  | 114.09      | 109.97   |
| 31  | b     | 308 | CLA  | CHD-C1D-ND  | -4.40 | 120.41      | 124.45   |
| 31  | B     | 835 | CLA  | C2C-C1C-NC  | 4.40  | 114.09      | 109.97   |
| 31  | 6     | 311 | CLA  | C1C-C2C-C3C | -4.40 | 102.33      | 106.96   |
| 31  | 8     | 321 | CLA  | C4D-CHA-C1A | -4.40 | 115.90      | 121.25   |
| 31  | 3     | 309 | CLA  | C2C-C1C-NC  | 4.40  | 114.09      | 109.97   |
| 31  | 9     | 311 | CLA  | C2D-C1D-ND  | 4.40  | 113.34      | 110.10   |
| 31  | B     | 828 | CLA  | O2D-CGD-CBD | 4.39  | 119.08      | 111.27   |
| 31  | B     | 828 | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 31  | 2     | 308 | CLA  | CHD-C1D-ND  | -4.39 | 120.42      | 124.45   |
| 31  | 8     | 313 | CLA  | C2C-C1C-NC  | 4.39  | 114.09      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 317 | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 31  | 2     | 305 | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 31  | 5     | 311 | CLA  | O2D-CGD-O1D | -4.39 | 115.25      | 123.84   |
| 31  | A     | 816 | CLA  | CHD-C4C-C3C | -4.39 | 118.39      | 124.84   |
| 31  | B     | 831 | CLA  | CHD-C4C-C3C | -4.39 | 118.39      | 124.84   |
| 31  | 7     | 321 | CLA  | CHD-C4C-C3C | -4.39 | 118.39      | 124.84   |
| 31  | B     | 845 | CLA  | CHD-C1D-ND  | -4.39 | 120.42      | 124.45   |
| 31  | a     | 319 | CLA  | C4D-CHA-C1A | -4.39 | 115.91      | 121.25   |
| 31  | A     | 820 | CLA  | CHD-C1D-ND  | -4.39 | 120.42      | 124.45   |
| 31  | 8     | 314 | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 31  | b     | 311 | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 31  | A     | 852 | CLA  | CHD-C1D-ND  | -4.39 | 120.42      | 124.45   |
| 31  | 5     | 313 | CLA  | C1C-C2C-C3C | -4.39 | 102.34      | 106.96   |
| 31  | 3     | 308 | CLA  | C2C-C1C-NC  | 4.39  | 114.08      | 109.97   |
| 31  | 2     | 304 | CLA  | CHD-C4C-C3C | -4.39 | 118.39      | 124.84   |
| 36  | 9     | 303 | LUT  | C8-C9-C10   | -4.39 | 112.21      | 118.94   |
| 31  | 5     | 312 | CLA  | C1C-C2C-C3C | -4.38 | 102.35      | 106.96   |
| 31  | A     | 829 | CLA  | O2D-CGD-CBD | 4.38  | 119.06      | 111.27   |
| 31  | A     | 828 | CLA  | C1C-C2C-C3C | -4.38 | 102.35      | 106.96   |
| 31  | B     | 814 | CLA  | C2C-C1C-NC  | 4.38  | 114.08      | 109.97   |
| 32  | 7     | 317 | CHL  | C1C-C2C-C3C | -4.38 | 103.64      | 107.11   |
| 31  | b     | 308 | CLA  | C1C-C2C-C3C | -4.38 | 102.35      | 106.96   |
| 31  | 7     | 315 | CLA  | C2D-C1D-ND  | 4.38  | 113.33      | 110.10   |
| 31  | 8     | 318 | CLA  | C1C-C2C-C3C | -4.38 | 102.35      | 106.96   |
| 31  | 7     | 313 | CLA  | CHD-C4C-C3C | -4.38 | 118.41      | 124.84   |
| 31  | 8     | 313 | CLA  | C1C-C2C-C3C | -4.38 | 102.36      | 106.96   |
| 31  | b     | 305 | CLA  | C2C-C1C-NC  | 4.38  | 114.07      | 109.97   |
| 31  | B     | 841 | CLA  | O2D-CGD-CBD | 4.37  | 119.04      | 111.27   |
| 31  | b     | 306 | CLA  | CHD-C4C-C3C | -4.37 | 118.41      | 124.84   |
| 35  | 7     | 303 | QTB  | C01-C02-C03 | -4.37 | 116.80      | 122.92   |
| 31  | A     | 846 | CLA  | C2C-C1C-NC  | 4.37  | 114.07      | 109.97   |
| 31  | 5     | 312 | CLA  | O2D-CGD-CBD | 4.37  | 119.04      | 111.27   |
| 31  | 9     | 319 | CLA  | C1C-C2C-C3C | -4.37 | 102.36      | 106.96   |
| 32  | 3     | 315 | CHL  | CGD-CBD-CAD | 4.37  | 124.89      | 110.73   |
| 31  | A     | 816 | CLA  | C2D-C1D-ND  | 4.37  | 113.32      | 110.10   |
| 31  | 2     | 315 | CLA  | C1C-C2C-C3C | -4.37 | 102.36      | 106.96   |
| 31  | B     | 835 | CLA  | C1C-C2C-C3C | -4.37 | 102.36      | 106.96   |
| 31  | K     | 205 | CLA  | C1C-C2C-C3C | -4.37 | 102.36      | 106.96   |
| 31  | A     | 832 | CLA  | C2D-C1D-ND  | 4.37  | 113.32      | 110.10   |
| 31  | A     | 822 | CLA  | CHD-C1D-ND  | -4.37 | 120.44      | 124.45   |
| 31  | B     | 815 | CLA  | C1C-C2C-C3C | -4.37 | 102.37      | 106.96   |
| 31  | B     | 844 | CLA  | C2C-C1C-NC  | 4.36  | 114.06      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 834 | CLA  | C1C-C2C-C3C | -4.36 | 102.37      | 106.96   |
| 31  | 9     | 316 | CLA  | CHD-C4C-C3C | -4.36 | 118.43      | 124.84   |
| 31  | 4     | 309 | CLA  | O2D-CGD-CBD | 4.36  | 119.02      | 111.27   |
| 31  | B     | 830 | CLA  | C1C-C2C-C3C | -4.36 | 102.37      | 106.96   |
| 31  | 8     | 317 | CLA  | C1C-C2C-C3C | -4.36 | 102.37      | 106.96   |
| 31  | 2     | 314 | CLA  | CHD-C1D-ND  | -4.36 | 120.44      | 124.45   |
| 31  | 7     | 312 | CLA  | O2D-CGD-O1D | -4.36 | 115.31      | 123.84   |
| 31  | 4     | 318 | CLA  | C2C-C1C-NC  | 4.36  | 114.06      | 109.97   |
| 31  | 6     | 316 | CLA  | C1C-C2C-C3C | -4.36 | 102.37      | 106.96   |
| 31  | G     | 205 | CLA  | C2D-C1D-ND  | 4.36  | 113.32      | 110.10   |
| 36  | 5     | 304 | LUT  | C21-C26-C27 | -4.36 | 107.19      | 112.70   |
| 31  | A     | 828 | CLA  | C2C-C1C-NC  | 4.36  | 114.06      | 109.97   |
| 31  | 9     | 316 | CLA  | CHD-C1D-ND  | -4.36 | 120.45      | 124.45   |
| 31  | 6     | 311 | CLA  | C4D-CHA-C1A | -4.36 | 115.94      | 121.25   |
| 31  | F     | 305 | CLA  | C4D-CHA-C1A | -4.36 | 115.94      | 121.25   |
| 31  | 8     | 314 | CLA  | O2D-CGD-CBD | 4.36  | 119.01      | 111.27   |
| 31  | O     | 203 | CLA  | C1C-C2C-C3C | -4.36 | 102.37      | 106.96   |
| 31  | 7     | 316 | CLA  | C1C-C2C-C3C | -4.36 | 102.38      | 106.96   |
| 31  | 7     | 311 | CLA  | C2C-C1C-NC  | 4.36  | 114.05      | 109.97   |
| 31  | 8     | 307 | CLA  | CHD-C4C-C3C | -4.36 | 118.44      | 124.84   |
| 31  | 3     | 307 | CLA  | C4D-CHA-C1A | -4.36 | 115.95      | 121.25   |
| 31  | 9     | 314 | CLA  | O2D-CGD-O1D | -4.36 | 115.32      | 123.84   |
| 31  | G     | 205 | CLA  | C2C-C1C-NC  | 4.35  | 114.05      | 109.97   |
| 31  | 5     | 307 | CLA  | C2C-C1C-NC  | 4.35  | 114.05      | 109.97   |
| 31  | 2     | 304 | CLA  | CHD-C1D-ND  | -4.35 | 120.45      | 124.45   |
| 31  | 4     | 321 | CLA  | C2D-C1D-ND  | 4.35  | 113.31      | 110.10   |
| 31  | B     | 836 | CLA  | C1C-C2C-C3C | -4.35 | 102.38      | 106.96   |
| 31  | b     | 305 | CLA  | C2D-C1D-ND  | 4.35  | 113.31      | 110.10   |
| 31  | 6     | 310 | CLA  | C2D-C1D-ND  | 4.35  | 113.31      | 110.10   |
| 31  | A     | 826 | CLA  | C2C-C1C-NC  | 4.35  | 114.05      | 109.97   |
| 31  | B     | 838 | CLA  | C1C-C2C-C3C | -4.35 | 102.38      | 106.96   |
| 31  | 4     | 316 | CLA  | C1C-C2C-C3C | -4.35 | 102.38      | 106.96   |
| 31  | G     | 205 | CLA  | O1D-CGD-CBD | -4.35 | 115.58      | 124.48   |
| 31  | 9     | 319 | CLA  | CHD-C1D-ND  | -4.35 | 120.46      | 124.45   |
| 31  | b     | 307 | CLA  | CHD-C1D-ND  | -4.35 | 120.46      | 124.45   |
| 31  | 3     | 316 | CLA  | C2D-C1D-ND  | 4.35  | 113.31      | 110.10   |
| 31  | A     | 819 | CLA  | CHD-C4C-C3C | -4.35 | 118.45      | 124.84   |
| 31  | A     | 823 | CLA  | C1C-C2C-C3C | -4.35 | 102.39      | 106.96   |
| 31  | A     | 842 | CLA  | C2C-C1C-NC  | 4.35  | 114.04      | 109.97   |
| 32  | 5     | 317 | CHL  | CHD-C4C-C3C | -4.35 | 118.45      | 124.84   |
| 31  | F     | 301 | CLA  | C2D-C1D-ND  | 4.35  | 113.31      | 110.10   |
| 31  | A     | 842 | CLA  | C1C-C2C-C3C | -4.35 | 102.39      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 5     | 322 | CHL  | O2D-CGD-CBD | 4.35  | 118.99      | 111.27   |
| 31  | 5     | 323 | CLA  | CHD-C4C-C3C | -4.35 | 118.45      | 124.84   |
| 31  | 2     | 315 | CLA  | CHD-C4C-C3C | -4.35 | 118.45      | 124.84   |
| 31  | A     | 819 | CLA  | C2C-C1C-NC  | 4.34  | 114.04      | 109.97   |
| 31  | A     | 853 | CLA  | C1C-C2C-C3C | -4.34 | 102.39      | 106.96   |
| 31  | B     | 840 | CLA  | C1C-C2C-C3C | -4.34 | 102.39      | 106.96   |
| 31  | B     | 825 | CLA  | CHD-C1D-ND  | -4.34 | 120.46      | 124.45   |
| 31  | 7     | 321 | CLA  | CHD-C1D-ND  | -4.34 | 120.46      | 124.45   |
| 31  | L     | 305 | CLA  | O2D-CGD-CBD | 4.34  | 118.99      | 111.27   |
| 31  | 6     | 312 | CLA  | C2C-C1C-NC  | 4.34  | 114.04      | 109.97   |
| 31  | B     | 831 | CLA  | CHD-C1D-ND  | -4.34 | 120.46      | 124.45   |
| 31  | 8     | 321 | CLA  | C1C-C2C-C3C | -4.34 | 102.39      | 106.96   |
| 31  | A     | 827 | CLA  | CHD-C4C-C3C | -4.34 | 118.46      | 124.84   |
| 31  | B     | 830 | CLA  | C2C-C1C-NC  | 4.34  | 114.04      | 109.97   |
| 31  | 4     | 306 | CLA  | C2D-C1D-ND  | 4.34  | 113.30      | 110.10   |
| 31  | 2     | 312 | CLA  | C1C-C2C-C3C | -4.34 | 102.39      | 106.96   |
| 31  | 8     | 314 | CLA  | C4D-CHA-C1A | -4.34 | 115.97      | 121.25   |
| 31  | 8     | 310 | CLA  | CHD-C1D-ND  | -4.34 | 120.47      | 124.45   |
| 31  | 2     | 307 | CLA  | O1D-CGD-CBD | -4.34 | 115.60      | 124.48   |
| 31  | A     | 849 | CLA  | O2D-CGD-CBD | 4.34  | 118.98      | 111.27   |
| 31  | B     | 833 | CLA  | O2D-CGD-CBD | 4.34  | 118.97      | 111.27   |
| 31  | A     | 844 | CLA  | C2D-C1D-ND  | 4.34  | 113.30      | 110.10   |
| 31  | F     | 305 | CLA  | C2D-C1D-ND  | 4.34  | 113.30      | 110.10   |
| 31  | a     | 315 | CLA  | C2D-C1D-ND  | 4.34  | 113.30      | 110.10   |
| 31  | A     | 842 | CLA  | CHD-C4C-C3C | -4.34 | 118.47      | 124.84   |
| 31  | L     | 307 | CLA  | C1C-C2C-C3C | -4.33 | 102.40      | 106.96   |
| 31  | A     | 836 | CLA  | C2C-C1C-NC  | 4.33  | 114.03      | 109.97   |
| 31  | 4     | 308 | CLA  | O2D-CGD-CBD | 4.33  | 118.97      | 111.27   |
| 31  | 3     | 309 | CLA  | CHD-C4C-C3C | -4.33 | 118.47      | 124.84   |
| 31  | 2     | 312 | CLA  | C2D-C1D-ND  | 4.33  | 113.30      | 110.10   |
| 31  | a     | 316 | CLA  | C2C-C1C-NC  | 4.33  | 114.03      | 109.97   |
| 31  | B     | 815 | CLA  | CHD-C4C-C3C | -4.33 | 118.47      | 124.84   |
| 31  | A     | 836 | CLA  | C2D-C1D-ND  | 4.33  | 113.30      | 110.10   |
| 32  | 5     | 316 | CHL  | C4D-CHA-C1A | -4.33 | 115.98      | 121.25   |
| 31  | 4     | 318 | CLA  | C2D-C1D-ND  | 4.33  | 113.29      | 110.10   |
| 31  | A     | 856 | CLA  | C1C-C2C-C3C | -4.33 | 102.41      | 106.96   |
| 32  | 9     | 322 | CHL  | O2D-CGD-O1D | -4.33 | 115.38      | 123.84   |
| 31  | b     | 307 | CLA  | C4D-CHA-C1A | -4.33 | 115.98      | 121.25   |
| 31  | O     | 203 | CLA  | C2C-C1C-NC  | 4.32  | 114.02      | 109.97   |
| 32  | 6     | 319 | CHL  | C1C-C2C-C3C | -4.32 | 103.68      | 107.11   |
| 31  | 5     | 315 | CLA  | CHD-C1D-ND  | -4.32 | 120.48      | 124.45   |
| 31  | 2     | 305 | CLA  | C2D-C1D-ND  | 4.32  | 113.29      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | L     | 306 | CLA  | C2D-C1D-ND  | 4.32  | 113.29      | 110.10   |
| 31  | a     | 315 | CLA  | CHD-C4C-C3C | -4.32 | 118.49      | 124.84   |
| 31  | L     | 305 | CLA  | C2C-C1C-NC  | 4.32  | 114.02      | 109.97   |
| 31  | B     | 842 | CLA  | O2D-CGD-CBD | 4.32  | 118.94      | 111.27   |
| 31  | G     | 206 | CLA  | O2D-CGD-O1D | -4.32 | 115.40      | 123.84   |
| 31  | 2     | 309 | CLA  | C2C-C1C-NC  | 4.32  | 114.02      | 109.97   |
| 31  | A     | 836 | CLA  | CHD-C4C-C3C | -4.32 | 118.50      | 124.84   |
| 31  | 9     | 319 | CLA  | C2D-C1D-ND  | 4.32  | 113.28      | 110.10   |
| 36  | F     | 304 | LUT  | C19-C9-C8   | -4.32 | 111.28      | 118.08   |
| 31  | A     | 857 | CLA  | O2D-CGD-O1D | -4.31 | 115.40      | 123.84   |
| 31  | 6     | 313 | CLA  | C2D-C1D-ND  | 4.31  | 113.28      | 110.10   |
| 31  | 5     | 314 | CLA  | CHD-C1D-ND  | -4.31 | 120.49      | 124.45   |
| 31  | 6     | 310 | CLA  | C1C-C2C-C3C | -4.31 | 102.42      | 106.96   |
| 31  | A     | 832 | CLA  | CHD-C4C-C3C | -4.31 | 118.50      | 124.84   |
| 31  | 5     | 310 | CLA  | C2D-C1D-ND  | 4.31  | 113.28      | 110.10   |
| 31  | K     | 206 | CLA  | O2D-CGD-O1D | -4.31 | 115.41      | 123.84   |
| 31  | b     | 308 | CLA  | C2C-C1C-NC  | 4.31  | 114.01      | 109.97   |
| 31  | 7     | 316 | CLA  | CHD-C1D-ND  | -4.31 | 120.49      | 124.45   |
| 31  | 2     | 306 | CLA  | C1C-C2C-C3C | -4.31 | 102.43      | 106.96   |
| 31  | 9     | 314 | CLA  | C1C-C2C-C3C | -4.31 | 102.43      | 106.96   |
| 31  | A     | 821 | CLA  | C1C-C2C-C3C | -4.31 | 102.43      | 106.96   |
| 32  | a     | 317 | CHL  | O2D-CGD-CBD | 4.31  | 118.92      | 111.27   |
| 31  | 9     | 313 | CLA  | C1C-C2C-C3C | -4.31 | 102.43      | 106.96   |
| 32  | 7     | 318 | CHL  | C1-C2-C3    | -4.30 | 118.60      | 126.04   |
| 31  | 5     | 320 | CLA  | O2D-CGD-CBD | 4.30  | 118.92      | 111.27   |
| 31  | 2     | 304 | CLA  | C2D-C1D-ND  | 4.30  | 113.28      | 110.10   |
| 31  | 9     | 313 | CLA  | C2C-C1C-NC  | 4.30  | 114.00      | 109.97   |
| 31  | O     | 204 | CLA  | C1C-C2C-C3C | -4.30 | 102.43      | 106.96   |
| 36  | 9     | 305 | LUT  | C35-C15-C14 | -4.30 | 114.66      | 123.47   |
| 32  | 6     | 320 | CHL  | CHD-C4C-C3C | -4.30 | 118.52      | 124.84   |
| 31  | 9     | 316 | CLA  | C2D-C1D-ND  | 4.30  | 113.28      | 110.10   |
| 31  | 5     | 320 | CLA  | C1C-C2C-C3C | -4.30 | 102.43      | 106.96   |
| 31  | b     | 313 | CLA  | O2D-CGD-O1D | -4.30 | 115.43      | 123.84   |
| 31  | A     | 822 | CLA  | C2C-C1C-NC  | 4.30  | 114.00      | 109.97   |
| 31  | 3     | 316 | CLA  | C2C-C1C-NC  | 4.30  | 114.00      | 109.97   |
| 31  | 6     | 308 | CLA  | CHD-C1D-ND  | -4.30 | 120.50      | 124.45   |
| 31  | 4     | 319 | CLA  | C2D-C1D-ND  | 4.30  | 113.27      | 110.10   |
| 31  | A     | 826 | CLA  | CHD-C4C-C3C | -4.30 | 118.52      | 124.84   |
| 31  | a     | 310 | CLA  | CHD-C4C-C3C | -4.30 | 118.52      | 124.84   |
| 31  | 3     | 309 | CLA  | C1C-C2C-C3C | -4.30 | 102.44      | 106.96   |
| 31  | A     | 817 | CLA  | O2D-CGD-CBD | 4.30  | 118.91      | 111.27   |
| 31  | B     | 820 | CLA  | O2D-CGD-CBD | 4.30  | 118.91      | 111.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 309 | CLA  | CHD-C4C-C3C | -4.29 | 118.53      | 124.84   |
| 32  | 5     | 316 | CHL  | CHD-C4C-C3C | -4.29 | 118.53      | 124.84   |
| 31  | 3     | 307 | CLA  | O2D-CGD-O1D | -4.29 | 115.44      | 123.84   |
| 31  | B     | 828 | CLA  | C2C-C1C-NC  | 4.29  | 114.00      | 109.97   |
| 31  | 8     | 308 | CLA  | C4D-CHA-C1A | -4.29 | 116.02      | 121.25   |
| 31  | 3     | 313 | CLA  | C2C-C1C-NC  | 4.29  | 113.99      | 109.97   |
| 31  | 6     | 315 | CLA  | C2C-C1C-NC  | 4.29  | 113.99      | 109.97   |
| 31  | B     | 823 | CLA  | CHD-C1D-ND  | -4.29 | 120.51      | 124.45   |
| 31  | 5     | 314 | CLA  | C2D-C1D-ND  | 4.29  | 113.27      | 110.10   |
| 31  | 2     | 305 | CLA  | CHD-C4C-C3C | -4.29 | 118.53      | 124.84   |
| 31  | 9     | 313 | CLA  | O2D-CGD-O1D | -4.29 | 115.45      | 123.84   |
| 36  | 5     | 304 | LUT  | C32-C33-C34 | -4.29 | 112.36      | 118.94   |
| 31  | K     | 206 | CLA  | C2D-C1D-ND  | 4.29  | 113.26      | 110.10   |
| 31  | a     | 313 | CLA  | C2D-C1D-ND  | 4.29  | 113.26      | 110.10   |
| 31  | 4     | 305 | CLA  | CHD-C1D-ND  | -4.29 | 120.51      | 124.45   |
| 31  | b     | 311 | CLA  | C2D-C1D-ND  | 4.29  | 113.26      | 110.10   |
| 31  | A     | 851 | CLA  | C2C-C1C-NC  | 4.29  | 113.99      | 109.97   |
| 31  | 2     | 308 | CLA  | C1C-C2C-C3C | -4.29 | 102.45      | 106.96   |
| 31  | F     | 306 | CLA  | O2D-CGD-CBD | 4.29  | 118.88      | 111.27   |
| 31  | K     | 204 | CLA  | CHD-C4C-C3C | -4.29 | 118.54      | 124.84   |
| 31  | 4     | 318 | CLA  | C4D-CHA-C1A | -4.29 | 116.03      | 121.25   |
| 31  | L     | 305 | CLA  | C1C-C2C-C3C | -4.28 | 102.45      | 106.96   |
| 31  | B     | 840 | CLA  | CHD-C4C-C3C | -4.28 | 118.54      | 124.84   |
| 31  | 5     | 310 | CLA  | C1C-C2C-C3C | -4.28 | 102.45      | 106.96   |
| 31  | 3     | 307 | CLA  | CHD-C4C-C3C | -4.28 | 118.54      | 124.84   |
| 32  | 7     | 317 | CHL  | CHD-C4C-C3C | -4.28 | 118.55      | 124.84   |
| 31  | 4     | 311 | CLA  | C2C-C1C-NC  | 4.28  | 113.98      | 109.97   |
| 32  | a     | 318 | CHL  | O2D-CGD-O1D | -4.28 | 115.47      | 123.84   |
| 31  | 6     | 316 | CLA  | C2C-C1C-NC  | 4.28  | 113.98      | 109.97   |
| 31  | 5     | 318 | CLA  | O2D-CGD-CBD | 4.28  | 118.87      | 111.27   |
| 31  | 2     | 309 | CLA  | C1C-C2C-C3C | -4.28 | 102.46      | 106.96   |
| 31  | 3     | 319 | CLA  | O2D-CGD-O1D | -4.28 | 115.47      | 123.84   |
| 31  | a     | 309 | CLA  | C2C-C1C-NC  | 4.28  | 113.98      | 109.97   |
| 32  | 5     | 317 | CHL  | C1C-C2C-C3C | -4.28 | 103.72      | 107.11   |
| 31  | a     | 309 | CLA  | C1C-C2C-C3C | -4.27 | 102.46      | 106.96   |
| 31  | J     | 105 | CLA  | C4D-CHA-C1A | -4.27 | 116.05      | 121.25   |
| 31  | 8     | 320 | CLA  | C4D-CHA-C1A | -4.27 | 116.05      | 121.25   |
| 31  | 6     | 306 | CLA  | C1C-C2C-C3C | -4.27 | 102.47      | 106.96   |
| 31  | 3     | 320 | CLA  | C4D-CHA-C1A | -4.27 | 116.05      | 121.25   |
| 31  | 8     | 309 | CLA  | C1C-C2C-C3C | -4.27 | 102.47      | 106.96   |
| 31  | A     | 818 | CLA  | C2D-C1D-ND  | 4.27  | 113.25      | 110.10   |
| 31  | 4     | 320 | CLA  | C2D-C1D-ND  | 4.27  | 113.25      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 308 | CLA  | CHD-C4C-C3C | -4.27 | 118.57      | 124.84   |
| 31  | A     | 820 | CLA  | O2D-CGD-CBD | 4.27  | 118.85      | 111.27   |
| 31  | B     | 812 | CLA  | C4D-CHA-C1A | -4.26 | 116.06      | 121.25   |
| 31  | B     | 845 | CLA  | CHD-C4C-C3C | -4.26 | 118.58      | 124.84   |
| 31  | 7     | 322 | CLA  | CHD-C4C-C3C | -4.26 | 118.58      | 124.84   |
| 31  | 7     | 312 | CLA  | C2D-C1D-ND  | 4.26  | 113.24      | 110.10   |
| 31  | B     | 826 | CLA  | O2D-CGD-CBD | 4.26  | 118.84      | 111.27   |
| 31  | A     | 824 | CLA  | C1C-C2C-C3C | -4.26 | 102.48      | 106.96   |
| 31  | 2     | 314 | CLA  | C2D-C1D-ND  | 4.26  | 113.24      | 110.10   |
| 36  | 6     | 303 | LUT  | C10-C11-C12 | -4.26 | 109.93      | 123.22   |
| 31  | a     | 310 | CLA  | C1C-C2C-C3C | -4.26 | 102.48      | 106.96   |
| 31  | a     | 316 | CLA  | C1C-C2C-C3C | -4.26 | 102.48      | 106.96   |
| 31  | 9     | 312 | CLA  | C1C-C2C-C3C | -4.26 | 102.48      | 106.96   |
| 31  | 6     | 314 | CLA  | C4D-CHA-C1A | -4.26 | 116.07      | 121.25   |
| 31  | 4     | 311 | CLA  | C1C-C2C-C3C | -4.26 | 102.48      | 106.96   |
| 31  | F     | 305 | CLA  | O2D-CGD-O1D | -4.26 | 115.52      | 123.84   |
| 31  | B     | 823 | CLA  | O2D-CGD-CBD | 4.25  | 118.83      | 111.27   |
| 31  | O     | 204 | CLA  | C2C-C1C-NC  | 4.25  | 113.96      | 109.97   |
| 31  | B     | 821 | CLA  | O2D-CGD-O1D | -4.25 | 115.52      | 123.84   |
| 31  | 5     | 308 | CLA  | C2D-C1D-ND  | 4.25  | 113.24      | 110.10   |
| 31  | 7     | 314 | CLA  | C4D-CHA-C1A | -4.25 | 116.07      | 121.25   |
| 31  | b     | 306 | CLA  | CHD-C1D-ND  | -4.25 | 120.55      | 124.45   |
| 31  | 4     | 314 | CLA  | O2D-CGD-O1D | -4.25 | 115.52      | 123.84   |
| 31  | B     | 822 | CLA  | C2D-C1D-ND  | 4.25  | 113.24      | 110.10   |
| 31  | 9     | 314 | CLA  | O1D-CGD-CBD | -4.25 | 115.78      | 124.48   |
| 31  | G     | 205 | CLA  | O2D-CGD-CBD | 4.25  | 118.82      | 111.27   |
| 32  | 6     | 317 | CHL  | CHD-C4C-C3C | -4.25 | 118.59      | 124.84   |
| 31  | 2     | 310 | CLA  | C2D-C1D-ND  | 4.25  | 113.24      | 110.10   |
| 32  | 6     | 309 | CHL  | C1C-C2C-C3C | -4.25 | 103.74      | 107.11   |
| 31  | 7     | 309 | CLA  | C4D-CHA-C1A | -4.25 | 116.08      | 121.25   |
| 31  | 5     | 308 | CLA  | O2D-CGD-O1D | -4.25 | 115.53      | 123.84   |
| 31  | 2     | 306 | CLA  | C2C-C1C-NC  | 4.25  | 113.95      | 109.97   |
| 31  | 7     | 312 | CLA  | CHD-C1D-ND  | -4.24 | 120.55      | 124.45   |
| 31  | H     | 902 | CLA  | C2D-C1D-ND  | 4.24  | 113.23      | 110.10   |
| 31  | A     | 856 | CLA  | O2D-CGD-CBD | 4.24  | 118.81      | 111.27   |
| 31  | B     | 842 | CLA  | C1C-C2C-C3C | -4.24 | 102.50      | 106.96   |
| 31  | B     | 819 | CLA  | C2D-C1D-ND  | 4.24  | 113.23      | 110.10   |
| 31  | B     | 833 | CLA  | CHD-C4C-C3C | -4.24 | 118.61      | 124.84   |
| 31  | a     | 316 | CLA  | C2D-C1D-ND  | 4.24  | 113.23      | 110.10   |
| 31  | H     | 901 | CLA  | CHD-C1D-ND  | -4.24 | 120.56      | 124.45   |
| 31  | B     | 821 | CLA  | C2D-C1D-ND  | 4.24  | 113.22      | 110.10   |
| 31  | 7     | 322 | CLA  | C2D-C1D-ND  | 4.24  | 113.22      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 307 | CLA  | C4D-CHA-C1A | -4.23 | 116.10      | 121.25   |
| 31  | A     | 825 | CLA  | C1C-C2C-C3C | -4.23 | 102.50      | 106.96   |
| 31  | 3     | 312 | CLA  | CHD-C1D-ND  | -4.23 | 120.56      | 124.45   |
| 31  | 3     | 318 | CLA  | CHD-C1D-ND  | -4.23 | 120.56      | 124.45   |
| 31  | A     | 844 | CLA  | O2D-CGD-CBD | 4.23  | 118.79      | 111.27   |
| 31  | A     | 852 | CLA  | C1C-C2C-C3C | -4.23 | 102.51      | 106.96   |
| 31  | 3     | 308 | CLA  | C2D-C1D-ND  | 4.23  | 113.22      | 110.10   |
| 31  | 2     | 308 | CLA  | C2C-C1C-NC  | 4.23  | 113.93      | 109.97   |
| 31  | B     | 813 | CLA  | C2C-C1C-NC  | 4.23  | 113.93      | 109.97   |
| 31  | B     | 849 | CLA  | C2C-C1C-NC  | 4.23  | 113.93      | 109.97   |
| 31  | b     | 307 | CLA  | O1D-CGD-CBD | -4.23 | 115.83      | 124.48   |
| 31  | 2     | 312 | CLA  | C2C-C1C-NC  | 4.23  | 113.93      | 109.97   |
| 31  | 4     | 315 | CLA  | C1C-C2C-C3C | -4.23 | 102.51      | 106.96   |
| 31  | A     | 850 | CLA  | CHD-C4C-C3C | -4.23 | 118.63      | 124.84   |
| 31  | a     | 319 | CLA  | C2D-C1D-ND  | 4.23  | 113.22      | 110.10   |
| 31  | 6     | 322 | CLA  | C2D-C1D-ND  | 4.23  | 113.22      | 110.10   |
| 31  | 6     | 314 | CLA  | CHD-C4C-C3C | -4.22 | 118.63      | 124.84   |
| 36  | 3     | 305 | LUT  | C7-C6-C5    | -4.22 | 111.23      | 121.46   |
| 31  | 7     | 311 | CLA  | CHD-C4C-C3C | -4.22 | 118.63      | 124.84   |
| 31  | B     | 840 | CLA  | C2C-C1C-NC  | 4.22  | 113.93      | 109.97   |
| 31  | A     | 857 | CLA  | CHD-C1D-ND  | -4.22 | 120.58      | 124.45   |
| 31  | A     | 816 | CLA  | O2D-CGD-O1D | -4.22 | 115.59      | 123.84   |
| 31  | O     | 202 | CLA  | C2C-C1C-NC  | 4.22  | 113.92      | 109.97   |
| 31  | K     | 204 | CLA  | CHD-C1D-ND  | -4.22 | 120.58      | 124.45   |
| 31  | O     | 203 | CLA  | C2D-C1D-ND  | 4.22  | 113.21      | 110.10   |
| 28  | 6     | 305 | LHG  | O4-P-O5     | 4.22  | 133.09      | 112.24   |
| 32  | K     | 201 | CHL  | CHD-C4C-C3C | -4.22 | 118.64      | 124.84   |
| 32  | K     | 201 | CHL  | C3B-C4B-NB  | 4.22  | 114.66      | 109.21   |
| 31  | B     | 830 | CLA  | O2D-CGD-O1D | -4.22 | 115.60      | 123.84   |
| 32  | 5     | 317 | CHL  | CHD-C1D-ND  | -4.22 | 120.58      | 124.45   |
| 31  | A     | 855 | CLA  | C2C-C1C-NC  | 4.22  | 113.92      | 109.97   |
| 28  | 6     | 301 | LHG  | O4-P-O5     | 4.22  | 133.08      | 112.24   |
| 31  | B     | 839 | CLA  | C1C-C2C-C3C | -4.22 | 102.53      | 106.96   |
| 31  | b     | 306 | CLA  | C2D-C1D-ND  | 4.21  | 113.21      | 110.10   |
| 31  | B     | 842 | CLA  | CHD-C4C-C3C | -4.21 | 118.64      | 124.84   |
| 31  | B     | 820 | CLA  | C2C-C1C-NC  | 4.21  | 113.92      | 109.97   |
| 31  | 4     | 318 | CLA  | O2D-CGD-CBD | 4.21  | 118.75      | 111.27   |
| 32  | 6     | 318 | CHL  | C1C-C2C-C3C | -4.21 | 103.77      | 107.11   |
| 31  | 2     | 310 | CLA  | C4D-CHA-C1A | -4.21 | 116.12      | 121.25   |
| 28  | A     | 809 | LHG  | O4-P-O5     | 4.21  | 133.05      | 112.24   |
| 36  | 5     | 304 | LUT  | C7-C6-C5    | -4.21 | 111.27      | 121.46   |
| 36  | 2     | 301 | LUT  | C7-C6-C5    | -4.21 | 111.27      | 121.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 839 | CLA  | C2D-C1D-ND  | 4.21  | 113.20      | 110.10   |
| 31  | b     | 302 | CLA  | CHD-C4C-C3C | -4.20 | 118.66      | 124.84   |
| 31  | b     | 305 | CLA  | CHD-C4C-C3C | -4.20 | 118.66      | 124.84   |
| 31  | A     | 852 | CLA  | C2C-C1C-NC  | 4.20  | 113.91      | 109.97   |
| 31  | A     | 849 | CLA  | C4D-CHA-C1A | -4.20 | 116.14      | 121.25   |
| 31  | a     | 310 | CLA  | O2D-CGD-O1D | -4.20 | 115.62      | 123.84   |
| 31  | 6     | 312 | CLA  | C2D-C1D-ND  | 4.20  | 113.20      | 110.10   |
| 32  | a     | 320 | CHL  | CHD-C4C-C3C | -4.20 | 118.67      | 124.84   |
| 36  | 7     | 305 | LUT  | C1-C6-C5    | -4.20 | 116.70      | 122.61   |
| 31  | A     | 834 | CLA  | C4D-CHA-C1A | -4.20 | 116.14      | 121.25   |
| 31  | 4     | 309 | CLA  | CHD-C4C-C3C | -4.20 | 118.67      | 124.84   |
| 32  | 7     | 319 | CHL  | CHD-C4C-C3C | -4.20 | 118.67      | 124.84   |
| 28  | 7     | 307 | LHG  | O4-P-O5     | 4.19  | 132.98      | 112.24   |
| 31  | 3     | 310 | CLA  | O2D-CGD-CBD | 4.19  | 118.72      | 111.27   |
| 31  | 6     | 307 | CLA  | C4D-CHA-C1A | -4.19 | 116.14      | 121.25   |
| 36  | a     | 305 | LUT  | C1-C6-C5    | -4.19 | 116.71      | 122.61   |
| 36  | a     | 303 | LUT  | C7-C6-C5    | -4.19 | 111.31      | 121.46   |
| 36  | 7     | 305 | LUT  | C16-C1-C6   | -4.19 | 103.50      | 110.30   |
| 31  | 3     | 308 | CLA  | C4D-CHA-C1A | -4.19 | 116.15      | 121.25   |
| 31  | G     | 204 | CLA  | C1C-C2C-C3C | -4.19 | 102.55      | 106.96   |
| 31  | 4     | 306 | CLA  | CHD-C4C-C3C | -4.19 | 118.68      | 124.84   |
| 31  | B     | 821 | CLA  | O2D-CGD-CBD | 4.19  | 118.72      | 111.27   |
| 31  | A     | 817 | CLA  | C1C-C2C-C3C | -4.19 | 102.55      | 106.96   |
| 31  | 4     | 315 | CLA  | CHD-C1D-ND  | -4.19 | 120.60      | 124.45   |
| 31  | a     | 312 | CLA  | C2C-C1C-NC  | 4.19  | 113.90      | 109.97   |
| 32  | 4     | 310 | CHL  | C4D-CHA-C1A | -4.19 | 116.15      | 121.25   |
| 31  | B     | 824 | CLA  | C1C-C2C-C3C | -4.19 | 102.55      | 106.96   |
| 31  | 4     | 319 | CLA  | CHD-C4C-C3C | -4.19 | 118.69      | 124.84   |
| 31  | L     | 306 | CLA  | CHD-C4C-C3C | -4.19 | 118.69      | 124.84   |
| 31  | A     | 830 | CLA  | C2C-C1C-NC  | 4.19  | 113.89      | 109.97   |
| 31  | 3     | 317 | CLA  | C2D-C1D-ND  | 4.18  | 113.19      | 110.10   |
| 31  | 9     | 315 | CLA  | CHD-C4C-C3C | -4.18 | 118.69      | 124.84   |
| 31  | A     | 816 | CLA  | CHD-C1D-ND  | -4.18 | 120.61      | 124.45   |
| 31  | B     | 811 | CLA  | CHD-C1D-ND  | -4.18 | 120.61      | 124.45   |
| 31  | K     | 205 | CLA  | C2D-C1D-ND  | 4.18  | 113.18      | 110.10   |
| 31  | A     | 825 | CLA  | CHD-C1D-ND  | -4.18 | 120.61      | 124.45   |
| 32  | 7     | 318 | CHL  | CHD-C4C-C3C | -4.18 | 118.70      | 124.84   |
| 31  | 4     | 308 | CLA  | O1D-CGD-CBD | -4.18 | 115.94      | 124.48   |
| 31  | 7     | 316 | CLA  | C2C-C1C-NC  | 4.17  | 113.88      | 109.97   |
| 31  | A     | 844 | CLA  | CHD-C4C-C3C | -4.17 | 118.71      | 124.84   |
| 31  | B     | 819 | CLA  | CHD-C4C-C3C | -4.17 | 118.71      | 124.84   |
| 31  | 6     | 315 | CLA  | CHD-C1D-ND  | -4.17 | 120.62      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 837 | CLA  | C1C-C2C-C3C | -4.17 | 102.57      | 106.96   |
| 31  | 4     | 315 | CLA  | C2D-C1D-ND  | 4.17  | 113.18      | 110.10   |
| 31  | A     | 856 | CLA  | C2C-C1C-NC  | 4.17  | 113.88      | 109.97   |
| 31  | B     | 844 | CLA  | C1C-C2C-C3C | -4.17 | 102.57      | 106.96   |
| 32  | 7     | 318 | CHL  | CGD-CBD-CAD | 4.17  | 124.24      | 110.73   |
| 36  | L     | 304 | LUT  | C7-C6-C5    | -4.17 | 111.36      | 121.46   |
| 31  | A     | 814 | CLA  | C2C-C1C-NC  | 4.17  | 113.88      | 109.97   |
| 31  | B     | 832 | CLA  | C4D-CHA-C1A | -4.17 | 116.18      | 121.25   |
| 28  | a     | 306 | LHG  | O4-P-O5     | 4.17  | 132.84      | 112.24   |
| 36  | 3     | 304 | LUT  | C40-C33-C32 | -4.17 | 111.51      | 118.08   |
| 32  | 5     | 319 | CHL  | CGD-CBD-CAD | 4.16  | 124.22      | 110.73   |
| 31  | 8     | 308 | CLA  | O2D-CGD-O1D | -4.16 | 115.70      | 123.84   |
| 31  | 6     | 312 | CLA  | O1D-CGD-CBD | -4.16 | 115.97      | 124.48   |
| 31  | B     | 820 | CLA  | O2D-CGD-O1D | -4.16 | 115.70      | 123.84   |
| 31  | B     | 829 | CLA  | O2D-CGD-CBD | 4.16  | 118.67      | 111.27   |
| 31  | 9     | 318 | CLA  | C1C-C2C-C3C | -4.16 | 102.58      | 106.96   |
| 36  | 4     | 302 | LUT  | C35-C15-C14 | -4.16 | 114.95      | 123.47   |
| 31  | 7     | 309 | CLA  | O1D-CGD-CBD | -4.16 | 115.97      | 124.48   |
| 31  | A     | 823 | CLA  | C2C-C1C-NC  | 4.16  | 113.87      | 109.97   |
| 36  | F     | 304 | LUT  | C20-C13-C12 | -4.16 | 111.53      | 118.08   |
| 31  | 8     | 311 | CLA  | C2D-C1D-ND  | 4.16  | 113.17      | 110.10   |
| 31  | A     | 824 | CLA  | C2C-C1C-NC  | 4.16  | 113.87      | 109.97   |
| 31  | 5     | 309 | CLA  | C4D-CHA-C1A | -4.16 | 116.19      | 121.25   |
| 31  | B     | 824 | CLA  | C2D-C1D-ND  | 4.16  | 113.17      | 110.10   |
| 31  | 8     | 308 | CLA  | O1D-CGD-CBD | -4.15 | 115.98      | 124.48   |
| 31  | A     | 833 | CLA  | C4D-CHA-C1A | -4.15 | 116.19      | 121.25   |
| 31  | 2     | 311 | CLA  | C2C-C1C-NC  | 4.15  | 113.86      | 109.97   |
| 31  | 4     | 315 | CLA  | C2C-C1C-NC  | 4.15  | 113.86      | 109.97   |
| 31  | a     | 314 | CLA  | CHD-C4C-C3C | -4.15 | 118.74      | 124.84   |
| 31  | 5     | 320 | CLA  | C2C-C1C-NC  | 4.15  | 113.86      | 109.97   |
| 28  | 7     | 302 | LHG  | O4-P-O5     | 4.15  | 132.76      | 112.24   |
| 31  | b     | 310 | CLA  | C2D-C1D-ND  | 4.15  | 113.16      | 110.10   |
| 31  | A     | 854 | CLA  | CHD-C1D-ND  | -4.15 | 120.64      | 124.45   |
| 31  | 6     | 308 | CLA  | C2C-C1C-NC  | 4.15  | 113.86      | 109.97   |
| 31  | A     | 845 | CLA  | CHD-C4C-C3C | -4.15 | 118.74      | 124.84   |
| 31  | 4     | 321 | CLA  | CHD-C4C-C3C | -4.15 | 118.74      | 124.84   |
| 31  | B     | 839 | CLA  | CHD-C4C-C3C | -4.15 | 118.74      | 124.84   |
| 31  | 2     | 311 | CLA  | C1C-C2C-C3C | -4.15 | 102.60      | 106.96   |
| 31  | 4     | 311 | CLA  | C4D-CHA-C1A | -4.15 | 116.20      | 121.25   |
| 36  | 5     | 304 | LUT  | C19-C9-C8   | -4.15 | 111.54      | 118.08   |
| 31  | B     | 837 | CLA  | C4D-CHA-C1A | -4.15 | 116.20      | 121.25   |
| 31  | 8     | 320 | CLA  | CAA-C2A-C3A | -4.15 | 101.42      | 112.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 322 | CLA  | CHD-C4C-C3C | -4.15 | 118.75      | 124.84   |
| 31  | B     | 826 | CLA  | CHD-C1D-ND  | -4.15 | 120.64      | 124.45   |
| 31  | 2     | 311 | CLA  | C2D-C1D-ND  | 4.14  | 113.16      | 110.10   |
| 31  | 6     | 314 | CLA  | C2D-C1D-ND  | 4.14  | 113.16      | 110.10   |
| 31  | A     | 837 | CLA  | C2C-C1C-NC  | 4.14  | 113.85      | 109.97   |
| 31  | B     | 849 | CLA  | C1C-C2C-C3C | -4.14 | 102.60      | 106.96   |
| 31  | B     | 814 | CLA  | CHD-C1D-ND  | -4.14 | 120.65      | 124.45   |
| 31  | a     | 313 | CLA  | O2D-CGD-O1D | -4.14 | 115.74      | 123.84   |
| 31  | 3     | 320 | CLA  | CHD-C4C-C3C | -4.14 | 118.75      | 124.84   |
| 31  | A     | 852 | CLA  | CHD-C4C-C3C | -4.14 | 118.75      | 124.84   |
| 36  | F     | 304 | LUT  | C18-C5-C4   | -4.14 | 106.69      | 114.36   |
| 31  | a     | 312 | CLA  | C1C-C2C-C3C | -4.14 | 102.60      | 106.96   |
| 31  | a     | 314 | CLA  | C4D-CHA-C1A | -4.14 | 116.21      | 121.25   |
| 32  | 6     | 319 | CHL  | CHD-C1D-ND  | -4.14 | 120.65      | 124.45   |
| 31  | B     | 826 | CLA  | O2D-CGD-O1D | -4.14 | 115.75      | 123.84   |
| 31  | 9     | 312 | CLA  | O2D-CGD-CBD | 4.14  | 118.62      | 111.27   |
| 31  | 3     | 311 | CLA  | C2D-C1D-ND  | 4.14  | 113.15      | 110.10   |
| 32  | 7     | 317 | CHL  | O2D-CGD-CBD | 4.14  | 118.62      | 111.27   |
| 31  | 5     | 307 | CLA  | C1C-C2C-C3C | -4.13 | 102.61      | 106.96   |
| 31  | b     | 304 | CLA  | C2C-C1C-NC  | 4.13  | 113.84      | 109.97   |
| 31  | B     | 829 | CLA  | CHD-C4C-C3C | -4.13 | 118.77      | 124.84   |
| 32  | 7     | 324 | CHL  | C1C-C2C-C3C | -4.13 | 103.84      | 107.11   |
| 31  | B     | 828 | CLA  | C2D-C1D-ND  | 4.13  | 113.15      | 110.10   |
| 31  | A     | 854 | CLA  | CHD-C4C-C3C | -4.13 | 118.77      | 124.84   |
| 31  | b     | 304 | CLA  | C1C-C2C-C3C | -4.13 | 102.62      | 106.96   |
| 31  | 4     | 321 | CLA  | CHD-C1D-ND  | -4.13 | 120.66      | 124.45   |
| 31  | A     | 834 | CLA  | C2D-C1D-ND  | 4.13  | 113.14      | 110.10   |
| 31  | B     | 846 | CLA  | C2D-C1D-ND  | 4.13  | 113.14      | 110.10   |
| 31  | A     | 841 | CLA  | C1C-C2C-C3C | -4.12 | 102.62      | 106.96   |
| 31  | A     | 848 | CLA  | C2D-C1D-ND  | 4.12  | 113.14      | 110.10   |
| 31  | A     | 826 | CLA  | C1C-C2C-C3C | -4.12 | 102.62      | 106.96   |
| 31  | A     | 851 | CLA  | C2D-C1D-ND  | 4.12  | 113.14      | 110.10   |
| 31  | 7     | 311 | CLA  | C2D-C1D-ND  | 4.12  | 113.14      | 110.10   |
| 31  | 2     | 304 | CLA  | C4D-CHA-C1A | -4.12 | 116.24      | 121.25   |
| 31  | 9     | 313 | CLA  | CHD-C4C-C3C | -4.12 | 118.79      | 124.84   |
| 36  | 4     | 302 | LUT  | C12-C13-C14 | -4.12 | 112.62      | 118.94   |
| 31  | 8     | 312 | CLA  | C2D-C1D-ND  | 4.12  | 113.14      | 110.10   |
| 31  | B     | 814 | CLA  | CHD-C4C-C3C | -4.12 | 118.79      | 124.84   |
| 31  | A     | 817 | CLA  | O2D-CGD-O1D | -4.11 | 115.80      | 123.84   |
| 31  | L     | 307 | CLA  | CHA-C4D-ND  | 4.11  | 141.10      | 132.50   |
| 31  | A     | 817 | CLA  | C2C-C1C-NC  | 4.11  | 113.82      | 109.97   |
| 28  | 8     | 304 | LHG  | O4-P-O5     | 4.11  | 132.56      | 112.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 313 | CLA  | CHD-C4C-C3C | -4.11 | 118.80      | 124.84   |
| 28  | B     | 807 | LHG  | O4-P-O5     | 4.11  | 132.56      | 112.24   |
| 31  | 5     | 320 | CLA  | CHD-C4C-C3C | -4.11 | 118.80      | 124.84   |
| 31  | 6     | 312 | CLA  | CHD-C4C-C3C | -4.11 | 118.80      | 124.84   |
| 31  | 4     | 308 | CLA  | CHD-C4C-C3C | -4.11 | 118.80      | 124.84   |
| 31  | 9     | 313 | CLA  | O2D-CGD-CBD | 4.11  | 118.57      | 111.27   |
| 31  | b     | 310 | CLA  | CHD-C4C-C3C | -4.11 | 118.80      | 124.84   |
| 31  | a     | 309 | CLA  | O2D-CGD-O1D | -4.11 | 115.81      | 123.84   |
| 36  | 8     | 302 | LUT  | C19-C9-C8   | -4.11 | 111.61      | 118.08   |
| 31  | 2     | 305 | CLA  | CHD-C1D-ND  | -4.11 | 120.68      | 124.45   |
| 31  | 3     | 316 | CLA  | C1C-C2C-C3C | -4.10 | 102.64      | 106.96   |
| 31  | 2     | 310 | CLA  | O2D-CGD-O1D | -4.10 | 115.82      | 123.84   |
| 32  | 8     | 316 | CHL  | C1C-C2C-C3C | -4.10 | 103.86      | 107.11   |
| 36  | a     | 303 | LUT  | C19-C9-C8   | -4.10 | 111.62      | 118.08   |
| 31  | 3     | 316 | CLA  | CHD-C4C-C3C | -4.10 | 118.81      | 124.84   |
| 31  | 7     | 322 | CLA  | CHD-C1D-ND  | -4.10 | 120.69      | 124.45   |
| 31  | A     | 818 | CLA  | O2D-CGD-O1D | -4.10 | 115.83      | 123.84   |
| 31  | B     | 844 | CLA  | CHD-C4C-C3C | -4.10 | 118.82      | 124.84   |
| 31  | 3     | 318 | CLA  | CHD-C4C-C3C | -4.10 | 118.82      | 124.84   |
| 31  | B     | 825 | CLA  | CHD-C4C-C3C | -4.09 | 118.82      | 124.84   |
| 31  | 6     | 315 | CLA  | CHD-C4C-C3C | -4.09 | 118.82      | 124.84   |
| 31  | 6     | 308 | CLA  | O2D-CGD-O1D | -4.09 | 115.84      | 123.84   |
| 36  | 6     | 303 | LUT  | C7-C6-C5    | -4.09 | 111.55      | 121.46   |
| 31  | 3     | 314 | CLA  | CHD-C4C-C3C | -4.09 | 118.83      | 124.84   |
| 31  | 7     | 322 | CLA  | C1C-C2C-C3C | -4.09 | 102.66      | 106.96   |
| 36  | 4     | 302 | LUT  | C1-C6-C5    | -4.09 | 116.86      | 122.61   |
| 31  | 8     | 315 | CLA  | O2D-CGD-CBD | 4.09  | 118.53      | 111.27   |
| 36  | J     | 103 | LUT  | C35-C15-C14 | -4.09 | 115.10      | 123.47   |
| 31  | B     | 844 | CLA  | O2D-CGD-CBD | 4.09  | 118.53      | 111.27   |
| 31  | 8     | 308 | CLA  | C2C-C1C-NC  | 4.09  | 113.80      | 109.97   |
| 31  | A     | 857 | CLA  | C1C-C2C-C3C | -4.08 | 102.66      | 106.96   |
| 31  | B     | 841 | CLA  | O2D-CGD-O1D | -4.08 | 115.85      | 123.84   |
| 32  | 5     | 317 | CHL  | O1D-CGD-CBD | -4.08 | 116.13      | 124.48   |
| 31  | 8     | 310 | CLA  | CHD-C4C-NC  | 4.08  | 130.64      | 124.20   |
| 31  | B     | 830 | CLA  | O2D-CGD-CBD | 4.08  | 118.53      | 111.27   |
| 31  | A     | 836 | CLA  | C4D-CHA-C1A | -4.08 | 116.28      | 121.25   |
| 31  | 7     | 311 | CLA  | CHD-C1D-ND  | -4.08 | 120.70      | 124.45   |
| 31  | A     | 835 | CLA  | C2C-C1C-NC  | 4.08  | 113.79      | 109.97   |
| 31  | B     | 833 | CLA  | C1C-C2C-C3C | -4.08 | 102.67      | 106.96   |
| 32  | 8     | 319 | CHL  | CHD-C4C-C3C | -4.08 | 118.84      | 124.84   |
| 35  | F     | 303 | QTB  | C01-C02-C03 | -4.08 | 117.21      | 122.92   |
| 31  | H     | 901 | CLA  | C1C-C2C-C3C | -4.08 | 102.67      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 851 | CLA  | CHD-C1D-ND  | -4.08 | 120.71      | 124.45   |
| 31  | B     | 829 | CLA  | O2D-CGD-O1D | -4.07 | 115.88      | 123.84   |
| 28  | A     | 811 | LHG  | O4-P-O5     | 4.07  | 132.36      | 112.24   |
| 31  | a     | 316 | CLA  | O2D-CGD-O1D | -4.07 | 115.88      | 123.84   |
| 36  | 5     | 303 | LUT  | C19-C9-C8   | -4.07 | 111.67      | 118.08   |
| 31  | 8     | 310 | CLA  | CMC-C2C-C1C | 4.07  | 131.23      | 125.04   |
| 31  | A     | 843 | CLA  | O2D-CGD-O1D | -4.07 | 115.89      | 123.84   |
| 31  | K     | 206 | CLA  | C4D-CHA-C1A | -4.07 | 116.30      | 121.25   |
| 31  | B     | 825 | CLA  | C1C-C2C-C3C | -4.06 | 102.69      | 106.96   |
| 31  | B     | 846 | CLA  | C1C-C2C-C3C | -4.06 | 102.69      | 106.96   |
| 31  | 3     | 320 | CLA  | CHD-C1D-ND  | -4.06 | 120.72      | 124.45   |
| 31  | A     | 828 | CLA  | CHD-C4C-C3C | -4.06 | 118.87      | 124.84   |
| 31  | A     | 827 | CLA  | CHD-C1D-ND  | -4.06 | 120.72      | 124.45   |
| 31  | G     | 206 | CLA  | CHD-C4C-C3C | -4.06 | 118.87      | 124.84   |
| 31  | 5     | 311 | CLA  | CHD-C4C-C3C | -4.06 | 118.87      | 124.84   |
| 31  | 4     | 318 | CLA  | C1C-C2C-C3C | -4.06 | 102.69      | 106.96   |
| 31  | A     | 828 | CLA  | CHD-C1D-ND  | -4.06 | 120.72      | 124.45   |
| 31  | 4     | 311 | CLA  | C2D-C1D-ND  | 4.06  | 113.09      | 110.10   |
| 31  | B     | 839 | CLA  | O2D-CGD-CBD | 4.06  | 118.48      | 111.27   |
| 32  | A     | 840 | CHL  | CHD-C4C-C3C | -4.06 | 118.88      | 124.84   |
| 31  | B     | 827 | CLA  | CHD-C4C-C3C | -4.06 | 118.88      | 124.84   |
| 36  | 9     | 305 | LUT  | C12-C13-C14 | -4.06 | 112.72      | 118.94   |
| 31  | A     | 829 | CLA  | C4D-CHA-C1A | -4.06 | 116.31      | 121.25   |
| 31  | B     | 826 | CLA  | C4D-CHA-C1A | -4.05 | 116.31      | 121.25   |
| 31  | B     | 833 | CLA  | C2C-C1C-NC  | 4.05  | 113.77      | 109.97   |
| 31  | A     | 846 | CLA  | CHD-C1D-ND  | -4.05 | 120.73      | 124.45   |
| 31  | A     | 835 | CLA  | C1C-C2C-C3C | -4.05 | 102.70      | 106.96   |
| 31  | A     | 846 | CLA  | C4D-CHA-C1A | -4.05 | 116.32      | 121.25   |
| 31  | a     | 315 | CLA  | C4D-CHA-C1A | -4.05 | 116.32      | 121.25   |
| 31  | 6     | 306 | CLA  | C2D-C1D-ND  | 4.05  | 113.09      | 110.10   |
| 31  | 3     | 312 | CLA  | C4D-CHA-C1A | -4.05 | 116.32      | 121.25   |
| 31  | A     | 837 | CLA  | C1C-C2C-C3C | -4.05 | 102.70      | 106.96   |
| 31  | A     | 825 | CLA  | C2C-C1C-NC  | 4.05  | 113.76      | 109.97   |
| 31  | 4     | 320 | CLA  | CHD-C4C-C3C | -4.05 | 118.89      | 124.84   |
| 32  | A     | 840 | CHL  | CHD-C1D-ND  | -4.04 | 120.74      | 124.45   |
| 36  | a     | 303 | LUT  | C8-C7-C6    | -4.04 | 115.84      | 127.20   |
| 31  | 4     | 312 | CLA  | CHD-C1D-ND  | -4.04 | 120.74      | 124.45   |
| 31  | 2     | 304 | CLA  | C2C-C1C-NC  | 4.04  | 113.76      | 109.97   |
| 32  | a     | 318 | CHL  | C1C-C2C-C3C | -4.04 | 103.91      | 107.11   |
| 31  | 5     | 315 | CLA  | C4D-CHA-C1A | -4.04 | 116.33      | 121.25   |
| 31  | b     | 304 | CLA  | C4D-CHA-C1A | -4.04 | 116.33      | 121.25   |
| 31  | B     | 825 | CLA  | C2C-C1C-NC  | 4.04  | 113.76      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 854 | CLA  | O2D-CGD-O1D | -4.04 | 115.95      | 123.84   |
| 31  | 5     | 318 | CLA  | C4D-CHA-C1A | -4.03 | 116.34      | 121.25   |
| 31  | 6     | 310 | CLA  | CHD-C4C-C3C | -4.03 | 118.91      | 124.84   |
| 32  | A     | 831 | CHL  | CGD-CBD-CAD | 4.03  | 123.80      | 110.73   |
| 31  | 6     | 308 | CLA  | C1C-C2C-C3C | -4.03 | 102.72      | 106.96   |
| 31  | B     | 849 | CLA  | CHD-C4C-C3C | -4.03 | 118.91      | 124.84   |
| 31  | 9     | 315 | CLA  | O2D-CGD-O1D | -4.03 | 115.95      | 123.84   |
| 31  | B     | 836 | CLA  | CHD-C4C-C3C | -4.03 | 118.91      | 124.84   |
| 31  | K     | 206 | CLA  | CHD-C4C-C3C | -4.03 | 118.91      | 124.84   |
| 31  | 5     | 312 | CLA  | C2D-C1D-ND  | 4.03  | 113.08      | 110.10   |
| 31  | b     | 305 | CLA  | O2D-CGD-O1D | -4.03 | 115.96      | 123.84   |
| 31  | A     | 857 | CLA  | C4D-CHA-C1A | -4.03 | 116.34      | 121.25   |
| 31  | 2     | 307 | CLA  | C2D-C1D-ND  | 4.03  | 113.07      | 110.10   |
| 31  | A     | 824 | CLA  | C2D-C1D-ND  | 4.03  | 113.07      | 110.10   |
| 31  | G     | 206 | CLA  | C1C-C2C-C3C | -4.03 | 102.72      | 106.96   |
| 32  | 3     | 315 | CHL  | CHD-C4C-C3C | -4.02 | 118.92      | 124.84   |
| 31  | B     | 850 | CLA  | CAC-C3C-C4C | 4.02  | 130.03      | 124.81   |
| 31  | A     | 814 | CLA  | C1C-C2C-C3C | -4.02 | 102.73      | 106.96   |
| 31  | A     | 855 | CLA  | C1C-C2C-C3C | -4.02 | 102.73      | 106.96   |
| 31  | 8     | 313 | CLA  | C4D-CHA-C1A | -4.02 | 116.35      | 121.25   |
| 32  | A     | 831 | CHL  | C1C-C2C-C3C | -4.02 | 103.92      | 107.11   |
| 31  | B     | 842 | CLA  | C4D-CHA-C1A | -4.02 | 116.35      | 121.25   |
| 31  | 4     | 311 | CLA  | O2D-CGD-O1D | -4.02 | 115.97      | 123.84   |
| 31  | a     | 314 | CLA  | O1D-CGD-CBD | -4.02 | 116.26      | 124.48   |
| 31  | G     | 204 | CLA  | CHD-C1D-ND  | -4.02 | 120.76      | 124.45   |
| 31  | 8     | 318 | CLA  | CHD-C4C-C3C | -4.02 | 118.93      | 124.84   |
| 31  | B     | 814 | CLA  | C1C-C2C-C3C | -4.02 | 102.73      | 106.96   |
| 31  | 5     | 309 | CLA  | C2D-C1D-ND  | 4.02  | 113.06      | 110.10   |
| 31  | 6     | 314 | CLA  | O2D-CGD-O1D | -4.02 | 115.98      | 123.84   |
| 32  | a     | 317 | CHL  | CHD-C4C-C3C | -4.02 | 118.94      | 124.84   |
| 31  | 4     | 312 | CLA  | C4D-CHA-C1A | -4.02 | 116.36      | 121.25   |
| 31  | A     | 849 | CLA  | CHD-C1D-ND  | -4.02 | 120.76      | 124.45   |
| 31  | A     | 829 | CLA  | C1D-ND-C4D  | -4.01 | 103.48      | 106.33   |
| 31  | 9     | 314 | CLA  | CHD-C1D-ND  | -4.01 | 120.77      | 124.45   |
| 31  | b     | 307 | CLA  | C2D-C1D-ND  | 4.01  | 113.06      | 110.10   |
| 31  | B     | 835 | CLA  | CHD-C1D-ND  | -4.01 | 120.77      | 124.45   |
| 31  | 5     | 320 | CLA  | C2D-C1D-ND  | 4.01  | 113.06      | 110.10   |
| 31  | 2     | 305 | CLA  | O2D-CGD-O1D | -4.01 | 116.00      | 123.84   |
| 31  | 3     | 320 | CLA  | C2D-C1D-ND  | 4.01  | 113.06      | 110.10   |
| 31  | B     | 839 | CLA  | C2C-C1C-NC  | 4.01  | 113.73      | 109.97   |
| 31  | b     | 313 | CLA  | C2C-C1C-NC  | 4.01  | 113.73      | 109.97   |
| 28  | A     | 810 | LHG  | O4-P-O5     | 4.01  | 132.05      | 112.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 318 | CLA  | C4D-CHA-C1A | -4.00 | 116.38      | 121.25   |
| 31  | B     | 816 | CLA  | C4D-CHA-C1A | -4.00 | 116.38      | 121.25   |
| 31  | O     | 204 | CLA  | CHD-C1D-ND  | -4.00 | 120.78      | 124.45   |
| 31  | B     | 836 | CLA  | CHD-C1D-ND  | -4.00 | 120.78      | 124.45   |
| 32  | a     | 318 | CHL  | CGD-CBD-CAD | 4.00  | 123.69      | 110.73   |
| 32  | A     | 839 | CHL  | C4D-C3D-CAD | 4.00  | 112.81      | 108.10   |
| 31  | 3     | 314 | CLA  | C2D-C1D-ND  | 4.00  | 113.05      | 110.10   |
| 31  | A     | 825 | CLA  | C1-O2A-CGA  | 4.00  | 126.94      | 116.44   |
| 31  | G     | 205 | CLA  | C4D-CHA-C1A | -4.00 | 116.38      | 121.25   |
| 31  | 6     | 308 | CLA  | C4D-CHA-C1A | -4.00 | 116.38      | 121.25   |
| 31  | 2     | 304 | CLA  | C1C-C2C-C3C | -4.00 | 102.75      | 106.96   |
| 32  | b     | 309 | CHL  | CGD-CBD-CAD | 4.00  | 123.68      | 110.73   |
| 40  | 7     | 306 | XAT  | C39-C29-C30 | -4.00 | 117.33      | 122.92   |
| 31  | A     | 856 | CLA  | CHD-C4C-C3C | -4.00 | 118.97      | 124.84   |
| 32  | 7     | 324 | CHL  | CHD-C4C-C3C | -4.00 | 118.97      | 124.84   |
| 31  | G     | 204 | CLA  | C2D-C1D-ND  | 3.99  | 113.05      | 110.10   |
| 31  | B     | 814 | CLA  | O1D-CGD-CBD | -3.99 | 116.31      | 124.48   |
| 31  | 8     | 308 | CLA  | CHD-C1D-ND  | -3.99 | 120.78      | 124.45   |
| 32  | 3     | 315 | CHL  | CHD-C1D-ND  | -3.99 | 120.78      | 124.45   |
| 36  | L     | 304 | LUT  | C1-C6-C5    | -3.99 | 116.99      | 122.61   |
| 31  | A     | 830 | CLA  | CAC-C3C-C4C | 3.99  | 129.99      | 124.81   |
| 26  | A     | 803 | BCR  | C2-C1-C6    | 3.99  | 116.62      | 110.48   |
| 31  | A     | 848 | CLA  | O2D-CGD-O1D | -3.99 | 116.03      | 123.84   |
| 31  | 9     | 315 | CLA  | CHA-C4D-ND  | 3.99  | 140.85      | 132.50   |
| 31  | 6     | 313 | CLA  | CHD-C4C-C3C | -3.99 | 118.97      | 124.84   |
| 40  | 7     | 306 | XAT  | C19-C9-C10  | -3.99 | 117.33      | 122.92   |
| 36  | 6     | 304 | LUT  | C1-C6-C5    | -3.99 | 116.99      | 122.61   |
| 31  | B     | 847 | CLA  | CHD-C1D-ND  | -3.99 | 120.79      | 124.45   |
| 36  | 3     | 305 | LUT  | C19-C9-C8   | -3.99 | 111.79      | 118.08   |
| 31  | B     | 837 | CLA  | CHD-C1D-ND  | -3.99 | 120.79      | 124.45   |
| 32  | 9     | 320 | CHL  | CHD-C4C-C3C | -3.99 | 118.98      | 124.84   |
| 31  | A     | 827 | CLA  | O2D-CGD-CBD | 3.99  | 118.35      | 111.27   |
| 31  | B     | 845 | CLA  | C1-C2-C3    | -3.99 | 120.30      | 126.75   |
| 31  | B     | 843 | CLA  | C2D-C1D-ND  | 3.99  | 113.04      | 110.10   |
| 31  | B     | 850 | CLA  | O2D-CGD-CBD | 3.99  | 118.35      | 111.27   |
| 31  | 9     | 321 | CLA  | O2D-CGD-CBD | 3.99  | 118.35      | 111.27   |
| 31  | 6     | 312 | CLA  | O2D-CGD-CBD | 3.99  | 118.35      | 111.27   |
| 36  | b     | 301 | LUT  | C32-C33-C34 | -3.98 | 112.83      | 118.94   |
| 31  | 7     | 322 | CLA  | C4D-CHA-C1A | -3.98 | 116.40      | 121.25   |
| 31  | 5     | 315 | CLA  | C2D-C1D-ND  | 3.98  | 113.04      | 110.10   |
| 31  | 2     | 310 | CLA  | CHD-C4C-C3C | -3.98 | 118.99      | 124.84   |
| 31  | 9     | 315 | CLA  | C4D-CHA-C1A | -3.98 | 116.41      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 823 | CLA  | CHD-C4C-C3C | -3.98 | 118.99      | 124.84   |
| 36  | 6     | 303 | LUT  | C12-C13-C14 | -3.98 | 112.84      | 118.94   |
| 32  | 7     | 319 | CHL  | C1C-C2C-C3C | -3.97 | 103.96      | 107.11   |
| 31  | 3     | 317 | CLA  | C4-C3-C5    | 3.97  | 120.53      | 115.98   |
| 31  | A     | 820 | CLA  | C4D-CHA-C1A | -3.97 | 116.41      | 121.25   |
| 31  | a     | 314 | CLA  | CHD-C1D-ND  | -3.97 | 120.80      | 124.45   |
| 31  | B     | 841 | CLA  | C2C-C1C-NC  | 3.97  | 113.69      | 109.97   |
| 31  | 8     | 310 | CLA  | O2D-CGD-O1D | -3.97 | 116.07      | 123.84   |
| 31  | 2     | 313 | CLA  | C4D-CHA-C1A | -3.97 | 116.42      | 121.25   |
| 31  | 5     | 307 | CLA  | O1D-CGD-CBD | -3.97 | 116.36      | 124.48   |
| 31  | L     | 305 | CLA  | CHD-C4C-C3C | -3.97 | 119.01      | 124.84   |
| 31  | 3     | 318 | CLA  | C2D-C1D-ND  | 3.97  | 113.03      | 110.10   |
| 31  | 5     | 321 | CLA  | O2D-CGD-O1D | -3.97 | 116.08      | 123.84   |
| 36  | 6     | 304 | LUT  | C12-C13-C14 | -3.97 | 112.85      | 118.94   |
| 31  | 4     | 314 | CLA  | CHD-C1D-ND  | -3.97 | 120.81      | 124.45   |
| 31  | A     | 843 | CLA  | C4D-CHA-C1A | -3.96 | 116.42      | 121.25   |
| 31  | A     | 826 | CLA  | O2D-CGD-O1D | -3.96 | 116.09      | 123.84   |
| 31  | B     | 845 | CLA  | O2D-CGD-CBD | 3.96  | 118.31      | 111.27   |
| 31  | 8     | 317 | CLA  | CHD-C4C-NC  | 3.96  | 130.45      | 124.20   |
| 31  | A     | 844 | CLA  | C4D-CHA-C1A | -3.96 | 116.43      | 121.25   |
| 31  | 2     | 313 | CLA  | C2D-C1D-ND  | 3.96  | 113.02      | 110.10   |
| 31  | 4     | 314 | CLA  | C2D-C1D-ND  | 3.96  | 113.02      | 110.10   |
| 31  | a     | 319 | CLA  | CHD-C4C-C3C | -3.96 | 119.02      | 124.84   |
| 32  | a     | 320 | CHL  | CGD-CBD-CAD | 3.96  | 123.56      | 110.73   |
| 36  | 2     | 301 | LUT  | C7-C8-C9    | -3.96 | 120.25      | 126.23   |
| 31  | A     | 837 | CLA  | CHD-C4C-C3C | -3.96 | 119.02      | 124.84   |
| 31  | A     | 814 | CLA  | CHD-C1D-ND  | -3.96 | 120.82      | 124.45   |
| 31  | A     | 823 | CLA  | C2D-C1D-ND  | 3.96  | 113.02      | 110.10   |
| 31  | A     | 835 | CLA  | CHD-C1D-ND  | -3.96 | 120.82      | 124.45   |
| 31  | L     | 307 | CLA  | C2D-C1D-ND  | 3.95  | 113.02      | 110.10   |
| 31  | B     | 822 | CLA  | C2C-C1C-NC  | 3.95  | 113.67      | 109.97   |
| 36  | b     | 301 | LUT  | C7-C8-C9    | -3.95 | 120.26      | 126.23   |
| 31  | a     | 312 | CLA  | O2D-CGD-O1D | -3.95 | 116.11      | 123.84   |
| 31  | 5     | 312 | CLA  | CHD-C4C-C3C | -3.95 | 119.03      | 124.84   |
| 31  | B     | 850 | CLA  | CHD-C4C-C3C | -3.95 | 119.03      | 124.84   |
| 31  | 6     | 315 | CLA  | C4D-CHA-C1A | -3.95 | 116.44      | 121.25   |
| 31  | B     | 832 | CLA  | C2D-C1D-ND  | 3.95  | 113.01      | 110.10   |
| 31  | B     | 846 | CLA  | CHD-C4C-C3C | -3.95 | 119.04      | 124.84   |
| 31  | K     | 206 | CLA  | CHD-C1D-ND  | -3.95 | 120.83      | 124.45   |
| 32  | 9     | 320 | CHL  | O2D-CGD-O1D | -3.95 | 116.12      | 123.84   |
| 31  | 2     | 311 | CLA  | O2D-CGD-O1D | -3.95 | 116.12      | 123.84   |
| 32  | 6     | 317 | CHL  | CGD-CBD-CAD | 3.95  | 123.52      | 110.73   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 312 | CLA  | O2D-CGD-O1D | -3.95 | 116.12      | 123.84   |
| 31  | A     | 815 | CLA  | C2C-C1C-NC  | 3.95  | 113.67      | 109.97   |
| 31  | B     | 848 | CLA  | C2C-C1C-NC  | 3.95  | 113.67      | 109.97   |
| 31  | a     | 312 | CLA  | CHD-C1D-ND  | -3.95 | 120.83      | 124.45   |
| 31  | B     | 834 | CLA  | C2C-C1C-NC  | 3.95  | 113.67      | 109.97   |
| 31  | 2     | 308 | CLA  | C4D-CHA-C1A | -3.94 | 116.45      | 121.25   |
| 31  | B     | 830 | CLA  | O1D-CGD-CBD | -3.94 | 116.41      | 124.48   |
| 31  | O     | 202 | CLA  | CBD-CHA-C1A | 3.94  | 133.15      | 128.50   |
| 31  | 5     | 312 | CLA  | C4D-CHA-C1A | -3.94 | 116.45      | 121.25   |
| 31  | 7     | 316 | CLA  | CHD-C4C-C3C | -3.94 | 119.04      | 124.84   |
| 31  | H     | 902 | CLA  | CHD-C1D-ND  | -3.94 | 120.83      | 124.45   |
| 31  | 3     | 313 | CLA  | C2D-C1D-ND  | 3.94  | 113.01      | 110.10   |
| 31  | 6     | 311 | CLA  | C2D-C1D-ND  | 3.94  | 113.01      | 110.10   |
| 31  | A     | 815 | CLA  | CHD-C4C-C3C | -3.94 | 119.04      | 124.84   |
| 31  | L     | 307 | CLA  | CHD-C1D-ND  | -3.94 | 120.83      | 124.45   |
| 31  | 8     | 318 | CLA  | C4D-CHA-C1A | -3.94 | 116.45      | 121.25   |
| 31  | A     | 818 | CLA  | CHD-C4C-C3C | -3.94 | 119.05      | 124.84   |
| 31  | 4     | 314 | CLA  | CHD-C4C-C3C | -3.94 | 119.05      | 124.84   |
| 31  | a     | 319 | CLA  | CHD-C1D-ND  | -3.94 | 120.84      | 124.45   |
| 31  | B     | 823 | CLA  | O2D-CGD-O1D | -3.94 | 116.14      | 123.84   |
| 31  | F     | 301 | CLA  | C1C-C2C-C3C | -3.94 | 102.82      | 106.96   |
| 31  | 3     | 307 | CLA  | O2D-CGD-CBD | 3.93  | 118.26      | 111.27   |
| 36  | 6     | 304 | LUT  | C21-C26-C27 | -3.93 | 107.73      | 112.70   |
| 31  | B     | 848 | CLA  | C1C-C2C-C3C | -3.93 | 102.82      | 106.96   |
| 31  | 5     | 323 | CLA  | O2D-CGD-O1D | -3.93 | 116.15      | 123.84   |
| 31  | 2     | 309 | CLA  | C2D-C1D-ND  | 3.93  | 113.00      | 110.10   |
| 31  | A     | 833 | CLA  | CHD-C4C-C3C | -3.93 | 119.06      | 124.84   |
| 31  | H     | 903 | CLA  | CHD-C4C-C3C | -3.93 | 119.06      | 124.84   |
| 32  | 6     | 321 | CHL  | CGD-CBD-CAD | 3.93  | 123.47      | 110.73   |
| 31  | 2     | 309 | CLA  | CHD-C4C-C3C | -3.93 | 119.06      | 124.84   |
| 31  | H     | 902 | CLA  | C4D-CHA-C1A | -3.93 | 116.47      | 121.25   |
| 32  | A     | 839 | CHL  | CHD-C1D-ND  | -3.93 | 120.84      | 124.45   |
| 31  | A     | 847 | CLA  | O2D-CGD-O1D | -3.93 | 116.16      | 123.84   |
| 31  | B     | 834 | CLA  | O2D-CGD-O1D | -3.93 | 116.16      | 123.84   |
| 31  | B     | 824 | CLA  | CHD-C1D-ND  | -3.93 | 120.84      | 124.45   |
| 31  | 5     | 312 | CLA  | CHD-C1D-ND  | -3.93 | 120.84      | 124.45   |
| 31  | 8     | 312 | CLA  | CHD-C4C-C3C | -3.93 | 119.07      | 124.84   |
| 36  | 6     | 303 | LUT  | C7-C8-C9    | -3.93 | 120.30      | 126.23   |
| 31  | A     | 824 | CLA  | CHD-C1D-ND  | -3.93 | 120.85      | 124.45   |
| 31  | 9     | 318 | CLA  | C2C-C1C-NC  | 3.93  | 113.65      | 109.97   |
| 31  | A     | 818 | CLA  | O2D-CGD-CBD | 3.93  | 118.24      | 111.27   |
| 31  | A     | 842 | CLA  | O2D-CGD-O1D | -3.93 | 116.16      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 309 | CLA  | CHD-C4C-C3C | -3.92 | 119.07      | 124.84   |
| 31  | A     | 850 | CLA  | CHD-C1D-ND  | -3.92 | 120.85      | 124.45   |
| 31  | A     | 850 | CLA  | C4-C3-C5    | 3.92  | 120.47      | 115.98   |
| 31  | B     | 817 | CLA  | CHD-C1D-ND  | -3.92 | 120.85      | 124.45   |
| 31  | 3     | 312 | CLA  | O2D-CGD-O1D | -3.92 | 116.17      | 123.84   |
| 31  | B     | 815 | CLA  | CHD-C1D-ND  | -3.92 | 120.85      | 124.45   |
| 31  | 5     | 308 | CLA  | CHD-C1D-ND  | -3.92 | 120.85      | 124.45   |
| 31  | B     | 819 | CLA  | O2D-CGD-O1D | -3.92 | 116.18      | 123.84   |
| 31  | A     | 849 | CLA  | C2D-C1D-ND  | 3.92  | 112.99      | 110.10   |
| 31  | a     | 311 | CLA  | C2D-C1D-ND  | 3.92  | 112.99      | 110.10   |
| 31  | A     | 830 | CLA  | C1C-C2C-C3C | -3.92 | 102.84      | 106.96   |
| 31  | B     | 843 | CLA  | C4D-CHA-C1A | -3.92 | 116.48      | 121.25   |
| 31  | A     | 834 | CLA  | O1D-CGD-CBD | -3.91 | 116.47      | 124.48   |
| 31  | A     | 854 | CLA  | C4D-CHA-C1A | -3.91 | 116.49      | 121.25   |
| 31  | L     | 307 | CLA  | C4D-CHA-C1A | -3.91 | 116.49      | 121.25   |
| 31  | B     | 822 | CLA  | CHD-C1D-ND  | -3.91 | 120.86      | 124.45   |
| 30  | A     | 813 | CL0  | C2A-C1A-CHA | -3.91 | 117.02      | 123.86   |
| 31  | B     | 834 | CLA  | CHD-C1D-ND  | -3.91 | 120.86      | 124.45   |
| 31  | A     | 841 | CLA  | O2D-CGD-O1D | -3.91 | 116.19      | 123.84   |
| 31  | 3     | 307 | CLA  | C2C-C1C-NC  | 3.91  | 113.63      | 109.97   |
| 31  | 3     | 317 | CLA  | CHD-C4C-C3C | -3.91 | 119.10      | 124.84   |
| 31  | A     | 848 | CLA  | C4D-CHA-C1A | -3.91 | 116.50      | 121.25   |
| 31  | 5     | 310 | CLA  | O2D-CGD-O1D | -3.91 | 116.20      | 123.84   |
| 31  | B     | 818 | CLA  | CHD-C4C-C3C | -3.90 | 119.10      | 124.84   |
| 32  | 4     | 310 | CHL  | C4A-NA-C1A  | 3.90  | 108.46      | 106.71   |
| 31  | B     | 843 | CLA  | CHD-C1D-ND  | -3.90 | 120.87      | 124.45   |
| 32  | K     | 201 | CHL  | C2D-C1D-ND  | 3.90  | 112.98      | 110.10   |
| 31  | 2     | 307 | CLA  | CHD-C1D-ND  | -3.90 | 120.87      | 124.45   |
| 31  | B     | 811 | CLA  | C2C-C1C-NC  | 3.90  | 113.62      | 109.97   |
| 32  | 7     | 320 | CHL  | CGD-CBD-CAD | 3.90  | 123.36      | 110.73   |
| 31  | 7     | 315 | CLA  | O2D-CGD-O1D | -3.90 | 116.22      | 123.84   |
| 31  | 3     | 307 | CLA  | CHD-C1D-ND  | -3.90 | 120.87      | 124.45   |
| 31  | 9     | 321 | CLA  | C4D-CHA-C1A | -3.90 | 116.51      | 121.25   |
| 32  | 4     | 310 | CHL  | CHD-C1D-ND  | -3.90 | 120.87      | 124.45   |
| 31  | A     | 833 | CLA  | O2D-CGD-CBD | 3.89  | 118.19      | 111.27   |
| 31  | A     | 838 | CLA  | CHD-C4C-C3C | -3.89 | 119.12      | 124.84   |
| 31  | 9     | 321 | CLA  | O2D-CGD-O1D | -3.89 | 116.23      | 123.84   |
| 36  | 7     | 305 | LUT  | C21-C26-C27 | -3.89 | 107.78      | 112.70   |
| 31  | b     | 308 | CLA  | C4D-CHA-C1A | -3.89 | 116.51      | 121.25   |
| 36  | 3     | 305 | LUT  | C21-C26-C27 | -3.89 | 107.78      | 112.70   |
| 36  | 5     | 303 | LUT  | C1-C6-C5    | -3.89 | 117.14      | 122.61   |
| 31  | 2     | 312 | CLA  | C4D-CHA-C1A | -3.89 | 116.52      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 317 | CLA  | C2D-C1D-ND  | 3.88  | 112.97      | 110.10   |
| 31  | K     | 205 | CLA  | O2D-CGD-O1D | -3.88 | 116.24      | 123.84   |
| 31  | A     | 822 | CLA  | C1C-C2C-C3C | -3.88 | 102.87      | 106.96   |
| 31  | 3     | 319 | CLA  | C4D-CHA-C1A | -3.88 | 116.53      | 121.25   |
| 31  | A     | 849 | CLA  | CHD-C4C-C3C | -3.88 | 119.14      | 124.84   |
| 31  | H     | 902 | CLA  | CHD-C4C-C3C | -3.88 | 119.14      | 124.84   |
| 31  | 5     | 307 | CLA  | CHD-C4C-C3C | -3.88 | 119.14      | 124.84   |
| 31  | B     | 841 | CLA  | C4D-CHA-C1A | -3.88 | 116.53      | 121.25   |
| 31  | a     | 311 | CLA  | CHD-C1D-ND  | -3.88 | 120.89      | 124.45   |
| 31  | B     | 832 | CLA  | CHD-C4C-C3C | -3.88 | 119.14      | 124.84   |
| 31  | 8     | 308 | CLA  | C1C-C2C-C3C | -3.88 | 102.88      | 106.96   |
| 31  | 3     | 311 | CLA  | CHA-C4D-ND  | 3.88  | 140.61      | 132.50   |
| 31  | 6     | 316 | CLA  | C4D-CHA-C1A | -3.87 | 116.53      | 121.25   |
| 31  | 7     | 309 | CLA  | C1C-C2C-C3C | -3.87 | 102.89      | 106.96   |
| 31  | B     | 830 | CLA  | CHD-C4C-C3C | -3.87 | 119.15      | 124.84   |
| 31  | b     | 311 | CLA  | CHD-C4C-C3C | -3.87 | 119.15      | 124.84   |
| 31  | 9     | 318 | CLA  | CHD-C1D-ND  | -3.87 | 120.90      | 124.45   |
| 31  | 7     | 316 | CLA  | O2D-CGD-CBD | 3.87  | 118.14      | 111.27   |
| 31  | 3     | 317 | CLA  | CHD-C1D-ND  | -3.87 | 120.90      | 124.45   |
| 31  | B     | 811 | CLA  | O2D-CGD-O1D | -3.87 | 116.27      | 123.84   |
| 31  | 3     | 308 | CLA  | O2D-CGD-O1D | -3.87 | 116.28      | 123.84   |
| 31  | 3     | 319 | CLA  | CHD-C4C-NC  | 3.87  | 130.30      | 124.20   |
| 32  | 7     | 318 | CHL  | O1D-CGD-CBD | -3.87 | 116.57      | 124.48   |
| 31  | A     | 821 | CLA  | C4D-CHA-C1A | -3.87 | 116.54      | 121.25   |
| 31  | 4     | 315 | CLA  | CHA-C4D-ND  | 3.87  | 140.59      | 132.50   |
| 31  | 5     | 308 | CLA  | O1D-CGD-CBD | -3.87 | 116.57      | 124.48   |
| 31  | A     | 814 | CLA  | CHD-C4C-C3C | -3.87 | 119.16      | 124.84   |
| 31  | B     | 825 | CLA  | O2D-CGD-O1D | -3.86 | 116.28      | 123.84   |
| 31  | 3     | 314 | CLA  | O1D-CGD-CBD | -3.86 | 116.58      | 124.48   |
| 31  | 9     | 313 | CLA  | O1D-CGD-CBD | -3.86 | 116.58      | 124.48   |
| 31  | a     | 321 | CLA  | C2D-C1D-ND  | 3.86  | 112.95      | 110.10   |
| 31  | A     | 857 | CLA  | O2D-CGD-CBD | 3.86  | 118.13      | 111.27   |
| 31  | a     | 311 | CLA  | CHD-C4C-C3C | -3.86 | 119.17      | 124.84   |
| 31  | 6     | 311 | CLA  | CHD-C1D-ND  | -3.86 | 120.91      | 124.45   |
| 31  | 2     | 304 | CLA  | O2D-CGD-O1D | -3.86 | 116.29      | 123.84   |
| 31  | F     | 305 | CLA  | CHD-C4C-C3C | -3.86 | 119.17      | 124.84   |
| 31  | 9     | 318 | CLA  | C4D-CHA-C1A | -3.86 | 116.55      | 121.25   |
| 32  | a     | 318 | CHL  | CHD-C4C-NC  | 3.85  | 130.28      | 124.20   |
| 31  | A     | 815 | CLA  | CHD-C1D-ND  | -3.85 | 120.91      | 124.45   |
| 31  | 8     | 315 | CLA  | C2D-C1D-ND  | 3.85  | 112.94      | 110.10   |
| 31  | 4     | 321 | CLA  | O2D-CGD-O1D | -3.85 | 116.31      | 123.84   |
| 31  | 3     | 307 | CLA  | C1C-C2C-C3C | -3.85 | 102.91      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 310 | CLA  | CHD-C4C-C3C | -3.85 | 119.18      | 124.84   |
| 31  | a     | 322 | CLA  | C4D-CHA-C1A | -3.85 | 116.56      | 121.25   |
| 31  | 8     | 307 | CLA  | CHD-C1D-ND  | -3.85 | 120.92      | 124.45   |
| 31  | 8     | 312 | CLA  | C4D-CHA-C1A | -3.85 | 116.57      | 121.25   |
| 31  | 6     | 307 | CLA  | CHD-C4C-C3C | -3.85 | 119.18      | 124.84   |
| 32  | 9     | 320 | CHL  | C1C-C2C-C3C | -3.85 | 104.06      | 107.11   |
| 31  | B     | 821 | CLA  | CHD-C4C-C3C | -3.85 | 119.19      | 124.84   |
| 31  | 8     | 311 | CLA  | CHD-C4C-C3C | -3.85 | 119.19      | 124.84   |
| 42  | 4     | 304 | SQD  | O47-C7-C8   | 3.84  | 119.79      | 111.50   |
| 31  | 4     | 305 | CLA  | C2A-C3A-C4A | -3.84 | 95.66       | 101.87   |
| 31  | 4     | 316 | CLA  | C2C-C1C-NC  | 3.84  | 113.57      | 109.97   |
| 31  | 5     | 318 | CLA  | O1D-CGD-CBD | -3.84 | 116.62      | 124.48   |
| 31  | 6     | 310 | CLA  | CHA-C4D-ND  | 3.84  | 140.54      | 132.50   |
| 31  | 9     | 314 | CLA  | C4D-CHA-C1A | -3.84 | 116.57      | 121.25   |
| 31  | B     | 848 | CLA  | CHD-C4C-NC  | 3.84  | 130.25      | 124.20   |
| 31  | A     | 815 | CLA  | C1C-C2C-C3C | -3.84 | 102.92      | 106.96   |
| 31  | B     | 843 | CLA  | O2D-CGD-CBD | 3.84  | 118.09      | 111.27   |
| 31  | 8     | 321 | CLA  | CHD-C4C-NC  | 3.84  | 130.25      | 124.20   |
| 31  | 6     | 314 | CLA  | CHD-C1D-ND  | -3.84 | 120.93      | 124.45   |
| 31  | b     | 312 | CLA  | C2D-C1D-ND  | 3.83  | 112.93      | 110.10   |
| 31  | B     | 822 | CLA  | CHD-C4C-C3C | -3.83 | 119.20      | 124.84   |
| 32  | 5     | 317 | CHL  | CGD-CBD-CAD | 3.83  | 123.15      | 110.73   |
| 31  | O     | 203 | CLA  | CHD-C1D-ND  | -3.83 | 120.93      | 124.45   |
| 31  | 2     | 315 | CLA  | C4D-CHA-C1A | -3.83 | 116.58      | 121.25   |
| 31  | 5     | 308 | CLA  | CHD-C4C-C3C | -3.83 | 119.21      | 124.84   |
| 31  | B     | 823 | CLA  | C4D-CHA-C1A | -3.83 | 116.58      | 121.25   |
| 31  | 7     | 313 | CLA  | C4D-CHA-C1A | -3.83 | 116.58      | 121.25   |
| 31  | 9     | 319 | CLA  | CHA-C4D-ND  | 3.83  | 140.52      | 132.50   |
| 31  | F     | 301 | CLA  | O2D-CGD-O1D | -3.83 | 116.35      | 123.84   |
| 31  | B     | 849 | CLA  | O2D-CGD-O1D | -3.83 | 116.35      | 123.84   |
| 31  | 5     | 312 | CLA  | O1D-CGD-CBD | -3.83 | 116.65      | 124.48   |
| 31  | a     | 316 | CLA  | CHD-C4C-C3C | -3.83 | 119.21      | 124.84   |
| 31  | 5     | 315 | CLA  | CHD-C4C-C3C | -3.83 | 119.22      | 124.84   |
| 31  | 7     | 316 | CLA  | C2D-C1D-ND  | 3.83  | 112.92      | 110.10   |
| 31  | 3     | 318 | CLA  | O2D-CGD-O1D | -3.83 | 116.36      | 123.84   |
| 31  | 2     | 306 | CLA  | CHD-C4C-C3C | -3.82 | 119.22      | 124.84   |
| 31  | A     | 848 | CLA  | CHD-C1D-ND  | -3.82 | 120.94      | 124.45   |
| 31  | 9     | 313 | CLA  | CHD-C1D-ND  | -3.82 | 120.94      | 124.45   |
| 31  | 8     | 309 | CLA  | CHA-C4D-ND  | 3.82  | 140.50      | 132.50   |
| 31  | A     | 833 | CLA  | O1D-CGD-CBD | -3.82 | 116.66      | 124.48   |
| 36  | 6     | 304 | LUT  | C7-C6-C5    | -3.82 | 112.21      | 121.46   |
| 40  | 7     | 306 | XAT  | C35-C15-C14 | 3.82  | 131.30      | 123.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 6     | 304 | LUT  | C10-C11-C12 | -3.82 | 111.30      | 123.22   |
| 31  | 8     | 311 | CLA  | O2D-CGD-O1D | -3.82 | 116.37      | 123.84   |
| 31  | 7     | 321 | CLA  | O2D-CGD-O1D | -3.82 | 116.38      | 123.84   |
| 31  | B     | 835 | CLA  | C4D-CHA-C1A | -3.82 | 116.60      | 121.25   |
| 31  | 4     | 314 | CLA  | O2D-CGD-CBD | 3.82  | 118.05      | 111.27   |
| 31  | A     | 841 | CLA  | O2D-CGD-CBD | 3.81  | 118.04      | 111.27   |
| 31  | 2     | 311 | CLA  | CHD-C1D-ND  | -3.81 | 120.95      | 124.45   |
| 31  | a     | 314 | CLA  | C2D-C1D-ND  | 3.81  | 112.91      | 110.10   |
| 36  | 4     | 303 | LUT  | C7-C8-C9    | -3.81 | 120.48      | 126.23   |
| 31  | B     | 815 | CLA  | CHA-C4D-ND  | 3.81  | 140.47      | 132.50   |
| 32  | 6     | 317 | CHL  | CHD-C1D-ND  | -3.81 | 120.95      | 124.45   |
| 31  | A     | 818 | CLA  | CHB-C4A-NA  | 3.81  | 129.78      | 124.51   |
| 31  | 8     | 314 | CLA  | CHD-C1D-ND  | -3.81 | 120.95      | 124.45   |
| 31  | A     | 850 | CLA  | O2D-CGD-O1D | -3.81 | 116.39      | 123.84   |
| 31  | 2     | 315 | CLA  | O2D-CGD-O1D | -3.81 | 116.39      | 123.84   |
| 42  | 4     | 304 | SQD  | O9-S-O7     | -3.81 | 100.77      | 113.95   |
| 31  | B     | 828 | CLA  | C4D-CHA-C1A | -3.81 | 116.62      | 121.25   |
| 31  | 6     | 307 | CLA  | C2D-C1D-ND  | 3.81  | 112.91      | 110.10   |
| 31  | 4     | 306 | CLA  | C4D-CHA-C1A | -3.81 | 116.62      | 121.25   |
| 32  | 4     | 313 | CHL  | CGD-CBD-CAD | 3.81  | 123.06      | 110.73   |
| 31  | B     | 818 | CLA  | CHD-C1D-ND  | -3.81 | 120.96      | 124.45   |
| 31  | 4     | 308 | CLA  | CHD-C1D-ND  | -3.80 | 120.96      | 124.45   |
| 36  | F     | 304 | LUT  | C21-C26-C27 | -3.80 | 107.89      | 112.70   |
| 31  | A     | 829 | CLA  | C1-C2-C3    | -3.80 | 120.60      | 126.75   |
| 31  | A     | 854 | CLA  | C1C-C2C-C3C | -3.80 | 102.96      | 106.96   |
| 31  | 8     | 320 | CLA  | CHD-C1D-ND  | -3.80 | 120.96      | 124.45   |
| 31  | 5     | 318 | CLA  | C2D-C1D-ND  | 3.80  | 112.91      | 110.10   |
| 31  | 8     | 313 | CLA  | O2D-CGD-CBD | 3.80  | 118.02      | 111.27   |
| 31  | a     | 311 | CLA  | O2D-CGD-O1D | -3.80 | 116.41      | 123.84   |
| 31  | 4     | 305 | CLA  | C1-C2-C3    | -3.80 | 119.48      | 126.04   |
| 36  | b     | 301 | LUT  | C1-C6-C5    | -3.79 | 117.27      | 122.61   |
| 36  | 9     | 302 | LUT  | C19-C9-C8   | -3.79 | 112.10      | 118.08   |
| 31  | 4     | 315 | CLA  | C4D-CHA-C1A | -3.79 | 116.63      | 121.25   |
| 31  | 7     | 309 | CLA  | C2C-C1C-NC  | 3.79  | 113.53      | 109.97   |
| 31  | b     | 307 | CLA  | CHD-C4C-C3C | -3.79 | 119.26      | 124.84   |
| 31  | a     | 321 | CLA  | O2D-CGD-O1D | -3.79 | 116.42      | 123.84   |
| 31  | O     | 204 | CLA  | C4D-CHA-C1A | -3.79 | 116.63      | 121.25   |
| 26  | K     | 203 | BCR  | C2-C1-C6    | 3.79  | 116.32      | 110.48   |
| 31  | b     | 308 | CLA  | C2D-C1D-ND  | 3.79  | 112.90      | 110.10   |
| 31  | 2     | 311 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 31  | A     | 827 | CLA  | O2D-CGD-O1D | -3.79 | 116.42      | 123.84   |
| 31  | 3     | 311 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 305 | CLA  | C4C-C3C-C2C | -3.79 | 101.37      | 106.90   |
| 31  | 2     | 313 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 31  | 8     | 309 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 31  | 2     | 314 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 31  | 4     | 312 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 31  | 2     | 312 | CLA  | CHD-C4C-C3C | -3.79 | 119.27      | 124.84   |
| 31  | 6     | 306 | CLA  | C3D-C2D-C1D | -3.79 | 100.66      | 105.83   |
| 31  | 6     | 311 | CLA  | O2D-CGD-O1D | -3.79 | 116.44      | 123.84   |
| 31  | 5     | 323 | CLA  | CHD-C1D-ND  | -3.79 | 120.97      | 124.45   |
| 31  | b     | 313 | CLA  | C4D-CHA-C1A | -3.79 | 116.64      | 121.25   |
| 32  | 7     | 320 | CHL  | CHD-C4C-C3C | -3.79 | 119.28      | 124.84   |
| 31  | B     | 823 | CLA  | C2D-C1D-ND  | 3.78  | 112.89      | 110.10   |
| 31  | F     | 306 | CLA  | O2D-CGD-O1D | -3.78 | 116.45      | 123.84   |
| 31  | a     | 321 | CLA  | CHD-C4C-C3C | -3.78 | 119.28      | 124.84   |
| 36  | 2     | 301 | LUT  | C1-C6-C5    | -3.78 | 117.29      | 122.61   |
| 31  | A     | 850 | CLA  | C4D-CHA-C1A | -3.78 | 116.65      | 121.25   |
| 31  | a     | 310 | CLA  | O1D-CGD-CBD | -3.78 | 116.76      | 124.48   |
| 31  | J     | 105 | CLA  | CHD-C1D-ND  | -3.78 | 120.98      | 124.45   |
| 31  | 4     | 306 | CLA  | CHA-C4D-ND  | 3.77  | 140.39      | 132.50   |
| 31  | A     | 825 | CLA  | C4D-CHA-C1A | -3.77 | 116.66      | 121.25   |
| 31  | B     | 813 | CLA  | C4D-CHA-C1A | -3.77 | 116.66      | 121.25   |
| 31  | O     | 202 | CLA  | C2D-C1D-ND  | 3.77  | 112.88      | 110.10   |
| 31  | 7     | 313 | CLA  | CHD-C1D-ND  | -3.77 | 120.99      | 124.45   |
| 31  | B     | 815 | CLA  | O2D-CGD-O1D | -3.77 | 116.47      | 123.84   |
| 31  | B     | 824 | CLA  | CHD-C4C-C3C | -3.77 | 119.30      | 124.84   |
| 31  | 2     | 312 | CLA  | CHA-C4D-ND  | 3.77  | 140.38      | 132.50   |
| 36  | 3     | 305 | LUT  | C8-C7-C6    | -3.76 | 116.64      | 127.20   |
| 31  | G     | 205 | CLA  | CHD-C1D-ND  | -3.76 | 121.00      | 124.45   |
| 31  | B     | 816 | CLA  | CHD-C4C-C3C | -3.76 | 119.31      | 124.84   |
| 31  | O     | 203 | CLA  | CHD-C4C-C3C | -3.76 | 119.32      | 124.84   |
| 26  | 5     | 302 | BCR  | C2-C1-C6    | 3.76  | 116.26      | 110.48   |
| 31  | A     | 838 | CLA  | C2D-C1D-ND  | 3.75  | 112.87      | 110.10   |
| 31  | A     | 822 | CLA  | O2D-CGD-CBD | 3.75  | 117.93      | 111.27   |
| 32  | 9     | 322 | CHL  | CGD-CBD-CAD | 3.75  | 122.88      | 110.73   |
| 31  | B     | 812 | CLA  | C2C-C1C-NC  | 3.75  | 113.49      | 109.97   |
| 36  | J     | 103 | LUT  | C3-C4-C5    | 3.75  | 119.33      | 111.85   |
| 36  | a     | 305 | LUT  | C39-C29-C28 | -3.75 | 112.17      | 118.08   |
| 31  | 4     | 312 | CLA  | C2D-C1D-ND  | 3.75  | 112.86      | 110.10   |
| 31  | B     | 824 | CLA  | CHA-C4D-ND  | 3.75  | 140.34      | 132.50   |
| 31  | 3     | 319 | CLA  | O1D-CGD-CBD | -3.74 | 116.82      | 124.48   |
| 31  | B     | 843 | CLA  | CMB-C2B-C3B | 3.74  | 131.68      | 124.68   |
| 31  | B     | 850 | CLA  | C4D-CHA-C1A | -3.74 | 116.69      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 312 | CLA  | C4D-CHA-C1A | -3.74 | 116.69      | 121.25   |
| 36  | 4     | 302 | LUT  | C7-C6-C5    | -3.74 | 112.39      | 121.46   |
| 31  | B     | 834 | CLA  | CHA-C4D-ND  | 3.74  | 140.33      | 132.50   |
| 31  | B     | 825 | CLA  | C4D-CHA-C1A | -3.74 | 116.69      | 121.25   |
| 36  | J     | 103 | LUT  | C8-C7-C6    | -3.74 | 116.69      | 127.20   |
| 31  | 7     | 310 | CLA  | CHA-C4D-ND  | 3.74  | 140.33      | 132.50   |
| 31  | 5     | 320 | CLA  | C1B-CHB-C4A | -3.74 | 122.71      | 130.12   |
| 31  | B     | 843 | CLA  | O1D-CGD-CBD | -3.74 | 116.83      | 124.48   |
| 31  | B     | 849 | CLA  | CMB-C2B-C3B | 3.74  | 131.67      | 124.68   |
| 31  | A     | 835 | CLA  | O2D-CGD-O1D | -3.74 | 116.53      | 123.84   |
| 31  | A     | 832 | CLA  | O2D-CGD-CBD | 3.74  | 117.91      | 111.27   |
| 31  | B     | 819 | CLA  | C4D-CHA-C1A | -3.74 | 116.70      | 121.25   |
| 31  | 8     | 314 | CLA  | O1D-CGD-CBD | -3.73 | 116.84      | 124.48   |
| 31  | B     | 847 | CLA  | C4D-CHA-C1A | -3.73 | 116.70      | 121.25   |
| 31  | 5     | 311 | CLA  | C4D-CHA-C1A | -3.73 | 116.70      | 121.25   |
| 31  | 2     | 311 | CLA  | C4D-CHA-C1A | -3.73 | 116.71      | 121.25   |
| 31  | 5     | 314 | CLA  | C4D-CHA-C1A | -3.73 | 116.71      | 121.25   |
| 31  | 8     | 311 | CLA  | O1D-CGD-CBD | -3.73 | 116.85      | 124.48   |
| 31  | A     | 838 | CLA  | C4D-CHA-C1A | -3.73 | 116.71      | 121.25   |
| 36  | 9     | 302 | LUT  | C8-C7-C6    | -3.73 | 116.72      | 127.20   |
| 31  | 7     | 314 | CLA  | CHD-C4C-C3C | -3.73 | 119.15      | 124.98   |
| 31  | B     | 827 | CLA  | C4D-CHA-C1A | -3.73 | 116.71      | 121.25   |
| 31  | 2     | 306 | CLA  | C4D-CHA-C1A | -3.73 | 116.71      | 121.25   |
| 31  | 7     | 312 | CLA  | C1C-C2C-C3C | -3.73 | 103.04      | 106.96   |
| 32  | 6     | 318 | CHL  | CGD-CBD-CAD | 3.73  | 122.80      | 110.73   |
| 31  | 5     | 312 | CLA  | CHA-C4D-ND  | 3.73  | 140.29      | 132.50   |
| 32  | 4     | 313 | CHL  | CHD-C1D-ND  | -3.72 | 121.03      | 124.45   |
| 31  | 9     | 321 | CLA  | C2D-C1D-ND  | 3.72  | 112.85      | 110.10   |
| 36  | a     | 303 | LUT  | C1-C6-C5    | -3.72 | 117.37      | 122.61   |
| 31  | B     | 837 | CLA  | O2D-CGD-O1D | -3.72 | 116.56      | 123.84   |
| 30  | A     | 813 | CL0  | C1-O2A-CGA  | 3.72  | 126.20      | 116.44   |
| 31  | O     | 202 | CLA  | CHA-C4D-ND  | 3.72  | 140.28      | 132.50   |
| 31  | B     | 834 | CLA  | C3D-C2D-C1D | -3.72 | 100.76      | 105.83   |
| 31  | b     | 302 | CLA  | CHA-C4D-ND  | 3.72  | 140.27      | 132.50   |
| 31  | 7     | 309 | CLA  | O2D-CGD-O1D | -3.72 | 116.57      | 123.84   |
| 31  | O     | 204 | CLA  | C2D-C1D-ND  | 3.72  | 112.84      | 110.10   |
| 31  | 5     | 311 | CLA  | O1D-CGD-CBD | -3.72 | 116.88      | 124.48   |
| 31  | G     | 204 | CLA  | CHA-C4D-ND  | 3.71  | 140.27      | 132.50   |
| 31  | 2     | 310 | CLA  | CHA-C4D-ND  | 3.71  | 140.27      | 132.50   |
| 36  | 4     | 302 | LUT  | C7-C8-C9    | -3.71 | 120.62      | 126.23   |
| 36  | a     | 303 | LUT  | C30-C31-C32 | -3.71 | 111.63      | 123.22   |
| 31  | K     | 205 | CLA  | CHD-C4C-C3C | -3.71 | 119.38      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 313 | CLA  | O1D-CGD-CBD | -3.71 | 116.89      | 124.48   |
| 32  | 6     | 309 | CHL  | CGD-CBD-CAD | 3.71  | 122.76      | 110.73   |
| 31  | a     | 321 | CLA  | CHA-C4D-ND  | 3.71  | 140.26      | 132.50   |
| 31  | F     | 306 | CLA  | CHD-C1D-ND  | -3.71 | 121.05      | 124.45   |
| 31  | 6     | 313 | CLA  | CHD-C1D-ND  | -3.71 | 121.05      | 124.45   |
| 31  | b     | 305 | CLA  | C4D-CHA-C1A | -3.71 | 116.73      | 121.25   |
| 31  | b     | 312 | CLA  | C4D-CHA-C1A | -3.71 | 116.74      | 121.25   |
| 31  | 2     | 306 | CLA  | C2D-C1D-ND  | 3.71  | 112.84      | 110.10   |
| 31  | A     | 848 | CLA  | O1D-CGD-CBD | -3.71 | 116.90      | 124.48   |
| 31  | A     | 830 | CLA  | CHD-C1D-ND  | -3.71 | 121.05      | 124.45   |
| 31  | F     | 306 | CLA  | CHA-C4D-ND  | 3.70  | 140.25      | 132.50   |
| 31  | 4     | 318 | CLA  | CHA-C4D-ND  | 3.70  | 140.25      | 132.50   |
| 36  | a     | 305 | LUT  | C20-C13-C12 | -3.70 | 112.24      | 118.08   |
| 31  | 2     | 304 | CLA  | O1D-CGD-CBD | -3.70 | 116.91      | 124.48   |
| 32  | 7     | 318 | CHL  | CHD-C1D-ND  | -3.70 | 121.05      | 124.45   |
| 32  | b     | 309 | CHL  | CHD-C4C-C3C | -3.70 | 119.40      | 124.84   |
| 31  | 9     | 319 | CLA  | CHD-C4C-C3C | -3.70 | 119.40      | 124.84   |
| 31  | B     | 818 | CLA  | C4D-CHA-C1A | -3.70 | 116.74      | 121.25   |
| 32  | 7     | 317 | CHL  | CHD-C1D-ND  | -3.70 | 121.06      | 124.45   |
| 32  | 8     | 316 | CHL  | CGD-CBD-CAD | 3.70  | 122.71      | 110.73   |
| 32  | 5     | 322 | CHL  | O2D-CGD-O1D | -3.70 | 116.61      | 123.84   |
| 32  | 4     | 317 | CHL  | CGD-CBD-CAD | 3.70  | 122.71      | 110.73   |
| 31  | 4     | 305 | CLA  | CMB-C2B-C3B | 3.69  | 131.59      | 124.68   |
| 32  | 4     | 317 | CHL  | C4D-CHA-C1A | -3.69 | 116.76      | 121.25   |
| 32  | 6     | 320 | CHL  | CGD-CBD-CAD | 3.69  | 122.69      | 110.73   |
| 31  | A     | 835 | CLA  | CHA-C4D-ND  | 3.69  | 140.22      | 132.50   |
| 31  | B     | 835 | CLA  | CHD-C4C-C3C | -3.69 | 119.42      | 124.84   |
| 31  | 7     | 312 | CLA  | C2C-C1C-NC  | 3.69  | 113.43      | 109.97   |
| 31  | 8     | 320 | CLA  | C2D-C1D-ND  | 3.69  | 112.82      | 110.10   |
| 32  | a     | 317 | CHL  | C1-C2-C3    | -3.69 | 119.67      | 126.04   |
| 31  | B     | 824 | CLA  | O1D-CGD-CBD | -3.69 | 116.94      | 124.48   |
| 31  | 3     | 310 | CLA  | CHD-C4C-NC  | 3.69  | 130.01      | 124.20   |
| 31  | 3     | 308 | CLA  | CHD-C1D-ND  | -3.69 | 121.07      | 124.45   |
| 31  | A     | 847 | CLA  | CHD-C4C-C3C | -3.69 | 119.42      | 124.84   |
| 36  | 9     | 303 | LUT  | C21-C26-C27 | -3.69 | 108.04      | 112.70   |
| 31  | A     | 852 | CLA  | C4-C3-C5    | 3.69  | 120.20      | 115.98   |
| 31  | 8     | 315 | CLA  | O2D-CGD-O1D | -3.68 | 116.63      | 123.84   |
| 32  | K     | 201 | CHL  | C1D-ND-C4D  | -3.68 | 103.72      | 106.33   |
| 31  | L     | 305 | CLA  | C4D-CHA-C1A | -3.68 | 116.77      | 121.25   |
| 31  | 2     | 314 | CLA  | C4D-CHA-C1A | -3.68 | 116.77      | 121.25   |
| 31  | H     | 901 | CLA  | C2D-C1D-ND  | 3.68  | 112.82      | 110.10   |
| 31  | 4     | 307 | CLA  | C2D-C1D-ND  | 3.68  | 112.82      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 319 | CLA  | C4D-CHA-C1A | -3.68 | 116.77      | 121.25   |
| 31  | 5     | 310 | CLA  | CHA-C4D-ND  | 3.68  | 140.20      | 132.50   |
| 31  | 5     | 313 | CLA  | C2C-C1C-NC  | 3.68  | 113.42      | 109.97   |
| 31  | a     | 309 | CLA  | C4D-CHA-C1A | -3.68 | 116.77      | 121.25   |
| 31  | A     | 830 | CLA  | C4-C3-C5    | 3.68  | 121.46      | 115.27   |
| 31  | 5     | 318 | CLA  | CHD-C4C-C3C | -3.68 | 119.43      | 124.84   |
| 36  | a     | 305 | LUT  | C18-C5-C4   | -3.68 | 107.54      | 114.36   |
| 31  | 4     | 318 | CLA  | CHD-C1D-ND  | -3.67 | 121.08      | 124.45   |
| 31  | 8     | 320 | CLA  | CHD-C4C-C3C | -3.67 | 119.44      | 124.84   |
| 31  | 7     | 314 | CLA  | C2D-C1D-ND  | 3.67  | 112.81      | 110.10   |
| 31  | 7     | 316 | CLA  | O1D-CGD-CBD | -3.67 | 116.97      | 124.48   |
| 31  | 2     | 307 | CLA  | CHA-C4D-ND  | 3.67  | 140.18      | 132.50   |
| 31  | 6     | 310 | CLA  | CHD-C1D-ND  | -3.67 | 121.08      | 124.45   |
| 31  | a     | 322 | CLA  | C2D-C1D-ND  | 3.67  | 112.81      | 110.10   |
| 31  | 5     | 321 | CLA  | C2D-C1D-ND  | 3.67  | 112.81      | 110.10   |
| 31  | 2     | 307 | CLA  | CHD-C4C-C3C | -3.67 | 119.45      | 124.84   |
| 36  | 5     | 303 | LUT  | C12-C13-C14 | -3.67 | 113.31      | 118.94   |
| 31  | b     | 305 | CLA  | O1D-CGD-CBD | -3.67 | 116.98      | 124.48   |
| 31  | B     | 830 | CLA  | C2D-C1D-ND  | 3.67  | 112.81      | 110.10   |
| 32  | A     | 840 | CHL  | C1C-C2C-C3C | -3.67 | 104.20      | 107.11   |
| 31  | 4     | 312 | CLA  | CHA-C4D-ND  | 3.67  | 140.17      | 132.50   |
| 31  | 5     | 320 | CLA  | O2D-CGD-O1D | -3.66 | 116.67      | 123.84   |
| 31  | 3     | 313 | CLA  | CHD-C4C-C3C | -3.66 | 119.46      | 124.84   |
| 32  | 5     | 322 | CHL  | CGD-CBD-CAD | 3.66  | 122.60      | 110.73   |
| 31  | b     | 302 | CLA  | CHD-C1D-ND  | -3.66 | 121.09      | 124.45   |
| 31  | 8     | 320 | CLA  | O2D-CGD-O1D | -3.66 | 116.68      | 123.84   |
| 31  | 3     | 320 | CLA  | CHA-C4D-ND  | 3.66  | 140.16      | 132.50   |
| 31  | B     | 841 | CLA  | CHD-C4C-NC  | 3.66  | 129.97      | 124.20   |
| 32  | 8     | 319 | CHL  | CGD-CBD-CAD | 3.66  | 122.59      | 110.73   |
| 31  | A     | 855 | CLA  | C4-C3-C5    | 3.66  | 121.42      | 115.27   |
| 31  | 6     | 313 | CLA  | C4D-CHA-C1A | -3.66 | 116.80      | 121.25   |
| 31  | A     | 819 | CLA  | CHA-C4D-ND  | 3.66  | 140.15      | 132.50   |
| 31  | a     | 309 | CLA  | CHA-C4D-ND  | 3.66  | 140.15      | 132.50   |
| 31  | b     | 303 | CLA  | CHA-C4D-ND  | 3.66  | 140.15      | 132.50   |
| 36  | 9     | 302 | LUT  | C10-C11-C12 | -3.65 | 111.81      | 123.22   |
| 31  | 8     | 314 | CLA  | CHD-C4C-C3C | -3.65 | 119.47      | 124.84   |
| 36  | 9     | 305 | LUT  | C4-C5-C6    | -3.65 | 112.70      | 120.85   |
| 31  | 7     | 315 | CLA  | CHD-C4C-C3C | -3.65 | 119.47      | 124.84   |
| 31  | B     | 835 | CLA  | C1-O2A-CGA  | 3.65  | 126.02      | 116.44   |
| 31  | B     | 811 | CLA  | C1C-C2C-C3C | -3.65 | 103.12      | 106.96   |
| 31  | 8     | 310 | CLA  | C1C-C2C-C3C | -3.65 | 103.12      | 106.96   |
| 31  | A     | 843 | CLA  | C2D-C1D-ND  | 3.65  | 112.79      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 849 | CLA  | O2D-CGD-O1D | -3.65 | 116.71      | 123.84   |
| 31  | 2     | 315 | CLA  | CHD-C1D-ND  | -3.65 | 121.10      | 124.45   |
| 31  | 9     | 316 | CLA  | O2D-CGD-CBD | 3.65  | 117.75      | 111.27   |
| 31  | 6     | 306 | CLA  | C2C-C1C-NC  | 3.65  | 113.39      | 109.97   |
| 31  | B     | 828 | CLA  | CHD-C4C-NC  | 3.65  | 129.95      | 124.20   |
| 31  | 7     | 314 | CLA  | CHD-C1D-ND  | -3.65 | 121.10      | 124.45   |
| 31  | A     | 830 | CLA  | CHA-C4D-ND  | 3.65  | 140.12      | 132.50   |
| 31  | a     | 310 | CLA  | CHA-C4D-ND  | 3.65  | 140.12      | 132.50   |
| 32  | 9     | 320 | CHL  | CGD-CBD-CAD | 3.65  | 122.54      | 110.73   |
| 36  | 5     | 304 | LUT  | C1-C6-C5    | -3.65 | 117.48      | 122.61   |
| 31  | 5     | 323 | CLA  | C4D-CHA-C1A | -3.65 | 116.81      | 121.25   |
| 32  | a     | 317 | CHL  | O2D-CGD-O1D | -3.64 | 116.71      | 123.84   |
| 31  | F     | 306 | CLA  | CHD-C4C-C3C | -3.64 | 119.48      | 124.84   |
| 32  | 5     | 317 | CHL  | CHD-C4C-NC  | 3.64  | 129.94      | 124.20   |
| 31  | 5     | 310 | CLA  | C4D-CHA-C1A | -3.64 | 116.82      | 121.25   |
| 31  | B     | 819 | CLA  | CHA-C4D-ND  | 3.64  | 140.12      | 132.50   |
| 31  | b     | 312 | CLA  | CHA-C4D-ND  | 3.64  | 140.11      | 132.50   |
| 31  | A     | 856 | CLA  | O2D-CGD-O1D | -3.64 | 116.72      | 123.84   |
| 30  | A     | 813 | CL0  | CMC-C2C-C1C | 3.64  | 130.58      | 125.04   |
| 31  | A     | 848 | CLA  | O2D-CGD-CBD | 3.64  | 117.73      | 111.27   |
| 31  | a     | 322 | CLA  | CHD-C4C-C3C | -3.64 | 119.49      | 124.84   |
| 32  | 8     | 316 | CHL  | O1D-CGD-CBD | -3.64 | 117.04      | 124.48   |
| 31  | A     | 832 | CLA  | C4D-CHA-C1A | -3.64 | 116.82      | 121.25   |
| 31  | F     | 301 | CLA  | CHA-C4D-ND  | 3.64  | 140.10      | 132.50   |
| 31  | B     | 830 | CLA  | CHA-C4D-ND  | 3.63  | 140.10      | 132.50   |
| 32  | A     | 839 | CHL  | C3D-C2D-C1D | -3.63 | 100.87      | 105.83   |
| 31  | H     | 902 | CLA  | CHA-C4D-ND  | 3.63  | 140.10      | 132.50   |
| 31  | a     | 312 | CLA  | O1D-CGD-CBD | -3.63 | 117.05      | 124.48   |
| 31  | 7     | 311 | CLA  | C4D-CHA-C1A | -3.63 | 116.83      | 121.25   |
| 31  | G     | 206 | CLA  | O2D-CGD-CBD | 3.63  | 117.72      | 111.27   |
| 31  | 5     | 314 | CLA  | O2D-CGD-O1D | -3.63 | 116.74      | 123.84   |
| 32  | A     | 839 | CHL  | C2D-C1D-ND  | 3.63  | 112.78      | 110.10   |
| 31  | 6     | 322 | CLA  | CHA-C4D-ND  | 3.63  | 140.09      | 132.50   |
| 31  | 9     | 321 | CLA  | CHA-C4D-ND  | 3.63  | 140.09      | 132.50   |
| 31  | B     | 827 | CLA  | O2D-CGD-O1D | -3.63 | 116.74      | 123.84   |
| 31  | A     | 823 | CLA  | CHD-C4C-C3C | -3.63 | 119.51      | 124.84   |
| 31  | 8     | 315 | CLA  | CHD-C4C-C3C | -3.63 | 119.51      | 124.84   |
| 31  | 4     | 311 | CLA  | CHD-C4C-C3C | -3.63 | 119.51      | 124.84   |
| 31  | B     | 839 | CLA  | C4D-CHA-C1A | -3.62 | 116.84      | 121.25   |
| 31  | B     | 841 | CLA  | C1C-C2C-C3C | -3.62 | 103.15      | 106.96   |
| 32  | a     | 317 | CHL  | CGD-CBD-CAD | 3.62  | 122.47      | 110.73   |
| 31  | A     | 850 | CLA  | CHA-C4D-ND  | 3.62  | 140.07      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 313 | CLA  | CHA-C4D-ND  | 3.62  | 140.07      | 132.50   |
| 31  | B     | 837 | CLA  | CHA-C4D-ND  | 3.62  | 140.07      | 132.50   |
| 31  | A     | 819 | CLA  | CHD-C1D-ND  | -3.62 | 121.13      | 124.45   |
| 31  | B     | 826 | CLA  | C1-C2-C3    | -3.62 | 120.90      | 126.75   |
| 31  | A     | 851 | CLA  | CHA-C4D-ND  | 3.62  | 140.07      | 132.50   |
| 31  | 3     | 316 | CLA  | CHA-C4D-ND  | 3.62  | 140.07      | 132.50   |
| 36  | J     | 103 | LUT  | C2-C3-C4    | 3.62  | 115.26      | 110.30   |
| 31  | K     | 206 | CLA  | O1D-CGD-CBD | -3.62 | 117.08      | 124.48   |
| 31  | A     | 815 | CLA  | CMB-C2B-C3B | 3.62  | 131.44      | 124.68   |
| 31  | b     | 302 | CLA  | C4D-CHA-C1A | -3.62 | 116.85      | 121.25   |
| 31  | 7     | 315 | CLA  | CHD-C1D-ND  | -3.61 | 121.13      | 124.45   |
| 31  | b     | 313 | CLA  | O1D-CGD-CBD | -3.61 | 117.09      | 124.48   |
| 32  | 7     | 318 | CHL  | O2A-CGA-CBA | 3.61  | 123.24      | 111.91   |
| 36  | 3     | 304 | LUT  | C16-C1-C6   | -3.61 | 104.44      | 110.30   |
| 31  | 9     | 311 | CLA  | CHD-C4C-C3C | -3.61 | 119.53      | 124.84   |
| 31  | a     | 309 | CLA  | CHD-C1D-ND  | -3.61 | 121.14      | 124.45   |
| 31  | 6     | 316 | CLA  | O2D-CGD-O1D | -3.61 | 116.78      | 123.84   |
| 31  | O     | 204 | CLA  | CHD-C4C-C3C | -3.61 | 119.54      | 124.84   |
| 31  | A     | 845 | CLA  | CHA-C4D-ND  | 3.61  | 140.05      | 132.50   |
| 31  | O     | 203 | CLA  | CHA-C4D-ND  | 3.61  | 140.04      | 132.50   |
| 31  | 2     | 310 | CLA  | CHD-C1D-ND  | -3.61 | 121.14      | 124.45   |
| 32  | 6     | 309 | CHL  | CHD-C1D-ND  | -3.60 | 121.14      | 124.45   |
| 36  | 5     | 304 | LUT  | C10-C11-C12 | -3.60 | 111.97      | 123.22   |
| 31  | A     | 818 | CLA  | CAC-C3C-C4C | 3.60  | 129.48      | 124.81   |
| 31  | 7     | 310 | CLA  | CHD-C4C-C3C | -3.60 | 119.35      | 124.98   |
| 31  | 5     | 321 | CLA  | CHA-C4D-ND  | 3.60  | 140.03      | 132.50   |
| 32  | 6     | 319 | CHL  | O2D-CGD-O1D | -3.60 | 116.80      | 123.84   |
| 31  | 8     | 307 | CLA  | O2D-CGD-O1D | -3.60 | 116.80      | 123.84   |
| 30  | A     | 813 | CL0  | C4D-CHA-C1A | -3.60 | 116.87      | 121.25   |
| 31  | 3     | 307 | CLA  | CHA-C4D-ND  | 3.60  | 140.03      | 132.50   |
| 31  | A     | 836 | CLA  | CHA-C4D-ND  | 3.60  | 140.03      | 132.50   |
| 31  | 8     | 309 | CLA  | CHD-C1D-ND  | -3.60 | 121.15      | 124.45   |
| 31  | A     | 822 | CLA  | CHA-C4D-ND  | 3.60  | 140.02      | 132.50   |
| 31  | F     | 301 | CLA  | CHD-C1D-ND  | -3.60 | 121.15      | 124.45   |
| 31  | A     | 852 | CLA  | CHA-C4D-ND  | 3.60  | 140.02      | 132.50   |
| 31  | 9     | 313 | CLA  | CHA-C4D-ND  | 3.60  | 140.02      | 132.50   |
| 31  | a     | 312 | CLA  | C4D-CHA-C1A | -3.59 | 116.87      | 121.25   |
| 31  | 5     | 309 | CLA  | CHD-C1D-ND  | -3.59 | 121.15      | 124.45   |
| 31  | 3     | 314 | CLA  | O2D-CGD-CBD | 3.59  | 117.65      | 111.27   |
| 31  | B     | 845 | CLA  | O2D-CGD-O1D | -3.59 | 116.81      | 123.84   |
| 31  | A     | 841 | CLA  | CHD-C4C-C3C | -3.59 | 119.56      | 124.84   |
| 31  | H     | 901 | CLA  | CHD-C4C-C3C | -3.59 | 119.56      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 849 | CLA  | CHA-C4D-ND  | 3.59  | 140.01      | 132.50   |
| 36  | 4     | 303 | LUT  | C12-C13-C14 | -3.59 | 113.43      | 118.94   |
| 31  | B     | 820 | CLA  | C4D-CHA-C1A | -3.59 | 116.88      | 121.25   |
| 36  | 9     | 305 | LUT  | C8-C7-C6    | -3.59 | 117.12      | 127.20   |
| 31  | 4     | 321 | CLA  | O1D-CGD-CBD | -3.59 | 117.14      | 124.48   |
| 31  | b     | 307 | CLA  | CHA-C4D-ND  | 3.59  | 140.00      | 132.50   |
| 31  | B     | 815 | CLA  | C4D-CHA-C1A | -3.58 | 116.89      | 121.25   |
| 31  | B     | 829 | CLA  | CHA-C4D-ND  | 3.58  | 140.00      | 132.50   |
| 31  | B     | 826 | CLA  | CHD-C4C-NC  | 3.58  | 129.85      | 124.20   |
| 31  | 8     | 311 | CLA  | O2A-CGA-CBA | 3.58  | 123.15      | 111.91   |
| 32  | A     | 840 | CHL  | C3D-C2D-C1D | -3.58 | 100.94      | 105.83   |
| 31  | 9     | 318 | CLA  | CHA-C4D-ND  | 3.58  | 139.99      | 132.50   |
| 31  | b     | 311 | CLA  | C4D-CHA-C1A | -3.58 | 116.89      | 121.25   |
| 32  | b     | 309 | CHL  | CHD-C1D-ND  | -3.58 | 121.17      | 124.45   |
| 31  | b     | 313 | CLA  | C1C-C2C-C3C | -3.58 | 103.20      | 106.96   |
| 31  | B     | 843 | CLA  | CHD-C4C-C3C | -3.58 | 119.58      | 124.84   |
| 31  | B     | 812 | CLA  | CHD-C4C-C3C | -3.58 | 119.58      | 124.84   |
| 31  | 7     | 313 | CLA  | CHA-C4D-ND  | 3.58  | 139.98      | 132.50   |
| 31  | 7     | 316 | CLA  | CHA-C4D-ND  | 3.57  | 139.98      | 132.50   |
| 36  | 5     | 303 | LUT  | C30-C31-C32 | -3.57 | 112.07      | 123.22   |
| 31  | 9     | 311 | CLA  | C4D-CHA-C1A | -3.57 | 116.90      | 121.25   |
| 31  | 6     | 313 | CLA  | O2D-CGD-O1D | -3.57 | 116.86      | 123.84   |
| 32  | 6     | 318 | CHL  | CHD-C4C-C3C | -3.57 | 119.59      | 124.84   |
| 31  | 8     | 315 | CLA  | CHA-C4D-ND  | 3.57  | 139.97      | 132.50   |
| 31  | A     | 853 | CLA  | C4D-CHA-C1A | -3.57 | 116.91      | 121.25   |
| 31  | 3     | 308 | CLA  | CHA-C4D-ND  | 3.57  | 139.96      | 132.50   |
| 32  | A     | 831 | CHL  | CHD-C1D-ND  | -3.57 | 121.18      | 124.45   |
| 31  | b     | 313 | CLA  | CHD-C1D-ND  | -3.57 | 121.18      | 124.45   |
| 32  | 5     | 316 | CHL  | C1C-C2C-C3C | -3.57 | 104.28      | 107.11   |
| 31  | 2     | 306 | CLA  | CAA-C2A-C3A | -3.57 | 103.02      | 112.78   |
| 31  | 8     | 308 | CLA  | CMB-C2B-C3B | 3.56  | 131.34      | 124.68   |
| 31  | A     | 824 | CLA  | C4D-CHA-C1A | -3.56 | 116.91      | 121.25   |
| 31  | 9     | 316 | CLA  | O2D-CGD-O1D | -3.56 | 116.87      | 123.84   |
| 31  | A     | 852 | CLA  | O2D-CGD-CBD | 3.56  | 117.60      | 111.27   |
| 32  | 4     | 317 | CHL  | CHC-C1C-NC  | -3.56 | 118.80      | 124.20   |
| 31  | b     | 310 | CLA  | CHA-C4D-ND  | 3.56  | 139.95      | 132.50   |
| 31  | B     | 838 | CLA  | C2D-C1D-ND  | 3.56  | 112.73      | 110.10   |
| 31  | A     | 819 | CLA  | C4D-CHA-C1A | -3.56 | 116.92      | 121.25   |
| 31  | 7     | 321 | CLA  | C4D-CHA-C1A | -3.56 | 116.92      | 121.25   |
| 31  | B     | 827 | CLA  | CHD-C4C-NC  | 3.56  | 129.81      | 124.20   |
| 31  | B     | 813 | CLA  | O1D-CGD-CBD | -3.55 | 117.21      | 124.48   |
| 32  | A     | 831 | CHL  | C1-C2-C3    | -3.55 | 119.90      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 311 | CLA  | CHA-C4D-ND  | 3.55  | 139.93      | 132.50   |
| 31  | 9     | 316 | CLA  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |
| 31  | B     | 838 | CLA  | CHA-C4D-ND  | 3.55  | 139.93      | 132.50   |
| 31  | B     | 840 | CLA  | O2A-CGA-CBA | 3.55  | 123.04      | 111.91   |
| 31  | 4     | 309 | CLA  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |
| 31  | A     | 827 | CLA  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |
| 31  | K     | 205 | CLA  | C4D-CHA-C1A | -3.55 | 116.93      | 121.25   |
| 31  | 4     | 320 | CLA  | O2D-CGD-O1D | -3.54 | 116.91      | 123.84   |
| 31  | A     | 826 | CLA  | C4D-CHA-C1A | -3.54 | 116.94      | 121.25   |
| 31  | B     | 818 | CLA  | O2D-CGD-CBD | 3.54  | 117.56      | 111.27   |
| 32  | 7     | 317 | CHL  | CGD-CBD-CAD | 3.54  | 122.21      | 110.73   |
| 36  | J     | 103 | LUT  | C28-C29-C30 | -3.54 | 113.51      | 118.94   |
| 31  | O     | 204 | CLA  | CHA-C4D-ND  | 3.54  | 139.90      | 132.50   |
| 33  | 7     | 308 | DGD  | O6D-C1D-O3G | -3.54 | 101.59      | 109.97   |
| 31  | 3     | 309 | CLA  | C4D-CHA-C1A | -3.54 | 116.94      | 121.25   |
| 31  | 5     | 309 | CLA  | CHA-C4D-ND  | 3.54  | 139.90      | 132.50   |
| 31  | 5     | 315 | CLA  | CHA-C4D-ND  | 3.54  | 139.90      | 132.50   |
| 31  | A     | 824 | CLA  | CHA-C4D-ND  | 3.54  | 139.90      | 132.50   |
| 31  | 4     | 314 | CLA  | CHA-C4D-ND  | 3.54  | 139.90      | 132.50   |
| 31  | A     | 817 | CLA  | C4D-CHA-C1A | -3.54 | 116.95      | 121.25   |
| 31  | B     | 814 | CLA  | C4D-CHA-C1A | -3.54 | 116.95      | 121.25   |
| 31  | 4     | 318 | CLA  | CAC-C3C-C4C | 3.54  | 129.40      | 124.81   |
| 31  | 9     | 318 | CLA  | CHD-C4C-C3C | -3.53 | 119.64      | 124.84   |
| 36  | 4     | 303 | LUT  | C21-C26-C27 | -3.53 | 108.23      | 112.70   |
| 31  | 9     | 315 | CLA  | CHD-C1D-ND  | -3.53 | 121.21      | 124.45   |
| 32  | 6     | 321 | CHL  | CHD-C4C-C3C | -3.53 | 119.65      | 124.84   |
| 32  | 4     | 310 | CHL  | CGD-CBD-CAD | 3.53  | 122.17      | 110.73   |
| 31  | 6     | 315 | CLA  | O2D-CGD-O1D | -3.53 | 116.94      | 123.84   |
| 36  | 7     | 305 | LUT  | C2-C3-C4    | 3.53  | 115.14      | 110.30   |
| 31  | 8     | 311 | CLA  | CHA-C4D-ND  | 3.53  | 139.88      | 132.50   |
| 32  | 7     | 324 | CHL  | CGD-CBD-CAD | 3.53  | 122.17      | 110.73   |
| 31  | 2     | 313 | CLA  | CHA-C4D-ND  | 3.53  | 139.88      | 132.50   |
| 31  | A     | 854 | CLA  | CAC-C3C-C4C | 3.53  | 129.39      | 124.81   |
| 31  | 9     | 317 | CLA  | C3D-C2D-C1D | -3.53 | 101.02      | 105.83   |
| 32  | 5     | 319 | CHL  | CHD-C4C-C3C | -3.53 | 119.66      | 124.84   |
| 26  | O     | 201 | BCR  | C2-C1-C6    | 3.53  | 115.91      | 110.48   |
| 31  | F     | 301 | CLA  | CHD-C4C-C3C | -3.53 | 119.66      | 124.84   |
| 31  | b     | 306 | CLA  | CHA-C4D-ND  | 3.53  | 139.87      | 132.50   |
| 31  | B     | 832 | CLA  | CHA-C4D-ND  | 3.52  | 139.87      | 132.50   |
| 31  | 7     | 315 | CLA  | CHA-C4D-ND  | 3.52  | 139.87      | 132.50   |
| 32  | 8     | 319 | CHL  | CHD-C1D-ND  | -3.52 | 121.22      | 124.45   |
| 31  | 6     | 307 | CLA  | CHA-C4D-ND  | 3.52  | 139.87      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 307 | CLA  | C4D-CHA-C1A | -3.52 | 116.96      | 121.25   |
| 31  | A     | 851 | CLA  | CHD-C4C-C3C | -3.52 | 119.66      | 124.84   |
| 31  | A     | 855 | CLA  | CHD-C1D-ND  | -3.52 | 121.22      | 124.45   |
| 31  | B     | 820 | CLA  | CHA-C4D-ND  | 3.52  | 139.87      | 132.50   |
| 32  | 7     | 319 | CHL  | CHD-C4C-NC  | 3.52  | 129.75      | 124.20   |
| 36  | 2     | 301 | LUT  | C21-C26-C27 | -3.52 | 108.25      | 112.70   |
| 31  | A     | 819 | CLA  | O2D-CGD-O1D | -3.52 | 116.96      | 123.84   |
| 31  | 6     | 308 | CLA  | O1D-CGD-CBD | -3.52 | 117.29      | 124.48   |
| 31  | a     | 313 | CLA  | CHA-C4D-ND  | 3.52  | 139.86      | 132.50   |
| 31  | B     | 841 | CLA  | C1-C2-C3    | -3.52 | 119.96      | 126.04   |
| 31  | 4     | 311 | CLA  | CHA-C4D-ND  | 3.52  | 139.85      | 132.50   |
| 31  | B     | 815 | CLA  | O1D-CGD-CBD | -3.52 | 117.29      | 124.48   |
| 31  | B     | 822 | CLA  | CHA-C4D-ND  | 3.52  | 139.85      | 132.50   |
| 32  | K     | 201 | CHL  | C3D-C4D-ND  | 3.51  | 115.92      | 110.24   |
| 31  | B     | 818 | CLA  | O2D-CGD-O1D | -3.51 | 116.97      | 123.84   |
| 31  | 8     | 309 | CLA  | O2D-CGD-O1D | -3.51 | 116.97      | 123.84   |
| 31  | 5     | 323 | CLA  | O1D-CGD-CBD | -3.51 | 117.30      | 124.48   |
| 36  | 9     | 305 | LUT  | C10-C11-C12 | -3.51 | 112.26      | 123.22   |
| 31  | A     | 836 | CLA  | CHD-C4C-NC  | 3.51  | 129.73      | 124.20   |
| 31  | 5     | 321 | CLA  | CHD-C4C-C3C | -3.51 | 119.69      | 124.84   |
| 32  | 8     | 316 | CHL  | CHD-C4C-NC  | 3.51  | 129.73      | 124.20   |
| 26  | B     | 805 | BCR  | C15-C16-C17 | -3.51 | 116.29      | 123.47   |
| 32  | 6     | 320 | CHL  | CHD-C4C-NC  | 3.51  | 129.73      | 124.20   |
| 31  | 6     | 312 | CLA  | CHA-C4D-ND  | 3.51  | 139.83      | 132.50   |
| 31  | 6     | 314 | CLA  | CHA-C4D-ND  | 3.50  | 139.83      | 132.50   |
| 31  | 3     | 312 | CLA  | CHD-C4C-C3C | -3.50 | 119.69      | 124.84   |
| 31  | 4     | 307 | CLA  | CHD-C4C-C3C | -3.50 | 119.69      | 124.84   |
| 31  | B     | 819 | CLA  | O2D-CGD-CBD | 3.50  | 117.49      | 111.27   |
| 31  | H     | 901 | CLA  | C4D-CHA-C1A | -3.50 | 116.99      | 121.25   |
| 31  | 3     | 316 | CLA  | C4D-CHA-C1A | -3.50 | 116.99      | 121.25   |
| 31  | 2     | 306 | CLA  | C4-C3-C5    | 3.50  | 121.15      | 115.27   |
| 31  | 6     | 315 | CLA  | CHA-C4D-ND  | 3.49  | 139.81      | 132.50   |
| 31  | 7     | 312 | CLA  | CHA-C4D-ND  | 3.49  | 139.81      | 132.50   |
| 31  | 8     | 312 | CLA  | CHA-C4D-ND  | 3.49  | 139.81      | 132.50   |
| 31  | B     | 846 | CLA  | CHA-C4D-ND  | 3.49  | 139.81      | 132.50   |
| 31  | a     | 316 | CLA  | CHA-C4D-ND  | 3.49  | 139.81      | 132.50   |
| 31  | 2     | 306 | CLA  | CHA-C4D-ND  | 3.49  | 139.80      | 132.50   |
| 31  | 5     | 308 | CLA  | CHA-C4D-ND  | 3.49  | 139.80      | 132.50   |
| 31  | a     | 322 | CLA  | CHA-C4D-ND  | 3.49  | 139.80      | 132.50   |
| 31  | b     | 311 | CLA  | CHA-C4D-ND  | 3.49  | 139.80      | 132.50   |
| 31  | 8     | 321 | CLA  | O2D-CGD-O1D | -3.49 | 117.01      | 123.84   |
| 31  | 3     | 312 | CLA  | C2D-C1D-ND  | 3.49  | 112.68      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | H     | 901 | CLA  | CHA-C4D-ND  | 3.49  | 139.80      | 132.50   |
| 31  | B     | 833 | CLA  | C4D-CHA-C1A | -3.49 | 117.00      | 121.25   |
| 31  | B     | 850 | CLA  | CHA-C4D-ND  | 3.49  | 139.79      | 132.50   |
| 31  | 4     | 307 | CLA  | CHA-C4D-ND  | 3.49  | 139.79      | 132.50   |
| 36  | 8     | 303 | LUT  | C16-C1-C6   | -3.49 | 104.64      | 110.30   |
| 31  | A     | 820 | CLA  | CHA-C4D-ND  | 3.49  | 139.79      | 132.50   |
| 32  | 6     | 318 | CHL  | CHD-C1D-ND  | -3.49 | 121.25      | 124.45   |
| 31  | 3     | 318 | CLA  | CHA-C4D-ND  | 3.48  | 139.79      | 132.50   |
| 31  | b     | 308 | CLA  | O2D-CGD-O1D | -3.48 | 117.03      | 123.84   |
| 31  | 7     | 314 | CLA  | CHA-C4D-ND  | 3.48  | 139.79      | 132.50   |
| 31  | 7     | 321 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 31  | F     | 305 | CLA  | O1D-CGD-CBD | -3.48 | 117.36      | 124.48   |
| 31  | 5     | 309 | CLA  | CHD-C4C-C3C | -3.48 | 119.72      | 124.84   |
| 31  | b     | 305 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 31  | B     | 836 | CLA  | CMB-C2B-C3B | 3.48  | 131.19      | 124.68   |
| 31  | 7     | 312 | CLA  | C4D-CHA-C1A | -3.48 | 117.01      | 121.25   |
| 31  | 5     | 320 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 31  | A     | 847 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 31  | A     | 836 | CLA  | C4-C3-C5    | 3.48  | 121.12      | 115.27   |
| 31  | A     | 848 | CLA  | C4-C3-C5    | 3.48  | 121.12      | 115.27   |
| 31  | B     | 835 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 31  | B     | 844 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 31  | 9     | 321 | CLA  | O1D-CGD-CBD | -3.48 | 117.37      | 124.48   |
| 31  | F     | 305 | CLA  | CHA-C4D-ND  | 3.48  | 139.78      | 132.50   |
| 32  | 5     | 319 | CHL  | O2D-CGD-O1D | -3.48 | 117.04      | 123.84   |
| 31  | A     | 855 | CLA  | C4D-CHA-C1A | -3.48 | 117.02      | 121.25   |
| 31  | 3     | 317 | CLA  | CHA-C4D-ND  | 3.47  | 139.77      | 132.50   |
| 31  | 4     | 319 | CLA  | CHA-C4D-ND  | 3.47  | 139.77      | 132.50   |
| 31  | 4     | 321 | CLA  | CHA-C4D-ND  | 3.47  | 139.77      | 132.50   |
| 31  | A     | 825 | CLA  | CHD-C4C-NC  | 3.47  | 129.68      | 124.20   |
| 31  | B     | 836 | CLA  | C4D-CHA-C1A | -3.47 | 117.02      | 121.25   |
| 31  | O     | 204 | CLA  | O2D-CGD-O1D | -3.47 | 117.05      | 123.84   |
| 31  | 4     | 318 | CLA  | CHD-C4C-C3C | -3.47 | 119.74      | 124.84   |
| 31  | 4     | 308 | CLA  | CHA-C4D-ND  | 3.47  | 139.76      | 132.50   |
| 31  | B     | 834 | CLA  | O2D-CGD-CBD | 3.47  | 117.43      | 111.27   |
| 31  | a     | 319 | CLA  | O2D-CGD-O1D | -3.47 | 117.06      | 123.84   |
| 31  | B     | 846 | CLA  | CHD-C1D-ND  | -3.47 | 121.27      | 124.45   |
| 31  | 6     | 316 | CLA  | CHD-C4C-NC  | 3.47  | 129.66      | 124.20   |
| 32  | A     | 840 | CHL  | C4D-C3D-CAD | 3.46  | 112.18      | 108.10   |
| 32  | 6     | 321 | CHL  | CHD-C1D-ND  | -3.46 | 121.27      | 124.45   |
| 31  | H     | 903 | CLA  | C2D-C1D-ND  | 3.46  | 112.65      | 110.10   |
| 31  | A     | 825 | CLA  | O2D-CGD-O1D | -3.46 | 117.07      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 815 | CLA  | O2D-CGD-CBD | 3.46  | 117.42      | 111.27   |
| 31  | 5     | 314 | CLA  | CHD-C4C-NC  | 3.46  | 129.65      | 124.20   |
| 36  | 6     | 303 | LUT  | C18-C5-C4   | -3.46 | 107.95      | 114.36   |
| 31  | a     | 311 | CLA  | CHA-C4D-ND  | 3.46  | 139.73      | 132.50   |
| 31  | 4     | 315 | CLA  | CHD-C4C-C3C | -3.46 | 119.76      | 124.84   |
| 31  | G     | 205 | CLA  | CHD-C4C-NC  | 3.46  | 129.65      | 124.20   |
| 31  | 4     | 305 | CLA  | O1D-CGD-CBD | -3.46 | 117.41      | 124.48   |
| 31  | K     | 205 | CLA  | CHA-C4D-ND  | 3.46  | 139.73      | 132.50   |
| 31  | 9     | 311 | CLA  | CHA-C4D-ND  | 3.46  | 139.73      | 132.50   |
| 32  | A     | 831 | CHL  | C4D-C3D-CAD | 3.45  | 112.17      | 108.10   |
| 31  | F     | 301 | CLA  | CAC-C3C-C4C | 3.45  | 129.29      | 124.81   |
| 31  | A     | 844 | CLA  | CHA-C4D-ND  | 3.45  | 139.72      | 132.50   |
| 36  | 9     | 305 | LUT  | C1-C6-C5    | -3.45 | 117.75      | 122.61   |
| 31  | 8     | 313 | CLA  | CHA-C4D-ND  | 3.45  | 139.72      | 132.50   |
| 31  | 2     | 308 | CLA  | CHA-C4D-ND  | 3.45  | 139.72      | 132.50   |
| 31  | A     | 845 | CLA  | O2D-CGD-O1D | -3.45 | 117.09      | 123.84   |
| 36  | L     | 304 | LUT  | C7-C8-C9    | -3.45 | 121.02      | 126.23   |
| 31  | A     | 823 | CLA  | CHA-C4D-ND  | 3.45  | 139.71      | 132.50   |
| 32  | 6     | 309 | CHL  | CHD-C4C-C3C | -3.45 | 119.77      | 124.84   |
| 32  | A     | 840 | CHL  | C1-C2-C3    | -3.45 | 120.08      | 126.04   |
| 32  | 6     | 317 | CHL  | CHD-C4C-NC  | 3.45  | 129.63      | 124.20   |
| 31  | A     | 828 | CLA  | O2D-CGD-O1D | -3.44 | 117.10      | 123.84   |
| 36  | 3     | 304 | LUT  | C2-C3-C4    | 3.44  | 115.02      | 110.30   |
| 31  | 9     | 312 | CLA  | CHA-C4D-ND  | 3.44  | 139.70      | 132.50   |
| 31  | b     | 306 | CLA  | O2D-CGD-O1D | -3.44 | 117.11      | 123.84   |
| 31  | A     | 814 | CLA  | C4D-CHA-C1A | -3.44 | 117.06      | 121.25   |
| 31  | A     | 828 | CLA  | CHA-C4D-ND  | 3.44  | 139.70      | 132.50   |
| 31  | A     | 834 | CLA  | CHD-C4C-NC  | 3.44  | 129.62      | 124.20   |
| 31  | 3     | 314 | CLA  | C4-C3-C5    | 3.44  | 121.06      | 115.27   |
| 31  | B     | 815 | CLA  | C3D-C2D-C1D | -3.44 | 101.14      | 105.83   |
| 31  | 6     | 311 | CLA  | CHA-C4D-ND  | 3.44  | 139.70      | 132.50   |
| 36  | 9     | 302 | LUT  | C7-C6-C5    | -3.44 | 113.13      | 121.46   |
| 31  | 5     | 323 | CLA  | CHA-C4D-ND  | 3.44  | 139.69      | 132.50   |
| 31  | A     | 838 | CLA  | CHA-C4D-ND  | 3.44  | 139.69      | 132.50   |
| 31  | 8     | 315 | CLA  | C4D-CHA-C1A | -3.44 | 117.07      | 121.25   |
| 31  | A     | 818 | CLA  | C2C-C1C-NC  | 3.44  | 113.19      | 109.97   |
| 31  | B     | 832 | CLA  | O1D-CGD-CBD | -3.44 | 117.45      | 124.48   |
| 32  | 5     | 322 | CHL  | CHD-C1D-ND  | -3.44 | 121.30      | 124.45   |
| 31  | H     | 903 | CLA  | CHA-C4D-ND  | 3.43  | 139.69      | 132.50   |
| 31  | 4     | 309 | CLA  | O2D-CGD-O1D | -3.43 | 117.12      | 123.84   |
| 31  | B     | 817 | CLA  | CHB-C4A-NA  | 3.43  | 129.26      | 124.51   |
| 31  | 4     | 307 | CLA  | O2D-CGD-O1D | -3.43 | 117.12      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 843 | CLA  | CHD-C1D-ND  | -3.43 | 121.30      | 124.45   |
| 31  | H     | 903 | CLA  | CHD-C1D-ND  | -3.43 | 121.30      | 124.45   |
| 31  | 7     | 310 | CLA  | C4D-CHA-C1A | -3.43 | 117.07      | 121.25   |
| 31  | 8     | 314 | CLA  | CHA-C4D-ND  | 3.43  | 139.67      | 132.50   |
| 31  | 6     | 308 | CLA  | CHA-C4D-ND  | 3.43  | 139.67      | 132.50   |
| 31  | 8     | 307 | CLA  | CHA-C4D-ND  | 3.43  | 139.67      | 132.50   |
| 31  | B     | 817 | CLA  | CHD-C4C-NC  | 3.43  | 129.60      | 124.20   |
| 31  | 9     | 321 | CLA  | CHD-C4C-C3C | -3.43 | 119.80      | 124.84   |
| 32  | A     | 839 | CHL  | CHD-C4C-NC  | 3.43  | 129.60      | 124.20   |
| 36  | 6     | 303 | LUT  | C30-C31-C32 | -3.43 | 112.52      | 123.22   |
| 31  | B     | 837 | CLA  | C2D-C1D-ND  | 3.43  | 112.63      | 110.10   |
| 31  | 3     | 312 | CLA  | CHA-C4D-ND  | 3.43  | 139.67      | 132.50   |
| 32  | 5     | 322 | CHL  | CHD-C4C-C3C | -3.43 | 119.81      | 124.84   |
| 36  | 6     | 304 | LUT  | C18-C5-C4   | -3.43 | 108.01      | 114.36   |
| 31  | 6     | 306 | CLA  | CMB-C2B-C3B | 3.42  | 131.08      | 124.68   |
| 31  | 8     | 310 | CLA  | C4D-CHA-C1A | -3.42 | 117.08      | 121.25   |
| 31  | L     | 306 | CLA  | C4D-CHA-C1A | -3.42 | 117.08      | 121.25   |
| 31  | 2     | 311 | CLA  | CHA-C4D-ND  | 3.42  | 139.66      | 132.50   |
| 31  | A     | 857 | CLA  | CHD-C4C-NC  | 3.42  | 129.60      | 124.20   |
| 31  | 2     | 309 | CLA  | CHA-C4D-ND  | 3.42  | 139.66      | 132.50   |
| 32  | A     | 839 | CHL  | C1C-C2C-C3C | -3.42 | 104.40      | 107.11   |
| 31  | A     | 821 | CLA  | O2D-CGD-O1D | -3.42 | 117.15      | 123.84   |
| 31  | A     | 837 | CLA  | CHA-C4D-ND  | 3.42  | 139.66      | 132.50   |
| 31  | A     | 832 | CLA  | CHD-C4C-NC  | 3.42  | 129.59      | 124.20   |
| 36  | 8     | 302 | LUT  | C7-C6-C5    | -3.42 | 113.18      | 121.46   |
| 31  | A     | 842 | CLA  | C4D-CHA-C1A | -3.42 | 117.09      | 121.25   |
| 31  | A     | 830 | CLA  | O2D-CGD-CBD | 3.42  | 117.34      | 111.27   |
| 31  | b     | 303 | CLA  | O2D-CGD-O1D | -3.42 | 117.16      | 123.84   |
| 31  | 6     | 311 | CLA  | CHD-C4C-C3C | -3.42 | 119.82      | 124.84   |
| 31  | A     | 833 | CLA  | CHD-C1D-ND  | -3.42 | 121.31      | 124.45   |
| 32  | A     | 840 | CHL  | OBD-CAD-C3D | 3.42  | 136.75      | 128.52   |
| 31  | 5     | 318 | CLA  | CHA-C4D-ND  | 3.42  | 139.65      | 132.50   |
| 31  | A     | 834 | CLA  | O2D-CGD-CBD | 3.42  | 117.34      | 111.27   |
| 31  | A     | 830 | CLA  | O1D-CGD-CBD | -3.42 | 117.49      | 124.48   |
| 31  | b     | 303 | CLA  | C2D-C1D-ND  | 3.42  | 112.62      | 110.10   |
| 31  | 5     | 314 | CLA  | CHA-C4D-ND  | 3.42  | 139.65      | 132.50   |
| 31  | a     | 310 | CLA  | C4D-CHA-C1A | -3.41 | 117.09      | 121.25   |
| 31  | G     | 204 | CLA  | C4D-CHA-C1A | -3.41 | 117.09      | 121.25   |
| 31  | B     | 823 | CLA  | CHA-C4D-ND  | 3.41  | 139.64      | 132.50   |
| 31  | 2     | 314 | CLA  | CHA-C4D-ND  | 3.41  | 139.64      | 132.50   |
| 31  | 8     | 317 | CLA  | C1-C2-C3    | -3.41 | 121.23      | 126.75   |
| 36  | 5     | 303 | LUT  | C7-C6-C5    | -3.41 | 113.19      | 121.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 836 | CLA  | CHA-C4D-ND  | 3.41  | 139.64      | 132.50   |
| 31  | B     | 825 | CLA  | CAC-C3C-C4C | 3.41  | 129.24      | 124.81   |
| 31  | a     | 312 | CLA  | CHA-C4D-ND  | 3.41  | 139.63      | 132.50   |
| 31  | a     | 312 | CLA  | CHD-C4C-NC  | 3.41  | 129.58      | 124.20   |
| 31  | A     | 849 | CLA  | CHA-C4D-ND  | 3.41  | 139.63      | 132.50   |
| 31  | 4     | 307 | CLA  | C4D-CHA-C1A | -3.41 | 117.10      | 121.25   |
| 31  | J     | 105 | CLA  | CHD-C4C-NC  | 3.41  | 129.57      | 124.20   |
| 31  | 3     | 309 | CLA  | O2D-CGD-O1D | -3.41 | 117.17      | 123.84   |
| 31  | A     | 845 | CLA  | CMB-C2B-C3B | 3.41  | 131.06      | 124.68   |
| 31  | a     | 315 | CLA  | O2D-CGD-CBD | 3.41  | 117.33      | 111.27   |
| 26  | 3     | 301 | BCR  | C2-C1-C6    | 3.41  | 115.73      | 110.48   |
| 32  | 4     | 317 | CHL  | CHD-C1D-ND  | -3.41 | 121.32      | 124.45   |
| 31  | A     | 852 | CLA  | O2D-CGD-O1D | -3.41 | 117.17      | 123.84   |
| 31  | 9     | 314 | CLA  | CHA-C4D-ND  | 3.41  | 139.63      | 132.50   |
| 31  | A     | 854 | CLA  | CHA-C4D-ND  | 3.41  | 139.62      | 132.50   |
| 31  | B     | 845 | CLA  | CHA-C4D-ND  | 3.41  | 139.62      | 132.50   |
| 31  | F     | 301 | CLA  | C4D-CHA-C1A | -3.41 | 117.10      | 121.25   |
| 36  | b     | 301 | LUT  | C4-C5-C6    | -3.41 | 113.26      | 120.85   |
| 31  | B     | 850 | CLA  | O2D-CGD-O1D | -3.41 | 117.18      | 123.84   |
| 31  | 9     | 316 | CLA  | CHA-C4D-ND  | 3.41  | 139.62      | 132.50   |
| 31  | 2     | 312 | CLA  | O1D-CGD-CBD | -3.40 | 117.52      | 124.48   |
| 31  | B     | 828 | CLA  | O2D-CGD-O1D | -3.40 | 117.18      | 123.84   |
| 31  | 7     | 309 | CLA  | CHA-C4D-ND  | 3.40  | 139.62      | 132.50   |
| 32  | 4     | 313 | CHL  | CHD-C4C-C3C | -3.40 | 119.84      | 124.84   |
| 32  | 4     | 313 | CHL  | C4D-C3D-CAD | 3.40  | 112.11      | 108.10   |
| 31  | 7     | 311 | CLA  | O2D-CGD-O1D | -3.40 | 117.19      | 123.84   |
| 31  | 2     | 305 | CLA  | CHA-C4D-ND  | 3.40  | 139.62      | 132.50   |
| 31  | B     | 813 | CLA  | CHD-C4C-NC  | 3.40  | 129.56      | 124.20   |
| 31  | b     | 304 | CLA  | CHD-C4C-NC  | 3.40  | 129.56      | 124.20   |
| 36  | 2     | 301 | LUT  | C18-C5-C4   | -3.40 | 108.06      | 114.36   |
| 31  | a     | 316 | CLA  | C4D-CHA-C1A | -3.40 | 117.11      | 121.25   |
| 36  | a     | 305 | LUT  | C30-C31-C32 | -3.40 | 112.62      | 123.22   |
| 31  | 2     | 304 | CLA  | CHA-C4D-ND  | 3.40  | 139.60      | 132.50   |
| 31  | B     | 822 | CLA  | O2D-CGD-CBD | 3.40  | 117.30      | 111.27   |
| 31  | 7     | 310 | CLA  | C4C-C3C-C2C | -3.39 | 103.96      | 107.07   |
| 31  | B     | 838 | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 31  | B     | 820 | CLA  | CHD-C4C-NC  | 3.39  | 129.54      | 124.20   |
| 31  | 4     | 305 | CLA  | CMC-C2C-C1C | 3.39  | 130.20      | 125.04   |
| 31  | 4     | 309 | CLA  | CHA-C4D-ND  | 3.39  | 139.59      | 132.50   |
| 31  | B     | 816 | CLA  | O2D-CGD-O1D | -3.39 | 117.21      | 123.84   |
| 31  | 8     | 317 | CLA  | C4D-CHA-C1A | -3.39 | 117.13      | 121.25   |
| 31  | A     | 826 | CLA  | CHA-C4D-ND  | 3.39  | 139.59      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 308 | CLA  | CHA-C4D-ND  | 3.39  | 139.59      | 132.50   |
| 31  | B     | 838 | CLA  | CHD-C1D-ND  | -3.39 | 121.34      | 124.45   |
| 31  | A     | 816 | CLA  | CHD-C4C-NC  | 3.39  | 129.54      | 124.20   |
| 31  | A     | 821 | CLA  | CHD-C4C-NC  | 3.39  | 129.54      | 124.20   |
| 31  | 2     | 315 | CLA  | CHA-C4D-ND  | 3.38  | 139.58      | 132.50   |
| 31  | A     | 830 | CLA  | C4D-CHA-C1A | -3.38 | 117.13      | 121.25   |
| 36  | 7     | 305 | LUT  | C10-C11-C12 | -3.38 | 112.66      | 123.22   |
| 31  | A     | 821 | CLA  | CHA-C4D-ND  | 3.38  | 139.57      | 132.50   |
| 31  | A     | 836 | CLA  | CMD-C2D-C1D | 3.38  | 130.67      | 124.71   |
| 32  | 7     | 318 | CHL  | CHD-C4C-NC  | 3.38  | 129.53      | 124.20   |
| 32  | 7     | 317 | CHL  | CHD-C4C-NC  | 3.38  | 129.53      | 124.20   |
| 36  | 2     | 301 | LUT  | C8-C7-C6    | -3.38 | 117.71      | 127.20   |
| 32  | 7     | 317 | CHL  | C4D-C3D-CAD | 3.38  | 112.08      | 108.10   |
| 31  | 4     | 320 | CLA  | C1B-CHB-C4A | -3.38 | 123.43      | 130.12   |
| 31  | a     | 310 | CLA  | CHD-C1D-ND  | -3.38 | 121.35      | 124.45   |
| 32  | A     | 840 | CHL  | O2D-CGD-CBD | 3.38  | 117.27      | 111.27   |
| 31  | b     | 313 | CLA  | CHA-C4D-ND  | 3.38  | 139.56      | 132.50   |
| 32  | a     | 317 | CHL  | O2A-CGA-CBA | 3.38  | 122.50      | 111.91   |
| 31  | b     | 312 | CLA  | CHD-C4C-C3C | -3.38 | 119.88      | 124.84   |
| 31  | 3     | 309 | CLA  | CHA-C4D-ND  | 3.37  | 139.56      | 132.50   |
| 31  | 3     | 319 | CLA  | C1C-C2C-C3C | -3.37 | 103.41      | 106.96   |
| 31  | G     | 205 | CLA  | CHA-C4D-ND  | 3.37  | 139.55      | 132.50   |
| 31  | 3     | 317 | CLA  | C4D-CHA-C1A | -3.37 | 117.15      | 121.25   |
| 36  | a     | 305 | LUT  | C21-C26-C25 | 3.37  | 117.45      | 111.42   |
| 31  | B     | 822 | CLA  | O1D-CGD-CBD | -3.37 | 117.59      | 124.48   |
| 31  | L     | 307 | CLA  | O2D-CGD-O1D | -3.37 | 117.25      | 123.84   |
| 32  | a     | 320 | CHL  | CHD-C4C-NC  | 3.37  | 129.51      | 124.20   |
| 36  | 4     | 303 | LUT  | C10-C11-C12 | -3.37 | 112.72      | 123.22   |
| 31  | a     | 313 | CLA  | O1D-CGD-CBD | -3.36 | 117.60      | 124.48   |
| 31  | 3     | 308 | CLA  | CHD-C4C-NC  | 3.36  | 129.50      | 124.20   |
| 36  | 9     | 302 | LUT  | C21-C26-C27 | -3.36 | 108.45      | 112.70   |
| 31  | A     | 842 | CLA  | CHA-C4D-ND  | 3.36  | 139.54      | 132.50   |
| 31  | B     | 839 | CLA  | CHD-C4C-NC  | 3.36  | 129.50      | 124.20   |
| 31  | B     | 846 | CLA  | C4D-CHA-C1A | -3.36 | 117.16      | 121.25   |
| 31  | A     | 850 | CLA  | O1D-CGD-CBD | -3.36 | 117.60      | 124.48   |
| 31  | 9     | 319 | CLA  | O1D-CGD-CBD | -3.36 | 117.60      | 124.48   |
| 31  | A     | 830 | CLA  | CHD-C4C-C3C | -3.36 | 119.90      | 124.84   |
| 31  | 8     | 310 | CLA  | O1D-CGD-CBD | -3.36 | 117.61      | 124.48   |
| 31  | A     | 826 | CLA  | CHD-C1D-ND  | -3.36 | 121.36      | 124.45   |
| 32  | 8     | 319 | CHL  | CHD-C4C-NC  | 3.36  | 129.50      | 124.20   |
| 31  | B     | 838 | CLA  | CHD-C4C-C3C | -3.36 | 119.90      | 124.84   |
| 31  | B     | 822 | CLA  | C1C-C2C-C3C | -3.36 | 103.42      | 106.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | J     | 103 | LUT  | C7-C6-C5    | -3.36 | 113.33      | 121.46   |
| 31  | A     | 833 | CLA  | CHA-C4D-ND  | 3.36  | 139.52      | 132.50   |
| 31  | 7     | 312 | CLA  | O1D-CGD-CBD | -3.36 | 117.61      | 124.48   |
| 31  | A     | 853 | CLA  | CHD-C4C-NC  | 3.36  | 129.49      | 124.20   |
| 26  | 6     | 302 | BCR  | C24-C23-C22 | -3.35 | 121.17      | 126.23   |
| 32  | 8     | 319 | CHL  | C4D-C3D-CAD | 3.35  | 112.05      | 108.10   |
| 31  | b     | 313 | CLA  | O2A-CGA-CBA | 3.35  | 122.43      | 111.91   |
| 31  | a     | 314 | CLA  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 31  | B     | 844 | CLA  | O2D-CGD-O1D | -3.35 | 117.28      | 123.84   |
| 31  | B     | 850 | CLA  | C2C-C1C-NC  | 3.35  | 113.11      | 109.97   |
| 31  | A     | 825 | CLA  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 31  | a     | 319 | CLA  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 31  | 2     | 305 | CLA  | O1D-CGD-CBD | -3.35 | 117.63      | 124.48   |
| 31  | 7     | 309 | CLA  | CHD-C4C-NC  | 3.35  | 129.48      | 124.20   |
| 31  | B     | 828 | CLA  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 31  | A     | 855 | CLA  | CHA-C4D-ND  | 3.35  | 139.51      | 132.50   |
| 31  | b     | 303 | CLA  | CHD-C1D-ND  | -3.35 | 121.38      | 124.45   |
| 36  | F     | 304 | LUT  | C7-C6-C5    | -3.35 | 113.35      | 121.46   |
| 32  | 8     | 316 | CHL  | C4D-C3D-CAD | 3.35  | 112.04      | 108.10   |
| 31  | 3     | 313 | CLA  | CHA-C4D-ND  | 3.35  | 139.50      | 132.50   |
| 31  | 7     | 311 | CLA  | CHD-C4C-NC  | 3.35  | 129.47      | 124.20   |
| 31  | B     | 849 | CLA  | O1D-CGD-CBD | -3.34 | 117.64      | 124.48   |
| 31  | L     | 306 | CLA  | CHA-C4D-ND  | 3.34  | 139.50      | 132.50   |
| 32  | A     | 839 | CHL  | C4-C3-C5    | 3.34  | 120.90      | 115.27   |
| 31  | B     | 827 | CLA  | CHA-C4D-ND  | 3.34  | 139.49      | 132.50   |
| 31  | 3     | 311 | CLA  | O2D-CGD-O1D | -3.34 | 117.30      | 123.84   |
| 31  | B     | 825 | CLA  | CMC-C2C-C1C | 3.34  | 130.13      | 125.04   |
| 32  | a     | 317 | CHL  | C4D-C3D-CAD | 3.34  | 112.04      | 108.10   |
| 31  | A     | 827 | CLA  | CHD-C4C-NC  | 3.34  | 129.47      | 124.20   |
| 36  | 6     | 303 | LUT  | C35-C15-C14 | -3.34 | 116.63      | 123.47   |
| 36  | F     | 304 | LUT  | C30-C31-C32 | -3.34 | 112.79      | 123.22   |
| 36  | 4     | 303 | LUT  | C7-C6-C5    | -3.34 | 113.37      | 121.46   |
| 31  | F     | 305 | CLA  | CHD-C1D-ND  | -3.34 | 121.38      | 124.45   |
| 31  | O     | 202 | CLA  | CHD-C4C-C3C | -3.34 | 119.76      | 124.98   |
| 31  | 4     | 320 | CLA  | CHA-C4D-ND  | 3.34  | 139.49      | 132.50   |
| 26  | J     | 102 | BCR  | C2-C1-C6    | 3.34  | 115.62      | 110.48   |
| 31  | B     | 821 | CLA  | CHA-C4D-ND  | 3.34  | 139.48      | 132.50   |
| 32  | 8     | 316 | CHL  | CHD-C1D-ND  | -3.34 | 121.39      | 124.45   |
| 31  | 5     | 318 | CLA  | C4-C3-C5    | 3.34  | 120.89      | 115.27   |
| 31  | 2     | 306 | CLA  | O2D-CGD-O1D | -3.34 | 117.31      | 123.84   |
| 31  | 5     | 307 | CLA  | CMB-C2B-C3B | 3.34  | 130.92      | 124.68   |
| 31  | A     | 846 | CLA  | CHD-C4C-NC  | 3.34  | 129.46      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 311 | CLA  | CHA-C4D-ND  | 3.34  | 139.48      | 132.50   |
| 31  | 3     | 319 | CLA  | CMC-C2C-C1C | 3.34  | 130.12      | 125.04   |
| 36  | 6     | 304 | LUT  | C8-C7-C6    | -3.34 | 117.83      | 127.20   |
| 31  | B     | 813 | CLA  | CHA-C4D-ND  | 3.34  | 139.48      | 132.50   |
| 31  | a     | 313 | CLA  | C4-C3-C5    | 3.34  | 120.88      | 115.27   |
| 32  | A     | 839 | CHL  | C1-O2A-CGA  | 3.33  | 125.19      | 116.44   |
| 31  | A     | 823 | CLA  | O2D-CGD-O1D | -3.33 | 117.32      | 123.84   |
| 31  | A     | 844 | CLA  | O1D-CGD-CBD | -3.33 | 117.66      | 124.48   |
| 32  | a     | 317 | CHL  | CHD-C1D-ND  | -3.33 | 121.39      | 124.45   |
| 31  | A     | 843 | CLA  | CHA-C4D-ND  | 3.33  | 139.47      | 132.50   |
| 31  | 8     | 308 | CLA  | O2A-CGA-CBA | 3.33  | 122.36      | 111.91   |
| 31  | L     | 306 | CLA  | CHD-C4C-NC  | 3.33  | 129.45      | 124.20   |
| 32  | 6     | 320 | CHL  | C4D-C3D-CAD | 3.33  | 112.02      | 108.10   |
| 31  | B     | 826 | CLA  | CHA-C4D-ND  | 3.33  | 139.47      | 132.50   |
| 32  | 3     | 315 | CHL  | CHD-C4C-NC  | 3.33  | 129.45      | 124.20   |
| 31  | B     | 849 | CLA  | C3D-C2D-C1D | -3.33 | 101.29      | 105.83   |
| 37  | J     | 104 | LMG  | O6-C1-O1    | -3.33 | 102.09      | 109.97   |
| 32  | a     | 320 | CHL  | CHD-C1D-ND  | -3.33 | 121.40      | 124.45   |
| 43  | 5     | 306 | PTY  | C6-O7-C8    | 3.33  | 125.98      | 117.79   |
| 32  | K     | 201 | CHL  | O2D-CGD-O1D | -3.33 | 117.34      | 123.84   |
| 36  | 6     | 304 | LUT  | C17-C1-C6   | -3.32 | 104.91      | 110.30   |
| 31  | a     | 315 | CLA  | CHA-C4D-ND  | 3.32  | 139.45      | 132.50   |
| 31  | 8     | 313 | CLA  | CHD-C4C-NC  | 3.32  | 129.44      | 124.20   |
| 31  | K     | 204 | CLA  | C1-C2-C3    | -3.32 | 121.38      | 126.75   |
| 31  | A     | 817 | CLA  | CHD-C4C-NC  | 3.32  | 129.43      | 124.20   |
| 31  | 4     | 308 | CLA  | C4D-CHA-C1A | -3.32 | 117.21      | 121.25   |
| 31  | A     | 814 | CLA  | O2D-CGD-O1D | -3.32 | 117.35      | 123.84   |
| 31  | K     | 204 | CLA  | CHD-C4C-NC  | 3.32  | 129.43      | 124.20   |
| 31  | 3     | 314 | CLA  | CHA-C4D-ND  | 3.32  | 139.43      | 132.50   |
| 32  | 5     | 322 | CHL  | O1D-CGD-CBD | -3.31 | 117.70      | 124.48   |
| 31  | 7     | 321 | CLA  | CHD-C4C-NC  | 3.31  | 129.43      | 124.20   |
| 31  | A     | 856 | CLA  | C4D-CHA-C1A | -3.31 | 117.22      | 121.25   |
| 31  | 6     | 312 | CLA  | C4D-CHA-C1A | -3.31 | 117.22      | 121.25   |
| 31  | B     | 842 | CLA  | O2A-CGA-CBA | 3.31  | 122.30      | 111.91   |
| 31  | 7     | 312 | CLA  | CHD-C4C-NC  | 3.31  | 129.42      | 124.20   |
| 31  | B     | 847 | CLA  | CHD-C4C-NC  | 3.31  | 129.42      | 124.20   |
| 31  | 4     | 321 | CLA  | C4D-CHA-C1A | -3.31 | 117.22      | 121.25   |
| 31  | 2     | 307 | CLA  | CMB-C2B-C3B | 3.31  | 130.87      | 124.68   |
| 32  | K     | 201 | CHL  | CMB-C2B-C3B | 3.31  | 130.87      | 124.68   |
| 31  | A     | 832 | CLA  | O2D-CGD-O1D | -3.31 | 117.37      | 123.84   |
| 32  | A     | 840 | CHL  | C2D-C1D-ND  | 3.31  | 112.54      | 110.10   |
| 31  | K     | 206 | CLA  | CHA-C4D-ND  | 3.31  | 139.42      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 848 | CLA  | CHD-C4C-C3C | -3.31 | 119.98      | 124.84   |
| 31  | A     | 841 | CLA  | C3D-C2D-C1D | -3.30 | 101.32      | 105.83   |
| 31  | J     | 105 | CLA  | O2D-CGD-O1D | -3.30 | 117.38      | 123.84   |
| 31  | A     | 856 | CLA  | CHA-C4D-ND  | 3.30  | 139.41      | 132.50   |
| 31  | 5     | 307 | CLA  | O2D-CGD-O1D | -3.30 | 117.38      | 123.84   |
| 31  | A     | 850 | CLA  | CHD-C4C-NC  | 3.30  | 129.41      | 124.20   |
| 31  | B     | 843 | CLA  | CHA-C4D-ND  | 3.30  | 139.41      | 132.50   |
| 32  | 6     | 318 | CHL  | O2D-CGD-O1D | -3.30 | 117.38      | 123.84   |
| 31  | 8     | 318 | CLA  | CHA-C4D-ND  | 3.30  | 139.41      | 132.50   |
| 31  | 3     | 307 | CLA  | CMB-C2B-C3B | 3.30  | 130.86      | 124.68   |
| 31  | 8     | 321 | CLA  | CHA-C4D-ND  | 3.30  | 139.41      | 132.50   |
| 32  | 7     | 324 | CHL  | CHD-C1D-ND  | -3.30 | 121.42      | 124.45   |
| 30  | A     | 813 | CL0  | C4A-NA-C1A  | -3.30 | 105.22      | 106.71   |
| 31  | L     | 305 | CLA  | C3D-C2D-C1D | -3.30 | 101.33      | 105.83   |
| 31  | B     | 833 | CLA  | CHD-C4C-NC  | 3.30  | 129.40      | 124.20   |
| 31  | 2     | 311 | CLA  | O1D-CGD-CBD | -3.30 | 117.73      | 124.48   |
| 36  | 4     | 302 | LUT  | C30-C31-C32 | -3.30 | 112.92      | 123.22   |
| 32  | a     | 320 | CHL  | C4D-C3D-CAD | 3.30  | 111.98      | 108.10   |
| 31  | F     | 306 | CLA  | O1D-CGD-CBD | -3.30 | 117.73      | 124.48   |
| 31  | A     | 841 | CLA  | C4D-CHA-C1A | -3.30 | 117.23      | 121.25   |
| 31  | 2     | 304 | CLA  | CHD-C4C-NC  | 3.30  | 129.40      | 124.20   |
| 31  | A     | 857 | CLA  | CHA-C4D-ND  | 3.30  | 139.40      | 132.50   |
| 40  | 7     | 306 | XAT  | C20-C13-C14 | -3.30 | 118.30      | 122.92   |
| 31  | 2     | 308 | CLA  | CHD-C4C-NC  | 3.30  | 129.40      | 124.20   |
| 31  | B     | 833 | CLA  | CHA-C4D-ND  | 3.30  | 139.40      | 132.50   |
| 31  | A     | 829 | CLA  | CHB-C4A-NA  | 3.30  | 129.07      | 124.51   |
| 36  | 8     | 302 | LUT  | C17-C1-C6   | -3.30 | 104.95      | 110.30   |
| 31  | A     | 836 | CLA  | O2D-CGD-O1D | -3.30 | 117.39      | 123.84   |
| 31  | 5     | 307 | CLA  | CHA-C4D-ND  | 3.29  | 139.39      | 132.50   |
| 31  | B     | 821 | CLA  | C4D-CHA-C1A | -3.29 | 117.24      | 121.25   |
| 31  | 6     | 322 | CLA  | C4D-CHA-C1A | -3.29 | 117.24      | 121.25   |
| 32  | 7     | 319 | CHL  | C3D-C2D-C1D | -3.29 | 101.34      | 105.83   |
| 31  | A     | 822 | CLA  | CHD-C4C-NC  | 3.29  | 129.39      | 124.20   |
| 31  | A     | 835 | CLA  | C4D-CHA-C1A | -3.29 | 117.24      | 121.25   |
| 32  | 4     | 310 | CHL  | C4D-C3D-CAD | 3.29  | 111.97      | 108.10   |
| 31  | B     | 817 | CLA  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |
| 31  | B     | 813 | CLA  | CMB-C2B-C3B | 3.29  | 130.83      | 124.68   |
| 31  | B     | 833 | CLA  | C1-O2A-CGA  | 3.29  | 125.07      | 116.44   |
| 36  | 8     | 302 | LUT  | C2-C3-C4    | 3.29  | 114.81      | 110.30   |
| 36  | J     | 103 | LUT  | C8-C9-C10   | -3.29 | 113.90      | 118.94   |
| 31  | A     | 835 | CLA  | CMB-C2B-C3B | 3.29  | 130.83      | 124.68   |
| 32  | 7     | 324 | CHL  | C3D-C2D-C1D | -3.29 | 101.35      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 848 | CLA  | CHA-C4D-ND  | 3.29  | 139.37      | 132.50   |
| 31  | b     | 308 | CLA  | CHA-C4D-ND  | 3.29  | 139.37      | 132.50   |
| 31  | 3     | 311 | CLA  | CHD-C1D-ND  | -3.29 | 121.43      | 124.45   |
| 32  | A     | 839 | CHL  | CGD-CBD-CAD | 3.29  | 121.38      | 110.73   |
| 31  | 9     | 316 | CLA  | O1D-CGD-CBD | -3.29 | 117.76      | 124.48   |
| 31  | A     | 842 | CLA  | CMB-C2B-C3B | 3.28  | 130.82      | 124.68   |
| 31  | 3     | 313 | CLA  | O2D-CGD-O1D | -3.28 | 117.42      | 123.84   |
| 36  | 9     | 302 | LUT  | C30-C31-C32 | -3.28 | 112.98      | 123.22   |
| 32  | a     | 318 | CHL  | C4D-C3D-CAD | 3.28  | 111.96      | 108.10   |
| 32  | 6     | 319 | CHL  | O1D-CGD-CBD | -3.28 | 117.77      | 124.48   |
| 36  | J     | 103 | LUT  | C12-C13-C14 | -3.28 | 113.91      | 118.94   |
| 32  | 7     | 320 | CHL  | C4D-C3D-CAD | 3.28  | 111.96      | 108.10   |
| 32  | 5     | 322 | CHL  | C4D-C3D-CAD | 3.28  | 111.96      | 108.10   |
| 31  | b     | 304 | CLA  | CHA-C4D-ND  | 3.28  | 139.35      | 132.50   |
| 31  | A     | 818 | CLA  | C1C-C2C-C3C | -3.28 | 103.51      | 106.96   |
| 35  | 7     | 303 | QTB  | C09-C02-C03 | 3.28  | 123.97      | 118.94   |
| 31  | b     | 310 | CLA  | CHD-C4C-NC  | 3.28  | 129.37      | 124.20   |
| 36  | F     | 304 | LUT  | C1-C6-C7    | -3.27 | 106.51      | 115.78   |
| 32  | 6     | 320 | CHL  | CHD-C1D-ND  | -3.27 | 121.44      | 124.45   |
| 31  | 7     | 309 | CLA  | O2A-CGA-CBA | 3.27  | 122.18      | 111.91   |
| 31  | 8     | 320 | CLA  | CHA-C4D-ND  | 3.27  | 139.35      | 132.50   |
| 31  | 4     | 312 | CLA  | O1D-CGD-CBD | -3.27 | 117.79      | 124.48   |
| 31  | B     | 825 | CLA  | O1D-CGD-CBD | -3.27 | 117.79      | 124.48   |
| 31  | A     | 835 | CLA  | CHD-C4C-C3C | -3.27 | 120.03      | 124.84   |
| 31  | B     | 819 | CLA  | O1D-CGD-CBD | -3.27 | 117.79      | 124.48   |
| 31  | 2     | 308 | CLA  | O1D-CGD-CBD | -3.27 | 117.79      | 124.48   |
| 31  | A     | 827 | CLA  | CHA-C4D-ND  | 3.27  | 139.34      | 132.50   |
| 31  | B     | 818 | CLA  | CHA-C4D-ND  | 3.27  | 139.34      | 132.50   |
| 31  | K     | 204 | CLA  | O2D-CGD-O1D | -3.27 | 117.44      | 123.84   |
| 31  | 3     | 314 | CLA  | CHD-C4C-NC  | 3.27  | 129.35      | 124.20   |
| 31  | B     | 814 | CLA  | CHA-C4D-ND  | 3.27  | 139.34      | 132.50   |
| 31  | a     | 315 | CLA  | CHD-C4C-NC  | 3.27  | 129.35      | 124.20   |
| 31  | A     | 841 | CLA  | CHA-C4D-ND  | 3.27  | 139.33      | 132.50   |
| 31  | 4     | 315 | CLA  | O2D-CGD-O1D | -3.26 | 117.46      | 123.84   |
| 31  | J     | 105 | CLA  | CHA-C4D-ND  | 3.26  | 139.33      | 132.50   |
| 31  | A     | 853 | CLA  | O2D-CGD-CBD | 3.26  | 117.07      | 111.27   |
| 31  | 4     | 315 | CLA  | CAC-C3C-C4C | 3.26  | 129.04      | 124.81   |
| 36  | 5     | 303 | LUT  | C35-C15-C14 | -3.26 | 116.79      | 123.47   |
| 32  | 6     | 321 | CHL  | C4D-C3D-CAD | 3.26  | 111.94      | 108.10   |
| 31  | 9     | 312 | CLA  | CHD-C4C-NC  | 3.26  | 129.34      | 124.20   |
| 32  | 9     | 320 | CHL  | C4D-C3D-CAD | 3.26  | 111.94      | 108.10   |
| 31  | A     | 822 | CLA  | O2A-CGA-CBA | 3.26  | 122.14      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 817 | CLA  | O1D-CGD-CBD | -3.26 | 117.81      | 124.48   |
| 31  | B     | 840 | CLA  | CHD-C4C-NC  | 3.26  | 129.34      | 124.20   |
| 31  | b     | 305 | CLA  | CMB-C2B-C3B | 3.26  | 130.77      | 124.68   |
| 31  | 9     | 314 | CLA  | CHD-C4C-NC  | 3.25  | 129.33      | 124.20   |
| 32  | 6     | 319 | CHL  | CGD-CBD-CAD | 3.25  | 121.27      | 110.73   |
| 31  | B     | 842 | CLA  | CHA-C4D-ND  | 3.25  | 139.31      | 132.50   |
| 31  | H     | 903 | CLA  | O1D-CGD-CBD | -3.25 | 117.83      | 124.48   |
| 31  | 6     | 316 | CLA  | CHA-C4D-ND  | 3.25  | 139.30      | 132.50   |
| 31  | A     | 852 | CLA  | CMB-C2B-C3B | 3.25  | 130.76      | 124.68   |
| 32  | 4     | 317 | CHL  | CHD-C4C-C3C | -3.25 | 120.06      | 124.84   |
| 31  | G     | 204 | CLA  | CHD-C4C-C3C | -3.25 | 120.07      | 124.84   |
| 31  | B     | 834 | CLA  | C4D-CHA-C1A | -3.25 | 117.30      | 121.25   |
| 31  | 8     | 310 | CLA  | CHA-C4D-ND  | 3.25  | 139.29      | 132.50   |
| 31  | 9     | 318 | CLA  | C1-C2-C3    | -3.25 | 120.43      | 126.04   |
| 31  | A     | 820 | CLA  | CHD-C4C-NC  | 3.25  | 129.32      | 124.20   |
| 32  | 6     | 317 | CHL  | O2D-CGD-O1D | -3.25 | 117.49      | 123.84   |
| 36  | 5     | 304 | LUT  | C30-C31-C32 | -3.24 | 113.10      | 123.22   |
| 31  | B     | 845 | CLA  | C3D-C2D-C1D | -3.24 | 101.41      | 105.83   |
| 31  | b     | 304 | CLA  | O1D-CGD-CBD | -3.24 | 117.85      | 124.48   |
| 32  | 6     | 319 | CHL  | C4D-C3D-CAD | 3.24  | 111.92      | 108.10   |
| 31  | A     | 816 | CLA  | CHA-C4D-ND  | 3.24  | 139.28      | 132.50   |
| 31  | G     | 206 | CLA  | CHA-C4D-ND  | 3.24  | 139.28      | 132.50   |
| 31  | F     | 301 | CLA  | C1-C2-C3    | -3.24 | 120.44      | 126.04   |
| 32  | 3     | 315 | CHL  | C4D-C3D-CAD | 3.24  | 111.91      | 108.10   |
| 31  | 8     | 317 | CLA  | CHA-C4D-ND  | 3.24  | 139.27      | 132.50   |
| 31  | B     | 825 | CLA  | CHA-C4D-ND  | 3.24  | 139.27      | 132.50   |
| 32  | 4     | 310 | CHL  | O1D-CGD-CBD | -3.24 | 117.86      | 124.48   |
| 31  | O     | 203 | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 31  | 6     | 314 | CLA  | O1D-CGD-CBD | -3.24 | 117.86      | 124.48   |
| 31  | 2     | 309 | CLA  | O2D-CGD-O1D | -3.24 | 117.51      | 123.84   |
| 32  | a     | 317 | CHL  | CHD-C4C-NC  | 3.24  | 129.30      | 124.20   |
| 31  | B     | 848 | CLA  | O2D-CGD-O1D | -3.23 | 117.52      | 123.84   |
| 31  | B     | 834 | CLA  | C1-C2-C3    | -3.23 | 120.45      | 126.04   |
| 42  | 4     | 304 | SQD  | O8-S-C6     | 3.23  | 110.89      | 105.74   |
| 31  | B     | 818 | CLA  | O1D-CGD-CBD | -3.23 | 117.87      | 124.48   |
| 31  | b     | 311 | CLA  | O1D-CGD-CBD | -3.23 | 117.87      | 124.48   |
| 31  | A     | 829 | CLA  | C2C-C1C-NC  | 3.23  | 113.00      | 109.97   |
| 32  | 6     | 309 | CHL  | C4D-C3D-CAD | 3.23  | 111.90      | 108.10   |
| 31  | B     | 835 | CLA  | O2D-CGD-O1D | -3.23 | 117.52      | 123.84   |
| 31  | b     | 306 | CLA  | CHD-C4C-NC  | 3.23  | 129.29      | 124.20   |
| 31  | B     | 837 | CLA  | CHD-C4C-C3C | -3.23 | 120.10      | 124.84   |
| 31  | 2     | 313 | CLA  | O1D-CGD-CBD | -3.23 | 117.88      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 9     | 302 | LUT  | C1-C6-C5    | -3.22 | 118.07      | 122.61   |
| 36  | L     | 304 | LUT  | C30-C31-C32 | -3.22 | 113.16      | 123.22   |
| 31  | A     | 852 | CLA  | C3D-C2D-C1D | -3.22 | 101.43      | 105.83   |
| 32  | 9     | 322 | CHL  | C4D-C3D-CAD | 3.22  | 111.89      | 108.10   |
| 31  | B     | 831 | CLA  | CHA-C4D-ND  | 3.22  | 139.24      | 132.50   |
| 31  | 6     | 312 | CLA  | CHD-C4C-NC  | 3.22  | 129.28      | 124.20   |
| 31  | 3     | 318 | CLA  | CHD-C4C-NC  | 3.22  | 129.28      | 124.20   |
| 32  | 5     | 316 | CHL  | CHD-C4C-NC  | 3.22  | 129.28      | 124.20   |
| 31  | 9     | 317 | CLA  | C1D-ND-C4D  | -3.22 | 104.05      | 106.33   |
| 31  | B     | 831 | CLA  | CHD-C4C-NC  | 3.22  | 129.28      | 124.20   |
| 31  | 8     | 317 | CLA  | O2A-CGA-CBA | 3.22  | 122.01      | 111.91   |
| 31  | A     | 845 | CLA  | C4-C3-C5    | 3.22  | 120.69      | 115.27   |
| 36  | 7     | 305 | LUT  | C4-C5-C6    | -3.22 | 113.68      | 120.85   |
| 31  | 3     | 319 | CLA  | C2C-C1C-NC  | 3.22  | 112.99      | 109.97   |
| 31  | 9     | 319 | CLA  | C4D-CHA-C1A | -3.22 | 117.33      | 121.25   |
| 31  | 6     | 310 | CLA  | O2D-CGD-O1D | -3.22 | 117.55      | 123.84   |
| 32  | K     | 201 | CHL  | CAC-C3C-C4C | 3.22  | 128.98      | 124.81   |
| 32  | 7     | 324 | CHL  | C4D-C3D-CAD | 3.21  | 111.89      | 108.10   |
| 31  | A     | 843 | CLA  | CHD-C4C-C3C | -3.21 | 120.11      | 124.84   |
| 32  | 5     | 317 | CHL  | C4D-C3D-CAD | 3.21  | 111.88      | 108.10   |
| 31  | A     | 845 | CLA  | CHD-C4C-NC  | 3.21  | 129.27      | 124.20   |
| 31  | A     | 850 | CLA  | CMB-C2B-C3B | 3.21  | 130.69      | 124.68   |
| 31  | 4     | 308 | CLA  | CMB-C2B-C3B | 3.21  | 130.69      | 124.68   |
| 31  | B     | 811 | CLA  | CHD-C4C-NC  | 3.21  | 129.26      | 124.20   |
| 31  | a     | 314 | CLA  | CHD-C4C-NC  | 3.21  | 129.26      | 124.20   |
| 31  | b     | 308 | CLA  | CHD-C4C-C3C | -3.21 | 120.12      | 124.84   |
| 31  | a     | 309 | CLA  | CMB-C2B-C3B | 3.21  | 130.68      | 124.68   |
| 31  | A     | 841 | CLA  | C1-C2-C3    | -3.21 | 120.49      | 126.04   |
| 31  | A     | 824 | CLA  | O2D-CGD-O1D | -3.21 | 117.56      | 123.84   |
| 31  | 8     | 317 | CLA  | C3D-C2D-C1D | -3.21 | 101.45      | 105.83   |
| 31  | 4     | 311 | CLA  | CHD-C1D-ND  | -3.21 | 121.51      | 124.45   |
| 31  | A     | 842 | CLA  | CHD-C4C-NC  | 3.21  | 129.26      | 124.20   |
| 31  | B     | 813 | CLA  | C1-C2-C3    | -3.20 | 120.50      | 126.04   |
| 31  | 3     | 316 | CLA  | O2D-CGD-O1D | -3.20 | 117.57      | 123.84   |
| 31  | F     | 301 | CLA  | O1D-CGD-CBD | -3.20 | 117.93      | 124.48   |
| 31  | A     | 855 | CLA  | O2D-CGD-O1D | -3.20 | 117.57      | 123.84   |
| 31  | a     | 313 | CLA  | CHD-C4C-NC  | 3.20  | 129.25      | 124.20   |
| 31  | 3     | 320 | CLA  | CHD-C4C-NC  | 3.20  | 129.25      | 124.20   |
| 31  | 8     | 311 | CLA  | C4-C3-C5    | 3.20  | 120.66      | 115.27   |
| 31  | B     | 841 | CLA  | O1D-CGD-CBD | -3.20 | 117.93      | 124.48   |
| 31  | A     | 819 | CLA  | CHD-C4C-NC  | 3.20  | 129.25      | 124.20   |
| 31  | B     | 811 | CLA  | CHA-C4D-ND  | 3.20  | 139.19      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 8     | 303 | LUT  | C4-C5-C6    | -3.20 | 113.72      | 120.85   |
| 31  | B     | 828 | CLA  | C4-C3-C5    | 3.20  | 120.65      | 115.27   |
| 32  | 6     | 318 | CHL  | C4D-C3D-CAD | 3.20  | 111.86      | 108.10   |
| 31  | 8     | 315 | CLA  | C6-C5-C3    | -3.20 | 109.39      | 114.62   |
| 31  | b     | 312 | CLA  | CHD-C1D-ND  | -3.20 | 121.52      | 124.45   |
| 32  | 7     | 317 | CHL  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 31  | A     | 823 | CLA  | C1-C2-C3    | -3.19 | 120.52      | 126.04   |
| 31  | A     | 837 | CLA  | C4D-CHA-C1A | -3.19 | 117.36      | 121.25   |
| 31  | 7     | 322 | CLA  | CHA-C4D-ND  | 3.19  | 139.17      | 132.50   |
| 31  | B     | 831 | CLA  | C1-C2-C3    | -3.19 | 121.59      | 126.75   |
| 31  | B     | 839 | CLA  | O1D-CGD-CBD | -3.19 | 117.96      | 124.48   |
| 31  | A     | 834 | CLA  | CMB-C2B-C3B | 3.19  | 130.64      | 124.68   |
| 26  | 8     | 301 | BCR  | C3-C4-C5    | -3.19 | 108.38      | 114.08   |
| 31  | B     | 819 | CLA  | CHD-C4C-NC  | 3.19  | 129.23      | 124.20   |
| 31  | 8     | 318 | CLA  | O2D-CGD-O1D | -3.19 | 117.61      | 123.84   |
| 32  | 8     | 319 | CHL  | O2D-CGD-O1D | -3.19 | 117.61      | 123.84   |
| 26  | B     | 804 | BCR  | C2-C1-C6    | 3.19  | 115.39      | 110.48   |
| 31  | 2     | 308 | CLA  | O2D-CGD-O1D | -3.18 | 117.61      | 123.84   |
| 31  | 7     | 315 | CLA  | C4D-CHA-C1A | -3.18 | 117.38      | 121.25   |
| 31  | A     | 842 | CLA  | C4-C3-C5    | 3.18  | 120.62      | 115.27   |
| 36  | 7     | 305 | LUT  | C30-C31-C32 | -3.18 | 113.29      | 123.22   |
| 31  | A     | 846 | CLA  | O2D-CGD-O1D | -3.18 | 117.62      | 123.84   |
| 31  | B     | 829 | CLA  | C3D-C2D-C1D | -3.18 | 101.49      | 105.83   |
| 31  | b     | 305 | CLA  | CHD-C4C-NC  | 3.18  | 129.21      | 124.20   |
| 31  | B     | 816 | CLA  | CHA-C4D-ND  | 3.18  | 139.15      | 132.50   |
| 31  | B     | 814 | CLA  | CMB-C2B-C3B | 3.18  | 130.62      | 124.68   |
| 31  | B     | 845 | CLA  | CHD-C4C-NC  | 3.18  | 129.21      | 124.20   |
| 31  | 4     | 316 | CLA  | CMD-C2D-C3D | -3.17 | 120.31      | 127.61   |
| 31  | A     | 819 | CLA  | O2A-CGA-CBA | 3.17  | 121.87      | 111.91   |
| 31  | 4     | 318 | CLA  | O2D-CGD-O1D | -3.17 | 117.63      | 123.84   |
| 31  | B     | 836 | CLA  | O2D-CGD-O1D | -3.17 | 117.64      | 123.84   |
| 31  | 8     | 311 | CLA  | CMB-C2B-C3B | 3.17  | 130.61      | 124.68   |
| 31  | A     | 836 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |
| 31  | F     | 306 | CLA  | C4D-CHA-C1A | -3.17 | 117.39      | 121.25   |
| 31  | A     | 838 | CLA  | O1D-CGD-CBD | -3.17 | 118.00      | 124.48   |
| 32  | A     | 839 | CHL  | C2C-C3C-C4C | -3.17 | 104.23      | 106.49   |
| 31  | 9     | 316 | CLA  | CHD-C4C-NC  | 3.17  | 129.20      | 124.20   |
| 32  | A     | 840 | CHL  | C4-C3-C5    | 3.17  | 120.60      | 115.27   |
| 31  | A     | 846 | CLA  | CHA-C4D-ND  | 3.17  | 139.13      | 132.50   |
| 32  | 3     | 315 | CHL  | C3D-C2D-C1D | -3.17 | 101.50      | 105.83   |
| 31  | B     | 821 | CLA  | CMB-C2B-C3B | 3.17  | 130.61      | 124.68   |
| 31  | A     | 828 | CLA  | C1-C2-C3    | -3.17 | 120.56      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 829 | CLA  | O1D-CGD-CBD | -3.17 | 118.00      | 124.48   |
| 31  | 6     | 322 | CLA  | CHD-C4C-NC  | 3.17  | 129.19      | 124.20   |
| 31  | B     | 813 | CLA  | CMC-C2C-C1C | 3.17  | 129.86      | 125.04   |
| 31  | B     | 838 | CLA  | O1D-CGD-CBD | -3.17 | 118.01      | 124.48   |
| 31  | 6     | 313 | CLA  | O1D-CGD-CBD | -3.16 | 118.01      | 124.48   |
| 31  | 2     | 314 | CLA  | O2D-CGD-O1D | -3.16 | 117.65      | 123.84   |
| 31  | A     | 850 | CLA  | C3D-C2D-C1D | -3.16 | 101.51      | 105.83   |
| 31  | A     | 851 | CLA  | O2D-CGD-O1D | -3.16 | 117.65      | 123.84   |
| 32  | 7     | 317 | CHL  | C3D-C2D-C1D | -3.16 | 101.51      | 105.83   |
| 31  | 7     | 310 | CLA  | CHD-C1D-ND  | -3.16 | 121.55      | 124.45   |
| 31  | 8     | 310 | CLA  | CMB-C2B-C3B | 3.16  | 130.59      | 124.68   |
| 31  | a     | 312 | CLA  | CMC-C2C-C1C | 3.16  | 129.85      | 125.04   |
| 31  | B     | 844 | CLA  | CMB-C2B-C3B | 3.16  | 130.59      | 124.68   |
| 36  | 2     | 301 | LUT  | C4-C5-C6    | -3.16 | 113.81      | 120.85   |
| 31  | a     | 311 | CLA  | CHD-C4C-NC  | 3.16  | 129.18      | 124.20   |
| 31  | B     | 825 | CLA  | CHD-C4C-NC  | 3.15  | 129.17      | 124.20   |
| 31  | 3     | 314 | CLA  | C4D-CHA-C1A | -3.15 | 117.41      | 121.25   |
| 31  | A     | 852 | CLA  | CHD-C4C-NC  | 3.15  | 129.17      | 124.20   |
| 31  | B     | 844 | CLA  | C4D-CHA-C1A | -3.15 | 117.42      | 121.25   |
| 31  | B     | 839 | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 31  | H     | 902 | CLA  | O2D-CGD-O1D | -3.15 | 117.68      | 123.84   |
| 36  | b     | 301 | LUT  | C30-C31-C32 | -3.15 | 113.39      | 123.22   |
| 31  | B     | 814 | CLA  | C3D-C2D-C1D | -3.15 | 101.53      | 105.83   |
| 31  | A     | 819 | CLA  | C1-O2A-CGA  | 3.15  | 124.71      | 116.44   |
| 31  | 8     | 310 | CLA  | C2C-C1C-NC  | 3.15  | 112.92      | 109.97   |
| 31  | b     | 313 | CLA  | C1-C2-C3    | -3.15 | 120.60      | 126.04   |
| 36  | 5     | 303 | LUT  | C7-C8-C9    | -3.15 | 121.48      | 126.23   |
| 32  | A     | 839 | CHL  | CMD-C2D-C1D | 3.15  | 130.26      | 124.71   |
| 32  | 4     | 317 | CHL  | C4D-C3D-CAD | 3.15  | 111.81      | 108.10   |
| 31  | 3     | 307 | CLA  | O2A-CGA-CBA | 3.15  | 121.78      | 111.91   |
| 31  | 9     | 315 | CLA  | CHD-C4C-NC  | 3.15  | 129.16      | 124.20   |
| 31  | 7     | 314 | CLA  | C4C-C3C-C2C | -3.15 | 104.19      | 107.07   |
| 31  | A     | 855 | CLA  | CHD-C4C-NC  | 3.15  | 129.16      | 124.20   |
| 31  | B     | 829 | CLA  | CHD-C4C-NC  | 3.14  | 129.16      | 124.20   |
| 31  | 3     | 308 | CLA  | O1D-CGD-CBD | -3.14 | 118.05      | 124.48   |
| 31  | 3     | 310 | CLA  | CHB-C4A-NA  | 3.14  | 128.86      | 124.51   |
| 31  | a     | 321 | CLA  | CHD-C4C-NC  | 3.14  | 129.15      | 124.20   |
| 31  | 6     | 314 | CLA  | CHD-C4C-NC  | 3.14  | 129.15      | 124.20   |
| 31  | A     | 828 | CLA  | CMB-C2B-C3B | 3.14  | 130.55      | 124.68   |
| 31  | 8     | 321 | CLA  | CMB-C2B-C3B | 3.14  | 130.55      | 124.68   |
| 31  | A     | 844 | CLA  | CHD-C1D-ND  | -3.14 | 121.57      | 124.45   |
| 26  | 8     | 301 | BCR  | C2-C1-C6    | 3.14  | 115.31      | 110.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 817 | CLA  | CHA-C4D-ND  | 3.14  | 139.07      | 132.50   |
| 36  | 5     | 304 | LUT  | C35-C15-C14 | -3.14 | 117.04      | 123.47   |
| 31  | A     | 834 | CLA  | CHA-C4D-ND  | 3.14  | 139.07      | 132.50   |
| 31  | 3     | 309 | CLA  | CHD-C4C-NC  | 3.14  | 129.15      | 124.20   |
| 31  | A     | 857 | CLA  | O1D-CGD-CBD | -3.14 | 118.06      | 124.48   |
| 31  | A     | 832 | CLA  | CHA-C4D-ND  | 3.14  | 139.06      | 132.50   |
| 31  | 7     | 314 | CLA  | O2D-CGD-O1D | -3.14 | 117.71      | 123.84   |
| 31  | 9     | 319 | CLA  | O2D-CGD-O1D | -3.14 | 117.71      | 123.84   |
| 31  | O     | 203 | CLA  | C4-C3-C5    | 3.13  | 120.54      | 115.27   |
| 31  | A     | 850 | CLA  | O2D-CGD-CBD | 3.13  | 116.84      | 111.27   |
| 36  | 8     | 302 | LUT  | C1-C6-C5    | -3.13 | 118.20      | 122.61   |
| 31  | 4     | 314 | CLA  | CHD-C4C-NC  | 3.13  | 129.14      | 124.20   |
| 32  | 7     | 320 | CHL  | C3D-C2D-C1D | -3.13 | 101.56      | 105.83   |
| 31  | B     | 844 | CLA  | CHD-C4C-NC  | 3.13  | 129.14      | 124.20   |
| 31  | 6     | 307 | CLA  | CHD-C4C-NC  | 3.13  | 129.14      | 124.20   |
| 36  | L     | 304 | LUT  | C18-C5-C4   | -3.13 | 108.55      | 114.36   |
| 31  | B     | 848 | CLA  | CHA-C4D-ND  | 3.13  | 139.05      | 132.50   |
| 26  | 3     | 301 | BCR  | C3-C4-C5    | -3.13 | 108.49      | 114.08   |
| 31  | B     | 848 | CLA  | C4D-CHA-C1A | -3.13 | 117.44      | 121.25   |
| 31  | 2     | 313 | CLA  | O2D-CGD-O1D | -3.13 | 117.72      | 123.84   |
| 31  | 8     | 307 | CLA  | CHD-C4C-NC  | 3.13  | 129.13      | 124.20   |
| 31  | B     | 821 | CLA  | O1D-CGD-CBD | -3.13 | 118.08      | 124.48   |
| 32  | b     | 309 | CHL  | C4D-C3D-CAD | 3.13  | 111.78      | 108.10   |
| 32  | 5     | 316 | CHL  | C1-C2-C3    | -3.13 | 120.64      | 126.04   |
| 31  | 9     | 318 | CLA  | O2D-CGD-O1D | -3.13 | 117.73      | 123.84   |
| 31  | A     | 820 | CLA  | CMB-C2B-C3B | 3.13  | 130.53      | 124.68   |
| 32  | b     | 309 | CHL  | O2D-CGD-O1D | -3.13 | 117.73      | 123.84   |
| 32  | 7     | 319 | CHL  | C4D-C3D-CAD | 3.12  | 111.78      | 108.10   |
| 31  | B     | 812 | CLA  | C3D-C2D-C1D | -3.12 | 101.57      | 105.83   |
| 31  | a     | 309 | CLA  | O2A-CGA-CBA | 3.12  | 121.71      | 111.91   |
| 31  | 7     | 322 | CLA  | CHD-C4C-NC  | 3.12  | 129.12      | 124.20   |
| 32  | 3     | 315 | CHL  | C4-C3-C5    | 3.12  | 120.52      | 115.27   |
| 31  | K     | 206 | CLA  | CHD-C4C-NC  | 3.12  | 129.12      | 124.20   |
| 32  | 6     | 319 | CHL  | CHD-C4C-C3C | -3.12 | 120.25      | 124.84   |
| 36  | 5     | 303 | LUT  | C10-C11-C12 | -3.12 | 113.48      | 123.22   |
| 31  | A     | 826 | CLA  | O2D-CGD-CBD | 3.12  | 116.81      | 111.27   |
| 31  | B     | 822 | CLA  | C4D-CHA-C1A | -3.12 | 117.45      | 121.25   |
| 31  | 5     | 308 | CLA  | C4D-CHA-C1A | -3.12 | 117.45      | 121.25   |
| 32  | 8     | 319 | CHL  | C4D-CHA-C1A | -3.12 | 117.45      | 121.25   |
| 31  | 6     | 310 | CLA  | C4D-CHA-C1A | -3.12 | 117.45      | 121.25   |
| 32  | 6     | 319 | CHL  | C3D-C2D-C1D | -3.12 | 101.58      | 105.83   |
| 36  | J     | 103 | LUT  | C1-C6-C5    | -3.12 | 118.22      | 122.61   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 307 | CLA  | CHD-C4C-NC  | 3.12  | 129.11      | 124.20   |
| 31  | A     | 827 | CLA  | C1-C2-C3    | -3.11 | 120.66      | 126.04   |
| 31  | 7     | 313 | CLA  | CHD-C4C-NC  | 3.11  | 129.11      | 124.20   |
| 31  | B     | 812 | CLA  | O2A-CGA-CBA | 3.11  | 121.68      | 111.91   |
| 31  | B     | 833 | CLA  | O2D-CGD-O1D | -3.11 | 117.75      | 123.84   |
| 31  | 8     | 315 | CLA  | O1D-CGD-CBD | -3.11 | 118.12      | 124.48   |
| 32  | 5     | 317 | CHL  | C3D-C2D-C1D | -3.11 | 101.58      | 105.83   |
| 32  | 5     | 319 | CHL  | CHD-C1D-ND  | -3.11 | 121.59      | 124.45   |
| 32  | a     | 320 | CHL  | O2D-CGD-O1D | -3.11 | 117.76      | 123.84   |
| 31  | B     | 840 | CLA  | CHA-C4D-ND  | 3.11  | 139.01      | 132.50   |
| 31  | 2     | 315 | CLA  | CHD-C4C-NC  | 3.11  | 129.10      | 124.20   |
| 31  | A     | 856 | CLA  | CHD-C4C-NC  | 3.11  | 129.10      | 124.20   |
| 31  | A     | 854 | CLA  | O1D-CGD-CBD | -3.11 | 118.13      | 124.48   |
| 31  | A     | 822 | CLA  | C3D-C2D-C1D | -3.11 | 101.59      | 105.83   |
| 26  | 2     | 302 | BCR  | C11-C10-C9  | -3.11 | 122.88      | 127.31   |
| 31  | 5     | 311 | CLA  | CHD-C4C-NC  | 3.11  | 129.10      | 124.20   |
| 31  | B     | 850 | CLA  | C1C-C2C-C3C | -3.10 | 103.69      | 106.96   |
| 31  | G     | 204 | CLA  | O2D-CGD-O1D | -3.10 | 117.77      | 123.84   |
| 31  | 3     | 312 | CLA  | O1D-CGD-CBD | -3.10 | 118.13      | 124.48   |
| 36  | 9     | 305 | LUT  | C21-C26-C25 | 3.10  | 116.98      | 111.42   |
| 32  | 5     | 316 | CHL  | C3D-C2D-C1D | -3.10 | 101.59      | 105.83   |
| 31  | 5     | 323 | CLA  | CHD-C4C-NC  | 3.10  | 129.09      | 124.20   |
| 31  | b     | 303 | CLA  | CHD-C4C-C3C | -3.10 | 120.28      | 124.84   |
| 31  | 2     | 305 | CLA  | CHD-C4C-NC  | 3.10  | 129.09      | 124.20   |
| 31  | A     | 856 | CLA  | C3D-C2D-C1D | -3.10 | 101.60      | 105.83   |
| 31  | 8     | 312 | CLA  | CHD-C1D-ND  | -3.10 | 121.61      | 124.45   |
| 31  | A     | 845 | CLA  | C3D-C2D-C1D | -3.10 | 101.61      | 105.83   |
| 31  | B     | 813 | CLA  | C3D-C2D-C1D | -3.10 | 101.61      | 105.83   |
| 31  | B     | 847 | CLA  | CHA-C4D-ND  | 3.10  | 138.98      | 132.50   |
| 31  | 3     | 319 | CLA  | C1-C2-C3    | -3.10 | 120.69      | 126.04   |
| 32  | 4     | 317 | CHL  | O2D-CGD-O1D | -3.09 | 117.79      | 123.84   |
| 31  | 5     | 310 | CLA  | O1D-CGD-CBD | -3.09 | 118.15      | 124.48   |
| 31  | A     | 853 | CLA  | CHA-C4D-ND  | 3.09  | 138.97      | 132.50   |
| 31  | B     | 815 | CLA  | CHD-C4C-NC  | 3.09  | 129.08      | 124.20   |
| 36  | J     | 103 | LUT  | C17-C1-C6   | -3.09 | 105.28      | 110.30   |
| 36  | a     | 303 | LUT  | C17-C1-C6   | -3.09 | 105.28      | 110.30   |
| 31  | 8     | 315 | CLA  | C4-C3-C5    | 3.09  | 120.47      | 115.27   |
| 32  | 5     | 316 | CHL  | C4D-C3D-CAD | 3.09  | 111.74      | 108.10   |
| 31  | 8     | 310 | CLA  | C3D-C2D-C1D | -3.09 | 101.61      | 105.83   |
| 31  | 3     | 311 | CLA  | CMB-C2B-C3B | 3.09  | 130.46      | 124.68   |
| 31  | B     | 848 | CLA  | C3D-C2D-C1D | -3.09 | 101.61      | 105.83   |
| 31  | 3     | 310 | CLA  | CHA-C4D-ND  | 3.09  | 138.96      | 132.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 311 | CLA  | CMB-C2B-C3B | 3.09  | 130.46      | 124.68   |
| 31  | A     | 817 | CLA  | C3D-C2D-C1D | -3.09 | 101.61      | 105.83   |
| 31  | B     | 813 | CLA  | O2A-CGA-CBA | 3.09  | 121.60      | 111.91   |
| 36  | 5     | 303 | LUT  | C18-C5-C4   | -3.09 | 108.63      | 114.36   |
| 31  | B     | 820 | CLA  | O1D-CGD-CBD | -3.09 | 118.17      | 124.48   |
| 32  | 7     | 324 | CHL  | C1-C2-C3    | -3.09 | 120.70      | 126.04   |
| 40  | 7     | 306 | XAT  | C40-C33-C34 | -3.09 | 118.60      | 122.92   |
| 31  | B     | 845 | CLA  | C4D-CHA-C1A | -3.09 | 117.49      | 121.25   |
| 31  | 4     | 306 | CLA  | O2D-CGD-O1D | -3.09 | 117.80      | 123.84   |
| 32  | 7     | 324 | CHL  | CHD-C4C-NC  | 3.09  | 129.07      | 124.20   |
| 31  | 5     | 315 | CLA  | CHD-C4C-NC  | 3.09  | 129.06      | 124.20   |
| 31  | B     | 846 | CLA  | O2D-CGD-O1D | -3.08 | 117.81      | 123.84   |
| 31  | 2     | 309 | CLA  | C4D-CHA-C1A | -3.08 | 117.50      | 121.25   |
| 30  | A     | 813 | CL0  | CBC-CAC-C3C | -3.08 | 103.93      | 112.43   |
| 31  | 7     | 312 | CLA  | CMB-C2B-C3B | 3.08  | 130.45      | 124.68   |
| 31  | 4     | 309 | CLA  | CHD-C4C-NC  | 3.08  | 129.06      | 124.20   |
| 31  | A     | 822 | CLA  | C4D-CHA-C1A | -3.08 | 117.50      | 121.25   |
| 31  | 6     | 315 | CLA  | CHD-C4C-NC  | 3.08  | 129.06      | 124.20   |
| 31  | A     | 825 | CLA  | CMB-C2B-C3B | 3.08  | 130.44      | 124.68   |
| 31  | 6     | 311 | CLA  | CAC-C3C-C4C | 3.08  | 128.80      | 124.81   |
| 32  | K     | 201 | CHL  | CHB-C4A-NA  | 3.08  | 128.77      | 124.51   |
| 32  | K     | 201 | CHL  | C2A-C1A-CHA | -3.08 | 118.48      | 123.86   |
| 31  | A     | 818 | CLA  | O2A-CGA-CBA | 3.08  | 121.56      | 111.91   |
| 31  | 3     | 318 | CLA  | C4-C3-C5    | 3.08  | 119.50      | 115.98   |
| 31  | O     | 203 | CLA  | O2A-CGA-CBA | 3.07  | 121.56      | 111.91   |
| 31  | A     | 828 | CLA  | CHD-C4C-NC  | 3.07  | 129.05      | 124.20   |
| 26  | L     | 303 | BCR  | C2-C1-C6    | 3.07  | 115.21      | 110.48   |
| 31  | A     | 853 | CLA  | O2A-CGA-CBA | 3.07  | 121.55      | 111.91   |
| 31  | a     | 316 | CLA  | CHD-C4C-NC  | 3.07  | 129.04      | 124.20   |
| 31  | G     | 206 | CLA  | CHD-C4C-NC  | 3.07  | 129.04      | 124.20   |
| 31  | 5     | 311 | CLA  | CMB-C2B-C3B | 3.07  | 130.42      | 124.68   |
| 31  | 7     | 316 | CLA  | CHD-C4C-NC  | 3.07  | 129.04      | 124.20   |
| 31  | 5     | 320 | CLA  | CHD-C4C-NC  | 3.07  | 129.04      | 124.20   |
| 31  | B     | 826 | CLA  | O1D-CGD-CBD | -3.07 | 118.20      | 124.48   |
| 31  | 3     | 310 | CLA  | O2D-CGD-O1D | -3.07 | 117.84      | 123.84   |
| 31  | A     | 826 | CLA  | C4-C3-C5    | 3.07  | 120.43      | 115.27   |
| 31  | 4     | 321 | CLA  | CHD-C4C-NC  | 3.07  | 129.03      | 124.20   |
| 31  | 9     | 311 | CLA  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |
| 31  | A     | 818 | CLA  | CHD-C4C-NC  | 3.06  | 129.03      | 124.20   |
| 31  | b     | 308 | CLA  | CAC-C3C-C4C | 3.06  | 128.79      | 124.81   |
| 31  | 3     | 316 | CLA  | CHD-C4C-NC  | 3.06  | 129.03      | 124.20   |
| 31  | 7     | 311 | CLA  | O1D-CGD-CBD | -3.06 | 118.22      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 849 | CLA  | C4D-CHA-C1A | -3.06 | 117.52      | 121.25   |
| 36  | 9     | 303 | LUT  | C18-C5-C4   | -3.06 | 108.68      | 114.36   |
| 31  | A     | 815 | CLA  | C3D-C2D-C1D | -3.06 | 101.65      | 105.83   |
| 31  | B     | 817 | CLA  | CHA-C4D-ND  | 3.06  | 138.91      | 132.50   |
| 31  | B     | 819 | CLA  | CMD-C2D-C1D | 3.06  | 130.11      | 124.71   |
| 31  | A     | 847 | CLA  | C3D-C2D-C1D | -3.06 | 101.65      | 105.83   |
| 31  | A     | 820 | CLA  | C3D-C2D-C1D | -3.06 | 101.65      | 105.83   |
| 36  | 3     | 304 | LUT  | C18-C5-C4   | -3.06 | 108.69      | 114.36   |
| 31  | B     | 833 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 31  | A     | 854 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 31  | A     | 835 | CLA  | CAC-C3C-C4C | 3.06  | 128.78      | 124.81   |
| 31  | 8     | 318 | CLA  | CHD-C4C-NC  | 3.06  | 129.02      | 124.20   |
| 31  | H     | 901 | CLA  | O2D-CGD-O1D | -3.06 | 117.86      | 123.84   |
| 32  | 4     | 310 | CHL  | CHD-C4C-C3C | -3.06 | 120.35      | 124.84   |
| 31  | B     | 824 | CLA  | C4D-CHA-C1A | -3.06 | 117.53      | 121.25   |
| 31  | 4     | 306 | CLA  | CHD-C4C-NC  | 3.05  | 129.02      | 124.20   |
| 31  | B     | 840 | CLA  | C3D-C2D-C1D | -3.05 | 101.66      | 105.83   |
| 31  | A     | 823 | CLA  | CMB-C2B-C3B | 3.05  | 130.39      | 124.68   |
| 32  | 6     | 317 | CHL  | C4D-CHA-C1A | -3.05 | 117.53      | 121.25   |
| 32  | A     | 831 | CHL  | CAC-C3C-C4C | 3.05  | 128.77      | 124.81   |
| 31  | B     | 822 | CLA  | C4-C3-C5    | 3.05  | 120.41      | 115.27   |
| 32  | 9     | 322 | CHL  | CHD-C4C-C3C | -3.05 | 120.35      | 124.84   |
| 31  | 9     | 313 | CLA  | CHD-C4C-NC  | 3.05  | 129.01      | 124.20   |
| 31  | b     | 304 | CLA  | O2D-CGD-O1D | -3.05 | 117.87      | 123.84   |
| 31  | 7     | 316 | CLA  | C4D-CHA-C1A | -3.05 | 117.54      | 121.25   |
| 31  | B     | 850 | CLA  | C3D-C2D-C1D | -3.05 | 101.67      | 105.83   |
| 26  | 7     | 304 | BCR  | C28-C27-C26 | -3.05 | 108.63      | 114.08   |
| 31  | B     | 837 | CLA  | CAC-C3C-C4C | 3.05  | 128.76      | 124.81   |
| 31  | B     | 839 | CLA  | CHA-C4D-ND  | 3.05  | 138.88      | 132.50   |
| 36  | 3     | 304 | LUT  | C30-C31-C32 | -3.05 | 113.71      | 123.22   |
| 31  | A     | 841 | CLA  | C6-C5-C3    | -3.05 | 105.47      | 113.45   |
| 31  | A     | 815 | CLA  | C1-C2-C3    | -3.05 | 120.77      | 126.04   |
| 31  | 7     | 309 | CLA  | C1-C2-C3    | -3.05 | 120.77      | 126.04   |
| 31  | A     | 828 | CLA  | O1D-CGD-CBD | -3.05 | 118.25      | 124.48   |
| 31  | F     | 306 | CLA  | C3D-C2D-C1D | -3.05 | 101.67      | 105.83   |
| 31  | 2     | 309 | CLA  | CHD-C4C-NC  | 3.05  | 129.00      | 124.20   |
| 31  | 5     | 309 | CLA  | O2D-CGD-O1D | -3.05 | 117.88      | 123.84   |
| 31  | A     | 818 | CLA  | C4-C3-C5    | 3.04  | 120.39      | 115.27   |
| 36  | 5     | 303 | LUT  | C21-C26-C27 | -3.04 | 108.85      | 112.70   |
| 31  | A     | 832 | CLA  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 31  | 5     | 310 | CLA  | CHD-C1D-ND  | -3.04 | 121.66      | 124.45   |
| 31  | A     | 837 | CLA  | CHD-C4C-NC  | 3.04  | 129.00      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 851 | CLA  | C4D-CHA-C1A | -3.04 | 117.55      | 121.25   |
| 32  | 8     | 316 | CHL  | C3D-C2D-C1D | -3.04 | 101.68      | 105.83   |
| 31  | A     | 823 | CLA  | O1D-CGD-CBD | -3.04 | 118.26      | 124.48   |
| 31  | B     | 849 | CLA  | C1-C2-C3    | -3.04 | 121.83      | 126.75   |
| 31  | 6     | 313 | CLA  | CMB-C2B-C3B | 3.04  | 130.37      | 124.68   |
| 31  | 4     | 316 | CLA  | CHA-C4D-ND  | 3.04  | 138.86      | 132.50   |
| 32  | 7     | 318 | CHL  | C4D-C3D-CAD | 3.04  | 111.68      | 108.10   |
| 32  | b     | 309 | CHL  | CHD-C4C-NC  | 3.04  | 128.99      | 124.20   |
| 31  | B     | 834 | CLA  | O1D-CGD-CBD | -3.04 | 118.27      | 124.48   |
| 31  | A     | 849 | CLA  | CHD-C4C-NC  | 3.04  | 128.99      | 124.20   |
| 31  | b     | 313 | CLA  | CMB-C2B-C3B | 3.04  | 130.36      | 124.68   |
| 36  | a     | 303 | LUT  | C12-C13-C14 | -3.03 | 114.28      | 118.94   |
| 31  | A     | 838 | CLA  | O2D-CGD-O1D | -3.03 | 117.91      | 123.84   |
| 36  | b     | 301 | LUT  | C18-C5-C4   | -3.03 | 108.74      | 114.36   |
| 31  | A     | 821 | CLA  | C3D-C2D-C1D | -3.03 | 101.69      | 105.83   |
| 31  | 2     | 306 | CLA  | CHD-C4C-NC  | 3.03  | 128.98      | 124.20   |
| 31  | L     | 307 | CLA  | CHD-C4C-C3C | -3.03 | 120.38      | 124.84   |
| 31  | B     | 818 | CLA  | C3D-C2D-C1D | -3.03 | 101.69      | 105.83   |
| 31  | B     | 850 | CLA  | CHD-C1D-ND  | -3.03 | 121.67      | 124.45   |
| 31  | B     | 816 | CLA  | CMC-C2C-C1C | 3.03  | 129.65      | 125.04   |
| 31  | 3     | 319 | CLA  | CHA-C4D-ND  | 3.03  | 138.84      | 132.50   |
| 31  | 9     | 318 | CLA  | CHC-C1C-NC  | -3.03 | 119.61      | 124.20   |
| 31  | B     | 845 | CLA  | O2A-CGA-CBA | 3.03  | 121.41      | 111.91   |
| 31  | 3     | 320 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 31  | 4     | 309 | CLA  | O1D-CGD-CBD | -3.03 | 118.29      | 124.48   |
| 31  | B     | 823 | CLA  | O1D-CGD-CBD | -3.03 | 118.29      | 124.48   |
| 31  | 9     | 311 | CLA  | O2A-CGA-CBA | 3.03  | 121.40      | 111.91   |
| 31  | 6     | 311 | CLA  | O1D-CGD-CBD | -3.02 | 118.30      | 124.48   |
| 32  | b     | 309 | CHL  | C4D-CHA-C1A | -3.02 | 117.57      | 121.25   |
| 31  | O     | 202 | CLA  | C4C-C3C-C2C | -3.02 | 104.30      | 107.07   |
| 32  | 6     | 317 | CHL  | C4D-C3D-CAD | 3.02  | 111.66      | 108.10   |
| 36  | 3     | 305 | LUT  | C2-C3-C4    | 3.02  | 114.44      | 110.30   |
| 36  | 4     | 303 | LUT  | C2-C3-C4    | 3.02  | 114.44      | 110.30   |
| 31  | A     | 853 | CLA  | C3D-C2D-C1D | -3.02 | 101.71      | 105.83   |
| 31  | 3     | 318 | CLA  | CAA-C2A-C3A | -3.02 | 104.51      | 112.78   |
| 31  | B     | 841 | CLA  | CMB-C2B-C3B | 3.02  | 130.33      | 124.68   |
| 31  | A     | 818 | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 31  | 6     | 310 | CLA  | CHC-C1C-NC  | -3.02 | 119.62      | 124.20   |
| 31  | A     | 819 | CLA  | C3D-C2D-C1D | -3.02 | 101.71      | 105.83   |
| 26  | 3     | 303 | BCR  | C11-C10-C9  | -3.02 | 123.00      | 127.31   |
| 31  | B     | 812 | CLA  | O2D-CGD-O1D | -3.02 | 117.94      | 123.84   |
| 31  | 9     | 313 | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 849 | CLA  | CHD-C4C-NC  | 3.01  | 128.95      | 124.20   |
| 31  | 9     | 315 | CLA  | C3D-C2D-C1D | -3.01 | 101.72      | 105.83   |
| 32  | A     | 831 | CHL  | C3D-C2D-C1D | -3.01 | 101.72      | 105.83   |
| 31  | 4     | 316 | CLA  | CHC-C1C-NC  | -3.01 | 119.63      | 124.20   |
| 32  | 9     | 320 | CHL  | CHD-C4C-NC  | 3.01  | 128.95      | 124.20   |
| 32  | 6     | 309 | CHL  | CHD-C4C-NC  | 3.01  | 128.95      | 124.20   |
| 31  | F     | 305 | CLA  | CED-O2D-CGD | 3.01  | 122.75      | 115.94   |
| 31  | B     | 826 | CLA  | CMB-C2B-C3B | 3.01  | 130.31      | 124.68   |
| 36  | 5     | 304 | LUT  | C17-C1-C6   | -3.01 | 105.42      | 110.30   |
| 31  | A     | 815 | CLA  | CAC-C3C-C4C | 3.01  | 128.71      | 124.81   |
| 31  | B     | 841 | CLA  | C3D-C2D-C1D | -3.01 | 101.72      | 105.83   |
| 31  | B     | 841 | CLA  | CHA-C4D-ND  | 3.01  | 138.79      | 132.50   |
| 31  | B     | 816 | CLA  | C3D-C2D-C1D | -3.01 | 101.73      | 105.83   |
| 31  | 6     | 307 | CLA  | C1-C2-C3    | -3.01 | 121.89      | 126.75   |
| 31  | A     | 824 | CLA  | CHD-C4C-C3C | -3.01 | 120.42      | 124.84   |
| 32  | 9     | 320 | CHL  | C3D-C2D-C1D | -3.01 | 101.73      | 105.83   |
| 31  | 3     | 319 | CLA  | O2A-CGA-CBA | 3.01  | 121.34      | 111.91   |
| 31  | B     | 820 | CLA  | C4-C3-C5    | 3.01  | 120.33      | 115.27   |
| 31  | A     | 842 | CLA  | C1-C2-C3    | -3.01 | 120.84      | 126.04   |
| 31  | 9     | 312 | CLA  | O2D-CGD-O1D | -3.00 | 117.96      | 123.84   |
| 32  | 6     | 318 | CHL  | C3D-C2D-C1D | -3.00 | 101.73      | 105.83   |
| 31  | A     | 824 | CLA  | CMB-C2B-C3B | 3.00  | 130.30      | 124.68   |
| 31  | 5     | 315 | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 31  | a     | 312 | CLA  | CMB-C2B-C3B | 3.00  | 130.29      | 124.68   |
| 31  | 3     | 319 | CLA  | C3D-C2D-C1D | -3.00 | 101.73      | 105.83   |
| 32  | 4     | 310 | CHL  | CMD-C2D-C1D | 3.00  | 130.00      | 124.71   |
| 31  | a     | 319 | CLA  | CHD-C4C-NC  | 3.00  | 128.93      | 124.20   |
| 36  | a     | 303 | LUT  | C18-C5-C4   | -3.00 | 108.80      | 114.36   |
| 32  | 6     | 320 | CHL  | CHC-C1C-NC  | -3.00 | 119.65      | 124.20   |
| 26  | L     | 301 | BCR  | C2-C1-C6    | 3.00  | 115.10      | 110.48   |
| 31  | 7     | 312 | CLA  | C4-C3-C5    | 3.00  | 120.31      | 115.27   |
| 31  | B     | 831 | CLA  | C3D-C2D-C1D | -3.00 | 101.74      | 105.83   |
| 31  | 8     | 311 | CLA  | C3D-C2D-C1D | -3.00 | 101.74      | 105.83   |
| 31  | B     | 848 | CLA  | CMB-C2B-C3B | 3.00  | 130.28      | 124.68   |
| 31  | B     | 830 | CLA  | CHD-C1D-ND  | -2.99 | 121.70      | 124.45   |
| 31  | A     | 835 | CLA  | C3D-C2D-C1D | -2.99 | 101.75      | 105.83   |
| 31  | 3     | 313 | CLA  | C4-C3-C5    | 2.99  | 120.31      | 115.27   |
| 31  | B     | 842 | CLA  | CHD-C4C-NC  | 2.99  | 128.92      | 124.20   |
| 31  | 2     | 308 | CLA  | C3D-C2D-C1D | -2.99 | 101.75      | 105.83   |
| 31  | B     | 834 | CLA  | C4C-C3C-C2C | -2.99 | 102.54      | 106.90   |
| 31  | a     | 311 | CLA  | CHB-C4A-NA  | 2.99  | 128.65      | 124.51   |
| 31  | a     | 322 | CLA  | CHD-C4C-NC  | 2.99  | 128.91      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 307 | CLA  | O2A-CGA-CBA | 2.99  | 121.29      | 111.91   |
| 31  | 4     | 316 | CLA  | CHD-C4C-C3C | -2.99 | 120.45      | 124.84   |
| 31  | a     | 319 | CLA  | C4-C3-C5    | 2.99  | 120.30      | 115.27   |
| 31  | A     | 854 | CLA  | C3D-C2D-C1D | -2.99 | 101.75      | 105.83   |
| 32  | 5     | 319 | CHL  | C3D-C2D-C1D | -2.99 | 101.75      | 105.83   |
| 32  | a     | 320 | CHL  | C3D-C2D-C1D | -2.99 | 101.76      | 105.83   |
| 32  | b     | 309 | CHL  | C3D-C2D-C1D | -2.99 | 101.76      | 105.83   |
| 31  | 3     | 307 | CLA  | CMC-C2C-C1C | 2.99  | 129.59      | 125.04   |
| 31  | A     | 818 | CLA  | CHA-C4D-ND  | 2.98  | 138.74      | 132.50   |
| 31  | A     | 842 | CLA  | C3D-C2D-C1D | -2.98 | 101.76      | 105.83   |
| 31  | A     | 826 | CLA  | CHD-C4C-NC  | 2.98  | 128.90      | 124.20   |
| 31  | B     | 827 | CLA  | C4-C3-C5    | 2.98  | 120.29      | 115.27   |
| 32  | 5     | 319 | CHL  | C4D-C3D-CAD | 2.98  | 111.61      | 108.10   |
| 31  | 9     | 314 | CLA  | CMB-C2B-C3B | 2.98  | 130.26      | 124.68   |
| 31  | B     | 823 | CLA  | CHD-C4C-NC  | 2.98  | 128.90      | 124.20   |
| 26  | L     | 303 | BCR  | C24-C23-C22 | -2.98 | 121.74      | 126.23   |
| 32  | A     | 840 | CHL  | CHD-C4C-NC  | 2.98  | 128.89      | 124.20   |
| 31  | 8     | 313 | CLA  | C3D-C2D-C1D | -2.98 | 101.77      | 105.83   |
| 31  | H     | 903 | CLA  | CHD-C4C-NC  | 2.98  | 128.89      | 124.20   |
| 31  | L     | 305 | CLA  | CHA-C4D-ND  | 2.98  | 138.72      | 132.50   |
| 31  | 5     | 321 | CLA  | CHC-C1C-NC  | -2.97 | 119.69      | 124.20   |
| 26  | O     | 201 | BCR  | C3-C4-C5    | -2.97 | 108.77      | 114.08   |
| 31  | 8     | 311 | CLA  | CHD-C4C-NC  | 2.97  | 128.89      | 124.20   |
| 31  | A     | 835 | CLA  | O1D-CGD-CBD | -2.97 | 118.40      | 124.48   |
| 31  | B     | 811 | CLA  | C4-C3-C5    | 2.97  | 120.27      | 115.27   |
| 31  | 3     | 319 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 32  | 6     | 320 | CHL  | C3D-C2D-C1D | -2.97 | 101.78      | 105.83   |
| 31  | 4     | 320 | CLA  | CHD-C4C-NC  | 2.97  | 128.89      | 124.20   |
| 31  | B     | 848 | CLA  | C1-C2-C3    | -2.97 | 120.91      | 126.04   |
| 32  | 7     | 318 | CHL  | C3D-C2D-C1D | -2.97 | 101.78      | 105.83   |
| 31  | K     | 204 | CLA  | O2A-CGA-CBA | 2.97  | 121.23      | 111.91   |
| 31  | B     | 829 | CLA  | C4-C3-C5    | 2.97  | 120.27      | 115.27   |
| 31  | B     | 830 | CLA  | CHD-C4C-NC  | 2.97  | 128.88      | 124.20   |
| 31  | b     | 311 | CLA  | O2D-CGD-O1D | -2.97 | 118.04      | 123.84   |
| 31  | 8     | 309 | CLA  | C3D-C2D-C1D | -2.96 | 101.78      | 105.83   |
| 32  | A     | 840 | CHL  | CGD-CBD-CAD | 2.96  | 120.34      | 110.73   |
| 31  | b     | 312 | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 32  | 7     | 319 | CHL  | CMB-C2B-C3B | 2.96  | 130.22      | 124.68   |
| 31  | B     | 815 | CLA  | C1-C2-C3    | -2.96 | 120.92      | 126.04   |
| 31  | 2     | 310 | CLA  | CHD-C4C-NC  | 2.96  | 128.87      | 124.20   |
| 31  | 7     | 321 | CLA  | C3D-C2D-C1D | -2.96 | 101.79      | 105.83   |
| 31  | 2     | 306 | CLA  | O2A-CGA-CBA | 2.96  | 121.21      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 5     | 316 | CHL  | C2C-C3C-C4C | -2.96 | 104.38      | 106.49   |
| 31  | 6     | 308 | CLA  | C3D-C2D-C1D | -2.96 | 101.79      | 105.83   |
| 31  | 9     | 315 | CLA  | O1D-CGD-CBD | -2.96 | 118.43      | 124.48   |
| 32  | 5     | 317 | CHL  | C4D-CHA-C1A | -2.96 | 117.65      | 121.25   |
| 31  | A     | 841 | CLA  | CMB-C2B-C3B | 2.96  | 130.22      | 124.68   |
| 31  | 7     | 309 | CLA  | CMB-C2B-C3B | 2.96  | 130.22      | 124.68   |
| 31  | B     | 812 | CLA  | C1-C2-C3    | -2.96 | 120.92      | 126.04   |
| 36  | 3     | 304 | LUT  | C12-C13-C14 | -2.96 | 114.40      | 118.94   |
| 32  | 9     | 322 | CHL  | C4D-CHA-C1A | -2.96 | 117.65      | 121.25   |
| 31  | A     | 837 | CLA  | CAC-C3C-C4C | 2.96  | 128.65      | 124.81   |
| 31  | B     | 823 | CLA  | C4-C3-C5    | 2.96  | 120.25      | 115.27   |
| 31  | A     | 844 | CLA  | CHD-C4C-NC  | 2.96  | 128.86      | 124.20   |
| 36  | 8     | 302 | LUT  | C10-C11-C12 | -2.96 | 113.99      | 123.22   |
| 31  | a     | 309 | CLA  | C1-C2-C3    | -2.96 | 120.93      | 126.04   |
| 31  | a     | 321 | CLA  | C4D-CHA-C1A | -2.95 | 117.65      | 121.25   |
| 31  | B     | 827 | CLA  | C3D-C2D-C1D | -2.95 | 101.80      | 105.83   |
| 32  | 6     | 317 | CHL  | C3D-C2D-C1D | -2.95 | 101.80      | 105.83   |
| 36  | 9     | 305 | LUT  | C17-C1-C6   | -2.95 | 105.51      | 110.30   |
| 31  | 7     | 321 | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 31  | A     | 837 | CLA  | C3D-C2D-C1D | -2.95 | 101.81      | 105.83   |
| 31  | A     | 855 | CLA  | C3D-C2D-C1D | -2.95 | 101.81      | 105.83   |
| 32  | 8     | 319 | CHL  | C3D-C2D-C1D | -2.95 | 101.81      | 105.83   |
| 32  | 5     | 322 | CHL  | CHD-C4C-NC  | 2.95  | 128.85      | 124.20   |
| 31  | A     | 814 | CLA  | CMB-C2B-C3B | 2.95  | 130.19      | 124.68   |
| 36  | J     | 103 | LUT  | C21-C26-C27 | -2.94 | 108.98      | 112.70   |
| 31  | B     | 844 | CLA  | C3D-C2D-C1D | -2.94 | 101.81      | 105.83   |
| 31  | 3     | 319 | CLA  | CAA-C2A-C1A | -2.94 | 102.33      | 111.97   |
| 31  | 8     | 308 | CLA  | CHD-C4C-NC  | 2.94  | 128.84      | 124.20   |
| 31  | A     | 836 | CLA  | C3D-C2D-C1D | -2.94 | 101.81      | 105.83   |
| 31  | 5     | 311 | CLA  | C3D-C2D-C1D | -2.94 | 101.81      | 105.83   |
| 36  | 6     | 304 | LUT  | C35-C15-C14 | -2.94 | 117.45      | 123.47   |
| 36  | 5     | 303 | LUT  | C8-C7-C6    | -2.94 | 118.94      | 127.20   |
| 31  | G     | 205 | CLA  | CMB-C2B-C3B | 2.94  | 130.18      | 124.68   |
| 31  | B     | 817 | CLA  | O2A-CGA-CBA | 2.94  | 121.14      | 111.91   |
| 31  | a     | 316 | CLA  | O1D-CGD-CBD | -2.94 | 118.47      | 124.48   |
| 36  | 3     | 305 | LUT  | C12-C13-C14 | -2.94 | 114.43      | 118.94   |
| 31  | B     | 829 | CLA  | C4D-CHA-C1A | -2.94 | 117.67      | 121.25   |
| 31  | B     | 833 | CLA  | C3D-C2D-C1D | -2.94 | 101.82      | 105.83   |
| 31  | 8     | 321 | CLA  | C3D-C2D-C1D | -2.94 | 101.82      | 105.83   |
| 26  | 2     | 302 | BCR  | C15-C16-C17 | -2.94 | 117.45      | 123.47   |
| 31  | 3     | 313 | CLA  | CHD-C4C-NC  | 2.94  | 128.83      | 124.20   |
| 32  | 7     | 320 | CHL  | O2A-CGA-CBA | 2.94  | 121.13      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 842 | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 31  | B     | 835 | CLA  | C3D-C2D-C1D | -2.94 | 101.82      | 105.83   |
| 31  | A     | 833 | CLA  | CHD-C4C-NC  | 2.94  | 128.83      | 124.20   |
| 31  | B     | 839 | CLA  | C1-C2-C3    | -2.94 | 120.97      | 126.04   |
| 32  | 7     | 320 | CHL  | CHD-C4C-NC  | 2.94  | 128.83      | 124.20   |
| 31  | A     | 845 | CLA  | C4D-CHA-C1A | -2.94 | 117.68      | 121.25   |
| 36  | 3     | 305 | LUT  | C30-C31-C32 | -2.93 | 114.06      | 123.22   |
| 31  | 6     | 306 | CLA  | CHD-C4C-C3C | -2.93 | 120.53      | 124.84   |
| 36  | 5     | 304 | LUT  | C8-C7-C6    | -2.93 | 118.96      | 127.20   |
| 31  | A     | 817 | CLA  | CMB-C2B-C3B | 2.93  | 130.17      | 124.68   |
| 31  | B     | 812 | CLA  | CHA-C4D-ND  | 2.93  | 138.63      | 132.50   |
| 31  | 6     | 307 | CLA  | O1D-CGD-CBD | -2.93 | 118.48      | 124.48   |
| 31  | 5     | 323 | CLA  | C3D-C2D-C1D | -2.93 | 101.83      | 105.83   |
| 31  | A     | 841 | CLA  | O2A-CGA-CBA | 2.93  | 121.11      | 111.91   |
| 31  | 6     | 315 | CLA  | CHC-C1C-NC  | -2.93 | 119.76      | 124.20   |
| 32  | a     | 318 | CHL  | C3D-C2D-C1D | -2.93 | 101.83      | 105.83   |
| 31  | O     | 203 | CLA  | C4D-CHA-C1A | -2.93 | 117.68      | 121.25   |
| 31  | 5     | 321 | CLA  | CHD-C1D-ND  | -2.93 | 121.76      | 124.45   |
| 31  | 5     | 312 | CLA  | CHD-C4C-NC  | 2.93  | 128.82      | 124.20   |
| 31  | B     | 821 | CLA  | CHD-C4C-NC  | 2.93  | 128.82      | 124.20   |
| 31  | 2     | 308 | CLA  | CMB-C2B-C3B | 2.93  | 130.15      | 124.68   |
| 31  | A     | 854 | CLA  | CHD-C4C-NC  | 2.93  | 128.81      | 124.20   |
| 31  | G     | 204 | CLA  | CAC-C3C-C4C | 2.93  | 128.61      | 124.81   |
| 31  | L     | 305 | CLA  | C1-C2-C3    | -2.93 | 120.98      | 126.04   |
| 31  | G     | 206 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 32  | 6     | 309 | CHL  | O2A-CGA-CBA | 2.92  | 121.08      | 111.91   |
| 31  | B     | 820 | CLA  | C1-C2-C3    | -2.92 | 120.99      | 126.04   |
| 31  | A     | 828 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 31  | 8     | 318 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 31  | 9     | 319 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 36  | 8     | 303 | LUT  | C30-C31-C32 | -2.92 | 114.09      | 123.22   |
| 31  | A     | 827 | CLA  | O1D-CGD-CBD | -2.92 | 118.50      | 124.48   |
| 31  | 4     | 319 | CLA  | CHD-C4C-NC  | 2.92  | 128.81      | 124.20   |
| 36  | 6     | 304 | LUT  | C4-C5-C6    | -2.92 | 114.33      | 120.85   |
| 31  | A     | 820 | CLA  | CMC-C2C-C1C | 2.92  | 129.49      | 125.04   |
| 31  | 7     | 313 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 31  | 8     | 314 | CLA  | O2A-CGA-CBA | 2.92  | 121.08      | 111.91   |
| 31  | 2     | 310 | CLA  | O1D-CGD-CBD | -2.92 | 118.50      | 124.48   |
| 32  | 9     | 320 | CHL  | CHD-C1D-ND  | -2.92 | 121.77      | 124.45   |
| 31  | B     | 837 | CLA  | CMD-C2D-C1D | 2.92  | 129.86      | 124.71   |
| 31  | A     | 846 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 31  | 8     | 314 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 318 | CLA  | C3D-C2D-C1D | -2.92 | 101.84      | 105.83   |
| 31  | A     | 853 | CLA  | O1D-CGD-CBD | -2.92 | 118.51      | 124.48   |
| 31  | 9     | 312 | CLA  | C3D-C2D-C1D | -2.92 | 101.85      | 105.83   |
| 31  | O     | 204 | CLA  | CHD-C4C-NC  | 2.92  | 128.80      | 124.20   |
| 31  | 7     | 314 | CLA  | CHD-C4C-NC  | 2.92  | 128.80      | 124.20   |
| 31  | O     | 203 | CLA  | O1D-CGD-CBD | -2.92 | 118.51      | 124.48   |
| 31  | 2     | 311 | CLA  | CAC-C3C-C4C | 2.92  | 128.60      | 124.81   |
| 26  | 6     | 302 | BCR  | C11-C10-C9  | -2.92 | 123.15      | 127.31   |
| 31  | B     | 834 | CLA  | C1C-C2C-C3C | -2.92 | 103.89      | 106.96   |
| 32  | a     | 320 | CHL  | CHC-C1C-NC  | -2.92 | 119.78      | 124.20   |
| 31  | 6     | 316 | CLA  | C1-C2-C3    | -2.92 | 122.03      | 126.75   |
| 37  | G     | 202 | LMG  | O6-C1-O1    | -2.92 | 103.07      | 109.97   |
| 31  | B     | 816 | CLA  | CHD-C4C-NC  | 2.92  | 128.80      | 124.20   |
| 31  | B     | 835 | CLA  | CAC-C3C-C4C | 2.92  | 128.59      | 124.81   |
| 31  | A     | 857 | CLA  | C4-C3-C5    | 2.91  | 120.17      | 115.27   |
| 31  | 6     | 315 | CLA  | CMC-C2C-C1C | 2.91  | 129.47      | 125.04   |
| 36  | L     | 304 | LUT  | C10-C11-C12 | -2.91 | 114.13      | 123.22   |
| 26  | G     | 201 | BCR  | C27-C26-C25 | 2.91  | 126.96      | 122.73   |
| 31  | A     | 821 | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 31  | 4     | 309 | CLA  | C3D-C2D-C1D | -2.91 | 101.86      | 105.83   |
| 31  | A     | 832 | CLA  | C3D-C2D-C1D | -2.91 | 101.86      | 105.83   |
| 31  | 6     | 313 | CLA  | CHD-C4C-NC  | 2.91  | 128.79      | 124.20   |
| 30  | A     | 813 | CL0  | C4-C3-C5    | 2.91  | 120.17      | 115.27   |
| 31  | 5     | 318 | CLA  | CHD-C4C-NC  | 2.91  | 128.79      | 124.20   |
| 31  | a     | 312 | CLA  | C4-C3-C5    | 2.91  | 120.16      | 115.27   |
| 30  | A     | 813 | CL0  | CHC-C1C-C2C | -2.91 | 118.68      | 126.72   |
| 31  | B     | 838 | CLA  | C4D-CHA-C1A | -2.91 | 117.71      | 121.25   |
| 31  | L     | 306 | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 31  | A     | 818 | CLA  | O1D-CGD-CBD | -2.91 | 118.53      | 124.48   |
| 31  | A     | 828 | CLA  | C4D-CHA-C1A | -2.91 | 117.71      | 121.25   |
| 31  | K     | 204 | CLA  | CMC-C2C-C1C | 2.91  | 129.47      | 125.04   |
| 31  | A     | 843 | CLA  | C1-C2-C3    | -2.91 | 121.02      | 126.04   |
| 31  | 3     | 312 | CLA  | C1-C2-C3    | -2.91 | 121.02      | 126.04   |
| 31  | 3     | 317 | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 31  | A     | 826 | CLA  | O1D-CGD-CBD | -2.90 | 118.54      | 124.48   |
| 31  | 7     | 310 | CLA  | CHC-C1C-NC  | -2.90 | 119.80      | 124.20   |
| 31  | B     | 847 | CLA  | C3D-C2D-C1D | -2.90 | 101.87      | 105.83   |
| 31  | 8     | 309 | CLA  | C1-C2-C3    | -2.90 | 122.05      | 126.75   |
| 31  | 3     | 310 | CLA  | C3D-C2D-C1D | -2.90 | 101.87      | 105.83   |
| 32  | 6     | 319 | CHL  | C1D-CHD-C4C | -2.90 | 119.80      | 126.06   |
| 31  | 4     | 312 | CLA  | CHD-C4C-NC  | 2.90  | 128.78      | 124.20   |
| 31  | b     | 302 | CLA  | CHD-C4C-NC  | 2.90  | 128.78      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 846 | CLA  | C1-O2A-CGA  | 2.90  | 124.05      | 116.44   |
| 31  | B     | 835 | CLA  | O2A-C1-C2   | -2.90 | 101.01      | 108.64   |
| 31  | 4     | 311 | CLA  | O1D-CGD-CBD | -2.90 | 118.55      | 124.48   |
| 31  | A     | 820 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 31  | L     | 305 | CLA  | CHD-C4C-NC  | 2.90  | 128.77      | 124.20   |
| 32  | 7     | 324 | CHL  | C4-C3-C5    | 2.90  | 120.15      | 115.27   |
| 31  | B     | 834 | CLA  | CMB-C2B-C3B | 2.90  | 130.10      | 124.68   |
| 31  | G     | 204 | CLA  | CMB-C2B-C3B | 2.90  | 130.10      | 124.68   |
| 31  | a     | 309 | CLA  | C3D-C2D-C1D | -2.90 | 101.88      | 105.83   |
| 31  | B     | 832 | CLA  | CHD-C4C-NC  | 2.90  | 128.77      | 124.20   |
| 32  | 4     | 313 | CHL  | C3D-C2D-C1D | -2.90 | 101.88      | 105.83   |
| 31  | a     | 309 | CLA  | CHC-C1C-NC  | -2.90 | 119.81      | 124.20   |
| 31  | B     | 820 | CLA  | C3D-C2D-C1D | -2.90 | 101.88      | 105.83   |
| 31  | A     | 814 | CLA  | CHA-C4D-ND  | 2.90  | 138.56      | 132.50   |
| 31  | A     | 857 | CLA  | CMC-C2C-C1C | 2.90  | 129.45      | 125.04   |
| 32  | A     | 840 | CHL  | CMD-C2D-C1D | 2.90  | 129.82      | 124.71   |
| 31  | 3     | 317 | CLA  | CHD-C4C-NC  | 2.89  | 128.76      | 124.20   |
| 31  | 6     | 312 | CLA  | CMB-C2B-C3B | 2.89  | 130.09      | 124.68   |
| 36  | b     | 301 | LUT  | C8-C7-C6    | -2.89 | 119.08      | 127.20   |
| 31  | A     | 847 | CLA  | CHD-C4C-NC  | 2.89  | 128.76      | 124.20   |
| 31  | B     | 832 | CLA  | CHD-C1D-ND  | -2.89 | 121.80      | 124.45   |
| 31  | 4     | 315 | CLA  | CMC-C2C-C1C | 2.89  | 129.44      | 125.04   |
| 31  | B     | 812 | CLA  | C1C-C2C-C3C | -2.89 | 103.92      | 106.96   |
| 31  | 3     | 307 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | 4     | 314 | CLA  | O1D-CGD-CBD | -2.89 | 118.57      | 124.48   |
| 31  | K     | 204 | CLA  | CHC-C1C-NC  | -2.89 | 119.82      | 124.20   |
| 31  | A     | 852 | CLA  | O1D-CGD-CBD | -2.89 | 118.57      | 124.48   |
| 31  | a     | 312 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | 2     | 315 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | a     | 310 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | 6     | 307 | CLA  | CMC-C2C-C1C | 2.89  | 129.44      | 125.04   |
| 31  | A     | 816 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | A     | 830 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | 9     | 314 | CLA  | C3D-C2D-C1D | -2.89 | 101.89      | 105.83   |
| 31  | B     | 844 | CLA  | C1-C2-C3    | -2.88 | 121.06      | 126.04   |
| 31  | b     | 302 | CLA  | C3D-C2D-C1D | -2.88 | 101.90      | 105.83   |
| 31  | 4     | 308 | CLA  | CHD-C4C-NC  | 2.88  | 128.75      | 124.20   |
| 31  | B     | 836 | CLA  | C3D-C2D-C1D | -2.88 | 101.90      | 105.83   |
| 31  | K     | 205 | CLA  | CHD-C4C-NC  | 2.88  | 128.75      | 124.20   |
| 32  | 6     | 321 | CHL  | C1D-CHD-C4C | -2.88 | 119.84      | 126.06   |
| 31  | B     | 840 | CLA  | C4D-CHA-C1A | -2.88 | 117.74      | 121.25   |
| 31  | 8     | 317 | CLA  | O2D-CGD-O1D | -2.88 | 118.21      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 313 | CLA  | C3D-C2D-C1D | -2.88 | 101.90      | 105.83   |
| 31  | A     | 838 | CLA  | CHD-C1D-ND  | -2.88 | 121.81      | 124.45   |
| 32  | 5     | 317 | CHL  | CHC-C1C-NC  | -2.88 | 119.83      | 124.20   |
| 31  | B     | 836 | CLA  | CHD-C4C-NC  | 2.88  | 128.74      | 124.20   |
| 31  | A     | 847 | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 31  | B     | 817 | CLA  | C1-C2-C3    | -2.88 | 121.07      | 126.04   |
| 31  | B     | 829 | CLA  | CMD-C2D-C1D | 2.88  | 129.78      | 124.71   |
| 31  | B     | 815 | CLA  | C4-C3-C5    | 2.88  | 120.11      | 115.27   |
| 31  | 2     | 307 | CLA  | C4D-CHA-C1A | -2.88 | 117.75      | 121.25   |
| 32  | 8     | 316 | CHL  | C4-C3-C5    | 2.88  | 120.11      | 115.27   |
| 31  | A     | 820 | CLA  | CMD-C2D-C1D | 2.88  | 129.78      | 124.71   |
| 31  | A     | 824 | CLA  | CAC-C3C-C4C | 2.88  | 128.54      | 124.81   |
| 31  | 4     | 305 | CLA  | CHC-C1C-NC  | -2.88 | 119.84      | 124.20   |
| 31  | 5     | 323 | CLA  | C1-C2-C3    | -2.87 | 121.07      | 126.04   |
| 31  | b     | 312 | CLA  | CAC-C3C-C4C | 2.87  | 128.54      | 124.81   |
| 31  | 3     | 307 | CLA  | CAC-C3C-C4C | 2.87  | 128.54      | 124.81   |
| 31  | 8     | 315 | CLA  | CHD-C4C-NC  | 2.87  | 128.73      | 124.20   |
| 31  | 3     | 320 | CLA  | CHC-C1C-NC  | -2.87 | 119.84      | 124.20   |
| 31  | A     | 843 | CLA  | CAC-C3C-C4C | 2.87  | 128.54      | 124.81   |
| 31  | A     | 851 | CLA  | C3D-C2D-C1D | -2.87 | 101.91      | 105.83   |
| 31  | A     | 821 | CLA  | C4-C3-C5    | 2.87  | 120.10      | 115.27   |
| 27  | 5     | 301 | LMT  | C3'-C4'-C5' | -2.87 | 104.34      | 110.93   |
| 31  | 6     | 315 | CLA  | CMB-C2B-C3B | 2.87  | 130.05      | 124.68   |
| 42  | 4     | 304 | SQD  | O7-S-C6     | 2.87  | 110.35      | 106.94   |
| 31  | B     | 822 | CLA  | CMB-C2B-C3B | 2.87  | 130.05      | 124.68   |
| 31  | 9     | 318 | CLA  | C3D-C2D-C1D | -2.87 | 101.92      | 105.83   |
| 31  | A     | 815 | CLA  | C4-C3-C5    | 2.87  | 120.10      | 115.27   |
| 31  | F     | 301 | CLA  | C3D-C2D-C1D | -2.87 | 101.92      | 105.83   |
| 31  | b     | 303 | CLA  | CAC-C3C-C4C | 2.87  | 128.53      | 124.81   |
| 31  | A     | 822 | CLA  | CMB-C2B-C3B | 2.87  | 130.04      | 124.68   |
| 31  | 4     | 312 | CLA  | CHC-C1C-NC  | -2.87 | 119.85      | 124.20   |
| 31  | 3     | 317 | CLA  | O2D-CGD-O1D | -2.87 | 118.23      | 123.84   |
| 36  | 9     | 302 | LUT  | C18-C5-C4   | -2.87 | 109.04      | 114.36   |
| 31  | 8     | 321 | CLA  | O1D-CGD-CBD | -2.87 | 118.62      | 124.48   |
| 32  | 6     | 321 | CHL  | CHD-C4C-NC  | 2.87  | 128.72      | 124.20   |
| 31  | 5     | 313 | CLA  | C3D-C2D-C1D | -2.87 | 101.92      | 105.83   |
| 31  | A     | 838 | CLA  | CAC-C3C-C4C | 2.86  | 128.53      | 124.81   |
| 31  | 7     | 313 | CLA  | CHC-C1C-NC  | -2.86 | 119.86      | 124.20   |
| 31  | B     | 822 | CLA  | C3D-C2D-C1D | -2.86 | 101.92      | 105.83   |
| 31  | 8     | 312 | CLA  | O2D-CGD-O1D | -2.86 | 118.24      | 123.84   |
| 31  | 8     | 310 | CLA  | C4-C3-C5    | 2.86  | 120.09      | 115.27   |
| 32  | A     | 840 | CHL  | CMB-C2B-C3B | 2.86  | 130.03      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 818 | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 31  | 4     | 315 | CLA  | CMB-C2B-C3B | 2.86  | 130.03      | 124.68   |
| 31  | 9     | 316 | CLA  | C3D-C2D-C1D | -2.86 | 101.93      | 105.83   |
| 31  | A     | 833 | CLA  | C3D-C2D-C1D | -2.86 | 101.93      | 105.83   |
| 31  | F     | 305 | CLA  | C3D-C2D-C1D | -2.86 | 101.93      | 105.83   |
| 31  | 9     | 313 | CLA  | C3D-C2D-C1D | -2.86 | 101.93      | 105.83   |
| 31  | 3     | 312 | CLA  | CHD-C4C-NC  | 2.86  | 128.71      | 124.20   |
| 31  | 5     | 312 | CLA  | C1-C2-C3    | -2.86 | 122.12      | 126.75   |
| 32  | 5     | 316 | CHL  | CGD-CBD-CAD | 2.86  | 120.00      | 110.73   |
| 31  | A     | 846 | CLA  | C4-C3-C5    | 2.86  | 120.08      | 115.27   |
| 31  | b     | 310 | CLA  | CMB-C2B-C3B | 2.86  | 130.03      | 124.68   |
| 31  | A     | 847 | CLA  | CMD-C2D-C1D | 2.86  | 129.75      | 124.71   |
| 38  | a     | 304 | AXT  | C3-C4-C5    | 2.86  | 117.55      | 111.85   |
| 31  | B     | 828 | CLA  | C3D-C2D-C1D | -2.86 | 101.93      | 105.83   |
| 32  | 6     | 321 | CHL  | CHC-C1C-NC  | -2.85 | 119.87      | 124.20   |
| 31  | 8     | 320 | CLA  | O1D-CGD-CBD | -2.85 | 118.64      | 124.48   |
| 31  | 5     | 321 | CLA  | O1D-CGD-CBD | -2.85 | 118.64      | 124.48   |
| 31  | 8     | 312 | CLA  | CHD-C4C-NC  | 2.85  | 128.70      | 124.20   |
| 31  | 7     | 321 | CLA  | O2A-CGA-CBA | 2.85  | 120.86      | 111.91   |
| 31  | A     | 815 | CLA  | CHD-C4C-NC  | 2.85  | 128.69      | 124.20   |
| 31  | 8     | 320 | CLA  | CHD-C4C-NC  | 2.85  | 128.69      | 124.20   |
| 31  | A     | 842 | CLA  | O1D-CGD-CBD | -2.85 | 118.66      | 124.48   |
| 31  | 4     | 308 | CLA  | C3D-C2D-C1D | -2.85 | 101.94      | 105.83   |
| 31  | B     | 842 | CLA  | C3D-C2D-C1D | -2.85 | 101.95      | 105.83   |
| 31  | a     | 321 | CLA  | CMD-C2D-C1D | 2.85  | 129.73      | 124.71   |
| 31  | 6     | 312 | CLA  | C1-C2-C3    | -2.85 | 121.12      | 126.04   |
| 31  | A     | 819 | CLA  | O1D-CGD-CBD | -2.85 | 118.66      | 124.48   |
| 31  | A     | 814 | CLA  | C3D-C2D-C1D | -2.84 | 101.95      | 105.83   |
| 31  | 4     | 305 | CLA  | CMD-C2D-C3D | -2.84 | 121.08      | 127.61   |
| 31  | B     | 812 | CLA  | CMB-C2B-C3B | 2.84  | 129.99      | 124.68   |
| 31  | A     | 844 | CLA  | C1-C2-C3    | -2.84 | 122.16      | 126.75   |
| 31  | 4     | 308 | CLA  | C4-C3-C5    | 2.84  | 120.05      | 115.27   |
| 31  | G     | 206 | CLA  | C4D-CHA-C1A | -2.84 | 117.79      | 121.25   |
| 31  | 4     | 311 | CLA  | CHC-C1C-NC  | -2.84 | 119.89      | 124.20   |
| 31  | B     | 828 | CLA  | O1D-CGD-CBD | -2.84 | 118.67      | 124.48   |
| 31  | 7     | 312 | CLA  | C3D-C2D-C1D | -2.84 | 101.96      | 105.83   |
| 32  | A     | 840 | CHL  | C2C-C3C-C4C | -2.84 | 104.47      | 106.49   |
| 31  | K     | 204 | CLA  | CHA-C4D-ND  | 2.84  | 138.43      | 132.50   |
| 31  | 5     | 320 | CLA  | CMD-C2D-C1D | 2.84  | 129.71      | 124.71   |
| 31  | 6     | 315 | CLA  | C3D-C2D-C1D | -2.83 | 101.96      | 105.83   |
| 31  | 9     | 317 | CLA  | CHD-C4C-C3C | -2.83 | 120.67      | 124.84   |
| 31  | B     | 844 | CLA  | O1D-CGD-CBD | -2.83 | 118.69      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 5     | 319 | CHL  | CHD-C4C-NC  | 2.83  | 128.67      | 124.20   |
| 31  | 2     | 312 | CLA  | C1B-CHB-C4A | -2.83 | 124.51      | 130.12   |
| 31  | A     | 852 | CLA  | O2A-CGA-CBA | 2.83  | 120.80      | 111.91   |
| 31  | A     | 832 | CLA  | O1D-CGD-CBD | -2.83 | 118.69      | 124.48   |
| 31  | b     | 311 | CLA  | CHD-C4C-NC  | 2.83  | 128.66      | 124.20   |
| 31  | b     | 304 | CLA  | CMB-C2B-C3B | 2.83  | 129.97      | 124.68   |
| 31  | 3     | 313 | CLA  | O2A-CGA-CBA | 2.83  | 120.79      | 111.91   |
| 31  | A     | 841 | CLA  | CMD-C2D-C1D | 2.83  | 129.70      | 124.71   |
| 31  | B     | 826 | CLA  | C3D-C2D-C1D | -2.83 | 101.97      | 105.83   |
| 31  | A     | 815 | CLA  | CHA-C4D-ND  | 2.83  | 138.41      | 132.50   |
| 31  | A     | 825 | CLA  | C3D-C2D-C1D | -2.83 | 101.97      | 105.83   |
| 31  | A     | 841 | CLA  | CAC-C3C-C4C | 2.83  | 128.48      | 124.81   |
| 31  | A     | 857 | CLA  | C3D-C2D-C1D | -2.83 | 101.97      | 105.83   |
| 32  | 4     | 310 | CHL  | C3D-C2D-C1D | -2.83 | 101.97      | 105.83   |
| 31  | 9     | 316 | CLA  | C1-C2-C3    | -2.83 | 122.18      | 126.75   |
| 31  | L     | 306 | CLA  | CMB-C2B-C3B | 2.83  | 129.96      | 124.68   |
| 32  | 4     | 317 | CHL  | C3D-C2D-C1D | -2.82 | 101.98      | 105.83   |
| 31  | a     | 314 | CLA  | CED-O2D-CGD | 2.82  | 122.33      | 115.94   |
| 31  | A     | 826 | CLA  | C3D-C2D-C1D | -2.82 | 101.98      | 105.83   |
| 31  | B     | 824 | CLA  | C3D-C2D-C1D | -2.82 | 101.98      | 105.83   |
| 31  | 3     | 318 | CLA  | O2A-CGA-CBA | 2.82  | 120.77      | 111.91   |
| 31  | B     | 847 | CLA  | C4-C3-C5    | 2.82  | 120.02      | 115.27   |
| 31  | a     | 315 | CLA  | CMB-C2B-C3B | 2.82  | 129.96      | 124.68   |
| 31  | A     | 825 | CLA  | CMC-C2C-C1C | 2.82  | 129.34      | 125.04   |
| 35  | a     | 302 | QTB  | C09-C02-C03 | 2.82  | 123.27      | 118.94   |
| 31  | 7     | 309 | CLA  | CMD-C2D-C1D | 2.82  | 129.69      | 124.71   |
| 31  | B     | 850 | CLA  | CMC-C2C-C1C | 2.82  | 129.34      | 125.04   |
| 30  | A     | 813 | CL0  | C1B-CHB-C4A | -2.82 | 124.53      | 130.12   |
| 31  | 3     | 318 | CLA  | O1D-CGD-CBD | -2.82 | 118.71      | 124.48   |
| 31  | 8     | 309 | CLA  | C1D-CHD-C4C | -2.82 | 119.97      | 126.06   |
| 36  | 4     | 302 | LUT  | C18-C5-C4   | -2.82 | 109.13      | 114.36   |
| 31  | B     | 827 | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 31  | 3     | 308 | CLA  | CHC-C1C-NC  | -2.82 | 119.93      | 124.20   |
| 31  | 9     | 318 | CLA  | CAC-C3C-C4C | 2.82  | 128.47      | 124.81   |
| 31  | B     | 819 | CLA  | C3D-C2D-C1D | -2.82 | 101.98      | 105.83   |
| 31  | 4     | 319 | CLA  | CHC-C1C-NC  | -2.82 | 119.93      | 124.20   |
| 26  | 3     | 303 | BCR  | C2-C1-C6    | 2.82  | 114.82      | 110.48   |
| 28  | 7     | 307 | LHG  | O8-C23-C24  | 2.81  | 120.74      | 111.91   |
| 32  | 5     | 316 | CHL  | O2A-CGA-CBA | 2.81  | 120.74      | 111.91   |
| 31  | b     | 308 | CLA  | O1D-CGD-CBD | -2.81 | 118.73      | 124.48   |
| 31  | B     | 827 | CLA  | CMC-C2C-C1C | 2.81  | 129.32      | 125.04   |
| 31  | A     | 856 | CLA  | CMB-C2B-C3B | 2.81  | 129.94      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | b     | 301 | LUT  | C35-C15-C14 | -2.81 | 117.71      | 123.47   |
| 31  | A     | 824 | CLA  | C3D-C2D-C1D | -2.81 | 101.99      | 105.83   |
| 32  | a     | 320 | CHL  | O2A-CGA-CBA | 2.81  | 120.73      | 111.91   |
| 31  | A     | 829 | CLA  | C2A-C3A-C4A | 2.81  | 106.41      | 101.87   |
| 31  | 2     | 312 | CLA  | CHD-C4C-NC  | 2.81  | 128.63      | 124.20   |
| 31  | B     | 847 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 31  | 7     | 314 | CLA  | O2A-CGA-CBA | 2.81  | 120.73      | 111.91   |
| 31  | a     | 321 | CLA  | C3D-C2D-C1D | -2.81 | 102.00      | 105.83   |
| 32  | 5     | 322 | CHL  | CHC-C1C-NC  | -2.81 | 119.94      | 124.20   |
| 31  | 6     | 322 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 32  | A     | 831 | CHL  | C4-C3-C5    | 2.81  | 120.00      | 115.27   |
| 36  | b     | 301 | LUT  | C10-C11-C12 | -2.81 | 114.45      | 123.22   |
| 31  | a     | 316 | CLA  | C3D-C2D-C1D | -2.81 | 102.00      | 105.83   |
| 31  | L     | 306 | CLA  | C3D-C2D-C1D | -2.81 | 102.00      | 105.83   |
| 32  | 6     | 318 | CHL  | CHD-C4C-NC  | 2.81  | 128.63      | 124.20   |
| 31  | b     | 310 | CLA  | C3D-C2D-C1D | -2.81 | 102.00      | 105.83   |
| 31  | 9     | 315 | CLA  | CMD-C2D-C1D | 2.81  | 129.66      | 124.71   |
| 26  | G     | 203 | BCR  | C27-C26-C25 | 2.81  | 126.81      | 122.73   |
| 31  | 3     | 309 | CLA  | C3D-C2D-C1D | -2.81 | 102.00      | 105.83   |
| 31  | A     | 857 | CLA  | CAC-C3C-C4C | 2.81  | 128.45      | 124.81   |
| 31  | H     | 902 | CLA  | CHD-C4C-NC  | 2.81  | 128.63      | 124.20   |
| 31  | a     | 319 | CLA  | CHC-C1C-NC  | -2.81 | 119.94      | 124.20   |
| 31  | 8     | 311 | CLA  | CMD-C2D-C1D | 2.81  | 129.66      | 124.71   |
| 31  | a     | 322 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 31  | A     | 838 | CLA  | CHD-C4C-NC  | 2.81  | 128.62      | 124.20   |
| 31  | 6     | 307 | CLA  | O2D-CGD-O1D | -2.80 | 118.35      | 123.84   |
| 31  | 3     | 309 | CLA  | C4-C3-C5    | 2.80  | 119.99      | 115.27   |
| 31  | A     | 823 | CLA  | C3D-C2D-C1D | -2.80 | 102.00      | 105.83   |
| 31  | K     | 205 | CLA  | O1D-CGD-CBD | -2.80 | 118.75      | 124.48   |
| 31  | a     | 309 | CLA  | CMC-C2C-C1C | 2.80  | 129.31      | 125.04   |
| 31  | 3     | 319 | CLA  | CAC-C3C-C4C | 2.80  | 128.44      | 124.81   |
| 31  | B     | 850 | CLA  | C1-C2-C3    | -2.80 | 121.20      | 126.04   |
| 31  | A     | 837 | CLA  | C1-C2-C3    | -2.80 | 121.20      | 126.04   |
| 32  | 6     | 321 | CHL  | C3D-C2D-C1D | -2.80 | 102.01      | 105.83   |
| 31  | A     | 830 | CLA  | CMC-C2C-C1C | 2.80  | 129.30      | 125.04   |
| 31  | 6     | 306 | CLA  | CMD-C2D-C3D | -2.80 | 121.17      | 127.61   |
| 32  | 7     | 320 | CHL  | O1D-CGD-CBD | -2.80 | 118.75      | 124.48   |
| 32  | 5     | 322 | CHL  | C4D-CHA-C1A | -2.80 | 117.84      | 121.25   |
| 31  | B     | 835 | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 32  | 5     | 316 | CHL  | O1D-CGD-CBD | -2.80 | 118.76      | 124.48   |
| 31  | 2     | 304 | CLA  | C3D-C2D-C1D | -2.80 | 102.01      | 105.83   |
| 36  | F     | 304 | LUT  | C10-C11-C12 | -2.80 | 114.48      | 123.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | K     | 201 | CHL  | CMD-C2D-C3D | -2.80 | 121.18      | 127.61   |
| 31  | 4     | 312 | CLA  | CMD-C2D-C1D | 2.80  | 129.64      | 124.71   |
| 31  | 7     | 309 | CLA  | C3D-C2D-C1D | -2.80 | 102.01      | 105.83   |
| 36  | 9     | 303 | LUT  | C12-C13-C14 | -2.80 | 114.65      | 118.94   |
| 31  | 4     | 315 | CLA  | C3D-C2D-C1D | -2.80 | 102.02      | 105.83   |
| 31  | B     | 844 | CLA  | CAC-C3C-C4C | 2.80  | 128.44      | 124.81   |
| 32  | A     | 831 | CHL  | CHD-C4C-C3C | -2.80 | 120.73      | 124.84   |
| 31  | O     | 203 | CLA  | CHC-C1C-NC  | -2.80 | 119.96      | 124.20   |
| 31  | L     | 305 | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 31  | A     | 827 | CLA  | C3D-C2D-C1D | -2.80 | 102.02      | 105.83   |
| 31  | A     | 817 | CLA  | C1-O2A-CGA  | 2.79  | 123.78      | 116.44   |
| 31  | 2     | 312 | CLA  | C3D-C2D-C1D | -2.79 | 102.02      | 105.83   |
| 31  | A     | 817 | CLA  | CAC-C3C-C4C | 2.79  | 128.44      | 124.81   |
| 31  | 2     | 311 | CLA  | CHD-C4C-NC  | 2.79  | 128.61      | 124.20   |
| 31  | A     | 816 | CLA  | CAC-C3C-C4C | 2.79  | 128.44      | 124.81   |
| 36  | 8     | 302 | LUT  | C30-C31-C32 | -2.79 | 114.50      | 123.22   |
| 31  | 2     | 313 | CLA  | CMB-C2B-C3B | 2.79  | 129.90      | 124.68   |
| 31  | 6     | 313 | CLA  | C3D-C2D-C1D | -2.79 | 102.02      | 105.83   |
| 36  | 9     | 302 | LUT  | C4-C5-C6    | -2.79 | 114.62      | 120.85   |
| 31  | b     | 307 | CLA  | CHD-C4C-NC  | 2.79  | 128.60      | 124.20   |
| 31  | 7     | 316 | CLA  | CMC-C2C-C1C | 2.79  | 129.29      | 125.04   |
| 31  | 8     | 307 | CLA  | C3D-C2D-C1D | -2.79 | 102.02      | 105.83   |
| 31  | 2     | 307 | CLA  | C1-C2-C3    | -2.79 | 121.22      | 126.04   |
| 36  | 3     | 304 | LUT  | C4-C5-C6    | -2.79 | 114.63      | 120.85   |
| 31  | K     | 205 | CLA  | C3D-C2D-C1D | -2.79 | 102.03      | 105.83   |
| 31  | F     | 305 | CLA  | CHD-C4C-NC  | 2.79  | 128.60      | 124.20   |
| 31  | 8     | 317 | CLA  | CMD-C2D-C1D | 2.79  | 129.63      | 124.71   |
| 31  | 3     | 316 | CLA  | C3D-C2D-C1D | -2.79 | 102.03      | 105.83   |
| 31  | 8     | 308 | CLA  | C3D-C2D-C1D | -2.79 | 102.03      | 105.83   |
| 31  | 8     | 309 | CLA  | O1D-CGD-CBD | -2.79 | 118.78      | 124.48   |
| 31  | 6     | 313 | CLA  | CHC-C1C-NC  | -2.79 | 119.97      | 124.20   |
| 31  | 9     | 319 | CLA  | CHD-C4C-NC  | 2.79  | 128.60      | 124.20   |
| 31  | H     | 903 | CLA  | CHC-C1C-NC  | -2.79 | 119.98      | 124.20   |
| 31  | 7     | 321 | CLA  | O1D-CGD-CBD | -2.79 | 118.78      | 124.48   |
| 31  | B     | 834 | CLA  | CHD-C4C-NC  | 2.78  | 128.59      | 124.20   |
| 36  | 4     | 302 | LUT  | C10-C11-C12 | -2.78 | 114.53      | 123.22   |
| 32  | 6     | 320 | CHL  | C4D-CHA-C1A | -2.78 | 117.86      | 121.25   |
| 31  | B     | 832 | CLA  | C3B-C4B-NB  | 2.78  | 112.81      | 109.21   |
| 31  | A     | 851 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 31  | 9     | 321 | CLA  | CMD-C2D-C1D | 2.78  | 129.62      | 124.71   |
| 31  | 8     | 315 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 31  | O     | 204 | CLA  | O1D-CGD-CBD | -2.78 | 118.79      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 830 | CLA  | C4-C3-C5    | 2.78  | 119.95      | 115.27   |
| 31  | 9     | 312 | CLA  | O1D-CGD-CBD | -2.78 | 118.79      | 124.48   |
| 31  | b     | 308 | CLA  | CHC-C1C-NC  | -2.78 | 119.98      | 124.20   |
| 32  | a     | 317 | CHL  | C3D-C2D-C1D | -2.78 | 102.04      | 105.83   |
| 31  | 2     | 313 | CLA  | CHD-C4C-NC  | 2.78  | 128.58      | 124.20   |
| 31  | 4     | 307 | CLA  | CHD-C4C-NC  | 2.78  | 128.58      | 124.20   |
| 31  | 8     | 318 | CLA  | C1-C2-C3    | -2.78 | 122.25      | 126.75   |
| 26  | 6     | 302 | BCR  | C27-C26-C25 | 2.78  | 126.77      | 122.73   |
| 31  | A     | 823 | CLA  | C4D-CHA-C1A | -2.78 | 117.87      | 121.25   |
| 36  | 3     | 304 | LUT  | C21-C26-C27 | -2.78 | 109.19      | 112.70   |
| 26  | G     | 201 | BCR  | C7-C8-C9    | -2.78 | 122.04      | 126.23   |
| 31  | B     | 818 | CLA  | CAC-C3C-C4C | 2.78  | 128.41      | 124.81   |
| 31  | B     | 821 | CLA  | C3D-C2D-C1D | -2.78 | 102.04      | 105.83   |
| 31  | 9     | 311 | CLA  | CHD-C4C-NC  | 2.78  | 128.58      | 124.20   |
| 31  | A     | 818 | CLA  | C1-C2-C3    | -2.78 | 121.24      | 126.04   |
| 31  | 5     | 308 | CLA  | CHD-C4C-NC  | 2.78  | 128.58      | 124.20   |
| 32  | 7     | 318 | CHL  | C4-C3-C5    | 2.78  | 119.94      | 115.27   |
| 32  | a     | 320 | CHL  | O1D-CGD-CBD | -2.78 | 118.80      | 124.48   |
| 31  | B     | 811 | CLA  | C3D-C2D-C1D | -2.78 | 102.04      | 105.83   |
| 28  | a     | 306 | LHG  | O8-C23-C24  | 2.77  | 120.61      | 111.91   |
| 31  | 6     | 316 | CLA  | C3D-C2D-C1D | -2.77 | 102.05      | 105.83   |
| 36  | 8     | 303 | LUT  | C21-C26-C25 | 2.77  | 116.38      | 111.42   |
| 31  | B     | 850 | CLA  | C4-C3-C5    | 2.77  | 119.93      | 115.27   |
| 31  | F     | 306 | CLA  | C1-C2-C3    | -2.77 | 122.27      | 126.75   |
| 31  | 7     | 315 | CLA  | C3D-C2D-C1D | -2.77 | 102.05      | 105.83   |
| 31  | 3     | 316 | CLA  | C1-C2-C3    | -2.77 | 122.27      | 126.75   |
| 31  | 2     | 314 | CLA  | CHD-C4C-NC  | 2.77  | 128.57      | 124.20   |
| 31  | B     | 846 | CLA  | O2A-CGA-CBA | 2.77  | 120.60      | 111.91   |
| 40  | 7     | 306 | XAT  | C12-C13-C14 | 2.77  | 123.19      | 118.94   |
| 31  | 6     | 322 | CLA  | CMB-C2B-C3B | 2.77  | 129.86      | 124.68   |
| 31  | A     | 817 | CLA  | C4-C3-C5    | 2.77  | 119.92      | 115.27   |
| 31  | B     | 825 | CLA  | C3D-C2D-C1D | -2.77 | 102.06      | 105.83   |
| 31  | A     | 823 | CLA  | CHD-C4C-NC  | 2.77  | 128.56      | 124.20   |
| 31  | B     | 814 | CLA  | CHB-C4A-NA  | 2.77  | 128.34      | 124.51   |
| 31  | 9     | 311 | CLA  | C4-C3-C5    | 2.76  | 119.92      | 115.27   |
| 32  | 5     | 322 | CHL  | C3D-C2D-C1D | -2.76 | 102.06      | 105.83   |
| 31  | 5     | 310 | CLA  | CHC-C1C-NC  | -2.76 | 120.01      | 124.20   |
| 31  | 5     | 307 | CLA  | CHD-C4C-NC  | 2.76  | 128.56      | 124.20   |
| 31  | 4     | 316 | CLA  | O2A-CGA-CBA | 2.76  | 120.58      | 111.91   |
| 31  | B     | 836 | CLA  | C1-O2A-CGA  | 2.76  | 123.70      | 116.44   |
| 31  | 4     | 314 | CLA  | C1B-CHB-C4A | -2.76 | 124.64      | 130.12   |
| 31  | B     | 840 | CLA  | CMB-C2B-C3B | 2.76  | 129.85      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 323 | CLA  | CHC-C1C-NC  | -2.76 | 120.01      | 124.20   |
| 31  | B     | 816 | CLA  | CAC-C3C-C4C | 2.76  | 128.40      | 124.81   |
| 31  | H     | 902 | CLA  | CHC-C1C-NC  | -2.76 | 120.01      | 124.20   |
| 32  | 7     | 317 | CHL  | CMD-C2D-C1D | 2.76  | 129.58      | 124.71   |
| 31  | 3     | 308 | CLA  | C3D-C2D-C1D | -2.76 | 102.06      | 105.83   |
| 31  | B     | 849 | CLA  | O2D-CGD-CBD | 2.76  | 116.17      | 111.27   |
| 31  | 6     | 310 | CLA  | CHD-C4C-NC  | 2.76  | 128.55      | 124.20   |
| 31  | a     | 315 | CLA  | C3D-C2D-C1D | -2.76 | 102.06      | 105.83   |
| 31  | 7     | 310 | CLA  | C1D-CHD-C4C | -2.76 | 120.11      | 126.06   |
| 32  | 7     | 319 | CHL  | C2D-C1D-ND  | 2.76  | 112.14      | 110.10   |
| 31  | B     | 814 | CLA  | CHD-C4C-NC  | 2.76  | 128.55      | 124.20   |
| 31  | 6     | 307 | CLA  | CMD-C2D-C1D | 2.76  | 129.57      | 124.71   |
| 31  | 4     | 320 | CLA  | C3D-C2D-C1D | -2.76 | 102.07      | 105.83   |
| 31  | 7     | 310 | CLA  | C3D-C2D-C1D | -2.76 | 102.07      | 105.83   |
| 36  | 2     | 301 | LUT  | C30-C31-C32 | -2.76 | 114.61      | 123.22   |
| 31  | 8     | 307 | CLA  | CMB-C2B-C3B | 2.76  | 129.84      | 124.68   |
| 31  | b     | 313 | CLA  | CHD-C4C-C3C | -2.76 | 120.79      | 124.84   |
| 31  | 5     | 309 | CLA  | CHD-C4C-NC  | 2.76  | 128.55      | 124.20   |
| 31  | 8     | 320 | CLA  | O2A-CGA-CBA | 2.76  | 120.56      | 111.91   |
| 31  | B     | 827 | CLA  | O1D-CGD-CBD | -2.76 | 118.85      | 124.48   |
| 31  | B     | 818 | CLA  | C3B-C4B-NB  | 2.76  | 112.77      | 109.21   |
| 31  | 2     | 310 | CLA  | C3D-C2D-C1D | -2.75 | 102.07      | 105.83   |
| 31  | G     | 204 | CLA  | C3D-C2D-C1D | -2.75 | 102.07      | 105.83   |
| 31  | 8     | 315 | CLA  | C3D-C2D-C1D | -2.75 | 102.07      | 105.83   |
| 31  | 6     | 312 | CLA  | C3D-C2D-C1D | -2.75 | 102.07      | 105.83   |
| 31  | 6     | 308 | CLA  | O2A-CGA-CBA | 2.75  | 120.55      | 111.91   |
| 31  | 6     | 310 | CLA  | C3D-C2D-C1D | -2.75 | 102.07      | 105.83   |
| 31  | B     | 838 | CLA  | CAC-C3C-C4C | 2.75  | 128.38      | 124.81   |
| 31  | 8     | 314 | CLA  | C1-C2-C3    | -2.75 | 121.28      | 126.04   |
| 31  | B     | 839 | CLA  | C3D-C2D-C1D | -2.75 | 102.08      | 105.83   |
| 31  | 5     | 312 | CLA  | C3D-C2D-C1D | -2.75 | 102.08      | 105.83   |
| 31  | B     | 824 | CLA  | C4-C3-C5    | 2.75  | 119.90      | 115.27   |
| 31  | 9     | 315 | CLA  | CHC-C1C-NC  | -2.75 | 120.03      | 124.20   |
| 31  | B     | 818 | CLA  | CHD-C4C-NC  | 2.75  | 128.54      | 124.20   |
| 26  | L     | 301 | BCR  | C29-C30-C25 | 2.75  | 114.71      | 110.48   |
| 36  | 8     | 303 | LUT  | C7-C6-C5    | -2.75 | 114.80      | 121.46   |
| 31  | 2     | 310 | CLA  | CHC-C1C-NC  | -2.75 | 120.03      | 124.20   |
| 31  | 4     | 318 | CLA  | CHD-C4C-NC  | 2.75  | 128.53      | 124.20   |
| 31  | b     | 305 | CLA  | C3D-C2D-C1D | -2.75 | 102.08      | 105.83   |
| 31  | 4     | 306 | CLA  | C3D-C2D-C1D | -2.75 | 102.08      | 105.83   |
| 31  | B     | 816 | CLA  | CHC-C1C-NC  | -2.75 | 120.03      | 124.20   |
| 31  | A     | 829 | CLA  | O2A-CGA-CBA | 2.75  | 120.53      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 9     | 320 | CHL  | O2A-CGA-CBA | 2.75  | 120.53      | 111.91   |
| 31  | 2     | 308 | CLA  | CHC-C1C-NC  | -2.75 | 120.04      | 124.20   |
| 31  | 4     | 319 | CLA  | C3D-C2D-C1D | -2.75 | 102.08      | 105.83   |
| 31  | A     | 853 | CLA  | CED-O2D-CGD | 2.75  | 122.15      | 115.94   |
| 31  | 8     | 317 | CLA  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 31  | B     | 821 | CLA  | C1-O2A-CGA  | 2.74  | 123.64      | 116.44   |
| 31  | b     | 311 | CLA  | C3D-C2D-C1D | -2.74 | 102.09      | 105.83   |
| 31  | O     | 202 | CLA  | C4D-CHA-C1A | -2.74 | 117.91      | 121.25   |
| 32  | 5     | 317 | CHL  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 31  | A     | 842 | CLA  | CMC-C2C-C1C | 2.74  | 129.21      | 125.04   |
| 31  | A     | 827 | CLA  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 31  | a     | 312 | CLA  | CHC-C1C-NC  | -2.74 | 120.04      | 124.20   |
| 31  | 8     | 307 | CLA  | O1D-CGD-CBD | -2.74 | 118.88      | 124.48   |
| 31  | A     | 850 | CLA  | CMD-C2D-C1D | 2.74  | 129.54      | 124.71   |
| 31  | 6     | 322 | CLA  | CMD-C2D-C1D | 2.74  | 129.54      | 124.71   |
| 33  | 7     | 308 | DGD  | C1E-O6E-C5E | 2.74  | 119.07      | 113.69   |
| 36  | 4     | 302 | LUT  | C17-C1-C6   | -2.74 | 105.86      | 110.30   |
| 26  | 5     | 302 | BCR  | C27-C26-C25 | 2.74  | 126.71      | 122.73   |
| 31  | L     | 307 | CLA  | C3D-C2D-C1D | -2.74 | 102.09      | 105.83   |
| 31  | A     | 853 | CLA  | C4-C3-C5    | 2.74  | 119.88      | 115.27   |
| 31  | 6     | 315 | CLA  | O1D-CGD-CBD | -2.74 | 118.88      | 124.48   |
| 31  | 3     | 313 | CLA  | CAC-C3C-C4C | 2.74  | 128.36      | 124.81   |
| 36  | J     | 103 | LUT  | C10-C11-C12 | -2.74 | 114.68      | 123.22   |
| 31  | 7     | 322 | CLA  | O2D-CGD-O1D | -2.74 | 118.49      | 123.84   |
| 31  | 5     | 320 | CLA  | CMC-C2C-C1C | 2.74  | 129.21      | 125.04   |
| 32  | 7     | 320 | CHL  | CHC-C1C-NC  | -2.74 | 120.05      | 124.20   |
| 31  | L     | 307 | CLA  | CMD-C2D-C1D | 2.73  | 129.53      | 124.71   |
| 31  | O     | 203 | CLA  | C3D-C2D-C1D | -2.73 | 102.10      | 105.83   |
| 36  | 3     | 304 | LUT  | C35-C15-C14 | -2.73 | 117.88      | 123.47   |
| 28  | A     | 811 | LHG  | O8-C23-C24  | 2.73  | 120.48      | 111.91   |
| 31  | 4     | 305 | CLA  | O2A-CGA-CBA | 2.73  | 120.48      | 111.91   |
| 31  | A     | 847 | CLA  | O1D-CGD-CBD | -2.73 | 118.89      | 124.48   |
| 31  | 8     | 307 | CLA  | CMC-C2C-C1C | 2.73  | 129.20      | 125.04   |
| 36  | F     | 304 | LUT  | C2-C3-C4    | 2.73  | 114.04      | 110.30   |
| 32  | b     | 309 | CHL  | CHC-C1C-NC  | -2.73 | 120.06      | 124.20   |
| 32  | 9     | 320 | CHL  | C2C-C3C-C4C | -2.73 | 104.54      | 106.49   |
| 31  | 3     | 317 | CLA  | C3D-C2D-C1D | -2.73 | 102.11      | 105.83   |
| 31  | B     | 822 | CLA  | C4C-C3C-C2C | -2.73 | 102.92      | 106.90   |
| 31  | a     | 313 | CLA  | CMD-C2D-C1D | 2.73  | 129.52      | 124.71   |
| 26  | B     | 805 | BCR  | C31-C1-C6   | 2.73  | 114.72      | 110.30   |
| 32  | 7     | 324 | CHL  | C2D-C1D-ND  | 2.73  | 112.11      | 110.10   |
| 31  | b     | 307 | CLA  | C3D-C2D-C1D | -2.73 | 102.11      | 105.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 821 | CLA  | O1D-CGD-CBD | -2.73 | 118.91      | 124.48   |
| 31  | b     | 310 | CLA  | CMD-C2D-C1D | 2.73  | 129.52      | 124.71   |
| 31  | b     | 310 | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 26  | A     | 805 | BCR  | C28-C27-C26 | -2.72 | 109.21      | 114.08   |
| 31  | A     | 826 | CLA  | CMB-C2B-C3B | 2.72  | 129.78      | 124.68   |
| 32  | 3     | 315 | CHL  | CHC-C1C-NC  | -2.72 | 120.07      | 124.20   |
| 31  | A     | 852 | CLA  | C4D-CHA-C1A | -2.72 | 117.93      | 121.25   |
| 31  | L     | 305 | CLA  | CMB-C2B-C3B | 2.72  | 129.77      | 124.68   |
| 28  | 7     | 302 | LHG  | O8-C23-C24  | 2.72  | 120.45      | 111.91   |
| 32  | 6     | 309 | CHL  | C4-C3-C5    | 2.72  | 119.85      | 115.27   |
| 31  | 7     | 309 | CLA  | CMC-C2C-C1C | 2.72  | 129.18      | 125.04   |
| 31  | b     | 306 | CLA  | CHC-C1C-NC  | -2.72 | 120.08      | 124.20   |
| 31  | 8     | 311 | CLA  | C4D-CHA-C1A | -2.72 | 117.94      | 121.25   |
| 31  | a     | 315 | CLA  | C1-C2-C3    | -2.72 | 121.34      | 126.04   |
| 31  | 4     | 309 | CLA  | C1-C2-C3    | -2.72 | 121.34      | 126.04   |
| 32  | 7     | 320 | CHL  | C4D-CHA-C1A | -2.72 | 117.94      | 121.25   |
| 31  | 5     | 314 | CLA  | O1D-CGD-CBD | -2.72 | 118.92      | 124.48   |
| 36  | 9     | 305 | LUT  | C30-C31-C32 | -2.72 | 114.73      | 123.22   |
| 31  | A     | 830 | CLA  | CMB-C2B-C3B | 2.72  | 129.76      | 124.68   |
| 31  | A     | 849 | CLA  | C3D-C2D-C1D | -2.72 | 102.12      | 105.83   |
| 31  | 5     | 313 | CLA  | CHD-C4C-C3C | -2.72 | 120.84      | 124.84   |
| 32  | a     | 318 | CHL  | O2A-CGA-CBA | 2.72  | 120.44      | 111.91   |
| 31  | 2     | 305 | CLA  | C3D-C2D-C1D | -2.72 | 102.12      | 105.83   |
| 31  | 5     | 310 | CLA  | CMC-C2C-C1C | 2.72  | 129.18      | 125.04   |
| 31  | 5     | 310 | CLA  | C3D-C2D-C1D | -2.72 | 102.12      | 105.83   |
| 31  | 5     | 313 | CLA  | O2D-CGD-O1D | -2.72 | 118.53      | 123.84   |
| 31  | F     | 305 | CLA  | CAC-C3C-C4C | 2.72  | 128.33      | 124.81   |
| 31  | B     | 843 | CLA  | CHC-C1C-NC  | -2.71 | 120.08      | 124.20   |
| 31  | B     | 835 | CLA  | O1D-CGD-CBD | -2.71 | 118.93      | 124.48   |
| 31  | b     | 304 | CLA  | C3D-C2D-C1D | -2.71 | 102.13      | 105.83   |
| 31  | A     | 832 | CLA  | C1-C2-C3    | -2.71 | 121.35      | 126.04   |
| 33  | 7     | 308 | DGD  | CDB-CCB-CBB | -2.71 | 100.65      | 114.42   |
| 31  | b     | 311 | CLA  | CHC-C1C-NC  | -2.71 | 120.09      | 124.20   |
| 31  | 5     | 309 | CLA  | CMD-C2D-C1D | 2.71  | 129.49      | 124.71   |
| 31  | B     | 811 | CLA  | CHB-C4A-NA  | 2.71  | 128.26      | 124.51   |
| 31  | 3     | 313 | CLA  | C3D-C2D-C1D | -2.71 | 102.13      | 105.83   |
| 26  | K     | 202 | BCR  | C27-C26-C25 | 2.71  | 126.67      | 122.73   |
| 31  | B     | 846 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 31  | 5     | 309 | CLA  | CAC-C3C-C4C | 2.71  | 128.33      | 124.81   |
| 31  | 9     | 315 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 31  | 6     | 312 | CLA  | CED-O2D-CGD | 2.71  | 122.07      | 115.94   |
| 31  | A     | 822 | CLA  | O2D-CGD-O1D | -2.71 | 118.54      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 8     | 302 | LUT  | C18-C5-C4   | -2.71 | 109.33      | 114.36   |
| 31  | 7     | 314 | CLA  | C4-C3-C5    | 2.71  | 119.83      | 115.27   |
| 31  | 7     | 311 | CLA  | C1-C2-C3    | -2.71 | 121.36      | 126.04   |
| 31  | 2     | 304 | CLA  | CMB-C2B-C3B | 2.71  | 129.75      | 124.68   |
| 31  | a     | 311 | CLA  | C3D-C2D-C1D | -2.71 | 102.14      | 105.83   |
| 31  | 2     | 308 | CLA  | O2A-CGA-CBA | 2.71  | 122.92      | 112.23   |
| 31  | 2     | 307 | CLA  | CHD-C4C-NC  | 2.71  | 128.47      | 124.20   |
| 31  | G     | 205 | CLA  | CHC-C1C-NC  | -2.70 | 120.10      | 124.20   |
| 31  | 9     | 321 | CLA  | C3D-C2D-C1D | -2.70 | 102.14      | 105.83   |
| 31  | J     | 105 | CLA  | CHB-C4A-NA  | 2.70  | 128.25      | 124.51   |
| 31  | A     | 820 | CLA  | C4-C3-C5    | 2.70  | 119.82      | 115.27   |
| 31  | a     | 309 | CLA  | CHD-C4C-NC  | 2.70  | 128.46      | 124.20   |
| 31  | O     | 203 | CLA  | CHD-C4C-NC  | 2.70  | 128.46      | 124.20   |
| 31  | 4     | 315 | CLA  | CHD-C4C-NC  | 2.70  | 128.46      | 124.20   |
| 31  | a     | 310 | CLA  | CHD-C4C-NC  | 2.70  | 128.46      | 124.20   |
| 31  | 5     | 307 | CLA  | C3D-C2D-C1D | -2.70 | 102.14      | 105.83   |
| 31  | 5     | 313 | CLA  | C4D-CHA-C1A | -2.70 | 117.96      | 121.25   |
| 31  | 9     | 321 | CLA  | O2A-CGA-CBA | 2.70  | 120.38      | 111.91   |
| 31  | b     | 308 | CLA  | CMC-C2C-C1C | 2.70  | 129.15      | 125.04   |
| 31  | 9     | 319 | CLA  | CED-O2D-CGD | 2.70  | 122.04      | 115.94   |
| 31  | 5     | 314 | CLA  | C3D-C2D-C1D | -2.70 | 102.15      | 105.83   |
| 31  | O     | 203 | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 31  | A     | 821 | CLA  | C1-C2-C3    | -2.70 | 121.38      | 126.04   |
| 31  | B     | 835 | CLA  | CHD-C4C-NC  | 2.70  | 128.46      | 124.20   |
| 36  | L     | 304 | LUT  | C4-C5-C6    | -2.70 | 114.83      | 120.85   |
| 31  | B     | 820 | CLA  | CMC-C2C-C1C | 2.70  | 129.15      | 125.04   |
| 32  | 6     | 318 | CHL  | O1D-CGD-CBD | -2.70 | 118.96      | 124.48   |
| 31  | O     | 202 | CLA  | CHD-C4C-NC  | 2.70  | 128.45      | 124.20   |
| 32  | 3     | 315 | CHL  | O2A-CGA-CBA | 2.70  | 120.37      | 111.91   |
| 31  | A     | 844 | CLA  | CMB-C2B-C3B | 2.70  | 129.72      | 124.68   |
| 31  | B     | 825 | CLA  | C1-C2-C3    | -2.69 | 121.38      | 126.04   |
| 31  | 9     | 316 | CLA  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 31  | 3     | 307 | CLA  | C1-C2-C3    | -2.69 | 121.38      | 126.04   |
| 31  | 3     | 313 | CLA  | CMC-C2C-C1C | 2.69  | 129.14      | 125.04   |
| 32  | 7     | 317 | CHL  | CHC-C1C-NC  | -2.69 | 120.12      | 124.20   |
| 31  | B     | 813 | CLA  | CMD-C2D-C1D | 2.69  | 129.46      | 124.71   |
| 31  | 6     | 307 | CLA  | O2A-CGA-CBA | 2.69  | 120.36      | 111.91   |
| 32  | 4     | 313 | CHL  | CHD-C4C-NC  | 2.69  | 128.45      | 124.20   |
| 31  | 6     | 311 | CLA  | CHC-C1C-NC  | -2.69 | 120.12      | 124.20   |
| 31  | B     | 824 | CLA  | CHD-C4C-NC  | 2.69  | 128.44      | 124.20   |
| 32  | 5     | 316 | CHL  | C4-C3-C5    | 2.69  | 119.80      | 115.27   |
| 36  | 8     | 303 | LUT  | C10-C11-C12 | -2.69 | 114.82      | 123.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 823 | CLA  | C3D-C2D-C1D | -2.69 | 102.16      | 105.83   |
| 32  | 9     | 322 | CHL  | O1D-CGD-CBD | -2.69 | 118.98      | 124.48   |
| 31  | B     | 819 | CLA  | C4-C3-C5    | 2.69  | 119.79      | 115.27   |
| 31  | 2     | 307 | CLA  | C4-C3-C5    | 2.69  | 119.79      | 115.27   |
| 32  | 6     | 321 | CHL  | C4D-CHA-C1A | -2.69 | 117.98      | 121.25   |
| 31  | B     | 834 | CLA  | C1D-CHD-C4C | -2.69 | 120.26      | 126.06   |
| 31  | 6     | 322 | CLA  | C3D-C2D-C1D | -2.69 | 102.17      | 105.83   |
| 31  | G     | 205 | CLA  | C3D-C2D-C1D | -2.68 | 102.17      | 105.83   |
| 31  | 7     | 311 | CLA  | C3D-C2D-C1D | -2.68 | 102.17      | 105.83   |
| 36  | 6     | 304 | LUT  | C30-C31-C32 | -2.68 | 114.84      | 123.22   |
| 31  | B     | 811 | CLA  | CAC-C3C-C4C | 2.68  | 128.29      | 124.81   |
| 31  | O     | 202 | CLA  | O2D-CGD-O1D | -2.68 | 118.00      | 124.09   |
| 36  | a     | 303 | LUT  | C35-C15-C14 | -2.68 | 117.98      | 123.47   |
| 31  | K     | 205 | CLA  | CMB-C2B-C3B | 2.68  | 129.70      | 124.68   |
| 31  | A     | 843 | CLA  | C3D-C2D-C1D | -2.68 | 102.17      | 105.83   |
| 26  | 5     | 302 | BCR  | C3-C4-C5    | -2.68 | 109.29      | 114.08   |
| 31  | F     | 301 | CLA  | O2A-CGA-CBA | 2.68  | 120.33      | 111.91   |
| 36  | a     | 303 | LUT  | C36-C21-C26 | 2.68  | 113.61      | 109.55   |
| 31  | O     | 204 | CLA  | CAC-C3C-C4C | 2.68  | 128.29      | 124.81   |
| 31  | 2     | 313 | CLA  | C3D-C2D-C1D | -2.68 | 102.17      | 105.83   |
| 31  | 6     | 314 | CLA  | C3D-C2D-C1D | -2.68 | 102.17      | 105.83   |
| 31  | 3     | 314 | CLA  | C3D-C2D-C1D | -2.68 | 102.17      | 105.83   |
| 31  | B     | 835 | CLA  | CMC-C2C-C1C | 2.68  | 129.12      | 125.04   |
| 26  | B     | 806 | BCR  | C27-C26-C25 | 2.68  | 126.62      | 122.73   |
| 31  | B     | 825 | CLA  | C4-C3-C5    | 2.68  | 119.78      | 115.27   |
| 32  | 8     | 316 | CHL  | C2D-C1D-ND  | 2.68  | 112.08      | 110.10   |
| 31  | a     | 313 | CLA  | CMB-C2B-C3B | 2.68  | 129.68      | 124.68   |
| 36  | 8     | 303 | LUT  | C22-C23-C24 | 2.67  | 114.78      | 111.74   |
| 31  | b     | 306 | CLA  | C3D-C2D-C1D | -2.67 | 102.18      | 105.83   |
| 31  | 2     | 306 | CLA  | C3D-C2D-C1D | -2.67 | 102.18      | 105.83   |
| 31  | O     | 202 | CLA  | CMD-C2D-C1D | 2.67  | 129.43      | 124.71   |
| 31  | 3     | 312 | CLA  | CAC-C3C-C4C | 2.67  | 128.28      | 124.81   |
| 31  | 8     | 310 | CLA  | CAC-C3C-C4C | 2.67  | 128.28      | 124.81   |
| 31  | 4     | 312 | CLA  | O2A-CGA-CBA | 2.67  | 120.29      | 111.91   |
| 31  | B     | 849 | CLA  | CMD-C2D-C1D | 2.67  | 129.42      | 124.71   |
| 32  | 6     | 320 | CHL  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 31  | A     | 837 | CLA  | O2D-CGD-O1D | -2.67 | 118.61      | 123.84   |
| 31  | 4     | 320 | CLA  | O1D-CGD-CBD | -2.67 | 119.02      | 124.48   |
| 31  | A     | 829 | CLA  | C1B-CHB-C4A | -2.67 | 124.83      | 130.12   |
| 31  | b     | 310 | CLA  | C4D-CHA-C1A | -2.67 | 118.00      | 121.25   |
| 31  | 6     | 313 | CLA  | CMC-C2C-C1C | 2.67  | 129.10      | 125.04   |
| 36  | 9     | 303 | LUT  | C16-C1-C6   | 2.67  | 114.63      | 110.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 822 | CLA  | O1D-CGD-CBD | -2.67 | 119.02      | 124.48   |
| 28  | 8     | 304 | LHG  | O8-C23-C24  | 2.67  | 120.28      | 111.91   |
| 32  | 7     | 324 | CHL  | O2A-CGA-CBA | 2.67  | 120.28      | 111.91   |
| 31  | H     | 902 | CLA  | C3D-C2D-C1D | -2.67 | 102.19      | 105.83   |
| 32  | A     | 840 | CHL  | O2A-CGA-CBA | 2.67  | 120.28      | 111.91   |
| 32  | 3     | 315 | CHL  | C2D-C1D-ND  | 2.67  | 112.07      | 110.10   |
| 31  | L     | 305 | CLA  | O1D-CGD-CBD | -2.67 | 119.03      | 124.48   |
| 31  | 6     | 316 | CLA  | O1D-CGD-CBD | -2.67 | 119.03      | 124.48   |
| 33  | B     | 808 | DGD  | CDB-CCB-CBB | -2.67 | 100.89      | 114.42   |
| 32  | 5     | 317 | CHL  | C2D-C1D-ND  | 2.67  | 112.07      | 110.10   |
| 31  | A     | 841 | CLA  | C4-C3-C5    | 2.67  | 119.76      | 115.27   |
| 32  | 6     | 309 | CHL  | C1-C2-C3    | -2.67 | 121.43      | 126.04   |
| 31  | A     | 817 | CLA  | CMC-C2C-C1C | 2.67  | 129.10      | 125.04   |
| 31  | 7     | 312 | CLA  | CMC-C2C-C1C | 2.67  | 129.10      | 125.04   |
| 31  | 3     | 311 | CLA  | C4-C3-C5    | 2.67  | 119.75      | 115.27   |
| 31  | B     | 844 | CLA  | CMD-C2D-C1D | 2.67  | 129.41      | 124.71   |
| 31  | 3     | 311 | CLA  | C3D-C2D-C1D | -2.67 | 102.19      | 105.83   |
| 31  | b     | 312 | CLA  | CHC-C1C-NC  | -2.66 | 120.16      | 124.20   |
| 31  | a     | 321 | CLA  | O2A-CGA-CBA | 2.66  | 120.27      | 111.91   |
| 31  | 2     | 309 | CLA  | C3D-C2D-C1D | -2.66 | 102.20      | 105.83   |
| 31  | L     | 307 | CLA  | CAC-C3C-C4C | 2.66  | 128.26      | 124.81   |
| 32  | 9     | 320 | CHL  | CMB-C2B-C3B | 2.66  | 129.66      | 124.68   |
| 31  | 6     | 307 | CLA  | CHC-C1C-NC  | -2.66 | 120.16      | 124.20   |
| 31  | 5     | 309 | CLA  | C3D-C2D-C1D | -2.66 | 102.20      | 105.83   |
| 31  | L     | 306 | CLA  | O1D-CGD-CBD | -2.66 | 119.04      | 124.48   |
| 36  | 9     | 303 | LUT  | C2-C3-C4    | 2.66  | 113.95      | 110.30   |
| 31  | B     | 827 | CLA  | CMD-C2D-C1D | 2.66  | 129.40      | 124.71   |
| 36  | 9     | 305 | LUT  | C18-C5-C4   | -2.66 | 109.43      | 114.36   |
| 31  | 2     | 307 | CLA  | C3D-C2D-C1D | -2.66 | 102.20      | 105.83   |
| 26  | 6     | 302 | BCR  | C7-C8-C9    | -2.66 | 122.22      | 126.23   |
| 31  | a     | 319 | CLA  | C3D-C2D-C1D | -2.66 | 102.20      | 105.83   |
| 31  | 9     | 311 | CLA  | C3D-C2D-C1D | -2.66 | 102.20      | 105.83   |
| 31  | 4     | 306 | CLA  | CHC-C1C-NC  | -2.66 | 120.17      | 124.20   |
| 31  | 6     | 306 | CLA  | C1D-ND-C4D  | -2.66 | 104.45      | 106.33   |
| 31  | G     | 206 | CLA  | CAC-C3C-C4C | 2.66  | 128.26      | 124.81   |
| 31  | K     | 206 | CLA  | C3D-C2D-C1D | -2.66 | 102.20      | 105.83   |
| 31  | 5     | 321 | CLA  | CAC-C3C-C4C | 2.66  | 128.26      | 124.81   |
| 30  | A     | 813 | CL0  | C1D-CHD-C4C | -2.66 | 120.33      | 126.06   |
| 31  | 5     | 323 | CLA  | O2A-CGA-CBA | 2.66  | 120.24      | 111.91   |
| 31  | 5     | 308 | CLA  | C3D-C2D-C1D | -2.66 | 102.21      | 105.83   |
| 32  | 4     | 317 | CHL  | CHD-C4C-NC  | 2.66  | 128.39      | 124.20   |
| 31  | 8     | 312 | CLA  | C1-C2-C3    | -2.66 | 122.46      | 126.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 838 | CLA  | C3D-C2D-C1D | -2.65 | 102.21      | 105.83   |
| 31  | 7     | 316 | CLA  | C3D-C2D-C1D | -2.65 | 102.21      | 105.83   |
| 36  | 9     | 303 | LUT  | C10-C11-C12 | -2.65 | 114.93      | 123.22   |
| 35  | a     | 302 | QTB  | C11-C10-C09 | 2.65  | 131.23      | 125.47   |
| 31  | A     | 853 | CLA  | C1-C2-C3    | -2.65 | 121.45      | 126.04   |
| 31  | A     | 816 | CLA  | C4-C3-C5    | 2.65  | 119.73      | 115.27   |
| 26  | K     | 203 | BCR  | C24-C23-C22 | -2.65 | 122.23      | 126.23   |
| 31  | 5     | 310 | CLA  | CAC-C3C-C4C | 2.65  | 128.25      | 124.81   |
| 31  | 9     | 318 | CLA  | CHD-C4C-NC  | 2.65  | 128.38      | 124.20   |
| 31  | B     | 834 | CLA  | CMD-C2D-C1D | 2.65  | 129.39      | 124.71   |
| 31  | 9     | 317 | CLA  | O2A-CGA-CBA | 2.65  | 120.23      | 111.91   |
| 31  | 4     | 308 | CLA  | CHC-C1C-NC  | -2.65 | 120.18      | 124.20   |
| 32  | 7     | 318 | CHL  | CHC-C1C-NC  | -2.65 | 120.18      | 124.20   |
| 31  | B     | 847 | CLA  | C1-C2-C3    | -2.65 | 121.46      | 126.04   |
| 31  | A     | 848 | CLA  | C4-C3-C2    | -2.65 | 116.88      | 123.68   |
| 32  | 4     | 317 | CHL  | C1D-CHD-C4C | -2.65 | 120.34      | 126.06   |
| 31  | B     | 842 | CLA  | CAC-C3C-C4C | 2.65  | 128.25      | 124.81   |
| 31  | G     | 204 | CLA  | CMD-C2D-C1D | 2.65  | 129.38      | 124.71   |
| 31  | A     | 852 | CLA  | CAC-C3C-C4C | 2.65  | 128.24      | 124.81   |
| 31  | H     | 901 | CLA  | CHD-C4C-NC  | 2.65  | 128.37      | 124.20   |
| 37  | a     | 301 | LMG  | O6-C1-O1    | -2.65 | 103.71      | 109.97   |
| 31  | 8     | 320 | CLA  | C4-C3-C5    | 2.64  | 119.72      | 115.27   |
| 32  | 5     | 317 | CHL  | CMD-C2D-C1D | 2.64  | 129.37      | 124.71   |
| 31  | A     | 830 | CLA  | O2A-CGA-CBA | 2.64  | 120.20      | 111.91   |
| 31  | A     | 856 | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 31  | B     | 818 | CLA  | CMC-C2C-C1C | 2.64  | 129.06      | 125.04   |
| 31  | B     | 830 | CLA  | C1-C2-C3    | -2.64 | 121.47      | 126.04   |
| 31  | 6     | 308 | CLA  | CHD-C4C-C3C | -2.64 | 120.96      | 124.84   |
| 31  | 5     | 315 | CLA  | C1-C2-C3    | -2.64 | 121.48      | 126.04   |
| 31  | B     | 817 | CLA  | C3D-C2D-C1D | -2.64 | 102.23      | 105.83   |
| 31  | 7     | 314 | CLA  | C1-C2-C3    | -2.64 | 121.48      | 126.04   |
| 31  | F     | 306 | CLA  | CAC-C3C-C4C | 2.64  | 128.24      | 124.81   |
| 31  | b     | 308 | CLA  | CHD-C4C-NC  | 2.64  | 128.36      | 124.20   |
| 31  | 6     | 311 | CLA  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 31  | B     | 814 | CLA  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 31  | 5     | 308 | CLA  | CHC-C1C-NC  | -2.64 | 120.20      | 124.20   |
| 31  | B     | 833 | CLA  | CMD-C2D-C1D | 2.64  | 129.36      | 124.71   |
| 31  | 4     | 306 | CLA  | CMD-C2D-C1D | 2.64  | 129.36      | 124.71   |
| 31  | A     | 815 | CLA  | O2A-CGA-CBA | 2.64  | 120.19      | 111.91   |
| 31  | 2     | 309 | CLA  | CMB-C2B-C3B | 2.64  | 129.61      | 124.68   |
| 32  | 6     | 309 | CHL  | C3D-C2D-C1D | -2.64 | 102.23      | 105.83   |
| 31  | G     | 204 | CLA  | C1-C2-C3    | -2.64 | 122.48      | 126.75   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 833 | CLA  | O1D-CGD-CBD | -2.64 | 119.09      | 124.48   |
| 31  | 5     | 320 | CLA  | CMB-C2B-C3B | 2.64  | 129.61      | 124.68   |
| 31  | 4     | 312 | CLA  | CMC-C2C-C1C | 2.64  | 129.05      | 125.04   |
| 31  | A     | 847 | CLA  | C4-C3-C5    | 2.64  | 119.70      | 115.27   |
| 32  | A     | 831 | CHL  | CHC-C1C-NC  | -2.64 | 120.20      | 124.20   |
| 31  | a     | 316 | CLA  | CAC-C3C-C4C | 2.64  | 128.23      | 124.81   |
| 31  | 3     | 316 | CLA  | CMB-C2B-C3B | 2.63  | 129.61      | 124.68   |
| 32  | 4     | 313 | CHL  | O2D-CGD-O1D | -2.63 | 118.69      | 123.84   |
| 31  | B     | 850 | CLA  | CMB-C2B-C3B | 2.63  | 129.61      | 124.68   |
| 31  | 2     | 311 | CLA  | CMC-C2C-C1C | 2.63  | 129.05      | 125.04   |
| 31  | 2     | 314 | CLA  | C3D-C2D-C1D | -2.63 | 102.24      | 105.83   |
| 32  | 5     | 316 | CHL  | CHD-C1D-ND  | -2.63 | 122.03      | 124.45   |
| 36  | 9     | 302 | LUT  | C17-C1-C6   | -2.63 | 106.03      | 110.30   |
| 31  | 8     | 314 | CLA  | CMB-C2B-C3B | 2.63  | 129.60      | 124.68   |
| 31  | B     | 828 | CLA  | CMD-C2D-C1D | 2.63  | 129.35      | 124.71   |
| 32  | 7     | 320 | CHL  | CMD-C2D-C1D | 2.63  | 129.35      | 124.71   |
| 31  | 9     | 317 | CLA  | CMD-C2D-C3D | -2.63 | 121.56      | 127.61   |
| 31  | 4     | 307 | CLA  | CMD-C2D-C1D | 2.63  | 129.35      | 124.71   |
| 31  | A     | 834 | CLA  | C3D-C2D-C1D | -2.63 | 102.24      | 105.83   |
| 31  | A     | 814 | CLA  | C4-C3-C5    | 2.63  | 119.69      | 115.27   |
| 31  | 8     | 308 | CLA  | CMC-C2C-C1C | 2.63  | 129.04      | 125.04   |
| 31  | 4     | 309 | CLA  | O2A-CGA-CBA | 2.63  | 120.16      | 111.91   |
| 26  | 3     | 302 | BCR  | C7-C8-C9    | -2.63 | 122.26      | 126.23   |
| 32  | 9     | 320 | CHL  | O1D-CGD-CBD | -2.63 | 119.11      | 124.48   |
| 31  | 3     | 309 | CLA  | O2A-CGA-CBA | 2.63  | 120.15      | 111.91   |
| 31  | 5     | 318 | CLA  | CMD-C2D-C1D | 2.63  | 129.34      | 124.71   |
| 31  | 5     | 310 | CLA  | CHD-C4C-NC  | 2.63  | 128.34      | 124.20   |
| 31  | 5     | 307 | CLA  | C1-C2-C3    | -2.63 | 121.50      | 126.04   |
| 31  | b     | 307 | CLA  | CHC-C1C-NC  | -2.63 | 120.22      | 124.20   |
| 31  | b     | 307 | CLA  | CED-O2D-CGD | 2.63  | 121.88      | 115.94   |
| 31  | 6     | 311 | CLA  | CHD-C4C-NC  | 2.63  | 128.34      | 124.20   |
| 31  | A     | 829 | CLA  | CMD-C2D-C3D | -2.63 | 121.57      | 127.61   |
| 31  | B     | 821 | CLA  | C1-C2-C3    | -2.63 | 121.50      | 126.04   |
| 31  | B     | 836 | CLA  | O1D-CGD-CBD | -2.62 | 119.11      | 124.48   |
| 30  | A     | 813 | CL0  | CHB-C4A-NA  | 2.62  | 128.14      | 124.51   |
| 31  | B     | 815 | CLA  | CHC-C1C-NC  | -2.62 | 120.22      | 124.20   |
| 36  | b     | 301 | LUT  | C22-C23-C24 | 2.62  | 114.72      | 111.74   |
| 32  | 7     | 317 | CHL  | C2D-C1D-ND  | 2.62  | 112.04      | 110.10   |
| 31  | B     | 836 | CLA  | C4-C3-C5    | 2.62  | 119.68      | 115.27   |
| 26  | 3     | 303 | BCR  | C27-C26-C25 | 2.62  | 126.54      | 122.73   |
| 31  | a     | 321 | CLA  | C5-C3-C4    | 2.62  | 120.39      | 114.60   |
| 31  | B     | 845 | CLA  | O1D-CGD-CBD | -2.62 | 119.12      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 4     | 315 | CLA  | CMD-C2D-C1D | 2.62  | 129.33      | 124.71   |
| 31  | 5     | 308 | CLA  | CED-O2D-CGD | 2.62  | 121.86      | 115.94   |
| 31  | A     | 848 | CLA  | CMB-C2B-C3B | 2.62  | 129.58      | 124.68   |
| 31  | 4     | 314 | CLA  | CHC-C1C-NC  | -2.62 | 120.23      | 124.20   |
| 32  | 7     | 324 | CHL  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 31  | G     | 205 | CLA  | CMC-C2C-C1C | 2.62  | 129.03      | 125.04   |
| 31  | a     | 316 | CLA  | C2A-C1A-CHA | -2.62 | 119.28      | 123.86   |
| 31  | 7     | 312 | CLA  | CAC-C3C-C4C | 2.62  | 128.21      | 124.81   |
| 31  | 2     | 315 | CLA  | CHC-C1C-NC  | -2.62 | 120.23      | 124.20   |
| 31  | 5     | 318 | CLA  | CMB-C2B-C3B | 2.62  | 129.58      | 124.68   |
| 31  | G     | 204 | CLA  | O2A-CGA-CBA | 2.62  | 120.12      | 111.91   |
| 31  | 8     | 312 | CLA  | CHC-C1C-NC  | -2.62 | 120.23      | 124.20   |
| 31  | 8     | 320 | CLA  | CAC-C3C-C4C | 2.62  | 128.21      | 124.81   |
| 31  | 4     | 308 | CLA  | CED-O2D-CGD | 2.62  | 121.86      | 115.94   |
| 31  | 8     | 309 | CLA  | C1-O2A-CGA  | 2.62  | 123.31      | 116.44   |
| 31  | A     | 823 | CLA  | C1D-CHD-C4C | -2.62 | 120.41      | 126.06   |
| 31  | 4     | 308 | CLA  | C1-C2-C3    | -2.62 | 121.52      | 126.04   |
| 31  | A     | 852 | CLA  | CMD-C2D-C1D | 2.62  | 129.32      | 124.71   |
| 31  | 2     | 308 | CLA  | CMD-C2D-C1D | 2.62  | 129.32      | 124.71   |
| 31  | 5     | 320 | CLA  | C3D-C2D-C1D | -2.62 | 102.26      | 105.83   |
| 31  | G     | 206 | CLA  | CMB-C2B-C3B | 2.62  | 129.57      | 124.68   |
| 31  | A     | 853 | CLA  | O2D-CGD-O1D | -2.62 | 118.72      | 123.84   |
| 37  | J     | 101 | LMG  | O6-C1-O1    | -2.62 | 103.78      | 109.97   |
| 32  | a     | 317 | CHL  | CAA-CBA-CGA | -2.62 | 105.61      | 113.25   |
| 31  | B     | 828 | CLA  | C11-C10-C8  | -2.62 | 107.47      | 115.92   |
| 31  | O     | 202 | CLA  | C3D-C2D-C1D | -2.62 | 102.26      | 105.83   |
| 31  | B     | 850 | CLA  | CHD-C4C-NC  | 2.61  | 128.32      | 124.20   |
| 32  | 6     | 319 | CHL  | CMD-C2D-C1D | 2.61  | 129.32      | 124.71   |
| 31  | B     | 834 | CLA  | C4-C3-C5    | 2.61  | 119.67      | 115.27   |
| 31  | 4     | 321 | CLA  | CED-O2D-CGD | 2.61  | 121.85      | 115.94   |
| 31  | b     | 313 | CLA  | C3D-C2D-C1D | -2.61 | 102.26      | 105.83   |
| 32  | 7     | 317 | CHL  | O2A-CGA-CBA | 2.61  | 120.11      | 111.91   |
| 31  | A     | 834 | CLA  | CED-O2D-CGD | 2.61  | 121.85      | 115.94   |
| 31  | B     | 832 | CLA  | CMD-C2D-C1D | 2.61  | 129.32      | 124.71   |
| 31  | 8     | 313 | CLA  | CMD-C2D-C1D | 2.61  | 129.32      | 124.71   |
| 32  | 9     | 322 | CHL  | CHD-C1D-ND  | -2.61 | 122.05      | 124.45   |
| 26  | K     | 202 | BCR  | C39-C30-C25 | 2.61  | 114.54      | 110.30   |
| 36  | 6     | 303 | LUT  | C8-C7-C6    | -2.61 | 119.87      | 127.20   |
| 31  | H     | 902 | CLA  | CMC-C2C-C1C | 2.61  | 129.02      | 125.04   |
| 36  | a     | 305 | LUT  | C4-C5-C6    | -2.61 | 115.03      | 120.85   |
| 31  | A     | 851 | CLA  | CHD-C4C-NC  | 2.61  | 128.32      | 124.20   |
| 31  | B     | 834 | CLA  | C3C-C4C-NC  | 2.61  | 113.50      | 110.57   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 2     | 301 | LUT  | C10-C11-C12 | -2.61 | 115.07      | 123.22   |
| 31  | B     | 832 | CLA  | C4-C3-C5    | 2.61  | 119.66      | 115.27   |
| 31  | 9     | 314 | CLA  | C1-C2-C3    | -2.61 | 121.53      | 126.04   |
| 31  | G     | 204 | CLA  | C5-C3-C4    | 2.61  | 120.36      | 114.60   |
| 32  | 5     | 316 | CHL  | OMC-CMC-C2C | -2.61 | 119.79      | 125.69   |
| 35  | 7     | 303 | QTB  | C03-C04-C05 | 2.61  | 131.36      | 123.22   |
| 32  | 4     | 310 | CHL  | CHD-C4C-NC  | 2.61  | 128.31      | 124.20   |
| 37  | G     | 202 | LMG  | O1-C7-C8    | -2.61 | 104.61      | 110.90   |
| 32  | A     | 840 | CHL  | C1D-CHD-C4C | -2.61 | 120.43      | 126.06   |
| 31  | 5     | 315 | CLA  | O2A-CGA-CBA | 2.61  | 120.09      | 111.91   |
| 31  | a     | 319 | CLA  | C1-O2A-CGA  | 2.61  | 123.28      | 116.44   |
| 31  | A     | 818 | CLA  | C3D-C2D-C1D | -2.61 | 102.28      | 105.83   |
| 31  | A     | 851 | CLA  | CMB-C2B-C3B | 2.61  | 129.55      | 124.68   |
| 31  | a     | 311 | CLA  | CMD-C2D-C1D | 2.61  | 129.31      | 124.71   |
| 31  | 9     | 321 | CLA  | CHD-C4C-NC  | 2.61  | 128.31      | 124.20   |
| 31  | 5     | 321 | CLA  | CHD-C4C-NC  | 2.61  | 128.31      | 124.20   |
| 31  | A     | 829 | CLA  | C5-C3-C4    | 2.61  | 120.36      | 114.60   |
| 31  | 4     | 314 | CLA  | C3D-C2D-C1D | -2.61 | 102.28      | 105.83   |
| 31  | 3     | 316 | CLA  | O2A-CGA-CBA | 2.60  | 120.08      | 111.91   |
| 31  | b     | 306 | CLA  | CED-O2D-CGD | 2.60  | 121.83      | 115.94   |
| 36  | 5     | 303 | LUT  | C1-C6-C7    | -2.60 | 108.41      | 115.78   |
| 31  | 2     | 315 | CLA  | CMC-C2C-C1C | 2.60  | 129.00      | 125.04   |
| 32  | 7     | 318 | CHL  | O2A-CGA-O1A | -2.60 | 117.02      | 123.59   |
| 31  | 8     | 308 | CLA  | O2A-CGA-O1A | -2.60 | 117.03      | 123.59   |
| 31  | 6     | 314 | CLA  | O2A-CGA-CBA | 2.60  | 120.07      | 111.91   |
| 31  | B     | 816 | CLA  | O1D-CGD-CBD | -2.60 | 119.16      | 124.48   |
| 31  | F     | 306 | CLA  | CHD-C4C-NC  | 2.60  | 128.30      | 124.20   |
| 31  | B     | 813 | CLA  | C4-C3-C5    | 2.60  | 119.64      | 115.27   |
| 31  | B     | 816 | CLA  | C1-C2-C3    | -2.60 | 121.55      | 126.04   |
| 31  | 3     | 313 | CLA  | CHC-C1C-NC  | -2.60 | 120.26      | 124.20   |
| 36  | J     | 103 | LUT  | C18-C5-C4   | -2.60 | 109.55      | 114.36   |
| 32  | 7     | 324 | CHL  | CMB-C2B-C3B | 2.60  | 129.53      | 124.68   |
| 32  | A     | 840 | CHL  | O2D-CGD-O1D | -2.60 | 118.76      | 123.84   |
| 31  | 4     | 315 | CLA  | O1D-CGD-CBD | -2.60 | 119.17      | 124.48   |
| 31  | 3     | 310 | CLA  | CMD-C2D-C1D | 2.60  | 129.29      | 124.71   |
| 31  | 8     | 312 | CLA  | C3D-C2D-C1D | -2.59 | 102.29      | 105.83   |
| 28  | 6     | 305 | LHG  | O8-C23-C24  | 2.59  | 120.05      | 111.91   |
| 31  | 3     | 320 | CLA  | C3D-C2D-C1D | -2.59 | 102.29      | 105.83   |
| 31  | 4     | 321 | CLA  | C3D-C2D-C1D | -2.59 | 102.29      | 105.83   |
| 31  | B     | 827 | CLA  | O2A-CGA-CBA | 2.59  | 120.05      | 111.91   |
| 31  | B     | 819 | CLA  | C1-C2-C3    | -2.59 | 121.56      | 126.04   |
| 31  | A     | 838 | CLA  | O2A-CGA-CBA | 2.59  | 120.05      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | F     | 306 | CLA  | O2A-CGA-CBA | 2.59  | 120.05      | 111.91   |
| 31  | A     | 814 | CLA  | CHD-C4C-NC  | 2.59  | 128.29      | 124.20   |
| 32  | 8     | 319 | CHL  | CMD-C2D-C1D | 2.59  | 129.28      | 124.71   |
| 31  | 2     | 306 | CLA  | CMD-C2D-C1D | 2.59  | 129.28      | 124.71   |
| 32  | 6     | 317 | CHL  | C2D-C1D-ND  | 2.59  | 112.01      | 110.10   |
| 31  | 8     | 314 | CLA  | CHD-C4C-NC  | 2.59  | 128.28      | 124.20   |
| 31  | B     | 829 | CLA  | CMB-C2B-C3B | 2.59  | 129.52      | 124.68   |
| 32  | K     | 201 | CHL  | C4D-CHA-C1A | -2.59 | 118.10      | 121.25   |
| 31  | 5     | 315 | CLA  | O1D-CGD-CBD | -2.59 | 119.19      | 124.48   |
| 31  | A     | 821 | CLA  | C6-C5-C3    | -2.59 | 106.67      | 113.45   |
| 31  | b     | 303 | CLA  | CHC-C1C-NC  | -2.59 | 120.28      | 124.20   |
| 31  | 2     | 311 | CLA  | C3D-C2D-C1D | -2.59 | 102.30      | 105.83   |
| 31  | 7     | 309 | CLA  | CAC-C3C-C4C | 2.59  | 128.17      | 124.81   |
| 31  | a     | 310 | CLA  | CHC-C1C-NC  | -2.59 | 120.28      | 124.20   |
| 31  | B     | 823 | CLA  | CHC-C1C-NC  | -2.59 | 120.28      | 124.20   |
| 32  | 9     | 320 | CHL  | C2D-C1D-ND  | 2.59  | 112.01      | 110.10   |
| 26  | J     | 102 | BCR  | C24-C23-C22 | -2.58 | 122.33      | 126.23   |
| 31  | B     | 842 | CLA  | C1-C2-C3    | -2.58 | 121.57      | 126.04   |
| 31  | 3     | 311 | CLA  | CHD-C4C-NC  | 2.58  | 128.28      | 124.20   |
| 31  | 4     | 311 | CLA  | CHD-C4C-NC  | 2.58  | 128.28      | 124.20   |
| 31  | B     | 843 | CLA  | C3D-C2D-C1D | -2.58 | 102.31      | 105.83   |
| 31  | 6     | 313 | CLA  | CMD-C2D-C1D | 2.58  | 129.27      | 124.71   |
| 36  | 4     | 302 | LUT  | C22-C23-C24 | 2.58  | 114.68      | 111.74   |
| 31  | 4     | 308 | CLA  | CMC-C2C-C1C | 2.58  | 128.97      | 125.04   |
| 31  | b     | 305 | CLA  | CMD-C2D-C1D | 2.58  | 129.26      | 124.71   |
| 31  | 9     | 313 | CLA  | CHC-C1C-NC  | -2.58 | 120.29      | 124.20   |
| 32  | 7     | 320 | CHL  | CHD-C1D-ND  | -2.58 | 122.08      | 124.45   |
| 32  | 6     | 320 | CHL  | C2D-C1D-ND  | 2.58  | 112.01      | 110.10   |
| 31  | 4     | 307 | CLA  | O2A-CGA-CBA | 2.58  | 120.00      | 111.91   |
| 31  | 5     | 315 | CLA  | C3D-C2D-C1D | -2.58 | 102.31      | 105.83   |
| 31  | 5     | 310 | CLA  | C1-C2-C3    | -2.58 | 121.58      | 126.04   |
| 26  | K     | 203 | BCR  | C15-C16-C17 | -2.58 | 118.19      | 123.47   |
| 31  | 9     | 315 | CLA  | C4-C3-C5    | 2.58  | 119.61      | 115.27   |
| 31  | K     | 204 | CLA  | C3D-C2D-C1D | -2.58 | 102.31      | 105.83   |
| 36  | b     | 301 | LUT  | C36-C21-C26 | 2.58  | 113.45      | 109.55   |
| 31  | A     | 856 | CLA  | O1D-CGD-CBD | -2.58 | 119.21      | 124.48   |
| 31  | 9     | 319 | CLA  | CAC-C3C-C4C | 2.58  | 128.15      | 124.81   |
| 32  | 5     | 319 | CHL  | CHC-C1C-NC  | -2.58 | 120.29      | 124.20   |
| 31  | 5     | 309 | CLA  | CHC-C1C-NC  | -2.58 | 120.30      | 124.20   |
| 31  | B     | 824 | CLA  | CMB-C2B-C3B | 2.58  | 129.50      | 124.68   |
| 31  | 6     | 311 | CLA  | C3D-C2D-C1D | -2.57 | 102.32      | 105.83   |
| 31  | A     | 845 | CLA  | CMC-C2C-C1C | 2.57  | 128.96      | 125.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 7     | 319 | CHL  | CMD-C2D-C1D | 2.57  | 129.25      | 124.71   |
| 26  | K     | 202 | BCR  | C24-C23-C22 | -2.57 | 122.35      | 126.23   |
| 31  | B     | 846 | CLA  | CHD-C4C-NC  | 2.57  | 128.26      | 124.20   |
| 31  | a     | 322 | CLA  | CMB-C2B-C3B | 2.57  | 129.49      | 124.68   |
| 31  | A     | 848 | CLA  | C3D-C2D-C1D | -2.57 | 102.32      | 105.83   |
| 31  | B     | 844 | CLA  | CMC-C2C-C1C | 2.57  | 128.96      | 125.04   |
| 32  | 7     | 324 | CHL  | CED-O2D-CGD | 2.57  | 121.76      | 115.94   |
| 31  | 5     | 320 | CLA  | O1D-CGD-CBD | -2.57 | 119.22      | 124.48   |
| 31  | 5     | 313 | CLA  | CMB-C2B-C3B | 2.57  | 129.49      | 124.68   |
| 30  | A     | 813 | CL0  | C4C-C3C-C2C | -2.57 | 103.15      | 106.90   |
| 31  | 8     | 308 | CLA  | CHC-C1C-NC  | -2.57 | 120.30      | 124.20   |
| 31  | B     | 843 | CLA  | CHD-C4C-NC  | 2.57  | 128.25      | 124.20   |
| 31  | B     | 820 | CLA  | CMB-C2B-C3B | 2.57  | 129.49      | 124.68   |
| 31  | 9     | 314 | CLA  | O2A-CGA-CBA | 2.57  | 119.97      | 111.91   |
| 31  | B     | 818 | CLA  | C1-C2-C3    | -2.57 | 121.60      | 126.04   |
| 36  | F     | 304 | LUT  | C4-C5-C6    | -2.57 | 115.12      | 120.85   |
| 31  | 2     | 307 | CLA  | O2A-CGA-CBA | 2.57  | 119.97      | 111.91   |
| 31  | 2     | 305 | CLA  | CHC-C1C-NC  | -2.57 | 120.31      | 124.20   |
| 31  | 4     | 305 | CLA  | C2A-C1A-CHA | -2.57 | 119.37      | 123.86   |
| 31  | a     | 314 | CLA  | C1-O2A-CGA  | 2.57  | 123.18      | 116.44   |
| 31  | F     | 301 | CLA  | C4-C3-C5    | 2.57  | 119.59      | 115.27   |
| 32  | 9     | 322 | CHL  | C3D-C2D-C1D | -2.57 | 102.33      | 105.83   |
| 31  | A     | 820 | CLA  | CHC-C1C-NC  | -2.57 | 120.31      | 124.20   |
| 31  | K     | 206 | CLA  | CMB-C2B-C3B | 2.57  | 129.48      | 124.68   |
| 31  | 9     | 321 | CLA  | CAA-C2A-C3A | -2.57 | 105.75      | 112.78   |
| 31  | 7     | 314 | CLA  | CHC-C1C-NC  | -2.57 | 120.31      | 124.20   |
| 31  | 9     | 318 | CLA  | O1D-CGD-CBD | -2.57 | 119.23      | 124.48   |
| 31  | 5     | 310 | CLA  | C4-C3-C5    | 2.57  | 119.59      | 115.27   |
| 31  | 9     | 312 | CLA  | CMB-C2B-C3B | 2.56  | 129.48      | 124.68   |
| 32  | 6     | 309 | CHL  | CMD-C2D-C1D | 2.56  | 129.23      | 124.71   |
| 31  | 3     | 309 | CLA  | CMB-C2B-C3B | 2.56  | 129.48      | 124.68   |
| 31  | A     | 814 | CLA  | O2A-CGA-CBA | 2.56  | 119.95      | 111.91   |
| 26  | 2     | 302 | BCR  | C33-C5-C6   | -2.56 | 121.65      | 124.53   |
| 31  | 4     | 306 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 31  | 7     | 316 | CLA  | CAC-C3C-C4C | 2.56  | 128.14      | 124.81   |
| 31  | B     | 825 | CLA  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 31  | 7     | 315 | CLA  | CHD-C4C-NC  | 2.56  | 128.24      | 124.20   |
| 31  | b     | 312 | CLA  | CHD-C4C-NC  | 2.56  | 128.24      | 124.20   |
| 31  | A     | 819 | CLA  | CMC-C2C-C1C | 2.56  | 128.94      | 125.04   |
| 31  | B     | 847 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 31  | 2     | 308 | CLA  | CED-O2D-CGD | 2.56  | 121.73      | 115.94   |
| 36  | 5     | 303 | LUT  | C4-C5-C6    | -2.56 | 115.14      | 120.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | L     | 305 | CLA  | CHC-C1C-NC  | -2.56 | 120.32      | 124.20   |
| 31  | 7     | 313 | CLA  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 31  | 8     | 320 | CLA  | C3D-C2D-C1D | -2.56 | 102.34      | 105.83   |
| 31  | A     | 834 | CLA  | C4-C3-C5    | 2.56  | 119.58      | 115.27   |
| 31  | A     | 856 | CLA  | C4-C3-C5    | 2.56  | 119.58      | 115.27   |
| 31  | 9     | 314 | CLA  | CED-O2D-CGD | 2.56  | 121.72      | 115.94   |
| 26  | G     | 201 | BCR  | C11-C10-C9  | -2.56 | 123.66      | 127.31   |
| 36  | 9     | 305 | LUT  | C7-C8-C9    | -2.56 | 122.37      | 126.23   |
| 31  | 8     | 309 | CLA  | CHC-C1C-NC  | -2.56 | 120.32      | 124.20   |
| 31  | b     | 302 | CLA  | CHC-C1C-NC  | -2.56 | 120.32      | 124.20   |
| 31  | A     | 838 | CLA  | CMB-C2B-C3B | 2.56  | 129.46      | 124.68   |
| 31  | B     | 835 | CLA  | C4-C3-C5    | 2.56  | 119.57      | 115.27   |
| 31  | 7     | 310 | CLA  | O2D-CGD-O1D | -2.56 | 118.84      | 123.84   |
| 31  | a     | 321 | CLA  | C1-C2-C3    | -2.55 | 122.62      | 126.75   |
| 31  | K     | 205 | CLA  | CMD-C2D-C1D | 2.55  | 129.22      | 124.71   |
| 31  | 4     | 320 | CLA  | CMB-C2B-C3B | 2.55  | 129.46      | 124.68   |
| 31  | B     | 824 | CLA  | C4-C3-C2    | -2.55 | 117.13      | 123.68   |
| 31  | B     | 824 | CLA  | C1D-CHD-C4C | -2.55 | 120.55      | 126.06   |
| 31  | A     | 844 | CLA  | C3D-C2D-C1D | -2.55 | 102.35      | 105.83   |
| 31  | B     | 812 | CLA  | C1D-CHD-C4C | -2.55 | 120.55      | 126.06   |
| 31  | 5     | 312 | CLA  | O2A-CGA-CBA | 2.55  | 119.92      | 111.91   |
| 36  | 4     | 302 | LUT  | C36-C21-C26 | 2.55  | 113.41      | 109.55   |
| 31  | 5     | 315 | CLA  | CMD-C2D-C1D | 2.55  | 129.21      | 124.71   |
| 32  | 6     | 309 | CHL  | C4D-CHA-C1A | -2.55 | 118.14      | 121.25   |
| 31  | K     | 204 | CLA  | CMB-C2B-C3B | 2.55  | 129.45      | 124.68   |
| 36  | 4     | 302 | LUT  | C4-C5-C6    | -2.55 | 115.16      | 120.85   |
| 37  | G     | 202 | LMG  | C38-C37-C36 | -2.55 | 101.47      | 114.42   |
| 31  | H     | 902 | CLA  | CMD-C2D-C1D | 2.55  | 129.21      | 124.71   |
| 31  | 7     | 311 | CLA  | CMC-C2C-C1C | 2.55  | 128.92      | 125.04   |
| 31  | 5     | 313 | CLA  | CMD-C2D-C3D | -2.55 | 121.75      | 127.61   |
| 31  | A     | 836 | CLA  | O1D-CGD-CBD | -2.55 | 119.27      | 124.48   |
| 31  | A     | 835 | CLA  | C1-O2A-CGA  | 2.55  | 123.13      | 116.44   |
| 31  | B     | 837 | CLA  | CMB-C2B-C3B | 2.55  | 129.44      | 124.68   |
| 31  | 7     | 314 | CLA  | C3D-C2D-C1D | -2.55 | 102.36      | 105.83   |
| 31  | 8     | 320 | CLA  | CHC-C1C-NC  | -2.55 | 120.34      | 124.20   |
| 31  | 9     | 312 | CLA  | CHC-C1C-NC  | -2.55 | 120.34      | 124.20   |
| 31  | 4     | 319 | CLA  | O2D-CGD-O1D | -2.55 | 118.86      | 123.84   |
| 32  | 6     | 309 | CHL  | O2D-CGD-O1D | -2.55 | 118.86      | 123.84   |
| 31  | B     | 828 | CLA  | C1-C2-C3    | -2.55 | 121.64      | 126.04   |
| 32  | a     | 317 | CHL  | CHC-C1C-NC  | -2.55 | 120.34      | 124.20   |
| 31  | F     | 305 | CLA  | CMC-C2C-C1C | 2.55  | 128.91      | 125.04   |
| 31  | 2     | 309 | CLA  | CMD-C2D-C1D | 2.54  | 129.20      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 33  | 7     | 308 | DGD  | O6D-C5D-C6D | -2.54 | 101.53      | 106.67   |
| 31  | a     | 312 | CLA  | O2A-CGA-CBA | 2.54  | 119.89      | 111.91   |
| 31  | A     | 849 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 31  | 2     | 315 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 31  | b     | 307 | CLA  | CMD-C2D-C1D | 2.54  | 129.20      | 124.71   |
| 31  | A     | 846 | CLA  | CHB-C4A-NA  | 2.54  | 128.03      | 124.51   |
| 31  | B     | 821 | CLA  | CMD-C2D-C1D | 2.54  | 129.19      | 124.71   |
| 31  | B     | 821 | CLA  | C4-C3-C5    | 2.54  | 119.55      | 115.27   |
| 31  | 4     | 307 | CLA  | CAC-C3C-C4C | 2.54  | 128.11      | 124.81   |
| 32  | 9     | 322 | CHL  | CHD-C4C-NC  | 2.54  | 128.21      | 124.20   |
| 31  | 4     | 318 | CLA  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 31  | 7     | 321 | CLA  | CHC-C1C-NC  | -2.54 | 120.35      | 124.20   |
| 31  | 4     | 309 | CLA  | C1-O2A-CGA  | 2.54  | 123.11      | 116.44   |
| 26  | 3     | 301 | BCR  | C27-C26-C25 | 2.54  | 126.42      | 122.73   |
| 32  | 4     | 317 | CHL  | O1D-CGD-CBD | -2.54 | 119.28      | 124.48   |
| 36  | b     | 301 | LUT  | C17-C1-C6   | -2.54 | 106.18      | 110.30   |
| 31  | A     | 849 | CLA  | CMD-C2D-C1D | 2.54  | 129.19      | 124.71   |
| 31  | 4     | 306 | CLA  | CMB-C2B-C3B | 2.54  | 129.43      | 124.68   |
| 32  | 4     | 313 | CHL  | CHC-C1C-NC  | -2.54 | 120.35      | 124.20   |
| 31  | 3     | 312 | CLA  | CMB-C2B-C3B | 2.54  | 129.43      | 124.68   |
| 31  | O     | 202 | CLA  | CHC-C1C-NC  | -2.54 | 120.35      | 124.20   |
| 31  | 8     | 310 | CLA  | CHC-C1C-NC  | -2.54 | 120.35      | 124.20   |
| 31  | a     | 313 | CLA  | C4-C3-C2    | -2.54 | 117.17      | 123.68   |
| 31  | B     | 816 | CLA  | C4-C3-C5    | 2.54  | 119.54      | 115.27   |
| 31  | 2     | 314 | CLA  | CHC-C1C-NC  | -2.54 | 120.36      | 124.20   |
| 26  | 2     | 302 | BCR  | C27-C26-C25 | 2.54  | 126.41      | 122.73   |
| 31  | 4     | 319 | CLA  | O1D-CGD-CBD | -2.54 | 119.30      | 124.48   |
| 26  | O     | 201 | BCR  | C24-C23-C22 | -2.54 | 122.40      | 126.23   |
| 32  | b     | 309 | CHL  | O1D-CGD-CBD | -2.53 | 119.30      | 124.48   |
| 28  | 7     | 302 | LHG  | C11-C10-C9  | -2.53 | 101.56      | 114.42   |
| 31  | B     | 814 | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 31  | 2     | 307 | CLA  | CED-O2D-CGD | 2.53  | 121.67      | 115.94   |
| 31  | 7     | 315 | CLA  | CMB-C2B-C3B | 2.53  | 129.42      | 124.68   |
| 31  | A     | 814 | CLA  | C1D-CHD-C4C | -2.53 | 120.59      | 126.06   |
| 32  | a     | 320 | CHL  | CMD-C2D-C1D | 2.53  | 129.18      | 124.71   |
| 31  | b     | 306 | CLA  | O1D-CGD-CBD | -2.53 | 119.30      | 124.48   |
| 31  | 9     | 315 | CLA  | O2A-CGA-CBA | 2.53  | 119.85      | 111.91   |
| 31  | A     | 843 | CLA  | C4-C3-C5    | 2.53  | 119.53      | 115.27   |
| 31  | 8     | 314 | CLA  | CMD-C2D-C1D | 2.53  | 129.18      | 124.71   |
| 31  | 6     | 316 | CLA  | CHC-C1C-NC  | -2.53 | 120.36      | 124.20   |
| 31  | 4     | 314 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 31  | B     | 812 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 313 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 31  | 5     | 315 | CLA  | CBC-CAC-C3C | -2.53 | 105.46      | 112.43   |
| 31  | A     | 829 | CLA  | CMC-C2C-C1C | 2.53  | 128.89      | 125.04   |
| 31  | 2     | 309 | CLA  | O1D-CGD-CBD | -2.53 | 119.31      | 124.48   |
| 32  | 6     | 320 | CHL  | CMB-C2B-C3B | 2.53  | 129.41      | 124.68   |
| 31  | 2     | 311 | CLA  | CHC-C1C-NC  | -2.53 | 120.37      | 124.20   |
| 31  | B     | 840 | CLA  | CMD-C2D-C1D | 2.53  | 129.17      | 124.71   |
| 31  | G     | 206 | CLA  | CMD-C2D-C1D | 2.53  | 129.17      | 124.71   |
| 32  | 5     | 316 | CHL  | CMD-C2D-C1D | 2.53  | 129.17      | 124.71   |
| 31  | A     | 814 | CLA  | CAC-C3C-C4C | 2.53  | 128.09      | 124.81   |
| 31  | B     | 850 | CLA  | C4C-C3C-C2C | -2.53 | 103.21      | 106.90   |
| 31  | H     | 902 | CLA  | CMB-C2B-C3B | 2.53  | 129.41      | 124.68   |
| 31  | b     | 312 | CLA  | C3D-C2D-C1D | -2.53 | 102.38      | 105.83   |
| 32  | 8     | 319 | CHL  | O1D-CGD-CBD | -2.53 | 119.31      | 124.48   |
| 31  | B     | 812 | CLA  | C4C-C3C-C2C | -2.53 | 103.22      | 106.90   |
| 32  | 3     | 315 | CHL  | CMD-C2D-C1D | 2.52  | 129.16      | 124.71   |
| 31  | 3     | 309 | CLA  | O1D-CGD-CBD | -2.52 | 119.32      | 124.48   |
| 31  | 4     | 307 | CLA  | C3D-C2D-C1D | -2.52 | 102.39      | 105.83   |
| 31  | B     | 843 | CLA  | C3B-C4B-NB  | 2.52  | 112.47      | 109.21   |
| 31  | 7     | 315 | CLA  | CAC-C3C-C4C | 2.52  | 128.08      | 124.81   |
| 31  | 3     | 313 | CLA  | CMD-C2D-C1D | 2.52  | 129.16      | 124.71   |
| 31  | 3     | 318 | CLA  | C1-C2-C3    | -2.52 | 121.68      | 126.04   |
| 31  | B     | 835 | CLA  | CHC-C1C-NC  | -2.52 | 120.38      | 124.20   |
| 32  | 7     | 324 | CHL  | CMD-C2D-C1D | 2.52  | 129.16      | 124.71   |
| 31  | b     | 303 | CLA  | O1D-CGD-CBD | -2.52 | 119.33      | 124.48   |
| 31  | B     | 832 | CLA  | C3D-C2D-C1D | -2.52 | 102.39      | 105.83   |
| 31  | 4     | 315 | CLA  | CHC-C1C-NC  | -2.52 | 120.38      | 124.20   |
| 32  | 4     | 313 | CHL  | O2A-CGA-CBA | 2.52  | 119.81      | 111.91   |
| 26  | 8     | 301 | BCR  | C27-C26-C25 | 2.52  | 126.39      | 122.73   |
| 31  | 5     | 314 | CLA  | CHC-C1C-NC  | -2.52 | 120.38      | 124.20   |
| 31  | 4     | 312 | CLA  | C3D-C2D-C1D | -2.52 | 102.39      | 105.83   |
| 31  | 6     | 308 | CLA  | CMC-C2C-C1C | 2.52  | 128.87      | 125.04   |
| 31  | B     | 824 | CLA  | O2A-CGA-CBA | 2.52  | 119.80      | 111.91   |
| 31  | 4     | 321 | CLA  | C5-C3-C4    | 2.52  | 120.16      | 114.60   |
| 31  | 6     | 312 | CLA  | O2A-CGA-CBA | 2.52  | 119.80      | 111.91   |
| 31  | 9     | 314 | CLA  | CHC-C1C-NC  | -2.52 | 120.39      | 124.20   |
| 31  | A     | 835 | CLA  | C4-C3-C5    | 2.52  | 119.50      | 115.27   |
| 31  | H     | 901 | CLA  | O1D-CGD-CBD | -2.51 | 119.34      | 124.48   |
| 31  | A     | 825 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 32  | 9     | 322 | CHL  | CHC-C1C-NC  | -2.51 | 120.39      | 124.20   |
| 31  | b     | 302 | CLA  | O2D-CGD-O1D | -2.51 | 118.92      | 123.84   |
| 31  | 2     | 315 | CLA  | CMB-C2B-C3B | 2.51  | 129.38      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 9     | 302 | LUT  | C7-C8-C9    | -2.51 | 122.44      | 126.23   |
| 31  | A     | 855 | CLA  | O1D-CGD-CBD | -2.51 | 119.35      | 124.48   |
| 31  | 8     | 318 | CLA  | CMD-C2D-C1D | 2.51  | 129.14      | 124.71   |
| 31  | B     | 838 | CLA  | CMB-C2B-C3B | 2.51  | 129.38      | 124.68   |
| 32  | A     | 831 | CHL  | C2D-C1D-ND  | 2.51  | 111.95      | 110.10   |
| 26  | B     | 805 | BCR  | C15-C14-C13 | -2.51 | 123.73      | 127.31   |
| 26  | K     | 203 | BCR  | C27-C26-C25 | 2.51  | 126.38      | 122.73   |
| 31  | B     | 818 | CLA  | O2A-CGA-CBA | 2.51  | 119.78      | 111.91   |
| 31  | 4     | 309 | CLA  | CMC-C2C-C1C | 2.51  | 128.86      | 125.04   |
| 31  | A     | 814 | CLA  | O1D-CGD-CBD | -2.51 | 119.35      | 124.48   |
| 31  | A     | 837 | CLA  | C4-C3-C5    | 2.51  | 119.49      | 115.27   |
| 31  | B     | 839 | CLA  | CAC-C3C-C4C | 2.51  | 128.06      | 124.81   |
| 31  | 5     | 318 | CLA  | C3D-C2D-C1D | -2.51 | 102.41      | 105.83   |
| 31  | A     | 852 | CLA  | CMC-C2C-C1C | 2.51  | 128.85      | 125.04   |
| 31  | 5     | 307 | CLA  | C1D-CHD-C4C | -2.51 | 120.65      | 126.06   |
| 31  | 6     | 306 | CLA  | O2D-CGD-O1D | -2.51 | 118.94      | 123.84   |
| 31  | B     | 844 | CLA  | C4-C3-C5    | 2.51  | 119.49      | 115.27   |
| 31  | b     | 306 | CLA  | CMD-C2D-C1D | 2.51  | 129.13      | 124.71   |
| 31  | 6     | 322 | CLA  | CMC-C2C-C1C | 2.51  | 128.85      | 125.04   |
| 31  | A     | 833 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 31  | 4     | 309 | CLA  | C1D-CHD-C4C | -2.50 | 120.66      | 126.06   |
| 31  | 4     | 314 | CLA  | CMD-C2D-C1D | 2.50  | 129.13      | 124.71   |
| 31  | A     | 847 | CLA  | C1D-CHD-C4C | -2.50 | 120.66      | 126.06   |
| 40  | 7     | 306 | XAT  | C15-C35-C34 | 2.50  | 128.60      | 123.47   |
| 31  | A     | 846 | CLA  | O2A-CGA-CBA | 2.50  | 119.76      | 111.91   |
| 32  | b     | 309 | CHL  | CMD-C2D-C1D | 2.50  | 129.12      | 124.71   |
| 32  | 4     | 313 | CHL  | CMD-C2D-C1D | 2.50  | 129.12      | 124.71   |
| 31  | 4     | 321 | CLA  | CHC-C1C-NC  | -2.50 | 120.41      | 124.20   |
| 31  | A     | 845 | CLA  | C1-C2-C3    | -2.50 | 121.71      | 126.04   |
| 31  | A     | 843 | CLA  | CMB-C2B-C3B | 2.50  | 129.36      | 124.68   |
| 31  | 4     | 320 | CLA  | CHC-C1C-NC  | -2.50 | 120.41      | 124.20   |
| 31  | 5     | 323 | CLA  | CMC-C2C-C1C | 2.50  | 128.85      | 125.04   |
| 31  | A     | 843 | CLA  | C3B-C4B-NB  | 2.50  | 112.44      | 109.21   |
| 31  | 4     | 309 | CLA  | C4-C3-C5    | 2.50  | 119.48      | 115.27   |
| 32  | 6     | 321 | CHL  | C2D-C1D-ND  | 2.50  | 111.95      | 110.10   |
| 26  | L     | 303 | BCR  | C27-C26-C25 | 2.50  | 126.36      | 122.73   |
| 31  | B     | 848 | CLA  | O2A-CGA-CBA | 2.50  | 119.75      | 111.91   |
| 31  | 8     | 309 | CLA  | C5-C3-C4    | 2.50  | 120.12      | 114.60   |
| 32  | 6     | 321 | CHL  | O2D-CGD-O1D | -2.50 | 118.95      | 123.84   |
| 31  | A     | 852 | CLA  | C1-C2-C3    | -2.50 | 121.72      | 126.04   |
| 31  | A     | 848 | CLA  | CHD-C4C-NC  | 2.50  | 128.14      | 124.20   |
| 31  | B     | 848 | CLA  | O1D-CGD-CBD | -2.50 | 119.37      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 6     | 312 | CLA  | CMC-C2C-C1C | 2.50  | 128.84      | 125.04   |
| 32  | 5     | 319 | CHL  | C4D-CHA-C1A | -2.50 | 118.21      | 121.25   |
| 31  | B     | 829 | CLA  | C1-C2-C3    | -2.50 | 121.72      | 126.04   |
| 31  | B     | 841 | CLA  | C4-C3-C5    | 2.50  | 119.47      | 115.27   |
| 31  | 3     | 311 | CLA  | CMD-C2D-C1D | 2.50  | 129.11      | 124.71   |
| 31  | b     | 302 | CLA  | CMD-C2D-C1D | 2.50  | 129.11      | 124.71   |
| 31  | A     | 854 | CLA  | CMC-C2C-C1C | 2.50  | 128.84      | 125.04   |
| 31  | 9     | 315 | CLA  | CMC-C2C-C1C | 2.50  | 128.84      | 125.04   |
| 31  | 9     | 318 | CLA  | CMC-C2C-C1C | 2.50  | 128.84      | 125.04   |
| 31  | 4     | 314 | CLA  | CED-O2D-CGD | 2.49  | 121.58      | 115.94   |
| 32  | 4     | 310 | CHL  | CAC-C3C-C4C | 2.49  | 128.05      | 124.81   |
| 31  | 3     | 312 | CLA  | CMC-C2C-C1C | 2.49  | 128.84      | 125.04   |
| 31  | 6     | 310 | CLA  | O2A-CGA-CBA | 2.49  | 119.73      | 111.91   |
| 31  | b     | 304 | CLA  | CHC-C1C-NC  | -2.49 | 120.42      | 124.20   |
| 31  | 8     | 313 | CLA  | CMC-C2C-C1C | 2.49  | 128.84      | 125.04   |
| 31  | 5     | 312 | CLA  | CHC-C1C-NC  | -2.49 | 120.42      | 124.20   |
| 31  | b     | 304 | CLA  | CMC-C2C-C1C | 2.49  | 128.84      | 125.04   |
| 31  | 4     | 311 | CLA  | CAC-C3C-C4C | 2.49  | 128.04      | 124.81   |
| 28  | 8     | 304 | LHG  | C11-C10-C9  | -2.49 | 101.77      | 114.42   |
| 31  | 9     | 318 | CLA  | CMD-C2D-C1D | 2.49  | 129.10      | 124.71   |
| 31  | 3     | 316 | CLA  | CMD-C2D-C1D | 2.49  | 129.10      | 124.71   |
| 31  | B     | 841 | CLA  | C1D-CHD-C4C | -2.49 | 120.69      | 126.06   |
| 31  | A     | 822 | CLA  | O2A-CGA-O1A | -2.49 | 117.31      | 123.59   |
| 31  | a     | 311 | CLA  | CHC-C1C-NC  | -2.49 | 120.43      | 124.20   |
| 31  | a     | 312 | CLA  | CAC-C3C-C4C | 2.49  | 128.04      | 124.81   |
| 31  | B     | 848 | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 31  | 9     | 311 | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 31  | 2     | 304 | CLA  | CMC-C2C-C1C | 2.49  | 128.83      | 125.04   |
| 31  | B     | 828 | CLA  | C6-C7-C8    | -2.49 | 107.88      | 115.92   |
| 31  | A     | 844 | CLA  | C1-O2A-CGA  | 2.49  | 122.97      | 116.44   |
| 31  | B     | 839 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 31  | A     | 836 | CLA  | O2A-CGA-CBA | 2.48  | 119.71      | 111.91   |
| 31  | 6     | 316 | CLA  | CMD-C2D-C1D | 2.48  | 129.09      | 124.71   |
| 31  | 5     | 315 | CLA  | CHC-C1C-NC  | -2.48 | 120.44      | 124.20   |
| 31  | 3     | 319 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 31  | B     | 834 | CLA  | CAC-C3C-C4C | 2.48  | 128.03      | 124.81   |
| 26  | M     | 101 | BCR  | C27-C26-C25 | 2.48  | 126.34      | 122.73   |
| 31  | A     | 851 | CLA  | O2A-CGA-CBA | 2.48  | 119.70      | 111.91   |
| 31  | B     | 848 | CLA  | CMD-C2D-C1D | 2.48  | 129.09      | 124.71   |
| 32  | a     | 318 | CHL  | C4D-CHA-C1A | -2.48 | 118.23      | 121.25   |
| 32  | A     | 831 | CHL  | C1D-CHD-C4C | -2.48 | 120.70      | 126.06   |
| 31  | 3     | 313 | CLA  | C1-C2-C3    | -2.48 | 121.75      | 126.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 829 | CLA  | CHA-C4D-ND  | 2.48  | 137.69      | 132.50   |
| 26  | A     | 803 | BCR  | C27-C26-C25 | 2.48  | 126.33      | 122.73   |
| 31  | B     | 831 | CLA  | CHC-C1C-NC  | -2.48 | 120.44      | 124.20   |
| 31  | a     | 311 | CLA  | CMC-C2C-C1C | 2.48  | 128.81      | 125.04   |
| 31  | 5     | 312 | CLA  | CMC-C2C-C1C | 2.48  | 128.81      | 125.04   |
| 31  | B     | 846 | CLA  | CAC-C3C-C4C | 2.48  | 128.03      | 124.81   |
| 30  | A     | 813 | CL0  | O2D-CGD-O1D | -2.48 | 118.99      | 123.84   |
| 31  | 9     | 317 | CLA  | C3B-C4B-NB  | 2.48  | 112.42      | 109.21   |
| 31  | 9     | 318 | CLA  | C4-C3-C5    | 2.48  | 119.44      | 115.27   |
| 31  | K     | 206 | CLA  | CHC-C1C-NC  | -2.48 | 120.44      | 124.20   |
| 31  | B     | 815 | CLA  | O2A-CGA-CBA | 2.48  | 119.68      | 111.91   |
| 26  | B     | 803 | BCR  | C27-C26-C25 | 2.48  | 126.33      | 122.73   |
| 31  | A     | 847 | CLA  | C4D-CHA-C1A | -2.48 | 118.23      | 121.25   |
| 28  | A     | 811 | LHG  | C11-C10-C9  | -2.48 | 101.85      | 114.42   |
| 32  | 8     | 316 | CHL  | O2A-CGA-CBA | 2.48  | 119.68      | 111.91   |
| 31  | B     | 813 | CLA  | CHC-C1C-NC  | -2.48 | 120.45      | 124.20   |
| 31  | 3     | 311 | CLA  | O1D-CGD-CBD | -2.47 | 119.42      | 124.48   |
| 37  | a     | 301 | LMG  | C38-C37-C36 | -2.47 | 101.86      | 114.42   |
| 31  | a     | 313 | CLA  | O2A-CGA-CBA | 2.47  | 119.67      | 111.91   |
| 31  | 8     | 315 | CLA  | CMD-C2D-C1D | 2.47  | 129.07      | 124.71   |
| 31  | B     | 826 | CLA  | O2A-CGA-CBA | 2.47  | 119.67      | 111.91   |
| 36  | 7     | 305 | LUT  | C18-C5-C4   | -2.47 | 109.77      | 114.36   |
| 32  | 5     | 319 | CHL  | O1D-CGD-CBD | -2.47 | 119.42      | 124.48   |
| 31  | 6     | 312 | CLA  | C4-C3-C5    | 2.47  | 119.43      | 115.27   |
| 31  | 3     | 308 | CLA  | CMB-C2B-C3B | 2.47  | 129.30      | 124.68   |
| 31  | A     | 835 | CLA  | CHD-C4C-NC  | 2.47  | 128.10      | 124.20   |
| 31  | A     | 838 | CLA  | CHC-C1C-NC  | -2.47 | 120.45      | 124.20   |
| 31  | 4     | 311 | CLA  | CMC-C2C-C1C | 2.47  | 128.80      | 125.04   |
| 31  | B     | 845 | CLA  | CMD-C2D-C1D | 2.47  | 129.07      | 124.71   |
| 31  | A     | 850 | CLA  | CMC-C2C-C1C | 2.47  | 128.80      | 125.04   |
| 31  | 5     | 314 | CLA  | CMC-C2C-C1C | 2.47  | 128.80      | 125.04   |
| 31  | O     | 204 | CLA  | C3D-C2D-C1D | -2.47 | 102.46      | 105.83   |
| 32  | 7     | 324 | CHL  | CHC-C1C-NC  | -2.47 | 120.46      | 124.20   |
| 36  | L     | 304 | LUT  | C36-C21-C26 | 2.47  | 113.28      | 109.55   |
| 31  | A     | 853 | CLA  | CMB-C2B-C3B | 2.47  | 129.30      | 124.68   |
| 31  | O     | 204 | CLA  | CMD-C2D-C1D | 2.47  | 129.06      | 124.71   |
| 36  | 8     | 303 | LUT  | C21-C26-C27 | -2.47 | 109.58      | 112.70   |
| 31  | G     | 206 | CLA  | O1D-CGD-CBD | -2.47 | 119.44      | 124.48   |
| 26  | K     | 202 | BCR  | C7-C8-C9    | -2.47 | 122.51      | 126.23   |
| 31  | B     | 837 | CLA  | C1-O2A-CGA  | 2.47  | 122.92      | 116.44   |
| 31  | A     | 819 | CLA  | CHC-C1C-NC  | -2.47 | 120.46      | 124.20   |
| 31  | A     | 822 | CLA  | C4-C3-C5    | 2.47  | 119.42      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 816 | CLA  | O1D-CGD-CBD | -2.47 | 119.44      | 124.48   |
| 31  | A     | 856 | CLA  | C1D-CHD-C4C | -2.46 | 120.74      | 126.06   |
| 32  | a     | 320 | CHL  | C4D-CHA-C1A | -2.46 | 118.25      | 121.25   |
| 31  | 9     | 314 | CLA  | C4-C3-C5    | 2.46  | 119.42      | 115.27   |
| 31  | 9     | 321 | CLA  | CAC-C3C-C4C | 2.46  | 128.01      | 124.81   |
| 31  | B     | 834 | CLA  | O2A-CGA-CBA | 2.46  | 119.64      | 111.91   |
| 31  | 2     | 313 | CLA  | CHC-C1C-NC  | -2.46 | 120.47      | 124.20   |
| 32  | 6     | 321 | CHL  | CMB-C2B-C3B | 2.46  | 129.29      | 124.68   |
| 31  | 6     | 311 | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 31  | 3     | 319 | CLA  | C2A-C1A-CHA | -2.46 | 119.55      | 123.86   |
| 31  | B     | 815 | CLA  | CMC-C2C-C1C | 2.46  | 128.79      | 125.04   |
| 32  | 6     | 318 | CHL  | C1D-CHD-C4C | -2.46 | 120.75      | 126.06   |
| 31  | A     | 857 | CLA  | C1-C2-C3    | -2.46 | 121.79      | 126.04   |
| 31  | B     | 817 | CLA  | C4-C3-C5    | 2.46  | 119.41      | 115.27   |
| 31  | 2     | 314 | CLA  | CMB-C2B-C3B | 2.46  | 129.28      | 124.68   |
| 32  | 6     | 319 | CHL  | CHD-C4C-NC  | 2.46  | 128.08      | 124.20   |
| 31  | b     | 311 | CLA  | CED-O2D-CGD | 2.46  | 121.50      | 115.94   |
| 31  | 4     | 311 | CLA  | C3D-C2D-C1D | -2.46 | 102.47      | 105.83   |
| 31  | 3     | 312 | CLA  | CMD-C2D-C1D | 2.46  | 129.05      | 124.71   |
| 31  | 7     | 311 | CLA  | CHC-C1C-NC  | -2.46 | 120.47      | 124.20   |
| 31  | b     | 306 | CLA  | CMB-C2B-C3B | 2.46  | 129.28      | 124.68   |
| 31  | B     | 824 | CLA  | CAC-C3C-C4C | 2.46  | 128.00      | 124.81   |
| 28  | B     | 807 | LHG  | C11-C10-C9  | -2.46 | 101.95      | 114.42   |
| 31  | B     | 822 | CLA  | CHD-C4C-NC  | 2.46  | 128.08      | 124.20   |
| 31  | b     | 305 | CLA  | CED-O2D-CGD | 2.46  | 121.50      | 115.94   |
| 28  | A     | 809 | LHG  | C11-C10-C9  | -2.46 | 101.95      | 114.42   |
| 31  | B     | 815 | CLA  | CMD-C2D-C1D | 2.46  | 129.04      | 124.71   |
| 36  | 4     | 303 | LUT  | C35-C15-C14 | -2.46 | 118.44      | 123.47   |
| 32  | 6     | 317 | CHL  | CMB-C2B-C3B | 2.45  | 129.27      | 124.68   |
| 31  | a     | 314 | CLA  | C1-C2-C3    | -2.45 | 122.78      | 126.75   |
| 31  | 6     | 311 | CLA  | CMD-C2D-C1D | 2.45  | 129.04      | 124.71   |
| 31  | 9     | 312 | CLA  | CMD-C2D-C1D | 2.45  | 129.04      | 124.71   |
| 31  | 6     | 307 | CLA  | CAC-C3C-C4C | 2.45  | 127.99      | 124.81   |
| 32  | 6     | 317 | CHL  | CHC-C1C-NC  | -2.45 | 120.48      | 124.20   |
| 31  | 4     | 316 | CLA  | CMC-C2C-C1C | 2.45  | 128.78      | 125.04   |
| 31  | 5     | 309 | CLA  | O2A-CGA-CBA | 2.45  | 119.61      | 111.91   |
| 28  | a     | 306 | LHG  | C11-C10-C9  | -2.45 | 101.97      | 114.42   |
| 31  | B     | 845 | CLA  | CHC-C1C-NC  | -2.45 | 120.48      | 124.20   |
| 31  | F     | 305 | CLA  | CHC-C1C-NC  | -2.45 | 120.48      | 124.20   |
| 31  | 5     | 318 | CLA  | C1-O2A-CGA  | 2.45  | 122.88      | 116.44   |
| 31  | 3     | 310 | CLA  | CMB-C2B-C3B | 2.45  | 129.26      | 124.68   |
| 31  | O     | 203 | CLA  | CMC-C2C-C1C | 2.45  | 128.77      | 125.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 825 | CLA  | CHC-C1C-NC  | -2.45 | 120.49      | 124.20   |
| 28  | A     | 809 | LHG  | C18-C17-C16 | -2.45 | 101.99      | 114.42   |
| 31  | H     | 901 | CLA  | C3D-C2D-C1D | -2.45 | 102.49      | 105.83   |
| 31  | 9     | 318 | CLA  | O2A-CGA-CBA | 2.45  | 119.59      | 111.91   |
| 31  | A     | 833 | CLA  | CAC-C3C-C4C | 2.45  | 127.99      | 124.81   |
| 32  | a     | 318 | CHL  | CMB-C2B-C3B | 2.45  | 129.26      | 124.68   |
| 31  | 6     | 314 | CLA  | CED-O2D-CGD | 2.45  | 121.47      | 115.94   |
| 31  | 6     | 316 | CLA  | O2A-CGA-CBA | 2.45  | 119.59      | 111.91   |
| 31  | 3     | 307 | CLA  | C4-C3-C5    | 2.45  | 119.39      | 115.27   |
| 31  | 3     | 313 | CLA  | O1D-CGD-CBD | -2.45 | 119.48      | 124.48   |
| 31  | 6     | 310 | CLA  | CMC-C2C-C1C | 2.45  | 128.76      | 125.04   |
| 31  | 9     | 313 | CLA  | CMD-C2D-C1D | 2.45  | 129.03      | 124.71   |
| 31  | 2     | 312 | CLA  | C1D-CHD-C4C | -2.45 | 120.78      | 126.06   |
| 31  | 3     | 312 | CLA  | C3D-C2D-C1D | -2.45 | 102.49      | 105.83   |
| 31  | A     | 819 | CLA  | CMB-C2B-C3B | 2.45  | 129.25      | 124.68   |
| 31  | B     | 832 | CLA  | C1-C2-C3    | -2.45 | 121.81      | 126.04   |
| 31  | 3     | 320 | CLA  | CMD-C2D-C1D | 2.44  | 129.02      | 124.71   |
| 31  | B     | 836 | CLA  | C3B-C4B-NB  | 2.44  | 112.37      | 109.21   |
| 36  | 3     | 305 | LUT  | C18-C5-C4   | -2.44 | 109.83      | 114.36   |
| 31  | 5     | 311 | CLA  | CMD-C2D-C1D | 2.44  | 129.02      | 124.71   |
| 31  | a     | 322 | CLA  | C3D-C2D-C1D | -2.44 | 102.50      | 105.83   |
| 28  | A     | 810 | LHG  | C11-C10-C9  | -2.44 | 102.02      | 114.42   |
| 28  | 7     | 307 | LHG  | C11-C10-C9  | -2.44 | 102.02      | 114.42   |
| 31  | 5     | 309 | CLA  | CMC-C2C-C1C | 2.44  | 128.76      | 125.04   |
| 31  | 6     | 311 | CLA  | CMC-C2C-C1C | 2.44  | 128.76      | 125.04   |
| 31  | L     | 307 | CLA  | CHC-C1C-NC  | -2.44 | 120.50      | 124.20   |
| 31  | A     | 814 | CLA  | C1-C2-C3    | -2.44 | 121.82      | 126.04   |
| 31  | 3     | 318 | CLA  | C3D-C2D-C1D | -2.44 | 102.50      | 105.83   |
| 31  | B     | 815 | CLA  | CED-O2D-CGD | 2.44  | 121.46      | 115.94   |
| 32  | K     | 201 | CHL  | C1C-C2C-C3C | -2.44 | 105.18      | 107.11   |
| 31  | 6     | 314 | CLA  | CHC-C1C-NC  | -2.44 | 120.50      | 124.20   |
| 31  | 2     | 305 | CLA  | CED-O2D-CGD | 2.44  | 121.46      | 115.94   |
| 31  | 5     | 310 | CLA  | CMB-C2B-C3B | 2.44  | 129.24      | 124.68   |
| 31  | 2     | 313 | CLA  | CMD-C2D-C1D | 2.44  | 129.01      | 124.71   |
| 24  | B     | 801 | PQN  | C11-C3-C4   | -2.44 | 115.89      | 118.50   |
| 31  | a     | 310 | CLA  | CMB-C2B-C3B | 2.44  | 129.24      | 124.68   |
| 31  | A     | 822 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 31  | 5     | 323 | CLA  | CED-O2D-CGD | 2.44  | 121.45      | 115.94   |
| 31  | 3     | 311 | CLA  | O2A-CGA-CBA | 2.44  | 119.56      | 111.91   |
| 31  | 5     | 320 | CLA  | CHC-C1C-NC  | -2.44 | 120.50      | 124.20   |
| 31  | B     | 840 | CLA  | C1-C2-C3    | -2.44 | 121.83      | 126.04   |
| 31  | A     | 841 | CLA  | CHD-C4C-NC  | 2.44  | 128.04      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 318 | CLA  | CED-O2D-CGD | 2.44  | 121.45      | 115.94   |
| 31  | 3     | 317 | CLA  | C1-C2-C3    | -2.44 | 121.83      | 126.04   |
| 31  | a     | 314 | CLA  | C3D-C2D-C1D | -2.44 | 102.51      | 105.83   |
| 31  | A     | 843 | CLA  | CHC-C1C-NC  | -2.43 | 120.51      | 124.20   |
| 31  | B     | 828 | CLA  | CMC-C2C-C1C | 2.43  | 128.75      | 125.04   |
| 31  | B     | 814 | CLA  | C1-O2A-CGA  | 2.43  | 122.83      | 116.44   |
| 36  | a     | 303 | LUT  | C4-C5-C6    | -2.43 | 115.42      | 120.85   |
| 31  | 9     | 317 | CLA  | O2D-CGD-O1D | -2.43 | 119.08      | 123.84   |
| 31  | A     | 829 | CLA  | CMB-C2B-C1B | -2.43 | 124.72      | 128.46   |
| 32  | 7     | 320 | CHL  | C4-C3-C5    | 2.43  | 119.36      | 115.27   |
| 31  | A     | 836 | CLA  | CHC-C1C-NC  | -2.43 | 120.51      | 124.20   |
| 31  | A     | 846 | CLA  | CHC-C1C-NC  | -2.43 | 120.51      | 124.20   |
| 32  | a     | 317 | CHL  | CED-O2D-CGD | 2.43  | 121.44      | 115.94   |
| 31  | 4     | 316 | CLA  | C3D-C2D-C1D | -2.43 | 102.51      | 105.83   |
| 32  | a     | 318 | CHL  | CMD-C2D-C1D | 2.43  | 129.00      | 124.71   |
| 32  | a     | 318 | CHL  | C2D-C1D-ND  | 2.43  | 111.90      | 110.10   |
| 32  | 5     | 317 | CHL  | C1D-CHD-C4C | -2.43 | 120.81      | 126.06   |
| 31  | 6     | 312 | CLA  | CMD-C2D-C1D | 2.43  | 129.00      | 124.71   |
| 31  | b     | 304 | CLA  | CMD-C2D-C1D | 2.43  | 129.00      | 124.71   |
| 31  | B     | 812 | CLA  | O1D-CGD-CBD | -2.43 | 119.52      | 124.48   |
| 31  | A     | 847 | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 31  | A     | 850 | CLA  | O2A-CGA-CBA | 2.43  | 119.53      | 111.91   |
| 31  | 4     | 308 | CLA  | CAC-C3C-C4C | 2.43  | 127.96      | 124.81   |
| 31  | B     | 829 | CLA  | CHC-C1C-NC  | -2.43 | 120.52      | 124.20   |
| 32  | 7     | 320 | CHL  | C2D-C1D-ND  | 2.43  | 111.89      | 110.10   |
| 31  | 8     | 317 | CLA  | C1D-CHD-C4C | -2.43 | 120.82      | 126.06   |
| 31  | 4     | 308 | CLA  | O2A-CGA-CBA | 2.43  | 119.52      | 111.91   |
| 32  | 7     | 317 | CHL  | CED-O2D-CGD | 2.43  | 121.42      | 115.94   |
| 39  | 7     | 301 | 3PH  | O13-P-O11   | -2.42 | 100.28      | 106.73   |
| 31  | A     | 824 | CLA  | CED-O2D-CGD | 2.42  | 121.42      | 115.94   |
| 31  | 9     | 315 | CLA  | C3B-C4B-NB  | 2.42  | 112.34      | 109.21   |
| 31  | 8     | 314 | CLA  | C6-C5-C3    | -2.42 | 110.66      | 114.62   |
| 31  | B     | 846 | CLA  | C3D-C2D-C1D | -2.42 | 102.52      | 105.83   |
| 36  | 4     | 302 | LUT  | C8-C7-C6    | -2.42 | 120.40      | 127.20   |
| 31  | H     | 901 | CLA  | CAC-C3C-C4C | 2.42  | 127.95      | 124.81   |
| 32  | 9     | 322 | CHL  | CAC-C3C-C4C | 2.42  | 127.95      | 124.81   |
| 31  | A     | 848 | CLA  | O2A-CGA-CBA | 2.42  | 119.51      | 111.91   |
| 28  | 8     | 304 | LHG  | C20-C19-C18 | -2.42 | 102.13      | 114.42   |
| 31  | A     | 815 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 31  | 4     | 316 | CLA  | O2D-CGD-O1D | -2.42 | 119.10      | 123.84   |
| 31  | 6     | 316 | CLA  | CMC-C2C-C1C | 2.42  | 128.73      | 125.04   |
| 31  | B     | 846 | CLA  | O1D-CGD-CBD | -2.42 | 119.53      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | J     | 105 | CLA  | C3D-C2D-C1D | -2.42 | 102.53      | 105.83   |
| 31  | A     | 816 | CLA  | CMC-C2C-C1C | 2.42  | 128.72      | 125.04   |
| 26  | 2     | 302 | BCR  | C15-C14-C13 | -2.42 | 123.86      | 127.31   |
| 31  | 3     | 311 | CLA  | CHC-C1C-NC  | -2.42 | 120.53      | 124.20   |
| 42  | 4     | 304 | SQD  | O48-C23-C24 | 2.42  | 119.50      | 111.91   |
| 31  | A     | 830 | CLA  | CHD-C4C-NC  | 2.42  | 128.01      | 124.20   |
| 31  | a     | 314 | CLA  | C5-C3-C4    | 2.42  | 119.94      | 114.60   |
| 31  | 8     | 320 | CLA  | C4-C3-C2    | -2.42 | 117.47      | 123.68   |
| 32  | 4     | 310 | CHL  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 31  | L     | 307 | CLA  | CED-O2D-CGD | 2.42  | 121.40      | 115.94   |
| 31  | B     | 834 | CLA  | C16-C15-C13 | -2.42 | 108.11      | 115.92   |
| 31  | B     | 836 | CLA  | CAC-C3C-C4C | 2.42  | 127.94      | 124.81   |
| 31  | B     | 838 | CLA  | C3D-C2D-C1D | -2.42 | 102.53      | 105.83   |
| 31  | a     | 319 | CLA  | O1D-CGD-CBD | -2.42 | 119.54      | 124.48   |
| 31  | A     | 824 | CLA  | C1-O2A-CGA  | 2.42  | 122.78      | 116.44   |
| 31  | 6     | 307 | CLA  | C3D-C2D-C1D | -2.42 | 102.53      | 105.83   |
| 26  | 3     | 301 | BCR  | C15-C16-C17 | -2.41 | 118.53      | 123.47   |
| 31  | 3     | 311 | CLA  | C3B-C4B-NB  | 2.41  | 112.33      | 109.21   |
| 31  | A     | 845 | CLA  | CAC-C3C-C4C | 2.41  | 127.94      | 124.81   |
| 31  | 3     | 314 | CLA  | CMC-C2C-C1C | 2.41  | 128.72      | 125.04   |
| 26  | L     | 302 | BCR  | C15-C16-C17 | -2.41 | 118.53      | 123.47   |
| 31  | B     | 842 | CLA  | CMB-C2B-C3B | 2.41  | 129.19      | 124.68   |
| 31  | 5     | 314 | CLA  | CMD-C2D-C1D | 2.41  | 128.97      | 124.71   |
| 31  | b     | 308 | CLA  | C3D-C2D-C1D | -2.41 | 102.54      | 105.83   |
| 31  | a     | 312 | CLA  | CMD-C2D-C1D | 2.41  | 128.97      | 124.71   |
| 31  | O     | 202 | CLA  | CMB-C2B-C3B | 2.41  | 129.19      | 124.68   |
| 31  | B     | 831 | CLA  | O2D-CGD-O1D | -2.41 | 119.12      | 123.84   |
| 31  | K     | 205 | CLA  | C1D-CHD-C4C | -2.41 | 120.85      | 126.06   |
| 31  | B     | 850 | CLA  | O1D-CGD-CBD | -2.41 | 119.55      | 124.48   |
| 31  | K     | 205 | CLA  | CAC-C3C-C4C | 2.41  | 127.94      | 124.81   |
| 31  | 8     | 314 | CLA  | CAC-C3C-C4C | 2.41  | 127.94      | 124.81   |
| 32  | 7     | 318 | CHL  | CMB-C2B-C3B | 2.41  | 129.19      | 124.68   |
| 31  | B     | 819 | CLA  | C3B-C4B-NB  | 2.41  | 112.33      | 109.21   |
| 31  | B     | 842 | CLA  | CMD-C2D-C1D | 2.41  | 128.96      | 124.71   |
| 32  | 8     | 319 | CHL  | C2D-C1D-ND  | 2.41  | 111.88      | 110.10   |
| 31  | 7     | 310 | CLA  | CHD-C4C-NC  | 2.41  | 128.00      | 124.20   |
| 31  | 7     | 321 | CLA  | CMD-C2D-C1D | 2.41  | 128.96      | 124.71   |
| 31  | A     | 841 | CLA  | O2A-CGA-O1A | -2.41 | 117.51      | 123.59   |
| 31  | B     | 827 | CLA  | C3B-C4B-NB  | 2.41  | 112.33      | 109.21   |
| 31  | 4     | 314 | CLA  | CAC-C3C-C4C | 2.41  | 127.94      | 124.81   |
| 32  | 6     | 318 | CHL  | C2D-C1D-ND  | 2.41  | 111.88      | 110.10   |
| 31  | a     | 321 | CLA  | CED-O2D-CGD | 2.41  | 121.39      | 115.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | F     | 301 | CLA  | CMB-C2B-C3B | 2.41  | 129.19      | 124.68   |
| 31  | 8     | 307 | CLA  | CHC-C1C-NC  | -2.41 | 120.55      | 124.20   |
| 32  | 6     | 319 | CHL  | CAC-C3C-C4C | 2.41  | 127.93      | 124.81   |
| 31  | B     | 817 | CLA  | O1D-CGD-CBD | -2.41 | 119.56      | 124.48   |
| 31  | 4     | 312 | CLA  | CAC-C3C-C4C | 2.41  | 127.93      | 124.81   |
| 32  | A     | 839 | CHL  | CMA-C3A-C4A | -2.41 | 105.31      | 111.77   |
| 31  | 2     | 312 | CLA  | CMD-C2D-C1D | 2.41  | 128.95      | 124.71   |
| 36  | F     | 304 | LUT  | C22-C23-C24 | 2.40  | 114.48      | 111.74   |
| 31  | 7     | 313 | CLA  | CMD-C2D-C1D | 2.40  | 128.95      | 124.71   |
| 31  | F     | 301 | CLA  | C6-C5-C3    | -2.40 | 107.15      | 113.45   |
| 36  | 5     | 304 | LUT  | C7-C8-C9    | -2.40 | 122.60      | 126.23   |
| 31  | A     | 834 | CLA  | O2A-CGA-CBA | 2.40  | 119.45      | 111.91   |
| 31  | A     | 832 | CLA  | CMD-C2D-C1D | 2.40  | 128.95      | 124.71   |
| 31  | 7     | 312 | CLA  | CMD-C2D-C1D | 2.40  | 128.95      | 124.71   |
| 31  | B     | 831 | CLA  | O2A-CGA-CBA | 2.40  | 119.45      | 111.91   |
| 32  | 6     | 319 | CHL  | C2D-C1D-ND  | 2.40  | 111.88      | 110.10   |
| 31  | 5     | 318 | CLA  | C6-C5-C3    | -2.40 | 107.15      | 113.45   |
| 36  | 3     | 305 | LUT  | C10-C11-C12 | -2.40 | 115.72      | 123.22   |
| 31  | 7     | 316 | CLA  | CHC-C1C-NC  | -2.40 | 120.56      | 124.20   |
| 31  | A     | 857 | CLA  | O2A-CGA-CBA | 2.40  | 119.44      | 111.91   |
| 31  | B     | 847 | CLA  | C3B-C4B-NB  | 2.40  | 112.31      | 109.21   |
| 31  | 5     | 321 | CLA  | CMC-C2C-C1C | 2.40  | 128.69      | 125.04   |
| 32  | a     | 320 | CHL  | C2D-C1D-ND  | 2.40  | 111.87      | 110.10   |
| 31  | B     | 819 | CLA  | C1-O2A-CGA  | 2.40  | 122.74      | 116.44   |
| 31  | 9     | 316 | CLA  | C5-C3-C4    | 2.40  | 119.91      | 114.60   |
| 31  | A     | 851 | CLA  | CMD-C2D-C1D | 2.40  | 128.94      | 124.71   |
| 31  | 8     | 317 | CLA  | C3B-C4B-NB  | 2.40  | 112.31      | 109.21   |
| 31  | 3     | 307 | CLA  | CHC-C1C-NC  | -2.40 | 120.56      | 124.20   |
| 32  | 7     | 324 | CHL  | C2C-C3C-C4C | -2.40 | 104.78      | 106.49   |
| 31  | B     | 831 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 31  | A     | 818 | CLA  | CMC-C2C-C1C | 2.40  | 128.69      | 125.04   |
| 31  | A     | 825 | CLA  | CMD-C2D-C1D | 2.40  | 128.94      | 124.71   |
| 31  | 7     | 313 | CLA  | O2D-CGD-O1D | -2.40 | 118.65      | 124.09   |
| 32  | 8     | 316 | CHL  | CHC-C1C-NC  | -2.40 | 120.57      | 124.20   |
| 31  | B     | 822 | CLA  | CMD-C2D-C1D | 2.40  | 128.94      | 124.71   |
| 31  | A     | 842 | CLA  | CHC-C1C-NC  | -2.40 | 120.57      | 124.20   |
| 31  | 9     | 321 | CLA  | C1D-CHD-C4C | -2.39 | 120.89      | 126.06   |
| 26  | 6     | 302 | BCR  | C16-C15-C14 | -2.39 | 118.57      | 123.47   |
| 26  | B     | 804 | BCR  | C27-C26-C25 | 2.39  | 126.20      | 122.73   |
| 31  | 3     | 319 | CLA  | C4-C3-C5    | 2.39  | 119.30      | 115.27   |
| 32  | 4     | 313 | CHL  | CAC-C3C-C4C | 2.39  | 127.91      | 124.81   |
| 31  | B     | 823 | CLA  | CMD-C2D-C1D | 2.39  | 128.93      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | 4     | 302 | LUT  | C1-C6-C7    | -2.39 | 109.01      | 115.78   |
| 31  | 4     | 321 | CLA  | CMC-C2C-C1C | 2.39  | 128.68      | 125.04   |
| 31  | B     | 824 | CLA  | CMD-C2D-C1D | 2.39  | 128.93      | 124.71   |
| 31  | 6     | 322 | CLA  | CHC-C1C-NC  | -2.39 | 120.58      | 124.20   |
| 31  | 3     | 319 | CLA  | CED-O2D-CGD | 2.39  | 121.34      | 115.94   |
| 31  | B     | 832 | CLA  | O2A-CGA-O1A | -2.39 | 117.56      | 123.59   |
| 31  | O     | 204 | CLA  | CHC-C1C-NC  | -2.39 | 120.58      | 124.20   |
| 31  | A     | 821 | CLA  | CHB-C4A-NA  | 2.39  | 127.81      | 124.51   |
| 31  | 8     | 312 | CLA  | CMB-C2B-C3B | 2.39  | 129.15      | 124.68   |
| 31  | B     | 843 | CLA  | CAC-C3C-C4C | 2.39  | 127.91      | 124.81   |
| 31  | 2     | 309 | CLA  | CAC-C3C-C4C | 2.39  | 127.91      | 124.81   |
| 31  | b     | 312 | CLA  | CMC-C2C-C1C | 2.39  | 128.67      | 125.04   |
| 31  | F     | 301 | CLA  | CED-O2D-CGD | 2.39  | 121.33      | 115.94   |
| 32  | 8     | 316 | CHL  | CMD-C2D-C1D | 2.39  | 128.92      | 124.71   |
| 31  | A     | 838 | CLA  | CMC-C2C-C1C | 2.38  | 128.67      | 125.04   |
| 31  | a     | 316 | CLA  | CMB-C2B-C3B | 2.38  | 129.14      | 124.68   |
| 32  | 4     | 310 | CHL  | CHC-C1C-NC  | -2.38 | 120.58      | 124.20   |
| 31  | 6     | 311 | CLA  | C1-C2-C3    | -2.38 | 121.92      | 126.04   |
| 31  | b     | 305 | CLA  | CMC-C2C-C1C | 2.38  | 128.67      | 125.04   |
| 31  | 3     | 307 | CLA  | CMD-C2D-C1D | 2.38  | 128.91      | 124.71   |
| 26  | A     | 804 | BCR  | C24-C23-C22 | -2.38 | 122.63      | 126.23   |
| 28  | A     | 809 | LHG  | C20-C19-C18 | -2.38 | 102.33      | 114.42   |
| 31  | b     | 313 | CLA  | C4C-C3C-C2C | -2.38 | 103.42      | 106.90   |
| 31  | L     | 307 | CLA  | C3D-C4D-CHA | -2.38 | 107.27      | 112.72   |
| 31  | L     | 306 | CLA  | CMC-C2C-C1C | 2.38  | 128.67      | 125.04   |
| 32  | 5     | 319 | CHL  | CMD-C2D-C1D | 2.38  | 128.91      | 124.71   |
| 31  | B     | 825 | CLA  | CHC-C1C-NC  | -2.38 | 120.59      | 124.20   |
| 31  | A     | 856 | CLA  | CMD-C2D-C1D | 2.38  | 128.91      | 124.71   |
| 31  | 4     | 307 | CLA  | O1D-CGD-CBD | -2.38 | 119.61      | 124.48   |
| 31  | B     | 826 | CLA  | CHC-C1C-NC  | -2.38 | 120.59      | 124.20   |
| 26  | 5     | 302 | BCR  | C34-C9-C10  | -2.38 | 119.59      | 122.92   |
| 31  | A     | 846 | CLA  | CMC-C2C-C1C | 2.38  | 128.66      | 125.04   |
| 31  | 6     | 307 | CLA  | CED-O2D-CGD | 2.38  | 121.32      | 115.94   |
| 31  | 6     | 308 | CLA  | CMB-C2B-C3B | 2.38  | 129.13      | 124.68   |
| 32  | 8     | 316 | CHL  | C2C-C3C-C4C | -2.38 | 104.79      | 106.49   |
| 31  | 8     | 312 | CLA  | CMC-C2C-C1C | 2.38  | 128.66      | 125.04   |
| 31  | b     | 302 | CLA  | CMB-C2B-C3B | 2.38  | 129.13      | 124.68   |
| 31  | 7     | 322 | CLA  | C3D-C2D-C1D | -2.38 | 102.59      | 105.83   |
| 31  | 8     | 311 | CLA  | CMC-C2C-C1C | 2.38  | 128.66      | 125.04   |
| 31  | 2     | 306 | CLA  | CAC-C3C-C4C | 2.38  | 127.89      | 124.81   |
| 36  | 5     | 303 | LUT  | C17-C1-C6   | -2.38 | 106.44      | 110.30   |
| 31  | B     | 819 | CLA  | O2A-CGA-CBA | 2.38  | 119.36      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 318 | CLA  | CMB-C2B-C3B | 2.38  | 129.12      | 124.68   |
| 31  | B     | 840 | CLA  | O2D-CGD-O1D | -2.37 | 119.19      | 123.84   |
| 31  | 2     | 312 | CLA  | CHC-C1C-NC  | -2.37 | 120.60      | 124.20   |
| 31  | 5     | 320 | CLA  | CAC-C3C-C4C | 2.37  | 127.89      | 124.81   |
| 31  | A     | 816 | CLA  | C1-C2-C3    | -2.37 | 121.94      | 126.04   |
| 31  | A     | 833 | CLA  | O2A-CGA-CBA | 2.37  | 119.35      | 111.91   |
| 31  | 7     | 309 | CLA  | C4-C3-C5    | 2.37  | 119.26      | 115.27   |
| 31  | a     | 322 | CLA  | CMD-C2D-C1D | 2.37  | 128.89      | 124.71   |
| 31  | 5     | 307 | CLA  | CAC-C3C-C4C | 2.37  | 127.89      | 124.81   |
| 31  | a     | 309 | CLA  | CMD-C2D-C1D | 2.37  | 128.89      | 124.71   |
| 32  | 6     | 319 | CHL  | O2A-CGA-CBA | 2.37  | 121.60      | 112.23   |
| 37  | G     | 202 | LMG  | O2-C2-C1    | -2.37 | 104.29      | 110.05   |
| 31  | B     | 837 | CLA  | CHC-C1C-NC  | -2.37 | 120.61      | 124.20   |
| 31  | K     | 206 | CLA  | C3B-C4B-NB  | 2.37  | 112.27      | 109.21   |
| 28  | A     | 811 | LHG  | C18-C17-C16 | -2.37 | 102.40      | 114.42   |
| 31  | B     | 831 | CLA  | CMB-C2B-C3B | 2.37  | 129.11      | 124.68   |
| 26  | 3     | 302 | BCR  | C27-C26-C25 | 2.37  | 126.17      | 122.73   |
| 31  | b     | 310 | CLA  | O1D-CGD-CBD | -2.37 | 119.64      | 124.48   |
| 31  | 7     | 315 | CLA  | CHC-C1C-NC  | -2.37 | 120.61      | 124.20   |
| 31  | 2     | 310 | CLA  | CMB-C2B-C3B | 2.37  | 129.10      | 124.68   |
| 31  | B     | 816 | CLA  | O2A-CGA-CBA | 2.37  | 119.33      | 111.91   |
| 31  | A     | 838 | CLA  | C3B-C4B-NB  | 2.37  | 112.27      | 109.21   |
| 31  | a     | 314 | CLA  | CMD-C2D-C1D | 2.37  | 128.88      | 124.71   |
| 31  | 4     | 315 | CLA  | C3D-C4D-CHA | -2.37 | 107.31      | 112.72   |
| 31  | B     | 840 | CLA  | O2A-CGA-O1A | -2.37 | 117.62      | 123.59   |
| 31  | B     | 812 | CLA  | CHD-C4C-NC  | 2.37  | 127.93      | 124.20   |
| 31  | 8     | 308 | CLA  | C4-C3-C5    | 2.37  | 119.25      | 115.27   |
| 31  | a     | 311 | CLA  | C4-C3-C5    | 2.36  | 119.25      | 115.27   |
| 26  | 3     | 303 | BCR  | C24-C23-C22 | -2.36 | 122.66      | 126.23   |
| 31  | a     | 315 | CLA  | O2A-CGA-CBA | 2.36  | 119.33      | 111.91   |
| 36  | 8     | 302 | LUT  | C1-C2-C3    | 2.36  | 118.98      | 113.64   |
| 31  | 4     | 306 | CLA  | O1D-CGD-CBD | -2.36 | 119.65      | 124.48   |
| 32  | 9     | 322 | CHL  | CMB-C2B-C3B | 2.36  | 129.10      | 124.68   |
| 32  | A     | 839 | CHL  | C1D-CHD-C4C | -2.36 | 120.96      | 126.06   |
| 31  | a     | 311 | CLA  | CAC-C3C-C4C | 2.36  | 127.88      | 124.81   |
| 31  | 8     | 318 | CLA  | C5-C3-C4    | 2.36  | 119.82      | 114.60   |
| 31  | 3     | 309 | CLA  | CHC-C1C-NC  | -2.36 | 120.62      | 124.20   |
| 31  | 9     | 311 | CLA  | C1-C2-C3    | -2.36 | 121.96      | 126.04   |
| 31  | A     | 844 | CLA  | C3B-C4B-NB  | 2.36  | 112.26      | 109.21   |
| 31  | A     | 828 | CLA  | C4-C3-C5    | 2.36  | 119.24      | 115.27   |
| 31  | F     | 305 | CLA  | CHB-C4A-NA  | 2.36  | 127.78      | 124.51   |
| 31  | a     | 321 | CLA  | C1D-CHD-C4C | -2.36 | 120.97      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 319 | CLA  | CMC-C2C-C1C | 2.36  | 128.63      | 125.04   |
| 31  | 8     | 315 | CLA  | CAC-C3C-C4C | 2.36  | 127.87      | 124.81   |
| 31  | a     | 315 | CLA  | CHC-C1C-NC  | -2.36 | 120.62      | 124.20   |
| 31  | 6     | 306 | CLA  | CMC-C2C-C1C | 2.36  | 128.63      | 125.04   |
| 28  | A     | 811 | LHG  | C20-C19-C18 | -2.36 | 102.45      | 114.42   |
| 32  | a     | 317 | CHL  | C2D-C1D-ND  | 2.36  | 111.84      | 110.10   |
| 32  | 5     | 316 | CHL  | CHB-C4A-NA  | 2.36  | 127.77      | 124.51   |
| 31  | B     | 839 | CLA  | C3B-C4B-NB  | 2.36  | 112.26      | 109.21   |
| 31  | 6     | 308 | CLA  | CMD-C2D-C1D | 2.36  | 128.87      | 124.71   |
| 31  | A     | 827 | CLA  | O2A-CGA-CBA | 2.36  | 119.31      | 111.91   |
| 36  | 3     | 304 | LUT  | C8-C7-C6    | 2.36  | 133.82      | 127.20   |
| 28  | A     | 810 | LHG  | O8-C23-C24  | 2.36  | 119.30      | 111.91   |
| 31  | 3     | 314 | CLA  | O2A-CGA-CBA | 2.36  | 119.30      | 111.91   |
| 31  | B     | 820 | CLA  | C1-O2A-CGA  | 2.36  | 122.62      | 116.44   |
| 31  | a     | 322 | CLA  | CAC-C3C-C4C | 2.36  | 127.87      | 124.81   |
| 31  | B     | 830 | CLA  | CMD-C2D-C1D | 2.36  | 128.86      | 124.71   |
| 31  | 5     | 308 | CLA  | CMC-C2C-C1C | 2.35  | 128.62      | 125.04   |
| 31  | B     | 837 | CLA  | C4-C3-C5    | 2.35  | 119.23      | 115.27   |
| 31  | 8     | 311 | CLA  | O2A-CGA-O1A | -2.35 | 117.65      | 123.59   |
| 31  | 9     | 314 | CLA  | CMD-C2D-C1D | 2.35  | 128.86      | 124.71   |
| 31  | 7     | 309 | CLA  | O2A-CGA-O1A | -2.35 | 117.65      | 123.59   |
| 32  | A     | 831 | CHL  | CMD-C2D-C1D | 2.35  | 128.86      | 124.71   |
| 31  | 4     | 306 | CLA  | C3D-C4D-CHA | -2.35 | 107.34      | 112.72   |
| 31  | 2     | 306 | CLA  | CMC-C2C-C1C | 2.35  | 128.62      | 125.04   |
| 33  | B     | 808 | DGD  | O6D-C1D-O3G | -2.35 | 104.41      | 109.97   |
| 31  | 4     | 318 | CLA  | CMD-C2D-C1D | 2.35  | 128.85      | 124.71   |
| 37  | J     | 104 | LMG  | O3-C3-C2    | -2.35 | 104.92      | 110.35   |
| 28  | a     | 306 | LHG  | C20-C19-C18 | -2.35 | 102.50      | 114.42   |
| 26  | 7     | 304 | BCR  | C15-C16-C17 | -2.35 | 118.66      | 123.47   |
| 32  | 6     | 317 | CHL  | CED-O2D-CGD | 2.35  | 121.25      | 115.94   |
| 31  | 8     | 312 | CLA  | O2A-CGA-CBA | 2.35  | 119.28      | 111.91   |
| 31  | 9     | 311 | CLA  | C1D-CHD-C4C | -2.35 | 120.99      | 126.06   |
| 31  | 3     | 310 | CLA  | C1-C2-C3    | -2.35 | 121.98      | 126.04   |
| 31  | 9     | 314 | CLA  | CMC-C2C-C1C | 2.35  | 128.61      | 125.04   |
| 31  | G     | 206 | CLA  | C3B-C4B-NB  | 2.35  | 112.24      | 109.21   |
| 31  | 3     | 318 | CLA  | CHC-C1C-NC  | -2.35 | 120.64      | 124.20   |
| 31  | 4     | 305 | CLA  | CHC-C1C-C2C | -2.35 | 120.23      | 126.72   |
| 31  | 4     | 309 | CLA  | C3B-C4B-NB  | 2.35  | 112.24      | 109.21   |
| 31  | 7     | 316 | CLA  | CMD-C2D-C1D | 2.35  | 128.85      | 124.71   |
| 31  | b     | 311 | CLA  | C1D-CHD-C4C | -2.34 | 121.00      | 126.06   |
| 31  | O     | 202 | CLA  | CMC-C2C-C1C | 2.34  | 128.61      | 125.04   |
| 33  | 7     | 308 | DGD  | C3G-C2G-C1G | -2.34 | 106.24      | 111.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | A     | 840 | CHL  | CHC-C1C-NC  | -2.34 | 120.65      | 124.20   |
| 31  | B     | 840 | CLA  | C6-C7-C8    | -2.34 | 108.34      | 115.92   |
| 31  | F     | 306 | CLA  | CMC-C2C-C1C | 2.34  | 128.61      | 125.04   |
| 31  | a     | 310 | CLA  | C1D-CHD-C4C | -2.34 | 121.00      | 126.06   |
| 32  | 9     | 320 | CHL  | C1D-CHD-C4C | -2.34 | 121.00      | 126.06   |
| 31  | b     | 303 | CLA  | CHD-C4C-NC  | 2.34  | 127.89      | 124.20   |
| 31  | A     | 844 | CLA  | CHC-C1C-NC  | -2.34 | 120.65      | 124.20   |
| 30  | A     | 813 | CL0  | CMB-C2B-C3B | 2.34  | 129.06      | 124.68   |
| 32  | 4     | 313 | CHL  | O1D-CGD-CBD | -2.34 | 119.69      | 124.48   |
| 31  | 8     | 309 | CLA  | O2A-CGA-CBA | 2.34  | 119.26      | 111.91   |
| 31  | O     | 204 | CLA  | CMC-C2C-C1C | 2.34  | 128.60      | 125.04   |
| 31  | B     | 826 | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 31  | B     | 830 | CLA  | C3D-C4D-CHA | -2.34 | 107.37      | 112.72   |
| 31  | A     | 823 | CLA  | CMD-C2D-C1D | 2.34  | 128.84      | 124.71   |
| 31  | A     | 837 | CLA  | CMD-C2D-C1D | 2.34  | 128.84      | 124.71   |
| 31  | 4     | 309 | CLA  | CMD-C2D-C1D | 2.34  | 128.84      | 124.71   |
| 31  | 5     | 321 | CLA  | CED-O2D-CGD | 2.34  | 121.23      | 115.94   |
| 31  | B     | 825 | CLA  | CMD-C2D-C1D | 2.34  | 128.84      | 124.71   |
| 31  | b     | 311 | CLA  | CMB-C2B-C3B | 2.34  | 129.06      | 124.68   |
| 31  | 5     | 313 | CLA  | CHC-C1C-NC  | -2.34 | 120.65      | 124.20   |
| 31  | B     | 849 | CLA  | CAC-C3C-C4C | 2.34  | 127.85      | 124.81   |
| 31  | 8     | 308 | CLA  | CAC-C3C-C4C | 2.34  | 127.84      | 124.81   |
| 31  | 7     | 310 | CLA  | CMC-C2C-C1C | 2.34  | 128.60      | 125.04   |
| 36  | a     | 303 | LUT  | C10-C11-C12 | -2.34 | 115.92      | 123.22   |
| 32  | A     | 831 | CHL  | CHD-C4C-NC  | 2.34  | 127.89      | 124.20   |
| 31  | 4     | 319 | CLA  | CMD-C2D-C1D | 2.34  | 128.83      | 124.71   |
| 31  | 8     | 318 | CLA  | CMB-C2B-C3B | 2.34  | 129.05      | 124.68   |
| 32  | 6     | 318 | CHL  | CMB-C2B-C3B | 2.34  | 129.05      | 124.68   |
| 31  | A     | 857 | CLA  | CAA-CBA-CGA | -2.34 | 106.42      | 113.25   |
| 31  | 5     | 323 | CLA  | C4-C3-C5    | 2.34  | 119.20      | 115.27   |
| 32  | 5     | 316 | CHL  | CHA-C4D-ND  | 2.34  | 137.38      | 132.50   |
| 31  | b     | 312 | CLA  | CMB-C2B-C3B | 2.34  | 129.05      | 124.68   |
| 31  | A     | 852 | CLA  | CAA-CBA-CGA | -2.34 | 106.43      | 113.25   |
| 31  | A     | 842 | CLA  | CED-O2D-CGD | 2.33  | 121.22      | 115.94   |
| 31  | 3     | 311 | CLA  | C1-C2-C3    | -2.33 | 122.01      | 126.04   |
| 31  | a     | 311 | CLA  | C1-O2A-CGA  | 2.33  | 122.57      | 116.44   |
| 31  | 3     | 314 | CLA  | CMB-C2B-C3B | 2.33  | 129.04      | 124.68   |
| 36  | F     | 304 | LUT  | C16-C1-C6   | -2.33 | 106.51      | 110.30   |
| 31  | 7     | 314 | CLA  | CMB-C2B-C3B | 2.33  | 129.04      | 124.68   |
| 31  | A     | 827 | CLA  | CMD-C2D-C1D | 2.33  | 128.82      | 124.71   |
| 36  | 3     | 304 | LUT  | C10-C11-C12 | -2.33 | 115.94      | 123.22   |
| 26  | M     | 101 | BCR  | C2-C1-C6    | 2.33  | 114.07      | 110.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | L     | 301 | BCR  | C11-C10-C9  | -2.33 | 123.98      | 127.31   |
| 31  | K     | 204 | CLA  | O1D-CGD-CBD | -2.33 | 119.71      | 124.48   |
| 31  | A     | 841 | CLA  | CHB-C4A-NA  | 2.33  | 127.74      | 124.51   |
| 31  | B     | 825 | CLA  | O2A-CGA-CBA | 2.33  | 119.22      | 111.91   |
| 31  | 4     | 309 | CLA  | CHC-C1C-NC  | -2.33 | 120.67      | 124.20   |
| 31  | 5     | 323 | CLA  | CMB-C2B-C3B | 2.33  | 129.04      | 124.68   |
| 31  | B     | 841 | CLA  | CAC-C3C-C4C | 2.33  | 127.83      | 124.81   |
| 31  | 3     | 312 | CLA  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 26  | 5     | 302 | BCR  | C11-C10-C9  | -2.33 | 123.98      | 127.31   |
| 28  | 6     | 301 | LHG  | O8-C23-C24  | 2.33  | 119.22      | 111.91   |
| 31  | A     | 814 | CLA  | CHC-C1C-NC  | -2.33 | 120.67      | 124.20   |
| 31  | B     | 814 | CLA  | CMD-C2D-C1D | 2.33  | 128.82      | 124.71   |
| 31  | H     | 902 | CLA  | CAC-C3C-C4C | 2.33  | 127.83      | 124.81   |
| 31  | B     | 815 | CLA  | CMB-C2B-C3B | 2.33  | 129.03      | 124.68   |
| 32  | a     | 317 | CHL  | OBD-CAD-C3D | 2.33  | 134.12      | 128.52   |
| 31  | G     | 204 | CLA  | CHD-C4C-NC  | 2.33  | 127.87      | 124.20   |
| 31  | a     | 309 | CLA  | C4-C3-C5    | 2.33  | 119.19      | 115.27   |
| 31  | b     | 308 | CLA  | CMB-C2B-C3B | 2.33  | 129.03      | 124.68   |
| 36  | 8     | 302 | LUT  | C21-C26-C27 | -2.33 | 109.76      | 112.70   |
| 31  | 8     | 321 | CLA  | CMD-C2D-C1D | 2.33  | 128.82      | 124.71   |
| 40  | 7     | 306 | XAT  | C32-C33-C34 | 2.33  | 122.51      | 118.94   |
| 31  | A     | 844 | CLA  | C5-C3-C4    | 2.33  | 119.74      | 114.60   |
| 32  | A     | 831 | CHL  | C2C-C3C-C4C | -2.33 | 104.83      | 106.49   |
| 31  | 3     | 312 | CLA  | O2A-CGA-CBA | 2.33  | 119.21      | 111.91   |
| 31  | J     | 105 | CLA  | CHC-C1C-NC  | -2.33 | 120.67      | 124.20   |
| 31  | 8     | 321 | CLA  | C3B-C4B-NB  | 2.33  | 112.22      | 109.21   |
| 31  | B     | 832 | CLA  | CMB-C2B-C3B | 2.33  | 129.03      | 124.68   |
| 32  | 7     | 320 | CHL  | CMB-C2B-C3B | 2.33  | 129.03      | 124.68   |
| 31  | 6     | 307 | CLA  | CMB-C2B-C3B | 2.33  | 129.03      | 124.68   |
| 31  | a     | 321 | CLA  | O1D-CGD-CBD | -2.33 | 119.73      | 124.48   |
| 31  | B     | 835 | CLA  | CMD-C2D-C1D | 2.32  | 128.81      | 124.71   |
| 31  | L     | 306 | CLA  | CMD-C2D-C1D | 2.32  | 128.81      | 124.71   |
| 31  | A     | 832 | CLA  | O2A-CGA-CBA | 2.32  | 119.20      | 111.91   |
| 31  | B     | 840 | CLA  | CHB-C4A-NA  | 2.32  | 127.72      | 124.51   |
| 31  | A     | 834 | CLA  | C7-C6-C5    | -2.32 | 107.05      | 113.36   |
| 31  | a     | 311 | CLA  | O2A-CGA-CBA | 2.32  | 119.19      | 111.91   |
| 31  | 3     | 312 | CLA  | C4-C3-C5    | 2.32  | 119.18      | 115.27   |
| 31  | A     | 832 | CLA  | C3B-C4B-NB  | 2.32  | 112.21      | 109.21   |
| 31  | F     | 301 | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |
| 31  | 3     | 311 | CLA  | CAC-C3C-C4C | 2.32  | 127.82      | 124.81   |
| 31  | 8     | 310 | CLA  | O2A-CGA-CBA | 2.32  | 119.19      | 111.91   |
| 31  | 3     | 311 | CLA  | CMC-C2C-C1C | 2.32  | 128.57      | 125.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 321 | CLA  | C4-C3-C5    | 2.32  | 119.17      | 115.27   |
| 31  | 4     | 307 | CLA  | C4-C3-C5    | 2.32  | 119.17      | 115.27   |
| 26  | 8     | 301 | BCR  | C15-C16-C17 | -2.32 | 118.72      | 123.47   |
| 31  | 3     | 320 | CLA  | CED-O2D-CGD | 2.32  | 121.18      | 115.94   |
| 31  | 6     | 315 | CLA  | CMD-C2D-C1D | 2.32  | 128.80      | 124.71   |
| 32  | 9     | 322 | CHL  | O2A-CGA-CBA | 2.32  | 121.39      | 112.23   |
| 31  | B     | 820 | CLA  | CMD-C2D-C1D | 2.32  | 128.80      | 124.71   |
| 26  | F     | 302 | BCR  | C27-C26-C25 | 2.32  | 126.10      | 122.73   |
| 31  | B     | 829 | CLA  | C3B-C4B-NB  | 2.32  | 112.21      | 109.21   |
| 31  | 2     | 314 | CLA  | CAC-C3C-C4C | 2.32  | 127.82      | 124.81   |
| 36  | 8     | 302 | LUT  | C4-C5-C6    | -2.32 | 115.69      | 120.85   |
| 31  | B     | 819 | CLA  | CBC-CAC-C3C | -2.32 | 106.05      | 112.43   |
| 31  | b     | 313 | CLA  | CED-O2D-CGD | 2.32  | 121.17      | 115.94   |
| 31  | B     | 832 | CLA  | O2A-CGA-CBA | 2.32  | 119.17      | 111.91   |
| 31  | 9     | 319 | CLA  | CMD-C2D-C1D | 2.32  | 128.79      | 124.71   |
| 31  | 4     | 305 | CLA  | C4-C3-C5    | 2.31  | 119.17      | 115.27   |
| 31  | A     | 829 | CLA  | CHD-C1D-C2D | 2.31  | 130.34      | 125.48   |
| 31  | B     | 842 | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 31  | 7     | 315 | CLA  | O1D-CGD-CBD | -2.31 | 119.75      | 124.48   |
| 31  | A     | 834 | CLA  | C3B-C4B-NB  | 2.31  | 112.20      | 109.21   |
| 31  | 9     | 319 | CLA  | CHC-C1C-NC  | -2.31 | 120.69      | 124.20   |
| 31  | B     | 838 | CLA  | CHD-C4C-NC  | 2.31  | 127.85      | 124.20   |
| 31  | 4     | 321 | CLA  | C1-C2-C3    | -2.31 | 123.01      | 126.75   |
| 31  | B     | 832 | CLA  | CHB-C4A-NA  | 2.31  | 127.71      | 124.51   |
| 31  | 5     | 312 | CLA  | C5-C3-C4    | 2.31  | 119.71      | 114.60   |
| 31  | A     | 845 | CLA  | CMD-C2D-C1D | 2.31  | 128.79      | 124.71   |
| 31  | 4     | 321 | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 32  | 7     | 320 | CHL  | CHA-C4D-ND  | 2.31  | 137.34      | 132.50   |
| 31  | 9     | 311 | CLA  | CAC-C3C-C4C | 2.31  | 127.81      | 124.81   |
| 31  | 5     | 311 | CLA  | CED-O2D-CGD | 2.31  | 121.16      | 115.94   |
| 31  | A     | 836 | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 31  | 4     | 306 | CLA  | C1D-CHD-C4C | -2.31 | 121.07      | 126.06   |
| 31  | 5     | 312 | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 31  | 2     | 310 | CLA  | CMC-C2C-C1C | 2.31  | 128.56      | 125.04   |
| 32  | 7     | 317 | CHL  | O1D-CGD-CBD | -2.31 | 119.76      | 124.48   |
| 31  | b     | 303 | CLA  | C3D-C2D-C1D | -2.31 | 102.68      | 105.83   |
| 26  | L     | 302 | BCR  | C28-C27-C26 | -2.31 | 109.95      | 114.08   |
| 31  | A     | 849 | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 31  | 9     | 319 | CLA  | CMB-C2B-C3B | 2.31  | 129.00      | 124.68   |
| 31  | 3     | 314 | CLA  | CMD-C2D-C1D | 2.31  | 128.78      | 124.71   |
| 32  | A     | 831 | CHL  | C1-O2A-CGA  | 2.31  | 122.50      | 116.44   |
| 32  | 7     | 318 | CHL  | C2D-C1D-ND  | 2.31  | 111.81      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 854 | CLA  | C3B-C4B-NB  | 2.31  | 112.19      | 109.21   |
| 31  | 8     | 309 | CLA  | C4C-C3C-C2C | -2.31 | 103.53      | 106.90   |
| 31  | A     | 847 | CLA  | C3B-C4B-NB  | 2.31  | 112.19      | 109.21   |
| 31  | 3     | 318 | CLA  | CMB-C2B-C3B | 2.31  | 128.99      | 124.68   |
| 31  | 5     | 321 | CLA  | CMB-C2B-C3B | 2.31  | 128.99      | 124.68   |
| 31  | A     | 854 | CLA  | CMD-C2D-C1D | 2.31  | 128.78      | 124.71   |
| 31  | A     | 822 | CLA  | CAC-C3C-C4C | 2.31  | 127.80      | 124.81   |
| 31  | 3     | 317 | CLA  | CAC-C3C-C4C | 2.31  | 127.80      | 124.81   |
| 36  | L     | 304 | LUT  | C1-C6-C7    | -2.31 | 109.25      | 115.78   |
| 31  | 3     | 308 | CLA  | CMC-C2C-C1C | 2.31  | 128.55      | 125.04   |
| 31  | A     | 846 | CLA  | CMD-C2D-C1D | 2.31  | 128.78      | 124.71   |
| 31  | 4     | 320 | CLA  | CMD-C2D-C1D | 2.31  | 128.78      | 124.71   |
| 31  | 3     | 317 | CLA  | CMD-C2D-C1D | 2.30  | 128.78      | 124.71   |
| 32  | A     | 839 | CHL  | CHB-C4A-NA  | 2.30  | 127.70      | 124.51   |
| 31  | O     | 204 | CLA  | CMB-C2B-C3B | 2.30  | 128.99      | 124.68   |
| 31  | 3     | 308 | CLA  | CMD-C2D-C1D | 2.30  | 128.77      | 124.71   |
| 31  | 3     | 314 | CLA  | C1-O2A-CGA  | 2.30  | 122.49      | 116.44   |
| 31  | A     | 824 | CLA  | C1D-CHD-C4C | -2.30 | 121.09      | 126.06   |
| 31  | B     | 837 | CLA  | CHD-C4C-NC  | 2.30  | 127.83      | 124.20   |
| 31  | 8     | 312 | CLA  | C5-C3-C4    | 2.30  | 119.69      | 114.60   |
| 31  | A     | 847 | CLA  | C1-O2A-CGA  | 2.30  | 122.48      | 116.44   |
| 28  | A     | 809 | LHG  | O8-C23-C24  | 2.30  | 119.13      | 111.91   |
| 32  | 6     | 318 | CHL  | CMD-C2D-C1D | 2.30  | 128.77      | 124.71   |
| 31  | B     | 814 | CLA  | C4C-C3C-C2C | -2.30 | 103.54      | 106.90   |
| 31  | 6     | 312 | CLA  | CAC-C3C-C4C | 2.30  | 127.80      | 124.81   |
| 26  | K     | 202 | BCR  | C15-C14-C13 | -2.30 | 124.03      | 127.31   |
| 31  | 7     | 312 | CLA  | O2A-CGA-CBA | 2.30  | 119.12      | 111.91   |
| 32  | 4     | 317 | CHL  | C2D-C1D-ND  | 2.30  | 111.80      | 110.10   |
| 31  | 2     | 307 | CLA  | CAC-C3C-C4C | 2.30  | 127.79      | 124.81   |
| 31  | 8     | 312 | CLA  | CAC-C3C-C4C | 2.30  | 127.79      | 124.81   |
| 31  | 8     | 313 | CLA  | CHC-C1C-NC  | -2.30 | 120.72      | 124.20   |
| 31  | 8     | 321 | CLA  | CHB-C4A-NA  | 2.30  | 127.69      | 124.51   |
| 26  | I     | 801 | BCR  | C28-C27-C26 | -2.30 | 109.98      | 114.08   |
| 31  | b     | 307 | CLA  | CMC-C2C-C1C | 2.29  | 128.53      | 125.04   |
| 31  | 2     | 315 | CLA  | CAC-C3C-C4C | 2.29  | 127.79      | 124.81   |
| 31  | B     | 829 | CLA  | C1-O2A-CGA  | 2.29  | 122.46      | 116.44   |
| 26  | A     | 804 | BCR  | C11-C10-C9  | -2.29 | 124.04      | 127.31   |
| 31  | F     | 306 | CLA  | CMD-C2D-C1D | 2.29  | 128.75      | 124.71   |
| 31  | A     | 830 | CLA  | C6-C7-C8    | -2.29 | 108.51      | 115.92   |
| 31  | 6     | 307 | CLA  | C3D-C4D-CHA | -2.29 | 107.48      | 112.72   |
| 31  | A     | 855 | CLA  | C4C-C3C-C2C | -2.29 | 103.56      | 106.90   |
| 31  | 6     | 313 | CLA  | CAC-C3C-C4C | 2.29  | 127.78      | 124.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | 7     | 324 | CHL  | CAC-C3C-C4C | 2.29  | 127.78      | 124.81   |
| 26  | B     | 803 | BCR  | C24-C23-C22 | -2.29 | 122.77      | 126.23   |
| 31  | A     | 838 | CLA  | C4-C3-C5    | 2.29  | 119.12      | 115.27   |
| 31  | A     | 824 | CLA  | CHD-C4C-NC  | 2.29  | 127.81      | 124.20   |
| 31  | a     | 310 | CLA  | C4C-C3C-C2C | -2.29 | 103.56      | 106.90   |
| 31  | B     | 843 | CLA  | CED-O2D-CGD | 2.29  | 121.12      | 115.94   |
| 36  | 8     | 303 | LUT  | C36-C21-C26 | 2.29  | 113.01      | 109.55   |
| 31  | B     | 813 | CLA  | CAC-C3C-C4C | 2.29  | 127.78      | 124.81   |
| 32  | 3     | 315 | CHL  | C1D-CHD-C4C | -2.29 | 121.12      | 126.06   |
| 31  | 2     | 306 | CLA  | O1D-CGD-CBD | -2.29 | 119.80      | 124.48   |
| 32  | b     | 309 | CHL  | CMB-C2B-C3B | 2.29  | 128.96      | 124.68   |
| 26  | G     | 203 | BCR  | C24-C23-C22 | -2.29 | 122.78      | 126.23   |
| 31  | 5     | 313 | CLA  | C2D-C1D-ND  | 2.29  | 111.79      | 110.10   |
| 31  | A     | 821 | CLA  | CMD-C2D-C1D | 2.29  | 128.75      | 124.71   |
| 31  | 5     | 308 | CLA  | C1D-CHD-C4C | -2.29 | 121.12      | 126.06   |
| 31  | 5     | 318 | CLA  | CAA-CBA-CGA | -2.29 | 106.57      | 113.25   |
| 31  | G     | 204 | CLA  | O1D-CGD-CBD | -2.29 | 119.81      | 124.48   |
| 35  | 9     | 304 | QTB  | C03-C04-C05 | 2.29  | 130.35      | 123.22   |
| 32  | 8     | 316 | CHL  | CMB-C2B-C3B | 2.29  | 128.96      | 124.68   |
| 32  | 8     | 316 | CHL  | C4-C3-C2    | -2.28 | 117.82      | 123.68   |
| 31  | 2     | 313 | CLA  | C3D-C4D-CHA | -2.28 | 107.50      | 112.72   |
| 31  | A     | 821 | CLA  | CMC-C2C-C1C | 2.28  | 128.52      | 125.04   |
| 32  | 6     | 309 | CHL  | CAC-C3C-C4C | 2.28  | 127.77      | 124.81   |
| 36  | 2     | 301 | LUT  | C17-C1-C6   | -2.28 | 106.59      | 110.30   |
| 31  | 8     | 310 | CLA  | C1-C2-C3    | -2.28 | 122.09      | 126.04   |
| 36  | 6     | 303 | LUT  | C22-C23-C24 | 2.28  | 114.34      | 111.74   |
| 31  | 5     | 312 | CLA  | CMD-C2D-C1D | 2.28  | 128.74      | 124.71   |
| 32  | 8     | 319 | CHL  | CHC-C1C-NC  | -2.28 | 120.74      | 124.20   |
| 35  | 7     | 303 | QTB  | C11-C10-C09 | 2.28  | 130.43      | 125.47   |
| 31  | B     | 842 | CLA  | C4-C3-C5    | 2.28  | 119.11      | 115.27   |
| 31  | 3     | 310 | CLA  | C4-C3-C5    | 2.28  | 119.11      | 115.27   |
| 31  | B     | 844 | CLA  | O2A-CGA-CBA | 2.28  | 119.07      | 111.91   |
| 31  | 4     | 311 | CLA  | CMB-C2B-C3B | 2.28  | 128.95      | 124.68   |
| 31  | a     | 312 | CLA  | C1-C2-C3    | -2.28 | 122.10      | 126.04   |
| 31  | A     | 833 | CLA  | CHC-C1C-NC  | -2.28 | 120.74      | 124.20   |
| 31  | A     | 829 | CLA  | CHD-C4C-C3C | -2.28 | 121.49      | 124.84   |
| 31  | B     | 849 | CLA  | C1D-CHD-C4C | -2.28 | 121.14      | 126.06   |
| 31  | 5     | 308 | CLA  | CAC-C3C-C4C | 2.28  | 127.77      | 124.81   |
| 31  | B     | 843 | CLA  | CMC-C2C-C1C | 2.28  | 128.51      | 125.04   |
| 26  | 3     | 301 | BCR  | C15-C14-C13 | -2.28 | 124.06      | 127.31   |
| 31  | a     | 309 | CLA  | C1D-CHD-C4C | -2.28 | 121.14      | 126.06   |
| 32  | 6     | 318 | CHL  | C2C-C3C-C4C | -2.28 | 104.86      | 106.49   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 831 | CLA  | CMD-C2D-C1D | 2.28  | 128.73      | 124.71   |
| 32  | 8     | 316 | CHL  | C4D-CHA-C1A | -2.28 | 118.48      | 121.25   |
| 31  | B     | 826 | CLA  | CMC-C2C-C1C | 2.28  | 128.51      | 125.04   |
| 31  | A     | 820 | CLA  | O2A-CGA-CBA | 2.28  | 119.06      | 111.91   |
| 31  | 8     | 309 | CLA  | CHD-C4C-NC  | 2.28  | 127.79      | 124.20   |
| 31  | B     | 849 | CLA  | C5-C3-C4    | 2.28  | 119.63      | 114.60   |
| 31  | B     | 838 | CLA  | C1D-CHD-C4C | -2.28 | 121.14      | 126.06   |
| 31  | 8     | 311 | CLA  | C3B-C4B-NB  | 2.28  | 112.15      | 109.21   |
| 31  | A     | 849 | CLA  | CHC-C1C-NC  | -2.28 | 120.75      | 124.20   |
| 31  | B     | 848 | CLA  | C4-C3-C5    | 2.28  | 119.10      | 115.27   |
| 31  | A     | 824 | CLA  | CMC-C2C-C1C | 2.28  | 128.50      | 125.04   |
| 28  | B     | 807 | LHG  | C27-C26-C25 | -2.28 | 102.87      | 114.42   |
| 31  | 5     | 310 | CLA  | C3B-C4B-NB  | 2.28  | 112.15      | 109.21   |
| 32  | 4     | 313 | CHL  | C2D-C1D-ND  | 2.28  | 111.78      | 110.10   |
| 26  | K     | 202 | BCR  | C11-C10-C9  | -2.28 | 124.06      | 127.31   |
| 32  | a     | 317 | CHL  | C4-C3-C5    | 2.27  | 119.10      | 115.27   |
| 28  | B     | 807 | LHG  | O8-C23-C24  | 2.27  | 119.05      | 111.91   |
| 31  | 7     | 314 | CLA  | CED-O2D-CGD | 2.27  | 121.08      | 115.94   |
| 31  | 6     | 314 | CLA  | CMB-C2B-C3B | 2.27  | 128.93      | 124.68   |
| 32  | a     | 320 | CHL  | CMB-C2B-C3B | 2.27  | 128.93      | 124.68   |
| 31  | a     | 315 | CLA  | CED-O2D-CGD | 2.27  | 121.08      | 115.94   |
| 31  | a     | 311 | CLA  | O1D-CGD-CBD | -2.27 | 119.83      | 124.48   |
| 31  | 3     | 317 | CLA  | O2A-CGA-CBA | 2.27  | 119.04      | 111.91   |
| 31  | 7     | 314 | CLA  | CMC-C2C-C1C | 2.27  | 128.50      | 125.04   |
| 26  | 3     | 303 | BCR  | C3-C4-C5    | -2.27 | 110.02      | 114.08   |
| 31  | B     | 837 | CLA  | C3D-C4D-CHA | -2.27 | 107.52      | 112.72   |
| 31  | H     | 901 | CLA  | CED-O2D-CGD | 2.27  | 121.08      | 115.94   |
| 31  | 8     | 315 | CLA  | CHB-C4A-NA  | 2.27  | 127.65      | 124.51   |
| 31  | 5     | 312 | CLA  | CAC-C3C-C4C | 2.27  | 127.76      | 124.81   |
| 31  | B     | 833 | CLA  | C1D-CHD-C4C | -2.27 | 121.16      | 126.06   |
| 31  | 2     | 311 | CLA  | CMB-C2B-C3B | 2.27  | 128.93      | 124.68   |
| 31  | 5     | 307 | CLA  | CHC-C1C-NC  | -2.27 | 120.76      | 124.20   |
| 31  | 3     | 320 | CLA  | CMC-C2C-C1C | 2.27  | 128.49      | 125.04   |
| 31  | 8     | 314 | CLA  | C4-C3-C5    | 2.27  | 119.09      | 115.27   |
| 31  | A     | 848 | CLA  | CAC-C3C-C4C | 2.27  | 127.75      | 124.81   |
| 28  | 6     | 305 | LHG  | C11-C10-C9  | -2.27 | 102.91      | 114.42   |
| 31  | 4     | 309 | CLA  | CMB-C2B-C3B | 2.27  | 128.92      | 124.68   |
| 32  | A     | 839 | CHL  | CMB-C2B-C3B | 2.27  | 128.92      | 124.68   |
| 31  | O     | 204 | CLA  | CAA-C2A-C3A | -2.27 | 110.81      | 116.10   |
| 31  | 6     | 310 | CLA  | C3D-C4D-CHA | -2.27 | 107.54      | 112.72   |
| 32  | 4     | 317 | CHL  | CMD-C2D-C1D | 2.27  | 128.71      | 124.71   |
| 31  | 4     | 312 | CLA  | C3D-C4D-CHA | -2.27 | 107.54      | 112.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 313 | CLA  | CMC-C2C-C1C | 2.27  | 128.49      | 125.04   |
| 31  | A     | 850 | CLA  | CAC-C3C-C4C | 2.27  | 127.75      | 124.81   |
| 31  | 3     | 313 | CLA  | CMB-C2B-C3B | 2.27  | 128.92      | 124.68   |
| 31  | a     | 316 | CLA  | CMC-C2C-C1C | 2.26  | 128.49      | 125.04   |
| 31  | 7     | 321 | CLA  | CMC-C2C-C1C | 2.26  | 128.49      | 125.04   |
| 31  | 2     | 307 | CLA  | CHC-C1C-NC  | -2.26 | 120.77      | 124.20   |
| 32  | 3     | 315 | CHL  | C4D-CHA-C1A | -2.26 | 118.49      | 121.25   |
| 31  | A     | 829 | CLA  | O2D-CGD-O1D | -2.26 | 119.41      | 123.84   |
| 31  | A     | 820 | CLA  | CAC-C3C-C4C | 2.26  | 127.75      | 124.81   |
| 31  | B     | 823 | CLA  | CMB-C2B-C3B | 2.26  | 128.91      | 124.68   |
| 31  | A     | 819 | CLA  | CMD-C2D-C1D | 2.26  | 128.70      | 124.71   |
| 31  | 2     | 314 | CLA  | CMC-C2C-C1C | 2.26  | 128.49      | 125.04   |
| 32  | 7     | 320 | CHL  | C2C-C3C-C4C | -2.26 | 104.88      | 106.49   |
| 36  | 2     | 301 | LUT  | C12-C13-C14 | -2.26 | 115.47      | 118.94   |
| 31  | 2     | 312 | CLA  | C3D-C4D-CHA | -2.26 | 107.55      | 112.72   |
| 26  | 8     | 301 | BCR  | C15-C14-C13 | -2.26 | 124.08      | 127.31   |
| 36  | a     | 303 | LUT  | C1-C2-C3    | 2.26  | 118.75      | 113.64   |
| 27  | A     | 808 | LMT  | O1'-C1'-C2' | 2.26  | 111.83      | 108.30   |
| 31  | a     | 311 | CLA  | C1-C2-C3    | -2.26 | 122.13      | 126.04   |
| 31  | 7     | 321 | CLA  | O2A-CGA-O1A | -2.26 | 117.89      | 123.59   |
| 31  | 6     | 316 | CLA  | C5-C3-C4    | 2.26  | 119.59      | 114.60   |
| 31  | b     | 305 | CLA  | CHC-C1C-NC  | -2.26 | 120.78      | 124.20   |
| 31  | A     | 822 | CLA  | CMD-C2D-C1D | 2.26  | 128.69      | 124.71   |
| 31  | B     | 825 | CLA  | CHB-C4A-NA  | 2.26  | 127.63      | 124.51   |
| 31  | B     | 837 | CLA  | C3D-C2D-C1D | -2.26 | 102.75      | 105.83   |
| 32  | 5     | 316 | CHL  | CMB-C2B-C3B | 2.26  | 128.90      | 124.68   |
| 31  | 4     | 312 | CLA  | CMB-C2B-C3B | 2.26  | 128.90      | 124.68   |
| 31  | A     | 830 | CLA  | C4-C3-C2    | -2.26 | 117.89      | 123.68   |
| 31  | B     | 819 | CLA  | CMB-C2B-C3B | 2.26  | 128.90      | 124.68   |
| 31  | b     | 308 | CLA  | CMD-C2D-C1D | 2.26  | 128.69      | 124.71   |
| 32  | 6     | 321 | CHL  | O1D-CGD-CBD | -2.26 | 119.87      | 124.48   |
| 31  | 8     | 309 | CLA  | C4D-CHA-C1A | -2.26 | 118.50      | 121.25   |
| 31  | B     | 817 | CLA  | O2A-CGA-O1A | -2.25 | 117.90      | 123.59   |
| 31  | 8     | 320 | CLA  | CMD-C2D-C1D | 2.25  | 128.69      | 124.71   |
| 31  | b     | 303 | CLA  | CMD-C2D-C1D | 2.25  | 128.69      | 124.71   |
| 32  | 8     | 316 | CHL  | C1-O2A-CGA  | 2.25  | 122.36      | 116.44   |
| 31  | B     | 828 | CLA  | CED-O2D-CGD | 2.25  | 121.04      | 115.94   |
| 37  | G     | 202 | LMG  | O3-C3-C2    | -2.25 | 105.14      | 110.35   |
| 31  | b     | 305 | CLA  | C3B-C4B-NB  | 2.25  | 112.12      | 109.21   |
| 31  | a     | 315 | CLA  | CMD-C2D-C1D | 2.25  | 128.68      | 124.71   |
| 32  | a     | 320 | CHL  | CHA-C4D-ND  | 2.25  | 137.21      | 132.50   |
| 31  | 3     | 309 | CLA  | CMD-C2D-C1D | 2.25  | 128.68      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 8     | 310 | CLA  | CED-O2D-CGD | 2.25  | 121.03      | 115.94   |
| 33  | B     | 808 | DGD  | CFB-CEB-CDB | -2.25 | 102.99      | 114.42   |
| 31  | B     | 845 | CLA  | C5-C3-C4    | 2.25  | 119.58      | 114.60   |
| 31  | 5     | 321 | CLA  | C3D-C2D-C1D | -2.25 | 102.76      | 105.83   |
| 31  | 3     | 317 | CLA  | CED-O2D-CGD | 2.25  | 121.03      | 115.94   |
| 31  | A     | 855 | CLA  | CAA-C2A-C3A | -2.25 | 106.61      | 112.78   |
| 31  | A     | 856 | CLA  | CHC-C1C-NC  | -2.25 | 120.79      | 124.20   |
| 31  | 2     | 304 | CLA  | CHC-C1C-NC  | -2.25 | 120.79      | 124.20   |
| 31  | a     | 316 | CLA  | CMD-C2D-C1D | 2.25  | 128.68      | 124.71   |
| 31  | 6     | 315 | CLA  | CAC-C3C-C4C | 2.25  | 127.73      | 124.81   |
| 31  | A     | 823 | CLA  | C4-C3-C5    | 2.25  | 119.06      | 115.27   |
| 31  | B     | 841 | CLA  | C4C-C3C-C2C | -2.25 | 103.62      | 106.90   |
| 31  | 5     | 311 | CLA  | CHC-C1C-NC  | -2.25 | 120.79      | 124.20   |
| 31  | 4     | 308 | CLA  | C6-C7-C8    | -2.25 | 108.64      | 115.92   |
| 31  | L     | 306 | CLA  | CAC-C3C-C4C | 2.25  | 127.73      | 124.81   |
| 31  | B     | 845 | CLA  | O2A-CGA-O1A | -2.25 | 117.92      | 123.59   |
| 31  | B     | 822 | CLA  | C1-C2-C3    | -2.25 | 122.15      | 126.04   |
| 31  | A     | 820 | CLA  | O1D-CGD-CBD | -2.25 | 119.88      | 124.48   |
| 31  | B     | 836 | CLA  | CHB-C4A-NA  | 2.25  | 127.62      | 124.51   |
| 27  | A     | 807 | LMT  | O1'-C1'-C2' | 2.25  | 111.81      | 108.30   |
| 31  | A     | 848 | CLA  | CHC-C1C-NC  | -2.25 | 120.79      | 124.20   |
| 31  | 8     | 311 | CLA  | CAC-C3C-C4C | 2.25  | 127.73      | 124.81   |
| 31  | 3     | 311 | CLA  | C3D-C4D-CHA | -2.25 | 107.58      | 112.72   |
| 31  | 6     | 313 | CLA  | C3B-C4B-NB  | 2.25  | 112.11      | 109.21   |
| 31  | B     | 841 | CLA  | O2A-CGA-CBA | 2.25  | 118.96      | 111.91   |
| 31  | a     | 309 | CLA  | CAC-C3C-C4C | 2.25  | 127.72      | 124.81   |
| 31  | 4     | 308 | CLA  | C3B-C4B-NB  | 2.25  | 112.11      | 109.21   |
| 31  | A     | 853 | CLA  | O2A-CGA-O1A | -2.25 | 117.92      | 123.59   |
| 31  | 5     | 320 | CLA  | O2A-CGA-CBA | 2.25  | 121.11      | 112.23   |
| 31  | G     | 205 | CLA  | CMD-C2D-C1D | 2.25  | 128.67      | 124.71   |
| 31  | B     | 831 | CLA  | CMC-C2C-C1C | 2.25  | 128.46      | 125.04   |
| 31  | b     | 310 | CLA  | CMC-C2C-C1C | 2.25  | 128.46      | 125.04   |
| 32  | 6     | 317 | CHL  | CMD-C2D-C1D | 2.25  | 128.67      | 124.71   |
| 31  | 4     | 318 | CLA  | CMC-C2C-C1C | 2.24  | 128.46      | 125.04   |
| 31  | A     | 815 | CLA  | C3B-C4B-NB  | 2.24  | 112.11      | 109.21   |
| 31  | 5     | 314 | CLA  | CMB-C2B-C3B | 2.24  | 128.88      | 124.68   |
| 31  | 8     | 309 | CLA  | CMD-C2D-C1D | 2.24  | 128.67      | 124.71   |
| 31  | a     | 314 | CLA  | CHC-C1C-NC  | -2.24 | 120.80      | 124.20   |
| 31  | 2     | 310 | CLA  | CMD-C2D-C1D | 2.24  | 128.67      | 124.71   |
| 31  | 3     | 314 | CLA  | C1-C2-C3    | -2.24 | 122.16      | 126.04   |
| 31  | a     | 316 | CLA  | C1D-CHD-C4C | -2.24 | 121.22      | 126.06   |
| 31  | 3     | 312 | CLA  | CED-O2D-CGD | 2.24  | 121.01      | 115.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 842 | CLA  | CMD-C2D-C1D | 2.24  | 128.66      | 124.71   |
| 31  | A     | 853 | CLA  | CMD-C2D-C1D | 2.24  | 128.66      | 124.71   |
| 31  | 3     | 310 | CLA  | O2A-CGA-CBA | 2.24  | 118.94      | 111.91   |
| 31  | b     | 312 | CLA  | CED-O2D-CGD | 2.24  | 121.01      | 115.94   |
| 31  | 4     | 309 | CLA  | CED-O2D-CGD | 2.24  | 121.01      | 115.94   |
| 31  | A     | 856 | CLA  | C1-C2-C3    | -2.24 | 122.17      | 126.04   |
| 31  | F     | 301 | CLA  | C1D-CHD-C4C | -2.24 | 121.22      | 126.06   |
| 31  | b     | 312 | CLA  | O1D-CGD-CBD | -2.24 | 119.90      | 124.48   |
| 31  | 8     | 314 | CLA  | CHC-C1C-NC  | -2.24 | 120.81      | 124.20   |
| 31  | 7     | 315 | CLA  | CMC-C2C-C1C | 2.24  | 128.45      | 125.04   |
| 26  | L     | 302 | BCR  | C29-C30-C25 | 2.24  | 113.93      | 110.48   |
| 31  | B     | 846 | CLA  | CHC-C1C-NC  | -2.24 | 120.81      | 124.20   |
| 31  | B     | 822 | CLA  | O2A-CGA-CBA | 2.24  | 118.93      | 111.91   |
| 31  | B     | 846 | CLA  | C4C-C3C-C2C | -2.24 | 103.64      | 106.90   |
| 32  | 6     | 320 | CHL  | CMD-C2D-C1D | 2.24  | 128.66      | 124.71   |
| 31  | a     | 321 | CLA  | CMB-C2B-C3B | 2.24  | 128.86      | 124.68   |
| 31  | 2     | 305 | CLA  | CMD-C2D-C1D | 2.24  | 128.66      | 124.71   |
| 31  | A     | 833 | CLA  | CMD-C2D-C1D | 2.24  | 128.66      | 124.71   |
| 31  | 9     | 316 | CLA  | CMD-C2D-C1D | 2.24  | 128.66      | 124.71   |
| 32  | 4     | 313 | CHL  | CED-O2D-CGD | 2.24  | 121.00      | 115.94   |
| 31  | J     | 105 | CLA  | CMC-C2C-C1C | 2.24  | 128.44      | 125.04   |
| 31  | A     | 820 | CLA  | C3B-C4B-NB  | 2.24  | 112.10      | 109.21   |
| 31  | 5     | 311 | CLA  | C3B-C4B-NB  | 2.24  | 112.10      | 109.21   |
| 31  | F     | 301 | CLA  | CHD-C4C-NC  | 2.24  | 127.73      | 124.20   |
| 36  | a     | 303 | LUT  | C22-C23-C24 | 2.24  | 114.28      | 111.74   |
| 31  | B     | 812 | CLA  | O2A-CGA-O1A | -2.24 | 117.95      | 123.59   |
| 31  | O     | 203 | CLA  | CMD-C2D-C1D | 2.24  | 128.65      | 124.71   |
| 26  | A     | 806 | BCR  | C15-C16-C17 | -2.23 | 118.90      | 123.47   |
| 31  | A     | 823 | CLA  | O2A-CGA-CBA | 2.23  | 118.92      | 111.91   |
| 31  | b     | 302 | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 31  | 5     | 307 | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 32  | 9     | 320 | CHL  | C3B-C4B-NB  | 2.23  | 112.10      | 109.21   |
| 31  | A     | 855 | CLA  | CAA-C2A-C1A | 2.23  | 119.29      | 111.97   |
| 35  | a     | 302 | QTB  | C03-C04-C05 | 2.23  | 130.18      | 123.22   |
| 32  | 6     | 319 | CHL  | CHA-C4D-ND  | 2.23  | 137.17      | 132.50   |
| 31  | B     | 836 | CLA  | C1D-CHD-C4C | -2.23 | 121.25      | 126.06   |
| 31  | b     | 303 | CLA  | CMC-C2C-C1C | 2.23  | 128.44      | 125.04   |
| 31  | A     | 818 | CLA  | C2A-C1A-CHA | -2.23 | 119.96      | 123.86   |
| 31  | 9     | 315 | CLA  | C1-O2A-CGA  | 2.23  | 122.29      | 116.44   |
| 31  | A     | 825 | CLA  | O2A-CGA-CBA | 2.23  | 118.90      | 111.91   |
| 31  | L     | 307 | CLA  | CHD-C4C-NC  | 2.23  | 127.72      | 124.20   |
| 31  | B     | 839 | CLA  | CMC-C2C-C1C | 2.23  | 128.43      | 125.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 819 | CLA  | C4-C3-C5    | 2.23  | 119.02      | 115.27   |
| 31  | 7     | 315 | CLA  | C7-C6-C5    | -2.23 | 109.65      | 114.49   |
| 31  | 5     | 320 | CLA  | C1D-CHD-C4C | -2.23 | 121.25      | 126.06   |
| 31  | 4     | 314 | CLA  | C3D-C4D-CHA | -2.23 | 107.63      | 112.72   |
| 31  | 2     | 309 | CLA  | CMC-C2C-C1C | 2.23  | 128.43      | 125.04   |
| 31  | 9     | 313 | CLA  | CAC-C3C-C4C | 2.23  | 127.70      | 124.81   |
| 31  | 3     | 309 | CLA  | CED-O2D-CGD | 2.22  | 120.97      | 115.94   |
| 31  | A     | 838 | CLA  | C1-C2-C3    | -2.22 | 122.20      | 126.04   |
| 37  | a     | 301 | LMG  | O2-C2-C1    | -2.22 | 104.64      | 110.05   |
| 31  | 4     | 316 | CLA  | CAA-CBA-CGA | -2.22 | 106.75      | 113.25   |
| 31  | 5     | 309 | CLA  | CMB-C2B-C3B | 2.22  | 128.84      | 124.68   |
| 31  | 5     | 321 | CLA  | C3D-C4D-CHA | -2.22 | 107.64      | 112.72   |
| 31  | 9     | 311 | CLA  | C3B-C4B-NB  | 2.22  | 112.08      | 109.21   |
| 31  | 3     | 309 | CLA  | CMC-C2C-C1C | 2.22  | 128.42      | 125.04   |
| 31  | b     | 306 | CLA  | C3D-C4D-CHA | -2.22 | 107.64      | 112.72   |
| 36  | 6     | 303 | LUT  | C1-C6-C7    | -2.22 | 109.49      | 115.78   |
| 31  | A     | 857 | CLA  | CHC-C1C-NC  | -2.22 | 120.83      | 124.20   |
| 31  | b     | 307 | CLA  | CMB-C2B-C3B | 2.22  | 128.84      | 124.68   |
| 26  | I     | 801 | BCR  | C29-C30-C25 | 2.22  | 113.90      | 110.48   |
| 31  | 8     | 315 | CLA  | CMC-C2C-C1C | 2.22  | 128.42      | 125.04   |
| 31  | 2     | 308 | CLA  | CMC-C2C-C1C | 2.22  | 128.42      | 125.04   |
| 26  | A     | 804 | BCR  | C27-C26-C25 | 2.22  | 125.96      | 122.73   |
| 31  | A     | 824 | CLA  | O2A-CGA-CBA | 2.22  | 118.88      | 111.91   |
| 31  | B     | 824 | CLA  | C3B-C4B-NB  | 2.22  | 112.08      | 109.21   |
| 33  | 7     | 308 | DGD  | CFB-CEB-CDB | -2.22 | 103.16      | 114.42   |
| 32  | 9     | 320 | CHL  | CED-O2D-CGD | 2.22  | 120.96      | 115.94   |
| 31  | a     | 313 | CLA  | C1-O2A-CGA  | 2.22  | 122.27      | 116.44   |
| 31  | a     | 313 | CLA  | C1-C2-C3    | -2.22 | 122.21      | 126.04   |
| 31  | A     | 815 | CLA  | O2D-CGD-O1D | -2.22 | 119.50      | 123.84   |
| 31  | A     | 822 | CLA  | C4C-C3C-C2C | -2.22 | 103.67      | 106.90   |
| 31  | L     | 305 | CLA  | C4-C3-C5    | 2.22  | 119.00      | 115.27   |
| 32  | 5     | 322 | CHL  | CMD-C2D-C1D | 2.22  | 128.62      | 124.71   |
| 31  | B     | 832 | CLA  | CHC-C1C-NC  | -2.22 | 120.84      | 124.20   |
| 31  | A     | 849 | CLA  | CED-O2D-CGD | 2.22  | 120.95      | 115.94   |
| 31  | 4     | 321 | CLA  | CAA-CBA-CGA | -2.22 | 106.78      | 113.25   |
| 28  | 8     | 304 | LHG  | C27-C26-C25 | -2.21 | 103.19      | 114.42   |
| 31  | B     | 832 | CLA  | CAC-C3C-C4C | 2.21  | 127.68      | 124.81   |
| 31  | 6     | 310 | CLA  | CED-O2D-CGD | 2.21  | 120.94      | 115.94   |
| 31  | A     | 814 | CLA  | C4C-C3C-C2C | -2.21 | 103.67      | 106.90   |
| 31  | 5     | 315 | CLA  | CMC-C2C-C1C | 2.21  | 128.41      | 125.04   |
| 36  | 9     | 302 | LUT  | C1-C6-C7    | -2.21 | 109.53      | 115.78   |
| 31  | 8     | 314 | CLA  | C3B-C4B-NB  | 2.21  | 112.07      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 310 | CLA  | CHC-C1C-NC  | -2.21 | 120.85      | 124.20   |
| 31  | A     | 822 | CLA  | C3B-C4B-NB  | 2.21  | 112.07      | 109.21   |
| 31  | B     | 831 | CLA  | C5-C3-C4    | 2.21  | 119.48      | 114.60   |
| 26  | A     | 805 | BCR  | C15-C14-C13 | -2.21 | 124.16      | 127.31   |
| 31  | B     | 813 | CLA  | O2A-CGA-O1A | -2.21 | 118.02      | 123.59   |
| 31  | 2     | 307 | CLA  | CMC-C2C-C1C | 2.21  | 128.40      | 125.04   |
| 31  | 5     | 315 | CLA  | CMB-C2B-C3B | 2.21  | 128.81      | 124.68   |
| 31  | A     | 828 | CLA  | CAC-C3C-C4C | 2.21  | 127.67      | 124.81   |
| 31  | A     | 824 | CLA  | CMD-C2D-C1D | 2.21  | 128.60      | 124.71   |
| 31  | 5     | 315 | CLA  | C3D-C4D-CHA | -2.21 | 107.68      | 112.72   |
| 31  | 2     | 307 | CLA  | C1D-CHD-C4C | -2.21 | 121.30      | 126.06   |
| 31  | F     | 306 | CLA  | CMB-C2B-C3B | 2.21  | 128.81      | 124.68   |
| 31  | B     | 817 | CLA  | C3B-C4B-NB  | 2.21  | 112.06      | 109.21   |
| 32  | 5     | 316 | CHL  | C2D-C1D-ND  | 2.21  | 111.73      | 110.10   |
| 31  | 9     | 312 | CLA  | C1D-CHD-C4C | -2.20 | 121.30      | 126.06   |
| 31  | B     | 845 | CLA  | CMB-C2B-C3B | 2.20  | 128.80      | 124.68   |
| 33  | 7     | 308 | DGD  | O2D-C2D-C1D | -2.20 | 104.69      | 110.05   |
| 31  | 5     | 310 | CLA  | O2A-CGA-CBA | 2.20  | 118.83      | 111.91   |
| 31  | B     | 850 | CLA  | CHC-C1C-NC  | -2.20 | 120.86      | 124.20   |
| 31  | 8     | 315 | CLA  | C1-C2-C3    | -2.20 | 122.23      | 126.04   |
| 31  | 6     | 316 | CLA  | CMB-C2B-C3B | 2.20  | 128.80      | 124.68   |
| 31  | G     | 206 | CLA  | C1D-CHD-C4C | -2.20 | 121.30      | 126.06   |
| 31  | B     | 827 | CLA  | CAC-C3C-C4C | 2.20  | 127.67      | 124.81   |
| 26  | J     | 102 | BCR  | C27-C26-C25 | 2.20  | 125.93      | 122.73   |
| 31  | 6     | 316 | CLA  | CED-O2D-CGD | 2.20  | 120.92      | 115.94   |
| 31  | B     | 845 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 31  | A     | 826 | CLA  | C3B-C4B-NB  | 2.20  | 112.06      | 109.21   |
| 26  | K     | 202 | BCR  | C15-C16-C17 | -2.20 | 118.97      | 123.47   |
| 31  | 7     | 315 | CLA  | O2A-CGA-CBA | 2.20  | 118.81      | 111.91   |
| 31  | 6     | 312 | CLA  | CHC-C1C-NC  | -2.20 | 120.86      | 124.20   |
| 31  | 8     | 320 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 31  | F     | 306 | CLA  | C5-C3-C4    | 2.20  | 119.46      | 114.60   |
| 26  | L     | 303 | BCR  | C15-C16-C17 | -2.20 | 118.97      | 123.47   |
| 31  | 5     | 311 | CLA  | CMC-C2C-C1C | 2.20  | 128.39      | 125.04   |
| 31  | B     | 846 | CLA  | C4-C3-C5    | 2.20  | 118.97      | 115.27   |
| 32  | 7     | 317 | CHL  | C2C-C3C-C4C | -2.20 | 104.92      | 106.49   |
| 26  | B     | 802 | BCR  | C15-C16-C17 | -2.20 | 118.97      | 123.47   |
| 31  | F     | 306 | CLA  | CHC-C1C-NC  | -2.20 | 120.87      | 124.20   |
| 31  | A     | 846 | CLA  | O1D-CGD-CBD | -2.20 | 119.99      | 124.48   |
| 31  | A     | 846 | CLA  | CMB-C2B-C3B | 2.20  | 128.79      | 124.68   |
| 31  | 2     | 308 | CLA  | C1D-CHD-C4C | -2.20 | 121.32      | 126.06   |
| 31  | L     | 305 | CLA  | CAC-C3C-C4C | 2.20  | 127.66      | 124.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 842 | CLA  | CHB-C4A-NA  | 2.20  | 127.55      | 124.51   |
| 31  | 5     | 307 | CLA  | C4-C3-C5    | 2.20  | 118.97      | 115.27   |
| 31  | 6     | 310 | CLA  | CMD-C2D-C1D | 2.20  | 128.58      | 124.71   |
| 31  | 8     | 307 | CLA  | C1D-CHD-C4C | -2.20 | 121.32      | 126.06   |
| 31  | 4     | 320 | CLA  | C1D-CHD-C4C | -2.20 | 121.32      | 126.06   |
| 28  | 8     | 304 | LHG  | C18-C17-C16 | -2.20 | 103.28      | 114.42   |
| 33  | B     | 808 | DGD  | O5D-C6D-C5D | -2.19 | 104.99      | 109.05   |
| 31  | K     | 205 | CLA  | C3B-C4B-NB  | 2.19  | 112.05      | 109.21   |
| 31  | A     | 819 | CLA  | C1D-CHD-C4C | -2.19 | 121.32      | 126.06   |
| 31  | F     | 301 | CLA  | C4C-C3C-C2C | -2.19 | 103.70      | 106.90   |
| 31  | a     | 315 | CLA  | C4-C3-C5    | 2.19  | 118.96      | 115.27   |
| 31  | 6     | 311 | CLA  | CMB-C2B-C3B | 2.19  | 128.78      | 124.68   |
| 32  | 5     | 322 | CHL  | CED-O2D-CGD | 2.19  | 120.90      | 115.94   |
| 31  | 5     | 310 | CLA  | C1-O2A-CGA  | 2.19  | 122.20      | 116.44   |
| 31  | H     | 902 | CLA  | C3D-C4D-CHA | -2.19 | 107.70      | 112.72   |
| 31  | 9     | 315 | CLA  | C1D-CHD-C4C | -2.19 | 121.33      | 126.06   |
| 31  | B     | 848 | CLA  | CAC-C3C-C4C | 2.19  | 127.66      | 124.81   |
| 31  | B     | 849 | CLA  | CMC-C2C-C1C | 2.19  | 128.38      | 125.04   |
| 31  | 9     | 315 | CLA  | C3D-C4D-CHA | -2.19 | 107.71      | 112.72   |
| 31  | B     | 839 | CLA  | C4-C3-C5    | 2.19  | 118.96      | 115.27   |
| 32  | 3     | 315 | CHL  | CMB-C2B-C3B | 2.19  | 128.78      | 124.68   |
| 31  | 9     | 321 | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.51   |
| 31  | J     | 105 | CLA  | O1D-CGD-CBD | -2.19 | 120.00      | 124.48   |
| 31  | 3     | 317 | CLA  | CHB-C4A-NA  | 2.19  | 127.54      | 124.51   |
| 32  | A     | 839 | CHL  | CAC-C3C-C4C | 2.19  | 127.65      | 124.81   |
| 31  | A     | 850 | CLA  | CBC-CAC-C3C | -2.19 | 106.39      | 112.43   |
| 32  | 6     | 319 | CHL  | CHC-C1C-NC  | -2.19 | 120.88      | 124.20   |
| 31  | 8     | 318 | CLA  | O1D-CGD-CBD | -2.19 | 120.00      | 124.48   |
| 36  | L     | 304 | LUT  | C17-C1-C6   | -2.19 | 106.75      | 110.30   |
| 26  | O     | 201 | BCR  | C28-C27-C26 | -2.19 | 110.17      | 114.08   |
| 26  | A     | 806 | BCR  | C38-C26-C27 | -2.19 | 109.41      | 113.62   |
| 31  | 2     | 314 | CLA  | C1D-CHD-C4C | -2.19 | 121.34      | 126.06   |
| 31  | B     | 831 | CLA  | C1-O2A-CGA  | 2.19  | 122.18      | 116.44   |
| 31  | A     | 824 | CLA  | CAA-C2A-C3A | -2.19 | 106.79      | 112.78   |
| 31  | 3     | 310 | CLA  | O1D-CGD-CBD | -2.19 | 120.01      | 124.48   |
| 36  | L     | 304 | LUT  | C22-C23-C24 | 2.19  | 114.23      | 111.74   |
| 26  | 3     | 302 | BCR  | C15-C16-C17 | -2.19 | 119.00      | 123.47   |
| 31  | 8     | 308 | CLA  | C4C-C3C-C2C | -2.19 | 103.71      | 106.90   |
| 31  | 6     | 322 | CLA  | C3D-C4D-CHA | -2.19 | 107.72      | 112.72   |
| 31  | 5     | 313 | CLA  | CAC-C3C-C4C | 2.18  | 127.64      | 124.81   |
| 27  | 5     | 301 | LMT  | O5B-C5B-C6B | 2.18  | 111.87      | 106.44   |
| 26  | L     | 302 | BCR  | C15-C14-C13 | -2.18 | 124.19      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 7     | 316 | CLA  | O2A-CGA-CBA | 2.18  | 120.86      | 112.23   |
| 31  | B     | 820 | CLA  | CHC-C1C-NC  | -2.18 | 120.89      | 124.20   |
| 31  | O     | 202 | CLA  | C3D-C4D-CHA | -2.18 | 107.73      | 112.72   |
| 31  | 9     | 316 | CLA  | CHC-C1C-NC  | -2.18 | 120.89      | 124.20   |
| 31  | 9     | 311 | CLA  | CHC-C1C-NC  | -2.18 | 120.89      | 124.20   |
| 31  | B     | 839 | CLA  | C2A-C1A-CHA | -2.18 | 120.04      | 123.86   |
| 31  | 4     | 309 | CLA  | C2A-C1A-CHA | -2.18 | 120.05      | 123.86   |
| 31  | B     | 842 | CLA  | O2A-CGA-O1A | -2.18 | 118.09      | 123.59   |
| 31  | 3     | 320 | CLA  | CMB-C2B-C3B | 2.18  | 128.76      | 124.68   |
| 31  | 4     | 314 | CLA  | CMB-C2B-C3B | 2.18  | 128.76      | 124.68   |
| 31  | H     | 902 | CLA  | O2A-CGA-CBA | 2.18  | 120.85      | 112.23   |
| 32  | 9     | 320 | CHL  | C4D-CHA-C1A | -2.18 | 118.60      | 121.25   |
| 33  | 7     | 308 | DGD  | C5B-C4B-C3B | -2.18 | 103.36      | 114.42   |
| 31  | 9     | 319 | CLA  | C3D-C4D-CHA | -2.18 | 107.74      | 112.72   |
| 31  | b     | 311 | CLA  | CMD-C2D-C1D | 2.18  | 128.55      | 124.71   |
| 31  | 4     | 318 | CLA  | CED-O2D-CGD | 2.18  | 120.86      | 115.94   |
| 31  | 8     | 308 | CLA  | C1-C2-C3    | -2.18 | 122.28      | 126.04   |
| 31  | A     | 855 | CLA  | CHC-C1C-NC  | -2.18 | 120.90      | 124.20   |
| 31  | 5     | 311 | CLA  | O2A-CGA-CBA | 2.18  | 120.84      | 112.23   |
| 31  | B     | 841 | CLA  | C2A-C1A-CHA | -2.18 | 120.05      | 123.86   |
| 35  | F     | 303 | QTB  | C03-C04-C05 | 2.18  | 130.01      | 123.22   |
| 26  | B     | 802 | BCR  | C28-C27-C26 | -2.18 | 110.19      | 114.08   |
| 26  | B     | 805 | BCR  | C11-C10-C9  | -2.18 | 124.20      | 127.31   |
| 31  | A     | 844 | CLA  | CMC-C2C-C1C | 2.18  | 128.35      | 125.04   |
| 36  | 4     | 303 | LUT  | C30-C31-C32 | -2.18 | 116.42      | 123.22   |
| 31  | A     | 830 | CLA  | CMD-C2D-C1D | 2.18  | 128.55      | 124.71   |
| 31  | B     | 830 | CLA  | C3B-C4B-NB  | 2.18  | 112.02      | 109.21   |
| 31  | a     | 310 | CLA  | C3C-C4C-NC  | 2.18  | 113.01      | 110.57   |
| 31  | B     | 838 | CLA  | C3B-C4B-NB  | 2.18  | 112.02      | 109.21   |
| 37  | J     | 104 | LMG  | O7-C10-O9   | -2.17 | 118.45      | 123.70   |
| 31  | 9     | 313 | CLA  | CMC-C2C-C1C | 2.17  | 128.35      | 125.04   |
| 31  | 3     | 319 | CLA  | C1D-CHD-C4C | -2.17 | 121.37      | 126.06   |
| 31  | A     | 828 | CLA  | CMD-C2D-C1D | 2.17  | 128.54      | 124.71   |
| 31  | 2     | 304 | CLA  | CMD-C2D-C1D | 2.17  | 128.54      | 124.71   |
| 31  | A     | 828 | CLA  | C3B-C4B-NB  | 2.17  | 112.02      | 109.21   |
| 31  | B     | 811 | CLA  | C1D-CHD-C4C | -2.17 | 121.37      | 126.06   |
| 31  | b     | 311 | CLA  | O2A-CGA-CBA | 2.17  | 120.82      | 112.23   |
| 31  | B     | 827 | CLA  | CHC-C1C-NC  | -2.17 | 120.91      | 124.20   |
| 31  | 3     | 314 | CLA  | CHC-C1C-NC  | -2.17 | 120.91      | 124.20   |
| 31  | H     | 901 | CLA  | CMB-C2B-C3B | 2.17  | 128.75      | 124.68   |
| 31  | 3     | 316 | CLA  | C3D-C4D-CHA | -2.17 | 107.75      | 112.72   |
| 31  | a     | 319 | CLA  | CED-O2D-CGD | 2.17  | 120.85      | 115.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | A     | 807 | LMT  | O5B-C5B-C4B | 2.17  | 113.64      | 109.69   |
| 32  | 6     | 318 | CHL  | C2A-C1A-CHA | -2.17 | 120.06      | 123.86   |
| 32  | 7     | 318 | CHL  | CMD-C2D-C1D | 2.17  | 128.54      | 124.71   |
| 31  | A     | 838 | CLA  | CHB-C4A-NA  | 2.17  | 127.52      | 124.51   |
| 31  | 8     | 318 | CLA  | CAC-C3C-C4C | 2.17  | 127.63      | 124.81   |
| 32  | 5     | 317 | CHL  | O2A-CGA-CBA | 2.17  | 120.81      | 112.23   |
| 31  | F     | 301 | CLA  | CMD-C2D-C1D | 2.17  | 128.54      | 124.71   |
| 31  | A     | 815 | CLA  | CMC-C2C-C1C | 2.17  | 128.35      | 125.04   |
| 31  | A     | 836 | CLA  | C3D-C4D-CHA | -2.17 | 107.76      | 112.72   |
| 31  | b     | 303 | CLA  | CMB-C2B-C3B | 2.17  | 128.74      | 124.68   |
| 31  | A     | 850 | CLA  | C3B-C4B-NB  | 2.17  | 112.02      | 109.21   |
| 31  | 7     | 309 | CLA  | CHC-C1C-NC  | -2.17 | 120.91      | 124.20   |
| 31  | 5     | 311 | CLA  | CAC-C3C-C4C | 2.17  | 127.62      | 124.81   |
| 31  | 2     | 310 | CLA  | O2A-CGA-CBA | 2.17  | 121.00      | 114.03   |
| 28  | a     | 306 | LHG  | C18-C17-C16 | -2.17 | 103.41      | 114.42   |
| 31  | 4     | 307 | CLA  | C1-C2-C3    | -2.17 | 122.29      | 126.04   |
| 31  | a     | 309 | CLA  | O2A-CGA-O1A | -2.17 | 118.12      | 123.59   |
| 31  | 9     | 314 | CLA  | C3B-C4B-NB  | 2.17  | 112.01      | 109.21   |
| 31  | 7     | 311 | CLA  | C4-C3-C5    | 2.17  | 118.92      | 115.27   |
| 26  | 5     | 302 | BCR  | C24-C23-C22 | -2.17 | 122.96      | 126.23   |
| 31  | 3     | 317 | CLA  | CHC-C1C-NC  | -2.17 | 120.92      | 124.20   |
| 31  | 9     | 317 | CLA  | CHC-C1C-NC  | -2.17 | 120.92      | 124.20   |
| 31  | 2     | 314 | CLA  | O1D-CGD-CBD | -2.17 | 120.05      | 124.48   |
| 31  | b     | 305 | CLA  | C3D-C4D-CHA | -2.17 | 107.77      | 112.72   |
| 31  | B     | 829 | CLA  | CMC-C2C-C1C | 2.17  | 128.34      | 125.04   |
| 31  | H     | 901 | CLA  | CMD-C2D-C1D | 2.17  | 128.53      | 124.71   |
| 32  | 9     | 322 | CHL  | CMD-C2D-C1D | 2.16  | 128.53      | 124.71   |
| 32  | 9     | 322 | CHL  | CHA-C4D-ND  | 2.16  | 137.03      | 132.50   |
| 32  | b     | 309 | CHL  | C2D-C1D-ND  | 2.16  | 111.70      | 110.10   |
| 26  | O     | 201 | BCR  | C15-C16-C17 | -2.16 | 119.04      | 123.47   |
| 26  | B     | 802 | BCR  | C31-C1-C6   | 2.16  | 113.81      | 110.30   |
| 31  | b     | 313 | CLA  | O2A-CGA-O1A | -2.16 | 118.13      | 123.59   |
| 31  | 4     | 314 | CLA  | O2A-CGA-CBA | 2.16  | 120.98      | 114.03   |
| 31  | 7     | 322 | CLA  | C3B-C4B-NB  | 2.16  | 112.01      | 109.21   |
| 31  | 4     | 311 | CLA  | O2A-CGA-CBA | 2.16  | 120.77      | 112.23   |
| 31  | B     | 842 | CLA  | C1D-CHD-C4C | -2.16 | 121.39      | 126.06   |
| 31  | A     | 843 | CLA  | C1-O2A-CGA  | 2.16  | 122.11      | 116.44   |
| 26  | L     | 303 | BCR  | C11-C10-C9  | -2.16 | 124.23      | 127.31   |
| 31  | 4     | 318 | CLA  | CMB-C2B-C3B | 2.16  | 128.72      | 124.68   |
| 31  | 6     | 308 | CLA  | CHD-C4C-NC  | 2.16  | 127.61      | 124.20   |
| 31  | A     | 828 | CLA  | CMC-C2C-C1C | 2.16  | 128.33      | 125.04   |
| 31  | B     | 824 | CLA  | CED-O2D-CGD | 2.16  | 120.82      | 115.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | G     | 203 | BCR  | C16-C15-C14 | -2.16 | 119.05      | 123.47   |
| 37  | J     | 101 | LMG  | O3-C3-C2    | -2.16 | 105.36      | 110.35   |
| 28  | 7     | 302 | LHG  | C20-C19-C18 | -2.16 | 103.46      | 114.42   |
| 31  | A     | 826 | CLA  | CMC-C2C-C1C | 2.16  | 128.33      | 125.04   |
| 26  | 8     | 301 | BCR  | C7-C8-C9    | -2.16 | 122.97      | 126.23   |
| 31  | A     | 816 | CLA  | O2A-CGA-CBA | 2.16  | 118.68      | 111.91   |
| 31  | 4     | 321 | CLA  | O2A-CGA-CBA | 2.16  | 118.68      | 111.91   |
| 32  | A     | 831 | CHL  | O2A-CGA-CBA | 2.16  | 118.68      | 111.91   |
| 31  | A     | 826 | CLA  | O2A-CGA-CBA | 2.16  | 118.68      | 111.91   |
| 31  | A     | 845 | CLA  | CHC-C1C-NC  | -2.16 | 120.93      | 124.20   |
| 32  | 6     | 318 | CHL  | CHA-C4D-ND  | 2.16  | 137.01      | 132.50   |
| 31  | 8     | 317 | CLA  | O2A-CGA-O1A | -2.16 | 118.15      | 123.59   |
| 31  | 4     | 321 | CLA  | C1D-CHD-C4C | -2.16 | 121.40      | 126.06   |
| 31  | A     | 821 | CLA  | C3B-C4B-NB  | 2.16  | 112.00      | 109.21   |
| 26  | A     | 806 | BCR  | C27-C26-C25 | 2.16  | 125.86      | 122.73   |
| 28  | A     | 809 | LHG  | C27-C26-C25 | -2.16 | 103.48      | 114.42   |
| 31  | A     | 843 | CLA  | CHD-C4C-NC  | 2.16  | 127.60      | 124.20   |
| 31  | A     | 817 | CLA  | CHB-C4A-NA  | 2.16  | 127.49      | 124.51   |
| 31  | a     | 321 | CLA  | C3D-C4D-CHA | -2.16 | 107.79      | 112.72   |
| 31  | 9     | 311 | CLA  | C3D-C4D-CHA | -2.16 | 107.79      | 112.72   |
| 31  | A     | 851 | CLA  | CHC-C1C-NC  | -2.16 | 120.93      | 124.20   |
| 32  | 5     | 319 | CHL  | CHA-C4D-ND  | 2.16  | 137.01      | 132.50   |
| 26  | I     | 801 | BCR  | C33-C5-C6   | -2.16 | 122.11      | 124.53   |
| 32  | 7     | 320 | CHL  | CAC-C3C-C4C | 2.15  | 127.61      | 124.81   |
| 31  | 7     | 311 | CLA  | O2A-CGA-CBA | 2.15  | 118.67      | 111.91   |
| 31  | 9     | 321 | CLA  | CED-O2D-CGD | 2.15  | 120.81      | 115.94   |
| 28  | 7     | 302 | LHG  | C27-C26-C25 | -2.15 | 103.50      | 114.42   |
| 31  | 4     | 309 | CLA  | CAC-C3C-C4C | 2.15  | 127.60      | 124.81   |
| 31  | B     | 812 | CLA  | C4-C3-C5    | 2.15  | 118.89      | 115.27   |
| 31  | 2     | 305 | CLA  | CMB-C2B-C3B | 2.15  | 128.70      | 124.68   |
| 31  | L     | 305 | CLA  | CMD-C2D-C1D | 2.15  | 128.50      | 124.71   |
| 35  | F     | 303 | QTB  | C11-C10-C09 | 2.15  | 130.14      | 125.47   |
| 32  | 5     | 322 | CHL  | C2D-C1D-ND  | 2.15  | 111.69      | 110.10   |
| 32  | 4     | 310 | CHL  | CMB-C2B-C3B | 2.15  | 128.70      | 124.68   |
| 31  | B     | 830 | CLA  | CMB-C2B-C3B | 2.15  | 128.70      | 124.68   |
| 31  | 8     | 321 | CLA  | CED-O2D-CGD | 2.15  | 120.80      | 115.94   |
| 31  | B     | 846 | CLA  | CMC-C2C-C1C | 2.15  | 128.31      | 125.04   |
| 31  | A     | 828 | CLA  | C1D-CHD-C4C | -2.15 | 121.42      | 126.06   |
| 31  | B     | 823 | CLA  | CMC-C2C-C1C | 2.15  | 128.31      | 125.04   |
| 31  | 6     | 306 | CLA  | CHD-C4C-NC  | 2.15  | 127.59      | 124.20   |
| 32  | 6     | 309 | CHL  | CHC-C1C-NC  | -2.15 | 120.94      | 124.20   |
| 31  | B     | 816 | CLA  | CMB-C2B-C3B | 2.15  | 128.70      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 9     | 311 | CLA  | CED-O2D-CGD | 2.15  | 120.80      | 115.94   |
| 31  | 3     | 319 | CLA  | CMD-C2D-C1D | 2.15  | 128.50      | 124.71   |
| 31  | 9     | 318 | CLA  | C3D-C4D-CHA | -2.15 | 107.81      | 112.72   |
| 31  | H     | 903 | CLA  | C3D-C2D-C1D | -2.15 | 102.90      | 105.83   |
| 26  | 7     | 304 | BCR  | C2-C1-C6    | 2.15  | 113.78      | 110.48   |
| 31  | 5     | 314 | CLA  | CED-O2D-CGD | 2.15  | 120.79      | 115.94   |
| 32  | 6     | 319 | CHL  | C1B-CHB-C4A | -2.15 | 125.87      | 130.12   |
| 31  | L     | 306 | CLA  | CED-O2D-CGD | 2.15  | 120.79      | 115.94   |
| 31  | A     | 832 | CLA  | CHC-C1C-NC  | -2.14 | 120.95      | 124.20   |
| 31  | A     | 841 | CLA  | C4C-C3C-C2C | -2.14 | 103.77      | 106.90   |
| 31  | 3     | 317 | CLA  | C1-O2A-CGA  | 2.14  | 122.07      | 116.44   |
| 31  | A     | 837 | CLA  | O2A-CGA-CBA | 2.14  | 118.64      | 111.91   |
| 31  | A     | 829 | CLA  | CHC-C1C-C2C | -2.14 | 120.79      | 126.72   |
| 31  | 8     | 317 | CLA  | CHB-C4A-NA  | 2.14  | 127.48      | 124.51   |
| 31  | 8     | 307 | CLA  | CAC-C3C-C4C | 2.14  | 127.59      | 124.81   |
| 32  | 7     | 324 | CHL  | CHA-C4D-ND  | 2.14  | 136.98      | 132.50   |
| 31  | 6     | 314 | CLA  | CMC-C2C-C1C | 2.14  | 128.30      | 125.04   |
| 31  | b     | 302 | CLA  | O1D-CGD-CBD | -2.14 | 120.10      | 124.48   |
| 31  | b     | 305 | CLA  | CAC-C3C-C4C | 2.14  | 127.59      | 124.81   |
| 31  | B     | 811 | CLA  | C4C-C3C-C2C | -2.14 | 103.78      | 106.90   |
| 31  | B     | 826 | CLA  | C3B-C4B-NB  | 2.14  | 111.98      | 109.21   |
| 31  | b     | 310 | CLA  | C1D-CHD-C4C | -2.14 | 121.44      | 126.06   |
| 31  | 3     | 310 | CLA  | C3B-C4B-NB  | 2.14  | 111.98      | 109.21   |
| 31  | 6     | 322 | CLA  | O1D-CGD-CBD | -2.14 | 120.11      | 124.48   |
| 32  | b     | 309 | CHL  | CED-O2D-CGD | 2.14  | 120.78      | 115.94   |
| 31  | B     | 850 | CLA  | O2A-CGA-CBA | 2.14  | 118.62      | 111.91   |
| 31  | B     | 817 | CLA  | C1D-CHD-C4C | -2.14 | 121.44      | 126.06   |
| 31  | B     | 814 | CLA  | C3B-C4B-NB  | 2.14  | 111.98      | 109.21   |
| 31  | A     | 846 | CLA  | C7-C6-C5    | -2.14 | 107.55      | 113.36   |
| 31  | B     | 847 | CLA  | CAC-C3C-C4C | 2.14  | 127.58      | 124.81   |
| 32  | 6     | 320 | CHL  | CED-O2D-CGD | 2.14  | 120.77      | 115.94   |
| 26  | A     | 805 | BCR  | C33-C5-C6   | -2.14 | 122.13      | 124.53   |
| 31  | 6     | 310 | CLA  | C1D-CHD-C4C | -2.14 | 121.45      | 126.06   |
| 26  | A     | 804 | BCR  | C15-C14-C13 | -2.14 | 124.26      | 127.31   |
| 31  | B     | 839 | CLA  | CMD-C2D-C1D | 2.14  | 128.48      | 124.71   |
| 31  | A     | 853 | CLA  | CHB-C4A-NA  | 2.14  | 127.47      | 124.51   |
| 31  | H     | 903 | CLA  | C3D-C4D-CHA | -2.14 | 107.84      | 112.72   |
| 31  | 5     | 318 | CLA  | C3D-C4D-CHA | -2.14 | 107.84      | 112.72   |
| 31  | A     | 849 | CLA  | CAC-C3C-C4C | 2.14  | 127.58      | 124.81   |
| 31  | A     | 827 | CLA  | CHC-C1C-NC  | -2.14 | 120.96      | 124.20   |
| 32  | 6     | 319 | CHL  | C2C-C3C-C4C | -2.14 | 104.97      | 106.49   |
| 31  | O     | 204 | CLA  | CED-O2D-CGD | 2.13  | 120.77      | 115.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 307 | CLA  | O2A-CGA-O1A | -2.13 | 118.20      | 123.59   |
| 31  | 5     | 318 | CLA  | C3B-C4B-NB  | 2.13  | 111.97      | 109.21   |
| 31  | A     | 854 | CLA  | C4C-C3C-C2C | -2.13 | 103.79      | 106.90   |
| 31  | 4     | 307 | CLA  | CMC-C2C-C1C | 2.13  | 128.29      | 125.04   |
| 31  | A     | 826 | CLA  | C1-O2A-CGA  | 2.13  | 122.04      | 116.44   |
| 32  | 6     | 309 | CHL  | O2A-CGA-O1A | -2.13 | 118.21      | 123.59   |
| 31  | B     | 818 | CLA  | CMD-C2D-C1D | 2.13  | 128.47      | 124.71   |
| 31  | K     | 206 | CLA  | CAC-C3C-C4C | 2.13  | 127.58      | 124.81   |
| 31  | 5     | 307 | CLA  | C3B-C4B-NB  | 2.13  | 111.97      | 109.21   |
| 31  | O     | 204 | CLA  | C3D-C4D-CHA | -2.13 | 107.84      | 112.72   |
| 31  | 4     | 321 | CLA  | CMD-C2D-C1D | 2.13  | 128.47      | 124.71   |
| 31  | B     | 849 | CLA  | C1-O2A-CGA  | 2.13  | 122.04      | 116.44   |
| 31  | B     | 826 | CLA  | C5-C3-C4    | 2.13  | 119.31      | 114.60   |
| 31  | 7     | 314 | CLA  | O1D-CGD-CBD | -2.13 | 120.12      | 124.48   |
| 32  | 5     | 322 | CHL  | CMB-C2B-C3B | 2.13  | 128.66      | 124.68   |
| 31  | 8     | 307 | CLA  | C3B-C4B-NB  | 2.13  | 111.96      | 109.21   |
| 31  | B     | 839 | CLA  | CED-O2D-CGD | 2.13  | 120.75      | 115.94   |
| 31  | B     | 832 | CLA  | CMC-C2C-C1C | 2.13  | 128.28      | 125.04   |
| 31  | A     | 855 | CLA  | C4-C3-C2    | -2.13 | 118.22      | 123.68   |
| 31  | B     | 842 | CLA  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 31  | A     | 825 | CLA  | O2A-C1-C2   | -2.13 | 103.04      | 108.64   |
| 32  | 5     | 319 | CHL  | CAC-C3C-C4C | 2.13  | 127.57      | 124.81   |
| 32  | 6     | 317 | CHL  | O2A-CGA-CBA | 2.13  | 120.64      | 112.23   |
| 31  | 3     | 320 | CLA  | O1D-CGD-CBD | -2.13 | 120.13      | 124.48   |
| 31  | 5     | 321 | CLA  | O2A-CGA-CBA | 2.13  | 120.64      | 112.23   |
| 31  | 4     | 321 | CLA  | C3D-C4D-CHA | -2.13 | 107.86      | 112.72   |
| 31  | 7     | 321 | CLA  | CED-O2D-CGD | 2.13  | 120.75      | 115.94   |
| 31  | 8     | 315 | CLA  | C1-O2A-CGA  | 2.13  | 122.02      | 116.44   |
| 31  | B     | 830 | CLA  | C3D-C2D-C1D | -2.13 | 102.93      | 105.83   |
| 32  | A     | 840 | CHL  | CHA-C4D-ND  | 2.13  | 136.95      | 132.50   |
| 31  | O     | 203 | CLA  | CED-O2D-CGD | 2.13  | 120.75      | 115.94   |
| 31  | 2     | 307 | CLA  | CMD-C2D-C1D | 2.13  | 128.46      | 124.71   |
| 31  | 5     | 309 | CLA  | C3D-C4D-CHA | -2.13 | 107.86      | 112.72   |
| 31  | 5     | 320 | CLA  | C3D-C4D-CHA | -2.13 | 107.86      | 112.72   |
| 31  | 9     | 312 | CLA  | C4C-C3C-C2C | -2.12 | 103.80      | 106.90   |
| 31  | 7     | 315 | CLA  | C3B-C4B-NB  | 2.12  | 111.96      | 109.21   |
| 31  | 4     | 311 | CLA  | C3D-C4D-CHA | -2.12 | 107.86      | 112.72   |
| 26  | K     | 203 | BCR  | C15-C14-C13 | -2.12 | 124.28      | 127.31   |
| 31  | b     | 307 | CLA  | CAC-C3C-C4C | 2.12  | 127.56      | 124.81   |
| 32  | 7     | 317 | CHL  | C4D-CHA-C1A | -2.12 | 118.67      | 121.25   |
| 32  | 5     | 316 | CHL  | C3B-C4B-NB  | 2.12  | 111.95      | 109.21   |
| 31  | 8     | 312 | CLA  | C1-O2A-CGA  | 2.12  | 122.01      | 116.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 815 | CLA  | C4C-C3C-C2C | -2.12 | 103.80      | 106.90   |
| 32  | A     | 831 | CHL  | C1B-CHB-C4A | -2.12 | 125.91      | 130.12   |
| 32  | 7     | 317 | CHL  | CMB-C2B-C3B | 2.12  | 128.65      | 124.68   |
| 31  | 6     | 311 | CLA  | C3D-C4D-CHA | -2.12 | 107.87      | 112.72   |
| 32  | 4     | 313 | CHL  | CHA-C4D-ND  | 2.12  | 136.94      | 132.50   |
| 31  | A     | 826 | CLA  | C4C-C3C-C2C | -2.12 | 103.81      | 106.90   |
| 32  | 4     | 317 | CHL  | CED-O2D-CGD | 2.12  | 120.73      | 115.94   |
| 31  | B     | 828 | CLA  | CMB-C2B-C3B | 2.12  | 128.65      | 124.68   |
| 31  | B     | 818 | CLA  | C1D-CHD-C4C | -2.12 | 121.48      | 126.06   |
| 31  | L     | 306 | CLA  | C3B-C4B-NB  | 2.12  | 111.95      | 109.21   |
| 31  | b     | 305 | CLA  | C1D-CHD-C4C | -2.12 | 121.48      | 126.06   |
| 31  | A     | 816 | CLA  | C1-O2A-CGA  | 2.12  | 122.00      | 116.44   |
| 31  | b     | 310 | CLA  | CAC-C3C-C4C | 2.12  | 127.56      | 124.81   |
| 31  | 9     | 316 | CLA  | O2A-CGA-CBA | 2.12  | 118.56      | 111.91   |
| 26  | 3     | 302 | BCR  | C33-C5-C6   | -2.12 | 122.15      | 124.53   |
| 32  | 7     | 318 | CHL  | CHA-C4D-ND  | 2.12  | 136.93      | 132.50   |
| 31  | H     | 901 | CLA  | CHC-C1C-NC  | -2.12 | 120.99      | 124.20   |
| 31  | 3     | 316 | CLA  | CHC-C1C-NC  | -2.12 | 120.99      | 124.20   |
| 31  | 3     | 307 | CLA  | C3D-C4D-CHA | -2.12 | 107.88      | 112.72   |
| 31  | b     | 313 | CLA  | C3D-C4D-CHA | -2.12 | 107.88      | 112.72   |
| 31  | B     | 836 | CLA  | CMD-C2D-C1D | 2.12  | 128.44      | 124.71   |
| 31  | 7     | 309 | CLA  | C3D-C4D-CHA | -2.12 | 107.88      | 112.72   |
| 31  | 6     | 314 | CLA  | CMD-C2D-C1D | 2.12  | 128.44      | 124.71   |
| 26  | K     | 203 | BCR  | C3-C4-C5    | -2.12 | 110.30      | 114.08   |
| 31  | a     | 322 | CLA  | C3D-C4D-CHA | -2.12 | 107.88      | 112.72   |
| 31  | 6     | 314 | CLA  | CAC-C3C-C4C | 2.12  | 127.56      | 124.81   |
| 28  | 6     | 305 | LHG  | C27-C26-C25 | -2.12 | 103.68      | 114.42   |
| 31  | K     | 204 | CLA  | C5-C3-C4    | 2.12  | 119.28      | 114.60   |
| 31  | b     | 311 | CLA  | C3D-C4D-CHA | -2.12 | 107.88      | 112.72   |
| 32  | a     | 317 | CHL  | C2C-C3C-C4C | -2.12 | 104.98      | 106.49   |
| 31  | A     | 835 | CLA  | O2A-CGA-CBA | 2.12  | 118.55      | 111.91   |
| 31  | A     | 843 | CLA  | CMD-C2D-C1D | 2.12  | 128.44      | 124.71   |
| 31  | B     | 823 | CLA  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 32  | 4     | 313 | CHL  | C1D-CHD-C4C | -2.11 | 121.50      | 126.06   |
| 26  | B     | 805 | BCR  | C29-C30-C25 | 2.11  | 113.74      | 110.48   |
| 31  | 6     | 307 | CLA  | C5-C3-C4    | 2.11  | 119.27      | 114.60   |
| 31  | 8     | 313 | CLA  | CMB-C2B-C3B | 2.11  | 128.63      | 124.68   |
| 28  | A     | 810 | LHG  | C27-C26-C25 | -2.11 | 103.69      | 114.42   |
| 31  | B     | 839 | CLA  | O2A-CGA-CBA | 2.11  | 118.54      | 111.91   |
| 26  | M     | 101 | BCR  | C16-C15-C14 | -2.11 | 119.14      | 123.47   |
| 31  | 3     | 312 | CLA  | CHC-C1C-NC  | -2.11 | 121.00      | 124.20   |
| 31  | 6     | 308 | CLA  | CHC-C1C-NC  | -2.11 | 121.00      | 124.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | L     | 305 | CLA  | CMC-C2C-C1C | 2.11  | 128.26      | 125.04   |
| 31  | A     | 834 | CLA  | C16-C15-C13 | -2.11 | 109.09      | 115.92   |
| 31  | B     | 828 | CLA  | O2A-CGA-CBA | 2.11  | 118.54      | 111.91   |
| 31  | b     | 312 | CLA  | C3D-C4D-CHA | -2.11 | 107.89      | 112.72   |
| 31  | A     | 837 | CLA  | CMC-C2C-C1C | 2.11  | 128.25      | 125.04   |
| 31  | A     | 833 | CLA  | CMB-C2B-C3B | 2.11  | 128.63      | 124.68   |
| 31  | 9     | 316 | CLA  | C3B-C4B-NB  | 2.11  | 111.94      | 109.21   |
| 32  | 7     | 320 | CHL  | C1-O2A-CGA  | 2.11  | 121.98      | 116.44   |
| 31  | A     | 853 | CLA  | C11-C10-C8  | -2.11 | 109.10      | 115.92   |
| 31  | 9     | 311 | CLA  | CBC-CAC-C3C | -2.11 | 106.61      | 112.43   |
| 36  | 8     | 303 | LUT  | C12-C13-C14 | -2.11 | 115.70      | 118.94   |
| 31  | 8     | 314 | CLA  | CED-O2D-CGD | 2.11  | 120.71      | 115.94   |
| 26  | B     | 806 | BCR  | C16-C15-C14 | -2.11 | 119.15      | 123.47   |
| 31  | 4     | 307 | CLA  | C2A-C1A-CHA | -2.11 | 120.17      | 123.86   |
| 32  | a     | 317 | CHL  | CMB-C2B-C3B | 2.11  | 128.62      | 124.68   |
| 31  | K     | 206 | CLA  | CMC-C2C-C1C | 2.11  | 128.25      | 125.04   |
| 31  | 4     | 307 | CLA  | C3D-C4D-CHA | -2.11 | 107.90      | 112.72   |
| 36  | 6     | 303 | LUT  | C36-C21-C26 | 2.11  | 112.74      | 109.55   |
| 26  | A     | 805 | BCR  | C15-C16-C17 | -2.11 | 119.16      | 123.47   |
| 31  | A     | 855 | CLA  | C1-O2A-CGA  | 2.11  | 121.97      | 116.44   |
| 32  | 6     | 318 | CHL  | CHC-C1C-NC  | -2.11 | 121.01      | 124.20   |
| 32  | 4     | 310 | CHL  | C3B-C4B-NB  | 2.11  | 111.93      | 109.21   |
| 31  | 7     | 322 | CLA  | O2A-CGA-CBA | 2.11  | 120.56      | 112.23   |
| 27  | A     | 808 | LMT  | O5B-C5B-C6B | 2.11  | 111.67      | 106.44   |
| 31  | A     | 817 | CLA  | CMD-C2D-C1D | 2.11  | 128.43      | 124.71   |
| 31  | 8     | 311 | CLA  | CED-O2D-CGD | 2.11  | 120.70      | 115.94   |
| 31  | B     | 819 | CLA  | C3D-C4D-CHA | -2.11 | 107.90      | 112.72   |
| 31  | 3     | 317 | CLA  | C3B-C4B-NB  | 2.11  | 111.93      | 109.21   |
| 31  | 8     | 318 | CLA  | CHC-C1C-NC  | -2.11 | 121.01      | 124.20   |
| 26  | 2     | 302 | BCR  | C24-C23-C22 | -2.11 | 123.05      | 126.23   |
| 31  | A     | 834 | CLA  | CMD-C2D-C1D | 2.11  | 128.42      | 124.71   |
| 31  | B     | 826 | CLA  | CMD-C2D-C1D | 2.11  | 128.42      | 124.71   |
| 31  | A     | 821 | CLA  | C11-C10-C8  | -2.11 | 109.11      | 115.92   |
| 26  | 5     | 302 | BCR  | C1-C6-C5    | -2.11 | 119.65      | 122.61   |
| 31  | A     | 841 | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 31  | B     | 819 | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 31  | 3     | 318 | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 32  | a     | 317 | CHL  | C4D-CHA-C1A | -2.10 | 118.69      | 121.25   |
| 31  | 8     | 309 | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 31  | B     | 816 | CLA  | C3B-C4B-NB  | 2.10  | 111.93      | 109.21   |
| 31  | a     | 315 | CLA  | C3B-C4B-NB  | 2.10  | 111.93      | 109.21   |
| 31  | b     | 303 | CLA  | C3B-C4B-NB  | 2.10  | 111.93      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | a     | 318 | CHL  | C3B-C4B-NB  | 2.10  | 111.93      | 109.21   |
| 32  | 4     | 313 | CHL  | C2C-C3C-C4C | -2.10 | 104.99      | 106.49   |
| 31  | a     | 321 | CLA  | CBC-CAC-C3C | -2.10 | 106.63      | 112.43   |
| 31  | A     | 851 | CLA  | O1D-CGD-CBD | -2.10 | 120.18      | 124.48   |
| 31  | B     | 837 | CLA  | C4D-C3D-CAD | 2.10  | 110.57      | 108.10   |
| 26  | G     | 203 | BCR  | C38-C26-C25 | -2.10 | 122.17      | 124.53   |
| 32  | 6     | 309 | CHL  | CMB-C2B-C3B | 2.10  | 128.61      | 124.68   |
| 31  | 9     | 311 | CLA  | O1D-CGD-CBD | -2.10 | 120.19      | 124.48   |
| 31  | A     | 816 | CLA  | CMD-C2D-C1D | 2.10  | 128.41      | 124.71   |
| 31  | 8     | 307 | CLA  | O2A-CGA-CBA | 2.10  | 120.53      | 112.23   |
| 31  | A     | 850 | CLA  | C1-O2A-CGA  | 2.10  | 121.95      | 116.44   |
| 32  | 7     | 319 | CHL  | C2C-C3C-C4C | -2.10 | 104.99      | 106.49   |
| 31  | a     | 322 | CLA  | O2A-CGA-CBA | 2.10  | 120.53      | 112.23   |
| 31  | a     | 321 | CLA  | CMC-C2C-C1C | 2.10  | 128.24      | 125.04   |
| 32  | 5     | 319 | CHL  | C2D-C1D-ND  | 2.10  | 111.65      | 110.10   |
| 31  | 8     | 309 | CLA  | C3C-C4C-NC  | 2.10  | 112.92      | 110.57   |
| 31  | 2     | 306 | CLA  | CHC-C1C-NC  | -2.10 | 121.02      | 124.20   |
| 31  | A     | 816 | CLA  | CHB-C4A-NA  | 2.10  | 127.41      | 124.51   |
| 31  | B     | 822 | CLA  | C6-C7-C8    | -2.10 | 109.14      | 115.92   |
| 31  | B     | 830 | CLA  | CMC-C2C-C1C | 2.10  | 128.23      | 125.04   |
| 31  | 5     | 323 | CLA  | CAC-C3C-C4C | 2.10  | 127.53      | 124.81   |
| 31  | 3     | 316 | CLA  | C5-C3-C4    | 2.10  | 119.23      | 114.60   |
| 31  | B     | 823 | CLA  | C1-C2-C3    | -2.10 | 122.42      | 126.04   |
| 32  | 6     | 320 | CHL  | O2A-CGA-CBA | 2.10  | 120.51      | 112.23   |
| 31  | 4     | 319 | CLA  | CMB-C2B-C3B | 2.10  | 128.60      | 124.68   |
| 31  | A     | 819 | CLA  | CHB-C4A-NA  | 2.09  | 127.41      | 124.51   |
| 36  | a     | 305 | LUT  | C16-C1-C6   | -2.09 | 106.90      | 110.30   |
| 31  | 7     | 311 | CLA  | CMD-C2D-C1D | 2.09  | 128.41      | 124.71   |
| 31  | O     | 203 | CLA  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 31  | b     | 308 | CLA  | C3D-C4D-CHA | -2.09 | 107.93      | 112.72   |
| 31  | 9     | 315 | CLA  | CED-O2D-CGD | 2.09  | 120.67      | 115.94   |
| 31  | 8     | 317 | CLA  | C5-C3-C4    | 2.09  | 119.23      | 114.60   |
| 31  | 8     | 314 | CLA  | C4C-C3C-C2C | -2.09 | 103.85      | 106.90   |
| 31  | A     | 842 | CLA  | CAC-C3C-C4C | 2.09  | 127.53      | 124.81   |
| 31  | B     | 819 | CLA  | C1D-CHD-C4C | -2.09 | 121.54      | 126.06   |
| 31  | A     | 853 | CLA  | CMC-C2C-C1C | 2.09  | 128.22      | 125.04   |
| 31  | A     | 832 | CLA  | C7-C6-C5    | -2.09 | 107.68      | 113.36   |
| 31  | 4     | 308 | CLA  | CMD-C2D-C1D | 2.09  | 128.40      | 124.71   |
| 31  | 5     | 323 | CLA  | CMD-C2D-C1D | 2.09  | 128.40      | 124.71   |
| 31  | 3     | 311 | CLA  | C1D-CHD-C4C | -2.09 | 121.55      | 126.06   |
| 31  | 7     | 312 | CLA  | C1-O2A-CGA  | 2.09  | 121.93      | 116.44   |
| 31  | 2     | 312 | CLA  | CMC-C2C-C1C | 2.09  | 128.22      | 125.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 830 | CLA  | O2A-CGA-CBA | 2.09  | 118.47      | 111.91   |
| 31  | A     | 823 | CLA  | CAC-C3C-C4C | 2.09  | 127.52      | 124.81   |
| 31  | 8     | 309 | CLA  | CAC-C3C-C4C | 2.09  | 127.52      | 124.81   |
| 31  | 2     | 304 | CLA  | CAC-C3C-C4C | 2.09  | 127.52      | 124.81   |
| 32  | b     | 309 | CHL  | CHA-C4D-ND  | 2.09  | 136.87      | 132.50   |
| 31  | L     | 307 | CLA  | CMC-C2C-C1C | 2.09  | 128.22      | 125.04   |
| 31  | A     | 851 | CLA  | CAC-C3C-C4C | 2.09  | 127.52      | 124.81   |
| 31  | G     | 204 | CLA  | CBA-CAA-C2A | -2.09 | 107.70      | 113.86   |
| 26  | K     | 202 | BCR  | C30-C25-C26 | -2.09 | 119.67      | 122.61   |
| 31  | b     | 313 | CLA  | CHC-C1C-NC  | -2.09 | 121.04      | 124.20   |
| 31  | 7     | 316 | CLA  | CED-O2D-CGD | 2.09  | 120.66      | 115.94   |
| 31  | a     | 316 | CLA  | CHB-C4A-NA  | 2.09  | 127.40      | 124.51   |
| 31  | B     | 811 | CLA  | C1-C2-C3    | -2.09 | 122.43      | 126.04   |
| 32  | 3     | 315 | CHL  | CHA-C4D-ND  | 2.09  | 136.86      | 132.50   |
| 26  | 3     | 301 | BCR  | C11-C10-C9  | -2.09 | 124.33      | 127.31   |
| 32  | 6     | 319 | CHL  | C4D-CHA-C1A | -2.09 | 118.71      | 121.25   |
| 31  | L     | 307 | CLA  | CMB-C2B-C3B | 2.09  | 128.58      | 124.68   |
| 31  | 2     | 308 | CLA  | O2A-CGA-O1A | -2.09 | 116.61      | 123.14   |
| 31  | b     | 303 | CLA  | C3D-C4D-CHA | -2.08 | 107.95      | 112.72   |
| 31  | A     | 814 | CLA  | CMC-C2C-C1C | 2.08  | 128.21      | 125.04   |
| 31  | 3     | 316 | CLA  | CAC-C3C-C4C | 2.08  | 127.52      | 124.81   |
| 31  | B     | 823 | CLA  | O2A-CGA-CBA | 2.08  | 118.45      | 111.91   |
| 31  | 6     | 310 | CLA  | O1D-CGD-CBD | -2.08 | 120.22      | 124.48   |
| 31  | 9     | 311 | CLA  | C2A-C1A-CHA | -2.08 | 120.22      | 123.86   |
| 31  | A     | 826 | CLA  | CHC-C1C-NC  | -2.08 | 121.04      | 124.20   |
| 31  | b     | 304 | CLA  | O2A-CGA-CBA | 2.08  | 120.46      | 112.23   |
| 31  | 6     | 306 | CLA  | C3B-C4B-NB  | 2.08  | 111.90      | 109.21   |
| 31  | 6     | 322 | CLA  | C1D-CHD-C4C | -2.08 | 121.56      | 126.06   |
| 31  | B     | 843 | CLA  | CMD-C2D-C1D | 2.08  | 128.38      | 124.71   |
| 31  | B     | 840 | CLA  | CMC-C2C-C1C | 2.08  | 128.21      | 125.04   |
| 31  | B     | 821 | CLA  | C3B-C4B-NB  | 2.08  | 111.90      | 109.21   |
| 31  | 7     | 310 | CLA  | C3D-C4D-CHA | -2.08 | 107.96      | 112.72   |
| 31  | 2     | 305 | CLA  | CMC-C2C-C1C | 2.08  | 128.21      | 125.04   |
| 26  | I     | 801 | BCR  | C38-C26-C27 | -2.08 | 109.62      | 113.62   |
| 31  | b     | 312 | CLA  | CMD-C2D-C1D | 2.08  | 128.38      | 124.71   |
| 31  | A     | 855 | CLA  | CBA-CAA-C2A | 2.08  | 120.00      | 113.86   |
| 31  | A     | 850 | CLA  | CHC-C1C-NC  | -2.08 | 121.05      | 124.20   |
| 31  | 2     | 314 | CLA  | CMD-C2D-C1D | 2.08  | 128.38      | 124.71   |
| 31  | B     | 824 | CLA  | C4C-C3C-C2C | -2.08 | 103.87      | 106.90   |
| 31  | 2     | 306 | CLA  | CMB-C2B-C3B | 2.08  | 128.57      | 124.68   |
| 31  | A     | 825 | CLA  | C4-C3-C5    | 2.08  | 118.77      | 115.27   |
| 31  | A     | 827 | CLA  | C4-C3-C5    | 2.08  | 118.77      | 115.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | O     | 203 | CLA  | C3D-C4D-CHA | -2.08 | 107.97      | 112.72   |
| 31  | A     | 819 | CLA  | C11-C10-C8  | -2.08 | 109.20      | 115.92   |
| 31  | 6     | 313 | CLA  | O2A-CGA-CBA | 2.08  | 120.44      | 112.23   |
| 32  | A     | 831 | CHL  | CHA-C4D-ND  | 2.08  | 136.84      | 132.50   |
| 31  | A     | 848 | CLA  | C3B-C4B-NB  | 2.08  | 111.89      | 109.21   |
| 31  | 6     | 316 | CLA  | C1B-CHB-C4A | -2.08 | 126.00      | 130.12   |
| 31  | B     | 841 | CLA  | CMC-C2C-C1C | 2.08  | 128.20      | 125.04   |
| 31  | 6     | 313 | CLA  | CED-O2D-CGD | 2.08  | 120.63      | 115.94   |
| 31  | 3     | 312 | CLA  | CHB-C4A-NA  | 2.08  | 127.38      | 124.51   |
| 31  | 3     | 320 | CLA  | C3D-C4D-CHA | -2.08 | 107.97      | 112.72   |
| 31  | A     | 827 | CLA  | C3B-C4B-NB  | 2.08  | 111.89      | 109.21   |
| 36  | 3     | 305 | LUT  | C35-C15-C14 | -2.08 | 119.22      | 123.47   |
| 31  | 5     | 308 | CLA  | CMD-C2D-C1D | 2.08  | 128.37      | 124.71   |
| 31  | 9     | 317 | CLA  | CMB-C2B-C3B | 2.07  | 128.56      | 124.68   |
| 31  | 7     | 315 | CLA  | C1D-CHD-C4C | -2.07 | 121.58      | 126.06   |
| 31  | A     | 824 | CLA  | C1-C2-C3    | -2.07 | 122.46      | 126.04   |
| 31  | 5     | 311 | CLA  | CBC-CAC-C3C | -2.07 | 106.72      | 112.43   |
| 31  | 2     | 310 | CLA  | CAC-C3C-C4C | 2.07  | 127.50      | 124.81   |
| 31  | B     | 820 | CLA  | C16-C15-C13 | -2.07 | 109.22      | 115.92   |
| 31  | B     | 846 | CLA  | C1D-CHD-C4C | -2.07 | 121.59      | 126.06   |
| 31  | a     | 314 | CLA  | CMB-C2B-C3B | 2.07  | 128.56      | 124.68   |
| 32  | 8     | 319 | CHL  | C2C-C3C-C4C | -2.07 | 105.01      | 106.49   |
| 31  | b     | 313 | CLA  | CMC-C2C-C1C | 2.07  | 128.19      | 125.04   |
| 31  | A     | 853 | CLA  | CAC-C3C-C4C | 2.07  | 127.50      | 124.81   |
| 31  | a     | 316 | CLA  | C3D-C4D-CHA | -2.07 | 107.99      | 112.72   |
| 31  | 3     | 313 | CLA  | O2A-CGA-O1A | -2.07 | 118.37      | 123.59   |
| 31  | 7     | 322 | CLA  | C4C-C3C-C2C | -2.07 | 103.88      | 106.90   |
| 32  | 4     | 310 | CHL  | CHA-C4D-ND  | 2.07  | 136.83      | 132.50   |
| 31  | A     | 849 | CLA  | C3B-C4B-NB  | 2.07  | 111.88      | 109.21   |
| 31  | H     | 902 | CLA  | O1D-CGD-CBD | -2.07 | 120.25      | 124.48   |
| 26  | L     | 302 | BCR  | C2-C1-C6    | 2.07  | 113.67      | 110.48   |
| 32  | 6     | 319 | CHL  | CMB-C2B-C3B | 2.07  | 128.55      | 124.68   |
| 31  | 5     | 313 | CLA  | C1D-ND-C4D  | -2.07 | 104.87      | 106.33   |
| 31  | 6     | 322 | CLA  | CAC-C3C-C4C | 2.07  | 127.49      | 124.81   |
| 31  | 7     | 310 | CLA  | CED-O2D-CGD | 2.07  | 120.61      | 115.94   |
| 31  | 2     | 315 | CLA  | CED-O2D-CGD | 2.07  | 120.61      | 115.94   |
| 31  | 4     | 308 | CLA  | C6-C5-C3    | -2.07 | 108.03      | 113.45   |
| 31  | A     | 826 | CLA  | CHB-C4A-NA  | 2.07  | 127.37      | 124.51   |
| 40  | 7     | 306 | XAT  | C28-C29-C30 | 2.07  | 122.11      | 118.94   |
| 31  | 4     | 307 | CLA  | CHC-C1C-NC  | -2.07 | 121.07      | 124.20   |
| 26  | A     | 806 | BCR  | C2-C1-C6    | 2.07  | 113.66      | 110.48   |
| 31  | B     | 823 | CLA  | C3B-C4B-NB  | 2.07  | 111.88      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 309 | CLA  | C6-C7-C8    | -2.07 | 109.24      | 115.92   |
| 31  | A     | 842 | CLA  | O2A-CGA-CBA | 2.07  | 118.39      | 111.91   |
| 31  | 7     | 321 | CLA  | C3B-C4B-NB  | 2.07  | 111.88      | 109.21   |
| 31  | a     | 319 | CLA  | CHB-C4A-NA  | 2.06  | 127.37      | 124.51   |
| 32  | 6     | 309 | CHL  | C3B-C4B-NB  | 2.06  | 111.88      | 109.21   |
| 31  | 3     | 316 | CLA  | O1D-CGD-CBD | -2.06 | 120.26      | 124.48   |
| 31  | 5     | 307 | CLA  | CMD-C2D-C1D | 2.06  | 128.35      | 124.71   |
| 26  | 5     | 302 | BCR  | C15-C16-C17 | -2.06 | 119.25      | 123.47   |
| 31  | A     | 857 | CLA  | CED-O2D-CGD | 2.06  | 120.61      | 115.94   |
| 32  | 9     | 320 | CHL  | CHA-C4D-ND  | 2.06  | 136.81      | 132.50   |
| 31  | B     | 819 | CLA  | CHC-C1C-NC  | -2.06 | 121.07      | 124.20   |
| 31  | 7     | 312 | CLA  | CHC-C1C-NC  | -2.06 | 121.07      | 124.20   |
| 32  | 6     | 317 | CHL  | C3B-C4B-NB  | 2.06  | 111.88      | 109.21   |
| 26  | B     | 804 | BCR  | C3-C4-C5    | -2.06 | 110.39      | 114.08   |
| 31  | 7     | 313 | CLA  | C3D-C4D-CHA | -2.06 | 108.00      | 112.72   |
| 31  | B     | 827 | CLA  | C1-C2-C3    | -2.06 | 122.48      | 126.04   |
| 31  | B     | 818 | CLA  | CHC-C1C-NC  | -2.06 | 121.08      | 124.20   |
| 26  | L     | 301 | BCR  | C40-C30-C25 | 2.06  | 113.64      | 110.30   |
| 31  | A     | 850 | CLA  | CHB-C4A-NA  | 2.06  | 127.36      | 124.51   |
| 31  | 3     | 312 | CLA  | C3D-C4D-CHA | -2.06 | 108.01      | 112.72   |
| 31  | B     | 830 | CLA  | CAC-C3C-C4C | 2.06  | 127.48      | 124.81   |
| 31  | 5     | 309 | CLA  | O1D-CGD-CBD | -2.06 | 120.27      | 124.48   |
| 31  | G     | 204 | CLA  | C3B-C4B-NB  | 2.06  | 111.87      | 109.21   |
| 31  | B     | 841 | CLA  | CMD-C2D-C1D | 2.06  | 128.34      | 124.71   |
| 26  | L     | 301 | BCR  | C27-C26-C25 | 2.06  | 125.72      | 122.73   |
| 32  | a     | 317 | CHL  | C1D-CHD-C4C | -2.06 | 121.61      | 126.06   |
| 31  | F     | 306 | CLA  | CHB-C4A-NA  | 2.06  | 127.36      | 124.51   |
| 31  | 5     | 312 | CLA  | C1D-CHD-C4C | -2.06 | 121.62      | 126.06   |
| 31  | B     | 841 | CLA  | C3C-C4C-NC  | 2.06  | 112.88      | 110.57   |
| 31  | 2     | 308 | CLA  | C4C-C3C-C2C | -2.06 | 103.90      | 106.90   |
| 31  | 2     | 313 | CLA  | O2A-CGA-CBA | 2.06  | 120.36      | 112.23   |
| 32  | 7     | 317 | CHL  | C6-C5-C3    | -2.06 | 108.06      | 113.45   |
| 31  | 8     | 312 | CLA  | C3D-C4D-CHA | -2.06 | 108.02      | 112.72   |
| 31  | 2     | 307 | CLA  | C3B-C4B-NB  | 2.06  | 111.87      | 109.21   |
| 31  | A     | 825 | CLA  | O1D-CGD-CBD | -2.06 | 120.28      | 124.48   |
| 31  | a     | 313 | CLA  | C3D-C4D-CHA | -2.06 | 108.02      | 112.72   |
| 31  | H     | 903 | CLA  | CMB-C2B-C3B | 2.06  | 128.53      | 124.68   |
| 33  | 7     | 308 | DGD  | CAB-C9B-C8B | -2.06 | 103.99      | 114.42   |
| 31  | 7     | 314 | CLA  | C3D-C4D-CHA | -2.06 | 108.02      | 112.72   |
| 31  | b     | 304 | CLA  | CED-O2D-CGD | 2.06  | 120.59      | 115.94   |
| 35  | F     | 303 | QTB  | C09-C02-C03 | 2.06  | 122.09      | 118.94   |
| 26  | B     | 806 | BCR  | C2-C1-C6    | 2.06  | 113.64      | 110.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | O     | 203 | CLA  | C1D-CHD-C4C | -2.06 | 121.62      | 126.06   |
| 31  | 2     | 312 | CLA  | CMB-C2B-C3B | 2.06  | 128.52      | 124.68   |
| 31  | A     | 847 | CLA  | CAC-C3C-C4C | 2.05  | 127.47      | 124.81   |
| 31  | 9     | 315 | CLA  | CHB-C4A-NA  | 2.05  | 127.35      | 124.51   |
| 37  | a     | 301 | LMG  | O3-C3-C2    | -2.05 | 105.60      | 110.35   |
| 31  | a     | 309 | CLA  | C3D-C4D-CHA | -2.05 | 108.03      | 112.72   |
| 31  | O     | 203 | CLA  | CAC-C3C-C4C | 2.05  | 127.47      | 124.81   |
| 31  | 4     | 306 | CLA  | CAC-C3C-C4C | 2.05  | 127.47      | 124.81   |
| 31  | A     | 830 | CLA  | C3B-C4B-NB  | 2.05  | 111.86      | 109.21   |
| 31  | A     | 822 | CLA  | C1D-CHD-C4C | -2.05 | 121.63      | 126.06   |
| 31  | B     | 832 | CLA  | C4D-C3D-CAD | 2.05  | 110.51      | 108.10   |
| 26  | 7     | 304 | BCR  | C29-C30-C25 | 2.05  | 113.64      | 110.48   |
| 36  | 2     | 301 | LUT  | C1-C2-C3    | 2.05  | 118.28      | 113.64   |
| 31  | A     | 847 | CLA  | CBC-CAC-C3C | -2.05 | 106.78      | 112.43   |
| 31  | 4     | 306 | CLA  | C2A-C1A-CHA | -2.05 | 120.27      | 123.86   |
| 31  | B     | 811 | CLA  | C3B-C4B-NB  | 2.05  | 111.86      | 109.21   |
| 31  | 7     | 321 | CLA  | C1D-CHD-C4C | -2.05 | 121.63      | 126.06   |
| 32  | 7     | 319 | CHL  | C1D-CHD-C4C | -2.05 | 121.63      | 126.06   |
| 31  | K     | 205 | CLA  | C3D-C4D-CHA | -2.05 | 108.03      | 112.72   |
| 31  | b     | 304 | CLA  | C3D-C4D-CHA | -2.05 | 108.03      | 112.72   |
| 31  | A     | 856 | CLA  | CAC-C3C-C4C | 2.05  | 127.47      | 124.81   |
| 31  | A     | 818 | CLA  | C4C-C3C-C2C | -2.05 | 103.91      | 106.90   |
| 27  | A     | 807 | LMT  | O5B-C5B-C6B | 2.05  | 111.53      | 106.44   |
| 31  | B     | 838 | CLA  | CMD-C2D-C1D | 2.05  | 128.32      | 124.71   |
| 33  | 7     | 308 | DGD  | C7B-C6B-C5B | -2.05 | 104.03      | 114.42   |
| 31  | 3     | 318 | CLA  | CAC-C3C-C4C | 2.05  | 127.47      | 124.81   |
| 31  | A     | 819 | CLA  | C1-C2-C3    | -2.05 | 122.50      | 126.04   |
| 31  | 8     | 317 | CLA  | O1D-CGD-CBD | -2.05 | 120.30      | 124.48   |
| 31  | B     | 827 | CLA  | C3D-C4D-CHA | -2.05 | 108.04      | 112.72   |
| 26  | A     | 803 | BCR  | C16-C15-C14 | -2.05 | 119.28      | 123.47   |
| 31  | A     | 845 | CLA  | C3B-C4B-NB  | 2.05  | 111.86      | 109.21   |
| 31  | 5     | 311 | CLA  | C1D-CHD-C4C | -2.05 | 121.64      | 126.06   |
| 32  | 7     | 318 | CHL  | C2C-C3C-C4C | -2.05 | 105.03      | 106.49   |
| 30  | A     | 813 | CL0  | O1D-CGD-CBD | -2.04 | 120.30      | 124.48   |
| 31  | A     | 833 | CLA  | CED-O2D-CGD | 2.04  | 120.56      | 115.94   |
| 31  | a     | 319 | CLA  | CMC-C2C-C1C | 2.04  | 128.15      | 125.04   |
| 32  | 7     | 317 | CHL  | CHA-C4D-ND  | 2.04  | 136.78      | 132.50   |
| 31  | K     | 206 | CLA  | CMD-C2D-C1D | 2.04  | 128.32      | 124.71   |
| 31  | B     | 830 | CLA  | CHB-C4A-NA  | 2.04  | 127.34      | 124.51   |
| 36  | 7     | 305 | LUT  | C8-C7-C6    | 2.04  | 132.94      | 127.20   |
| 32  | a     | 318 | CHL  | C2C-C3C-C4C | -2.04 | 105.03      | 106.49   |
| 31  | 2     | 314 | CLA  | C3B-C4B-NB  | 2.04  | 111.85      | 109.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | A     | 825 | CLA  | CAC-C3C-C4C | 2.04  | 127.46      | 124.81   |
| 31  | H     | 901 | CLA  | C3D-C4D-CHA | -2.04 | 108.05      | 112.72   |
| 31  | 2     | 310 | CLA  | C3D-C4D-CHA | -2.04 | 108.05      | 112.72   |
| 31  | 3     | 318 | CLA  | C3D-C4D-CHA | -2.04 | 108.05      | 112.72   |
| 26  | F     | 302 | BCR  | C38-C26-C27 | -2.04 | 109.69      | 113.62   |
| 31  | a     | 310 | CLA  | CMD-C2D-C1D | 2.04  | 128.31      | 124.71   |
| 31  | 6     | 322 | CLA  | CED-O2D-CGD | 2.04  | 120.55      | 115.94   |
| 31  | 3     | 316 | CLA  | C3B-C4B-NB  | 2.04  | 111.85      | 109.21   |
| 31  | 8     | 320 | CLA  | C1-O2A-CGA  | 2.04  | 121.80      | 116.44   |
| 31  | B     | 816 | CLA  | CBC-CAC-C3C | -2.04 | 106.81      | 112.43   |
| 31  | b     | 307 | CLA  | C3D-C4D-CHA | -2.04 | 108.06      | 112.72   |
| 31  | 8     | 315 | CLA  | C3D-C4D-CHA | -2.04 | 108.06      | 112.72   |
| 32  | 4     | 317 | CHL  | CMB-C2B-C3B | 2.04  | 128.49      | 124.68   |
| 26  | G     | 201 | BCR  | C38-C26-C27 | -2.04 | 109.70      | 113.62   |
| 28  | 7     | 307 | LHG  | C27-C26-C25 | -2.04 | 104.08      | 114.42   |
| 31  | 3     | 307 | CLA  | C4C-C3C-C2C | -2.04 | 103.93      | 106.90   |
| 31  | B     | 818 | CLA  | CMB-C2B-C3B | 2.04  | 128.49      | 124.68   |
| 32  | 4     | 310 | CHL  | C2C-C3C-C4C | -2.04 | 105.04      | 106.49   |
| 31  | L     | 306 | CLA  | CHC-C1C-NC  | -2.04 | 121.11      | 124.20   |
| 31  | A     | 851 | CLA  | C3B-C4B-NB  | 2.04  | 111.84      | 109.21   |
| 31  | 3     | 313 | CLA  | CAA-CBA-CGA | -2.04 | 107.30      | 113.25   |
| 31  | 6     | 313 | CLA  | C3D-C4D-CHA | -2.04 | 108.06      | 112.72   |
| 26  | A     | 805 | BCR  | C29-C30-C25 | 2.04  | 113.61      | 110.48   |
| 31  | 7     | 313 | CLA  | C1D-CHD-C4C | -2.04 | 121.67      | 126.06   |
| 31  | A     | 856 | CLA  | C3B-C4B-NB  | 2.04  | 111.84      | 109.21   |
| 31  | 8     | 320 | CLA  | C3B-C4B-NB  | 2.04  | 111.84      | 109.21   |
| 31  | B     | 837 | CLA  | C4C-C3C-C2C | -2.03 | 103.93      | 106.90   |
| 33  | B     | 808 | DGD  | CBB-CAB-C9B | -2.03 | 104.10      | 114.42   |
| 31  | 4     | 321 | CLA  | C3B-C4B-NB  | 2.03  | 111.84      | 109.21   |
| 31  | F     | 305 | CLA  | O2A-CGA-CBA | 2.03  | 120.27      | 112.23   |
| 31  | A     | 836 | CLA  | CMB-C2B-C3B | 2.03  | 128.48      | 124.68   |
| 32  | a     | 317 | CHL  | CMD-C2D-C1D | 2.03  | 128.30      | 124.71   |
| 31  | G     | 204 | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 31  | 8     | 313 | CLA  | CAC-C3C-C4C | 2.03  | 127.45      | 124.81   |
| 31  | A     | 835 | CLA  | CMC-C2C-C1C | 2.03  | 128.13      | 125.04   |
| 31  | a     | 311 | CLA  | C3B-C4B-NB  | 2.03  | 111.84      | 109.21   |
| 32  | A     | 839 | CHL  | CHA-C4D-ND  | 2.03  | 136.75      | 132.50   |
| 31  | A     | 849 | CLA  | O2A-CGA-CBA | 2.03  | 120.26      | 112.23   |
| 31  | A     | 830 | CLA  | CHC-C1C-NC  | -2.03 | 121.12      | 124.20   |
| 31  | A     | 822 | CLA  | CMC-C2C-C1C | 2.03  | 128.13      | 125.04   |
| 31  | 4     | 320 | CLA  | CMC-C2C-C1C | 2.03  | 128.13      | 125.04   |
| 31  | B     | 831 | CLA  | CAC-C3C-C4C | 2.03  | 127.45      | 124.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 5     | 318 | CLA  | CHB-C4A-NA  | 2.03  | 127.32      | 124.51   |
| 32  | 6     | 317 | CHL  | C2C-C3C-C4C | -2.03 | 105.04      | 106.49   |
| 31  | 7     | 310 | CLA  | CMD-C2D-C1D | 2.03  | 128.29      | 124.71   |
| 26  | 6     | 302 | BCR  | C33-C5-C6   | -2.03 | 122.25      | 124.53   |
| 31  | A     | 845 | CLA  | C3D-C4D-CHA | -2.03 | 108.08      | 112.72   |
| 32  | 7     | 324 | CHL  | O2A-CGA-O1A | -2.03 | 118.47      | 123.59   |
| 31  | b     | 302 | CLA  | C1D-CHD-C4C | -2.03 | 121.68      | 126.06   |
| 36  | a     | 303 | LUT  | C2-C3-C4    | 2.03  | 113.08      | 110.30   |
| 31  | 4     | 309 | CLA  | C3D-C4D-CHA | -2.03 | 108.08      | 112.72   |
| 31  | 7     | 312 | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 32  | 9     | 322 | CHL  | C3B-C4B-NB  | 2.03  | 111.83      | 109.21   |
| 31  | F     | 301 | CLA  | O2A-CGA-O1A | -2.03 | 118.47      | 123.59   |
| 36  | 6     | 303 | LUT  | C2-C3-C4    | 2.03  | 113.08      | 110.30   |
| 36  | 8     | 303 | LUT  | C3-C4-C5    | 2.03  | 115.89      | 111.85   |
| 31  | A     | 821 | CLA  | CAC-C3C-C4C | 2.03  | 127.44      | 124.81   |
| 31  | b     | 310 | CLA  | C3D-C4D-CHA | -2.03 | 108.08      | 112.72   |
| 26  | 2     | 302 | BCR  | C40-C30-C25 | 2.03  | 113.59      | 110.30   |
| 32  | a     | 317 | CHL  | C3B-C4B-NB  | 2.03  | 111.83      | 109.21   |
| 31  | 7     | 322 | CLA  | CHC-C1C-NC  | -2.03 | 121.13      | 124.20   |
| 31  | 5     | 307 | CLA  | O2A-CGA-O1A | -2.03 | 118.48      | 123.59   |
| 26  | B     | 802 | BCR  | C27-C26-C25 | 2.03  | 125.67      | 122.73   |
| 31  | 6     | 316 | CLA  | C3D-C4D-CHA | -2.03 | 108.09      | 112.72   |
| 31  | 5     | 310 | CLA  | C4C-C3C-C2C | -2.03 | 103.94      | 106.90   |
| 31  | 9     | 319 | CLA  | C1D-CHD-C4C | -2.03 | 121.69      | 126.06   |
| 32  | 7     | 324 | CHL  | C1D-CHD-C4C | -2.03 | 121.69      | 126.06   |
| 31  | 5     | 312 | CLA  | C3D-C4D-CHA | -2.03 | 108.09      | 112.72   |
| 32  | b     | 309 | CHL  | O2A-CGA-CBA | 2.03  | 120.24      | 112.23   |
| 31  | A     | 857 | CLA  | C6-C5-C3    | -2.03 | 108.14      | 113.45   |
| 31  | 6     | 311 | CLA  | CED-O2D-CGD | 2.03  | 120.52      | 115.94   |
| 31  | a     | 310 | CLA  | C3B-C4B-NB  | 2.03  | 111.83      | 109.21   |
| 31  | b     | 302 | CLA  | C3B-C4B-NB  | 2.03  | 111.83      | 109.21   |
| 31  | 8     | 309 | CLA  | CMB-C2B-C3B | 2.03  | 128.47      | 124.68   |
| 32  | 5     | 317 | CHL  | C1B-CHB-C4A | -2.02 | 126.11      | 130.12   |
| 31  | A     | 848 | CLA  | CED-O2D-CGD | 2.02  | 120.52      | 115.94   |
| 31  | B     | 821 | CLA  | CAC-C3C-C4C | 2.02  | 127.44      | 124.81   |
| 36  | 3     | 305 | LUT  | C1-C6-C7    | -2.02 | 110.05      | 115.78   |
| 31  | B     | 838 | CLA  | C3D-C4D-CHA | -2.02 | 108.09      | 112.72   |
| 31  | a     | 313 | CLA  | C3B-C4B-NB  | 2.02  | 111.83      | 109.21   |
| 32  | A     | 831 | CHL  | CMB-C2B-C3B | 2.02  | 128.47      | 124.68   |
| 26  | B     | 806 | BCR  | C30-C25-C26 | -2.02 | 119.76      | 122.61   |
| 31  | 8     | 315 | CLA  | CED-O2D-CGD | 2.02  | 120.51      | 115.94   |
| 31  | A     | 857 | CLA  | CMD-C2D-C1D | 2.02  | 128.28      | 124.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 828 | CLA  | CHC-C1C-NC  | -2.02 | 121.14      | 124.20   |
| 27  | 9     | 306 | LMT  | C1'-O5'-C5' | -2.02 | 109.72      | 113.69   |
| 31  | 8     | 318 | CLA  | C3B-C4B-NB  | 2.02  | 111.82      | 109.21   |
| 31  | B     | 831 | CLA  | C4C-C3C-C2C | -2.02 | 103.95      | 106.90   |
| 31  | 5     | 307 | CLA  | C4C-C3C-C2C | -2.02 | 103.95      | 106.90   |
| 26  | B     | 806 | BCR  | C10-C11-C12 | -2.02 | 116.91      | 123.22   |
| 32  | 5     | 322 | CHL  | O2A-CGA-CBA | 2.02  | 120.22      | 112.23   |
| 31  | A     | 844 | CLA  | C3D-C4D-CHA | -2.02 | 108.10      | 112.72   |
| 31  | G     | 204 | CLA  | C3D-C4D-CHA | -2.02 | 108.10      | 112.72   |
| 31  | 3     | 310 | CLA  | C1-O2A-CGA  | 2.02  | 121.74      | 116.44   |
| 31  | B     | 844 | CLA  | C3D-C4D-CHA | -2.02 | 108.10      | 112.72   |
| 31  | A     | 826 | CLA  | C1-C2-C3    | -2.02 | 122.55      | 126.04   |
| 31  | 8     | 318 | CLA  | C1D-CHD-C4C | -2.02 | 121.70      | 126.06   |
| 31  | a     | 314 | CLA  | C3D-C4D-CHA | -2.02 | 108.10      | 112.72   |
| 31  | 8     | 314 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 31  | 2     | 314 | CLA  | C3D-C4D-CHA | -2.02 | 108.10      | 112.72   |
| 31  | 5     | 310 | CLA  | C3D-C4D-CHA | -2.02 | 108.10      | 112.72   |
| 31  | 9     | 321 | CLA  | CMC-C2C-C1C | 2.02  | 128.11      | 125.04   |
| 31  | 7     | 314 | CLA  | CMD-C2D-C1D | 2.02  | 128.27      | 124.71   |
| 31  | A     | 837 | CLA  | CMB-C2B-C3B | 2.02  | 128.45      | 124.68   |
| 31  | B     | 840 | CLA  | C4-C3-C5    | 2.02  | 118.67      | 115.27   |
| 31  | a     | 319 | CLA  | C6-C5-C3    | -2.02 | 108.16      | 113.45   |
| 32  | A     | 839 | CHL  | O2A-C1-C2   | -2.02 | 103.33      | 108.64   |
| 31  | F     | 305 | CLA  | C3B-C4B-NB  | 2.02  | 111.82      | 109.21   |
| 32  | 6     | 319 | CHL  | C3B-C4B-NB  | 2.02  | 111.82      | 109.21   |
| 31  | a     | 314 | CLA  | CMC-C2C-C1C | 2.02  | 128.11      | 125.04   |
| 31  | B     | 845 | CLA  | CHB-C4A-NA  | 2.02  | 127.30      | 124.51   |
| 32  | 9     | 322 | CHL  | CHB-C4A-NA  | 2.02  | 127.30      | 124.51   |
| 31  | 4     | 307 | CLA  | CED-O2D-CGD | 2.02  | 120.50      | 115.94   |
| 31  | 6     | 315 | CLA  | C3D-C4D-CHA | -2.02 | 108.11      | 112.72   |
| 31  | G     | 205 | CLA  | CAC-C3C-C4C | 2.02  | 127.43      | 124.81   |
| 31  | B     | 830 | CLA  | C6-C5-C3    | -2.02 | 108.17      | 113.45   |
| 31  | A     | 830 | CLA  | C4C-C3C-C2C | -2.02 | 103.96      | 106.90   |
| 31  | A     | 843 | CLA  | C4C-C3C-C2C | -2.02 | 103.96      | 106.90   |
| 31  | b     | 302 | CLA  | CED-O2D-CGD | 2.02  | 120.50      | 115.94   |
| 31  | 8     | 315 | CLA  | CHC-C1C-NC  | -2.02 | 121.14      | 124.20   |
| 31  | A     | 846 | CLA  | C16-C15-C13 | -2.02 | 109.40      | 115.92   |
| 31  | b     | 305 | CLA  | O2A-CGA-CBA | 2.02  | 120.19      | 112.23   |
| 31  | a     | 322 | CLA  | O1D-CGD-CBD | -2.02 | 120.36      | 124.48   |
| 31  | 4     | 320 | CLA  | C3D-C4D-CHA | -2.01 | 108.11      | 112.72   |
| 31  | 5     | 307 | CLA  | C3D-C4D-CHA | -2.01 | 108.11      | 112.72   |
| 31  | A     | 841 | CLA  | C1D-CHD-C4C | -2.01 | 121.71      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | 3     | 316 | CLA  | C4C-C3C-C2C | -2.01 | 103.96      | 106.90   |
| 31  | H     | 903 | CLA  | CED-O2D-CGD | 2.01  | 120.49      | 115.94   |
| 31  | B     | 820 | CLA  | C3D-C4D-CHA | -2.01 | 108.12      | 112.72   |
| 31  | A     | 829 | CLA  | C3D-C4D-CHA | -2.01 | 108.12      | 112.72   |
| 31  | 9     | 313 | CLA  | C3D-C4D-CHA | -2.01 | 108.12      | 112.72   |
| 26  | L     | 303 | BCR  | C3-C4-C5    | -2.01 | 110.48      | 114.08   |
| 26  | A     | 806 | BCR  | C10-C11-C12 | -2.01 | 116.94      | 123.22   |
| 31  | A     | 832 | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 31  | 9     | 317 | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 26  | L     | 302 | BCR  | C33-C5-C6   | -2.01 | 122.27      | 124.53   |
| 31  | 5     | 318 | CLA  | CHC-C1C-NC  | -2.01 | 121.15      | 124.20   |
| 27  | 9     | 306 | LMT  | O5B-C5B-C6B | 2.01  | 111.44      | 106.44   |
| 31  | 8     | 308 | CLA  | C3B-C4B-NB  | 2.01  | 111.81      | 109.21   |
| 31  | 9     | 311 | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 31  | B     | 837 | CLA  | C1-C2-C3    | -2.01 | 122.57      | 126.04   |
| 31  | 5     | 310 | CLA  | C1D-CHD-C4C | -2.01 | 121.72      | 126.06   |
| 31  | b     | 302 | CLA  | C3D-C4D-CHA | -2.01 | 108.13      | 112.72   |
| 30  | A     | 813 | CL0  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 32  | 6     | 321 | CHL  | CMD-C2D-C1D | 2.01  | 128.25      | 124.71   |
| 31  | B     | 842 | CLA  | CHC-C1C-NC  | -2.01 | 121.16      | 124.20   |
| 31  | 2     | 309 | CLA  | O2A-CGA-CBA | 2.01  | 120.17      | 112.23   |
| 31  | 3     | 308 | CLA  | CHB-C4A-NA  | 2.01  | 127.29      | 124.51   |
| 31  | A     | 855 | CLA  | CMD-C2D-C1D | 2.01  | 128.25      | 124.71   |
| 31  | 6     | 310 | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 31  | A     | 844 | CLA  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 32  | 6     | 318 | CHL  | CAC-C3C-C4C | 2.01  | 127.42      | 124.81   |
| 31  | B     | 833 | CLA  | O2A-CGA-CBA | 2.01  | 118.21      | 111.91   |
| 31  | B     | 836 | CLA  | C4C-C3C-C2C | -2.01 | 103.97      | 106.90   |
| 31  | A     | 828 | CLA  | C7-C6-C5    | -2.01 | 107.91      | 113.36   |
| 31  | B     | 843 | CLA  | CMB-C2B-C1B | -2.01 | 125.38      | 128.46   |
| 31  | 4     | 316 | CLA  | C3C-C4C-NC  | 2.01  | 112.82      | 110.57   |
| 31  | a     | 319 | CLA  | C6-C7-C8    | -2.01 | 109.43      | 115.92   |
| 31  | A     | 832 | CLA  | C1-O2A-CGA  | 2.01  | 121.71      | 116.44   |
| 31  | B     | 838 | CLA  | CMC-C2C-C1C | 2.01  | 128.09      | 125.04   |
| 31  | B     | 813 | CLA  | CHB-C4A-NA  | 2.01  | 127.29      | 124.51   |
| 31  | 8     | 311 | CLA  | C1-C2-C3    | -2.01 | 122.57      | 126.04   |
| 31  | 7     | 312 | CLA  | C3B-C4B-NB  | 2.01  | 111.80      | 109.21   |
| 31  | 5     | 323 | CLA  | C3B-C4B-NB  | 2.01  | 111.80      | 109.21   |
| 31  | a     | 321 | CLA  | CAC-C3C-C4C | 2.01  | 127.41      | 124.81   |
| 31  | 3     | 309 | CLA  | C3D-C4D-CHA | -2.01 | 108.14      | 112.72   |
| 32  | a     | 317 | CHL  | C2A-C1A-CHA | -2.01 | 120.35      | 123.86   |
| 31  | 7     | 322 | CLA  | C3D-C4D-CHA | -2.00 | 108.14      | 112.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | B     | 824 | CLA  | CHC-C1C-NC  | -2.00 | 121.16      | 124.20   |
| 31  | 4     | 319 | CLA  | C1D-CHD-C4C | -2.00 | 121.73      | 126.06   |
| 31  | 3     | 308 | CLA  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 31  | 4     | 318 | CLA  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 31  | F     | 305 | CLA  | C3D-C4D-CHA | -2.00 | 108.14      | 112.72   |
| 31  | F     | 305 | CLA  | CMB-C2B-C3B | 2.00  | 128.43      | 124.68   |
| 31  | 4     | 319 | CLA  | C3D-C4D-CHA | -2.00 | 108.14      | 112.72   |
| 32  | 5     | 322 | CHL  | CHA-C4D-ND  | 2.00  | 136.69      | 132.50   |
| 32  | 6     | 321 | CHL  | CHA-C4D-ND  | 2.00  | 136.69      | 132.50   |
| 31  | H     | 901 | CLA  | C4C-C3C-C2C | -2.00 | 103.98      | 106.90   |
| 31  | 3     | 309 | CLA  | C1-O2A-CGA  | 2.00  | 121.70      | 116.44   |
| 31  | 5     | 314 | CLA  | C3D-C4D-CHA | -2.00 | 108.14      | 112.72   |
| 32  | 6     | 309 | CHL  | CHA-C4D-ND  | 2.00  | 136.69      | 132.50   |
| 31  | L     | 305 | CLA  | O2A-CGA-CBA | 2.00  | 118.19      | 111.91   |
| 31  | A     | 817 | CLA  | C1-C2-C3    | -2.00 | 122.58      | 126.04   |
| 33  | 7     | 308 | DGD  | CBB-CAB-C9B | -2.00 | 104.26      | 114.42   |
| 31  | B     | 837 | CLA  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 36  | F     | 304 | LUT  | C3-C4-C5    | 2.00  | 115.84      | 111.85   |
| 31  | a     | 321 | CLA  | CHC-C1C-NC  | -2.00 | 121.17      | 124.20   |
| 31  | 8     | 318 | CLA  | CHB-C4A-NA  | 2.00  | 127.28      | 124.51   |
| 31  | 2     | 311 | CLA  | C3D-C4D-CHA | -2.00 | 108.14      | 112.72   |
| 32  | 8     | 319 | CHL  | CMB-C2B-C3B | 2.00  | 128.42      | 124.68   |
| 31  | 8     | 314 | CLA  | C3D-C4D-CHA | -2.00 | 108.14      | 112.72   |
| 31  | 2     | 305 | CLA  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 32  | 7     | 320 | CHL  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 31  | 3     | 309 | CLA  | CHB-C4A-NA  | 2.00  | 127.28      | 124.51   |
| 31  | 4     | 318 | CLA  | CHC-C1C-NC  | -2.00 | 121.17      | 124.20   |
| 31  | 7     | 313 | CLA  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 32  | 5     | 322 | CHL  | C3B-C4B-NB  | 2.00  | 111.80      | 109.21   |
| 31  | 4     | 315 | CLA  | CED-O2D-CGD | 2.00  | 120.46      | 115.94   |
| 31  | 4     | 319 | CLA  | CED-O2D-CGD | 2.00  | 120.46      | 115.94   |
| 31  | J     | 105 | CLA  | CAC-C3C-C4C | 2.00  | 127.41      | 124.81   |
| 31  | 3     | 314 | CLA  | CAC-C3C-C4C | 2.00  | 127.41      | 124.81   |
| 31  | 9     | 314 | CLA  | CAC-C3C-C4C | 2.00  | 127.41      | 124.81   |
| 31  | a     | 309 | CLA  | C4C-C3C-C2C | -2.00 | 103.98      | 106.90   |
| 31  | a     | 322 | CLA  | CHC-C1C-NC  | -2.00 | 121.17      | 124.20   |

All (223) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30  | A     | 813 | CL0  | NC   |
| 31  | A     | 814 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | A     | 816 | CLA  | ND   |
| 31  | A     | 817 | CLA  | ND   |
| 31  | A     | 818 | CLA  | ND   |
| 31  | A     | 819 | CLA  | ND   |
| 31  | A     | 821 | CLA  | ND   |
| 31  | A     | 824 | CLA  | ND   |
| 31  | A     | 826 | CLA  | ND   |
| 31  | A     | 834 | CLA  | ND   |
| 31  | A     | 838 | CLA  | ND   |
| 31  | A     | 841 | CLA  | ND   |
| 31  | A     | 849 | CLA  | ND   |
| 31  | A     | 850 | CLA  | ND   |
| 31  | A     | 851 | CLA  | ND   |
| 31  | A     | 854 | CLA  | ND   |
| 31  | A     | 856 | CLA  | ND   |
| 31  | A     | 857 | CLA  | ND   |
| 31  | B     | 811 | CLA  | ND   |
| 31  | B     | 812 | CLA  | ND   |
| 31  | B     | 814 | CLA  | ND   |
| 31  | B     | 815 | CLA  | ND   |
| 31  | B     | 817 | CLA  | ND   |
| 31  | B     | 818 | CLA  | ND   |
| 31  | B     | 819 | CLA  | ND   |
| 31  | B     | 822 | CLA  | ND   |
| 31  | B     | 823 | CLA  | ND   |
| 31  | B     | 827 | CLA  | ND   |
| 31  | B     | 828 | CLA  | ND   |
| 31  | B     | 832 | CLA  | ND   |
| 31  | B     | 833 | CLA  | ND   |
| 31  | B     | 834 | CLA  | ND   |
| 31  | B     | 835 | CLA  | ND   |
| 31  | B     | 840 | CLA  | ND   |
| 31  | B     | 842 | CLA  | ND   |
| 31  | B     | 843 | CLA  | ND   |
| 31  | B     | 844 | CLA  | ND   |
| 31  | B     | 848 | CLA  | ND   |
| 31  | B     | 849 | CLA  | ND   |
| 31  | F     | 301 | CLA  | ND   |
| 31  | F     | 305 | CLA  | ND   |
| 31  | F     | 306 | CLA  | ND   |
| 31  | G     | 204 | CLA  | ND   |
| 31  | G     | 205 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | G     | 206 | CLA  | ND   |
| 31  | H     | 901 | CLA  | ND   |
| 31  | H     | 902 | CLA  | ND   |
| 31  | J     | 105 | CLA  | ND   |
| 31  | K     | 205 | CLA  | ND   |
| 31  | a     | 309 | CLA  | ND   |
| 31  | a     | 310 | CLA  | ND   |
| 31  | a     | 311 | CLA  | ND   |
| 31  | a     | 312 | CLA  | ND   |
| 31  | a     | 313 | CLA  | ND   |
| 31  | a     | 314 | CLA  | ND   |
| 31  | a     | 315 | CLA  | ND   |
| 31  | a     | 319 | CLA  | ND   |
| 31  | a     | 322 | CLA  | ND   |
| 31  | 3     | 307 | CLA  | ND   |
| 31  | 3     | 308 | CLA  | ND   |
| 31  | 3     | 309 | CLA  | ND   |
| 31  | 3     | 310 | CLA  | ND   |
| 31  | 3     | 311 | CLA  | ND   |
| 31  | 3     | 312 | CLA  | ND   |
| 31  | 3     | 313 | CLA  | ND   |
| 31  | 3     | 316 | CLA  | ND   |
| 31  | 3     | 317 | CLA  | ND   |
| 31  | 3     | 319 | CLA  | ND   |
| 31  | 3     | 320 | CLA  | ND   |
| 31  | 7     | 309 | CLA  | ND   |
| 31  | 7     | 310 | CLA  | ND   |
| 31  | 7     | 312 | CLA  | ND   |
| 31  | 7     | 313 | CLA  | ND   |
| 31  | 7     | 315 | CLA  | ND   |
| 31  | 7     | 316 | CLA  | ND   |
| 31  | 7     | 322 | CLA  | ND   |
| 31  | 8     | 307 | CLA  | ND   |
| 31  | 8     | 308 | CLA  | ND   |
| 31  | 8     | 309 | CLA  | ND   |
| 31  | 8     | 310 | CLA  | ND   |
| 31  | 8     | 311 | CLA  | ND   |
| 31  | 8     | 312 | CLA  | ND   |
| 31  | 8     | 313 | CLA  | ND   |
| 31  | 8     | 314 | CLA  | ND   |
| 31  | 8     | 315 | CLA  | ND   |
| 31  | 8     | 318 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | 8     | 321 | CLA  | ND   |
| 31  | 9     | 311 | CLA  | ND   |
| 31  | 9     | 312 | CLA  | ND   |
| 31  | 9     | 313 | CLA  | ND   |
| 31  | 9     | 314 | CLA  | ND   |
| 31  | 9     | 315 | CLA  | ND   |
| 31  | 9     | 316 | CLA  | ND   |
| 31  | 9     | 318 | CLA  | ND   |
| 31  | 9     | 321 | CLA  | ND   |
| 31  | L     | 307 | CLA  | ND   |
| 31  | O     | 202 | CLA  | ND   |
| 31  | O     | 203 | CLA  | ND   |
| 31  | O     | 204 | CLA  | ND   |
| 31  | b     | 302 | CLA  | ND   |
| 31  | b     | 303 | CLA  | ND   |
| 31  | b     | 304 | CLA  | ND   |
| 31  | b     | 305 | CLA  | ND   |
| 31  | b     | 307 | CLA  | ND   |
| 31  | b     | 310 | CLA  | ND   |
| 31  | b     | 311 | CLA  | ND   |
| 31  | b     | 313 | CLA  | ND   |
| 31  | 2     | 305 | CLA  | ND   |
| 31  | 2     | 306 | CLA  | ND   |
| 31  | 2     | 307 | CLA  | ND   |
| 31  | 2     | 308 | CLA  | ND   |
| 31  | 2     | 310 | CLA  | ND   |
| 31  | 2     | 311 | CLA  | ND   |
| 31  | 2     | 312 | CLA  | ND   |
| 31  | 2     | 313 | CLA  | ND   |
| 31  | 2     | 314 | CLA  | ND   |
| 31  | 2     | 315 | CLA  | ND   |
| 31  | 4     | 306 | CLA  | ND   |
| 31  | 4     | 307 | CLA  | ND   |
| 31  | 4     | 308 | CLA  | ND   |
| 31  | 4     | 309 | CLA  | ND   |
| 31  | 4     | 311 | CLA  | ND   |
| 31  | 4     | 312 | CLA  | ND   |
| 31  | 4     | 314 | CLA  | ND   |
| 31  | 4     | 315 | CLA  | ND   |
| 31  | 4     | 318 | CLA  | ND   |
| 31  | 4     | 319 | CLA  | ND   |
| 31  | 4     | 320 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | 4     | 321 | CLA  | ND   |
| 31  | 5     | 307 | CLA  | ND   |
| 31  | 5     | 308 | CLA  | ND   |
| 31  | 5     | 310 | CLA  | ND   |
| 31  | 5     | 311 | CLA  | ND   |
| 31  | 5     | 312 | CLA  | ND   |
| 31  | 5     | 315 | CLA  | ND   |
| 31  | 5     | 318 | CLA  | ND   |
| 31  | 5     | 323 | CLA  | ND   |
| 31  | 6     | 307 | CLA  | ND   |
| 31  | 6     | 308 | CLA  | ND   |
| 31  | 6     | 310 | CLA  | ND   |
| 31  | 6     | 311 | CLA  | ND   |
| 31  | 6     | 312 | CLA  | ND   |
| 31  | 6     | 313 | CLA  | ND   |
| 31  | 6     | 315 | CLA  | ND   |
| 31  | 6     | 316 | CLA  | ND   |
| 32  | A     | 831 | CHL  | NA   |
| 32  | A     | 831 | CHL  | NC   |
| 32  | A     | 839 | CHL  | NA   |
| 32  | A     | 839 | CHL  | NC   |
| 32  | A     | 840 | CHL  | NA   |
| 32  | A     | 840 | CHL  | ND   |
| 32  | K     | 201 | CHL  | NA   |
| 32  | K     | 201 | CHL  | ND   |
| 32  | K     | 201 | CHL  | NC   |
| 32  | a     | 317 | CHL  | NA   |
| 32  | a     | 317 | CHL  | NC   |
| 32  | a     | 318 | CHL  | NA   |
| 32  | a     | 318 | CHL  | NC   |
| 32  | a     | 320 | CHL  | NA   |
| 32  | a     | 320 | CHL  | ND   |
| 32  | a     | 320 | CHL  | NC   |
| 32  | 3     | 315 | CHL  | NA   |
| 32  | 3     | 315 | CHL  | NC   |
| 32  | 7     | 317 | CHL  | NA   |
| 32  | 7     | 317 | CHL  | ND   |
| 32  | 7     | 317 | CHL  | NC   |
| 32  | 7     | 318 | CHL  | NA   |
| 32  | 7     | 318 | CHL  | ND   |
| 32  | 7     | 318 | CHL  | NC   |
| 32  | 7     | 319 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | 7     | 319 | CHL  | ND   |
| 32  | 7     | 319 | CHL  | NC   |
| 32  | 7     | 320 | CHL  | NA   |
| 32  | 7     | 320 | CHL  | ND   |
| 32  | 7     | 320 | CHL  | NC   |
| 32  | 7     | 324 | CHL  | NA   |
| 32  | 7     | 324 | CHL  | NC   |
| 32  | 8     | 316 | CHL  | NA   |
| 32  | 8     | 316 | CHL  | ND   |
| 32  | 8     | 316 | CHL  | NC   |
| 32  | 8     | 319 | CHL  | NA   |
| 32  | 8     | 319 | CHL  | ND   |
| 32  | 8     | 319 | CHL  | NC   |
| 32  | 9     | 320 | CHL  | NA   |
| 32  | 9     | 320 | CHL  | ND   |
| 32  | 9     | 320 | CHL  | NC   |
| 32  | 9     | 322 | CHL  | NA   |
| 32  | 9     | 322 | CHL  | ND   |
| 32  | 9     | 322 | CHL  | NC   |
| 32  | b     | 309 | CHL  | NA   |
| 32  | b     | 309 | CHL  | NC   |
| 32  | 4     | 310 | CHL  | NA   |
| 32  | 4     | 310 | CHL  | NC   |
| 32  | 4     | 313 | CHL  | NA   |
| 32  | 4     | 313 | CHL  | NC   |
| 32  | 4     | 317 | CHL  | NA   |
| 32  | 4     | 317 | CHL  | ND   |
| 32  | 4     | 317 | CHL  | NC   |
| 32  | 5     | 316 | CHL  | NA   |
| 32  | 5     | 316 | CHL  | ND   |
| 32  | 5     | 316 | CHL  | NC   |
| 32  | 5     | 317 | CHL  | NA   |
| 32  | 5     | 317 | CHL  | NC   |
| 32  | 5     | 319 | CHL  | NA   |
| 32  | 5     | 319 | CHL  | NC   |
| 32  | 5     | 322 | CHL  | NA   |
| 32  | 5     | 322 | CHL  | ND   |
| 32  | 5     | 322 | CHL  | NC   |
| 32  | 6     | 309 | CHL  | NA   |
| 32  | 6     | 309 | CHL  | ND   |
| 32  | 6     | 309 | CHL  | NC   |
| 32  | 6     | 317 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 32  | 6     | 317 | CHL  | NC   |
| 32  | 6     | 318 | CHL  | NA   |
| 32  | 6     | 318 | CHL  | ND   |
| 32  | 6     | 318 | CHL  | NC   |
| 32  | 6     | 319 | CHL  | NC   |
| 32  | 6     | 320 | CHL  | NA   |
| 32  | 6     | 320 | CHL  | ND   |
| 32  | 6     | 320 | CHL  | NC   |
| 32  | 6     | 321 | CHL  | NA   |
| 32  | 6     | 321 | CHL  | ND   |
| 32  | 6     | 321 | CHL  | NC   |

All (2779) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | A     | 804 | BCR  | C7-C8-C9-C10    |
| 26  | A     | 804 | BCR  | C7-C8-C9-C34    |
| 26  | A     | 804 | BCR  | C20-C21-C22-C23 |
| 26  | A     | 805 | BCR  | C7-C8-C9-C34    |
| 26  | A     | 805 | BCR  | C20-C21-C22-C37 |
| 26  | A     | 806 | BCR  | C21-C22-C23-C24 |
| 26  | A     | 806 | BCR  | C37-C22-C23-C24 |
| 26  | B     | 802 | BCR  | C7-C8-C9-C34    |
| 26  | B     | 802 | BCR  | C21-C22-C23-C24 |
| 26  | B     | 802 | BCR  | C37-C22-C23-C24 |
| 26  | B     | 803 | BCR  | C7-C8-C9-C10    |
| 26  | B     | 803 | BCR  | C11-C10-C9-C8   |
| 26  | B     | 805 | BCR  | C7-C8-C9-C34    |
| 26  | B     | 805 | BCR  | C23-C24-C25-C30 |
| 26  | F     | 302 | BCR  | C7-C8-C9-C10    |
| 26  | F     | 302 | BCR  | C7-C8-C9-C34    |
| 26  | F     | 302 | BCR  | C37-C22-C23-C24 |
| 26  | G     | 201 | BCR  | C7-C8-C9-C10    |
| 26  | G     | 201 | BCR  | C7-C8-C9-C34    |
| 26  | G     | 201 | BCR  | C21-C22-C23-C24 |
| 26  | G     | 201 | BCR  | C37-C22-C23-C24 |
| 26  | G     | 203 | BCR  | C1-C6-C7-C8     |
| 26  | G     | 203 | BCR  | C18-C19-C20-C21 |
| 26  | G     | 203 | BCR  | C20-C21-C22-C37 |
| 26  | G     | 203 | BCR  | C21-C22-C23-C24 |
| 26  | G     | 203 | BCR  | C37-C22-C23-C24 |
| 26  | G     | 203 | BCR  | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | I     | 801 | BCR  | C1-C6-C7-C8     |
| 26  | I     | 801 | BCR  | C7-C8-C9-C34    |
| 26  | J     | 102 | BCR  | C7-C8-C9-C10    |
| 26  | J     | 102 | BCR  | C7-C8-C9-C34    |
| 26  | K     | 202 | BCR  | C7-C8-C9-C10    |
| 26  | K     | 202 | BCR  | C23-C24-C25-C26 |
| 26  | K     | 202 | BCR  | C23-C24-C25-C30 |
| 26  | K     | 203 | BCR  | C23-C24-C25-C30 |
| 26  | M     | 101 | BCR  | C7-C8-C9-C34    |
| 26  | M     | 101 | BCR  | C23-C24-C25-C30 |
| 26  | 3     | 301 | BCR  | C1-C6-C7-C8     |
| 26  | 3     | 301 | BCR  | C7-C8-C9-C10    |
| 26  | 3     | 301 | BCR  | C23-C24-C25-C30 |
| 26  | 3     | 302 | BCR  | C1-C6-C7-C8     |
| 26  | 3     | 303 | BCR  | C7-C8-C9-C10    |
| 26  | 7     | 304 | BCR  | C20-C21-C22-C23 |
| 26  | 7     | 304 | BCR  | C20-C21-C22-C37 |
| 26  | 8     | 301 | BCR  | C20-C21-C22-C37 |
| 26  | 8     | 301 | BCR  | C23-C24-C25-C30 |
| 26  | L     | 301 | BCR  | C7-C8-C9-C10    |
| 26  | L     | 301 | BCR  | C7-C8-C9-C34    |
| 26  | L     | 301 | BCR  | C21-C22-C23-C24 |
| 26  | L     | 301 | BCR  | C37-C22-C23-C24 |
| 26  | L     | 301 | BCR  | C23-C24-C25-C26 |
| 26  | L     | 301 | BCR  | C23-C24-C25-C30 |
| 26  | L     | 302 | BCR  | C1-C6-C7-C8     |
| 26  | L     | 302 | BCR  | C11-C10-C9-C34  |
| 26  | L     | 303 | BCR  | C17-C18-C19-C20 |
| 26  | L     | 303 | BCR  | C23-C24-C25-C30 |
| 26  | 2     | 302 | BCR  | C6-C7-C8-C9     |
| 26  | 5     | 302 | BCR  | C6-C7-C8-C9     |
| 26  | 5     | 302 | BCR  | C7-C8-C9-C34    |
| 26  | 5     | 302 | BCR  | C11-C10-C9-C8   |
| 26  | 5     | 302 | BCR  | C17-C18-C19-C20 |
| 26  | 5     | 302 | BCR  | C18-C19-C20-C21 |
| 26  | 5     | 302 | BCR  | C20-C21-C22-C23 |
| 26  | 5     | 302 | BCR  | C20-C21-C22-C37 |
| 26  | 5     | 302 | BCR  | C21-C22-C23-C24 |
| 26  | 5     | 302 | BCR  | C23-C24-C25-C30 |
| 26  | 6     | 302 | BCR  | C1-C6-C7-C8     |
| 26  | 6     | 302 | BCR  | C11-C12-C13-C14 |
| 27  | 9     | 306 | LMT  | C2'-C1'-O1'-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | 9     | 306 | LMT  | O5'-C1'-O1'-C1  |
| 27  | 5     | 301 | LMT  | C2-C1-O1'-C1'   |
| 28  | A     | 809 | LHG  | O1-C1-C2-C3     |
| 28  | A     | 809 | LHG  | C3-O3-P-O4      |
| 28  | A     | 810 | LHG  | O9-C7-O7-C5     |
| 28  | A     | 811 | LHG  | C3-O3-P-O5      |
| 28  | a     | 306 | LHG  | C4-O6-P-O4      |
| 28  | 7     | 302 | LHG  | C4-O6-P-O3      |
| 28  | 7     | 302 | LHG  | O9-C7-O7-C5     |
| 28  | 7     | 307 | LHG  | C4-O6-P-O5      |
| 28  | 5     | 305 | LHG  | O1-C1-C2-C3     |
| 28  | 5     | 305 | LHG  | C1-C2-C3-O3     |
| 28  | 5     | 305 | LHG  | O2-C2-C3-O3     |
| 28  | 5     | 305 | LHG  | C3-O3-P-O4      |
| 28  | 5     | 305 | LHG  | C3-O3-P-O5      |
| 28  | 5     | 305 | LHG  | C3-O3-P-O6      |
| 28  | 5     | 305 | LHG  | C4-O6-P-O4      |
| 28  | 6     | 301 | LHG  | C3-O3-P-O4      |
| 28  | 6     | 301 | LHG  | C3-O3-P-O6      |
| 28  | 6     | 305 | LHG  | C8-C7-O7-C5     |
| 31  | A     | 818 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 818 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 824 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 824 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 830 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 832 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 833 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 834 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 834 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 835 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 836 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 836 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 842 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 842 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 843 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 845 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 845 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 845 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 846 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 847 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 850 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 850 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 852 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 853 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 854 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 855 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 857 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 857 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 811 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 811 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 813 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 817 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 817 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 818 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 819 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 822 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 830 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 830 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 831 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 832 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 833 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 836 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 841 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 847 | CLA  | CBD-CGD-O2D-CED |
| 31  | F     | 301 | CLA  | CBD-CGD-O2D-CED |
| 31  | F     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 31  | F     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | F     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | G     | 204 | CLA  | CBD-CGD-O2D-CED |
| 31  | G     | 205 | CLA  | CBD-CGD-O2D-CED |
| 31  | G     | 206 | CLA  | CBD-CGD-O2D-CED |
| 31  | H     | 901 | CLA  | CBD-CGD-O2D-CED |
| 31  | H     | 901 | CLA  | O1D-CGD-O2D-CED |
| 31  | H     | 902 | CLA  | CHA-CBD-CGD-O2D |
| 31  | H     | 902 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | H     | 902 | CLA  | O1D-CGD-O2D-CED |
| 31  | H     | 903 | CLA  | C1A-C2A-CAA-CBA |
| 31  | H     | 903 | CLA  | C3A-C2A-CAA-CBA |
| 31  | H     | 903 | CLA  | CHA-CBD-CGD-O2D |
| 31  | H     | 903 | CLA  | CBD-CGD-O2D-CED |
| 31  | J     | 105 | CLA  | C1A-C2A-CAA-CBA |
| 31  | J     | 105 | CLA  | CHA-CBD-CGD-O2D |
| 31  | J     | 105 | CLA  | CBD-CGD-O2D-CED |
| 31  | K     | 205 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 309 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 31  | a     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 316 | CLA  | C3A-C2A-CAA-CBA |
| 31  | a     | 316 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 319 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 321 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 322 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 309 | CLA  | C6-C7-C8-C9     |
| 31  | 3     | 312 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 3     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 316 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 317 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 317 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 317 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 317 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 318 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 3     | 318 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 318 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 320 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 320 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 316 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 322 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 7     | 322 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 313 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 8     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 8     | 317 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 320 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 8     | 320 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 321 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 8     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 316 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 9     | 318 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 319 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 319 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 319 | CLA  | O1D-CGD-O2D-CED |
| 31  | L     | 306 | CLA  | CBD-CGD-O2D-CED |
| 31  | L     | 307 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | O     | 203 | CLA  | CHA-CBD-CGD-O2D |
| 31  | O     | 203 | CLA  | CBD-CGD-O2D-CED |
| 31  | O     | 203 | CLA  | C2-C3-C5-C6     |
| 31  | O     | 203 | CLA  | C4-C3-C5-C6     |
| 31  | O     | 204 | CLA  | CBD-CGD-O2D-CED |
| 31  | O     | 204 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 302 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 303 | CLA  | CHA-CBD-CGD-O1D |
| 31  | b     | 303 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 306 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 306 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 31  | b     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 31  | b     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 2     | 304 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 304 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 306 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 306 | CLA  | C2-C3-C5-C6     |
| 31  | 2     | 306 | CLA  | C4-C3-C5-C6     |
| 31  | 2     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 310 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 2     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 313 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 315 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 2     | 315 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 305 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 306 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 4     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 312 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 4     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 4     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 318 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 318 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 319 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 319 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 312 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 318 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 320 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 323 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 323 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 323 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 6     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 311 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 6     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 312 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 316 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 322 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 322 | CLA  | O1D-CGD-O2D-CED |
| 32  | A     | 831 | CHL  | C3A-C2A-CAA-CBA |
| 32  | A     | 831 | CHL  | C1C-C2C-CMC-OMC |
| 32  | A     | 831 | CHL  | C3C-C2C-CMC-OMC |
| 32  | A     | 839 | CHL  | C1C-C2C-CMC-OMC |
| 32  | A     | 839 | CHL  | C3C-C2C-CMC-OMC |
| 32  | A     | 839 | CHL  | CAD-CBD-CGD-O2D |
| 32  | A     | 839 | CHL  | CBD-CGD-O2D-CED |
| 32  | A     | 840 | CHL  | CHA-CBD-CGD-O1D |
| 32  | A     | 840 | CHL  | CBD-CGD-O2D-CED |
| 32  | A     | 840 | CHL  | O1D-CGD-O2D-CED |
| 32  | a     | 317 | CHL  | C3C-C2C-CMC-OMC |
| 32  | a     | 317 | CHL  | CHA-CBD-CGD-O1D |
| 32  | a     | 317 | CHL  | CBD-CGD-O2D-CED |
| 32  | a     | 317 | CHL  | O1D-CGD-O2D-CED |
| 32  | a     | 318 | CHL  | C3C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | a     | 320 | CHL  | C1C-C2C-CMC-OMC |
| 32  | a     | 320 | CHL  | CBD-CGD-O2D-CED |
| 32  | 3     | 315 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 3     | 315 | CHL  | C2-C3-C5-C6     |
| 32  | 3     | 315 | CHL  | C4-C3-C5-C6     |
| 32  | 7     | 317 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 7     | 317 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 7     | 317 | CHL  | CBD-CGD-O2D-CED |
| 32  | 7     | 317 | CHL  | O1D-CGD-O2D-CED |
| 32  | 7     | 317 | CHL  | C2-C3-C5-C6     |
| 32  | 7     | 317 | CHL  | C4-C3-C5-C6     |
| 32  | 7     | 318 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 7     | 318 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 7     | 318 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 7     | 320 | CHL  | CBD-CGD-O2D-CED |
| 32  | 7     | 324 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 7     | 324 | CHL  | CBD-CGD-O2D-CED |
| 32  | 7     | 324 | CHL  | O1D-CGD-O2D-CED |
| 32  | 8     | 316 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 8     | 316 | CHL  | CBD-CGD-O2D-CED |
| 32  | 8     | 319 | CHL  | CBD-CGD-O2D-CED |
| 32  | 9     | 320 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 9     | 320 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 9     | 320 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 9     | 320 | CHL  | CBD-CGD-O2D-CED |
| 32  | 9     | 322 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 9     | 322 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 9     | 322 | CHL  | CBD-CGD-O2D-CED |
| 32  | b     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 32  | b     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 32  | b     | 309 | CHL  | CHA-CBD-CGD-O1D |
| 32  | b     | 309 | CHL  | CBD-CGD-O2D-CED |
| 32  | b     | 309 | CHL  | O1D-CGD-O2D-CED |
| 32  | 4     | 310 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 4     | 313 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 4     | 313 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 4     | 313 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 4     | 313 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 4     | 313 | CHL  | CBD-CGD-O2D-CED |
| 32  | 4     | 317 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 4     | 317 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 4     | 317 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | 4     | 317 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 4     | 317 | CHL  | CBD-CGD-O2D-CED |
| 32  | 4     | 317 | CHL  | O1D-CGD-O2D-CED |
| 32  | 5     | 316 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 5     | 316 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 5     | 316 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 5     | 317 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 5     | 319 | CHL  | CBD-CGD-O2D-CED |
| 32  | 5     | 322 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 5     | 322 | CHL  | CBD-CGD-O2D-CED |
| 32  | 5     | 322 | CHL  | O1D-CGD-O2D-CED |
| 32  | 6     | 309 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 6     | 309 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 6     | 309 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 6     | 309 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 6     | 309 | CHL  | CBD-CGD-O2D-CED |
| 32  | 6     | 309 | CHL  | O1D-CGD-O2D-CED |
| 32  | 6     | 309 | CHL  | C2-C3-C5-C6     |
| 32  | 6     | 309 | CHL  | C4-C3-C5-C6     |
| 32  | 6     | 317 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 6     | 317 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 6     | 317 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 6     | 317 | CHL  | CBD-CGD-O2D-CED |
| 32  | 6     | 317 | CHL  | O1D-CGD-O2D-CED |
| 32  | 6     | 318 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 6     | 318 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 6     | 318 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 6     | 318 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 6     | 319 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 6     | 319 | CHL  | C3A-C2A-CAA-CBA |
| 32  | 6     | 319 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 6     | 319 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 6     | 320 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 6     | 320 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 6     | 320 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 6     | 320 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 6     | 320 | CHL  | CBD-CGD-O2D-CED |
| 32  | 6     | 320 | CHL  | O1D-CGD-O2D-CED |
| 32  | 6     | 321 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 6     | 321 | CHL  | CBD-CGD-O2D-CED |
| 32  | 6     | 321 | CHL  | O1D-CGD-O2D-CED |
| 34  | B     | 851 | LAP  | O2-C1-O1-C13    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | B     | 851 | LAP  | C15-O4-P9-O5    |
| 34  | B     | 851 | LAP  | C15-O4-P9-O6    |
| 35  | F     | 303 | QTB  | C01-C02-C03-C04 |
| 35  | F     | 303 | QTB  | C09-C02-C03-C04 |
| 35  | F     | 303 | QTB  | C01-C02-C09-C10 |
| 35  | F     | 303 | QTB  | C03-C02-C09-C10 |
| 35  | F     | 303 | QTB  | C02-C09-C10-C11 |
| 35  | a     | 302 | QTB  | C09-C10-C11-C12 |
| 35  | a     | 302 | QTB  | C09-C10-C11-C17 |
| 35  | 7     | 303 | QTB  | C01-C02-C09-C10 |
| 35  | 7     | 303 | QTB  | C04-C05-C06-C08 |
| 35  | 7     | 303 | QTB  | C02-C09-C10-C11 |
| 35  | 7     | 303 | QTB  | C09-C10-C11-C12 |
| 35  | 9     | 304 | QTB  | C03-C02-C09-C10 |
| 35  | 9     | 304 | QTB  | C03-C04-C05-C06 |
| 35  | 9     | 304 | QTB  | C04-C05-C06-C08 |
| 35  | 9     | 304 | QTB  | C04-C05-C06-O07 |
| 36  | F     | 304 | LUT  | C5-C6-C7-C8     |
| 36  | F     | 304 | LUT  | C7-C8-C9-C10    |
| 36  | F     | 304 | LUT  | C7-C8-C9-C19    |
| 36  | F     | 304 | LUT  | C11-C10-C9-C8   |
| 36  | F     | 304 | LUT  | C20-C13-C14-C15 |
| 36  | F     | 304 | LUT  | C39-C29-C30-C31 |
| 36  | F     | 304 | LUT  | C31-C32-C33-C34 |
| 36  | F     | 304 | LUT  | C31-C32-C33-C40 |
| 36  | F     | 304 | LUT  | C40-C33-C34-C35 |
| 36  | J     | 103 | LUT  | C5-C6-C7-C8     |
| 36  | J     | 103 | LUT  | C11-C10-C9-C19  |
| 36  | J     | 103 | LUT  | C11-C12-C13-C20 |
| 36  | J     | 103 | LUT  | C20-C13-C14-C15 |
| 36  | J     | 103 | LUT  | C27-C28-C29-C30 |
| 36  | J     | 103 | LUT  | C39-C29-C30-C31 |
| 36  | J     | 103 | LUT  | C40-C33-C34-C35 |
| 36  | J     | 103 | LUT  | C33-C34-C35-C15 |
| 36  | a     | 303 | LUT  | C5-C6-C7-C8     |
| 36  | a     | 303 | LUT  | C7-C8-C9-C19    |
| 36  | a     | 303 | LUT  | C11-C10-C9-C19  |
| 36  | a     | 303 | LUT  | C11-C12-C13-C20 |
| 36  | a     | 303 | LUT  | C20-C13-C14-C15 |
| 36  | a     | 303 | LUT  | C27-C28-C29-C30 |
| 36  | a     | 303 | LUT  | C28-C29-C30-C31 |
| 36  | a     | 303 | LUT  | C39-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | a     | 303 | LUT  | C31-C32-C33-C34 |
| 36  | a     | 303 | LUT  | C31-C32-C33-C40 |
| 36  | a     | 303 | LUT  | C40-C33-C34-C35 |
| 36  | a     | 305 | LUT  | C5-C6-C7-C8     |
| 36  | a     | 305 | LUT  | C7-C8-C9-C19    |
| 36  | a     | 305 | LUT  | C11-C10-C9-C19  |
| 36  | a     | 305 | LUT  | C20-C13-C14-C15 |
| 36  | a     | 305 | LUT  | C21-C26-C27-C28 |
| 36  | a     | 305 | LUT  | C25-C26-C27-C28 |
| 36  | a     | 305 | LUT  | C27-C28-C29-C30 |
| 36  | a     | 305 | LUT  | C27-C28-C29-C39 |
| 36  | a     | 305 | LUT  | C28-C29-C30-C31 |
| 36  | a     | 305 | LUT  | C40-C33-C34-C35 |
| 36  | 3     | 304 | LUT  | C11-C10-C9-C19  |
| 36  | 3     | 304 | LUT  | C11-C12-C13-C14 |
| 36  | 3     | 304 | LUT  | C20-C13-C14-C15 |
| 36  | 3     | 304 | LUT  | C39-C29-C30-C31 |
| 36  | 3     | 304 | LUT  | C40-C33-C34-C35 |
| 36  | 3     | 305 | LUT  | C5-C6-C7-C8     |
| 36  | 3     | 305 | LUT  | C7-C8-C9-C19    |
| 36  | 3     | 305 | LUT  | C11-C10-C9-C19  |
| 36  | 3     | 305 | LUT  | C11-C12-C13-C20 |
| 36  | 3     | 305 | LUT  | C20-C13-C14-C15 |
| 36  | 3     | 305 | LUT  | C27-C28-C29-C30 |
| 36  | 3     | 305 | LUT  | C39-C29-C30-C31 |
| 36  | 3     | 305 | LUT  | C40-C33-C34-C35 |
| 36  | 7     | 305 | LUT  | C11-C10-C9-C19  |
| 36  | 7     | 305 | LUT  | C20-C13-C14-C15 |
| 36  | 7     | 305 | LUT  | C39-C29-C30-C31 |
| 36  | 7     | 305 | LUT  | C40-C33-C34-C35 |
| 36  | 8     | 302 | LUT  | C5-C6-C7-C8     |
| 36  | 8     | 302 | LUT  | C7-C8-C9-C19    |
| 36  | 8     | 302 | LUT  | C11-C10-C9-C19  |
| 36  | 8     | 302 | LUT  | C11-C12-C13-C14 |
| 36  | 8     | 302 | LUT  | C20-C13-C14-C15 |
| 36  | 8     | 302 | LUT  | C27-C28-C29-C39 |
| 36  | 8     | 302 | LUT  | C39-C29-C30-C31 |
| 36  | 8     | 302 | LUT  | C31-C32-C33-C34 |
| 36  | 8     | 302 | LUT  | C31-C32-C33-C40 |
| 36  | 8     | 302 | LUT  | C40-C33-C34-C35 |
| 36  | 8     | 303 | LUT  | C20-C13-C14-C15 |
| 36  | 8     | 303 | LUT  | C39-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 8     | 303 | LUT  | C40-C33-C34-C35 |
| 36  | 9     | 302 | LUT  | C5-C6-C7-C8     |
| 36  | 9     | 302 | LUT  | C7-C8-C9-C10    |
| 36  | 9     | 302 | LUT  | C11-C10-C9-C19  |
| 36  | 9     | 302 | LUT  | C20-C13-C14-C15 |
| 36  | 9     | 302 | LUT  | C28-C29-C30-C31 |
| 36  | 9     | 302 | LUT  | C39-C29-C30-C31 |
| 36  | 9     | 302 | LUT  | C40-C33-C34-C35 |
| 36  | 9     | 303 | LUT  | C7-C8-C9-C10    |
| 36  | 9     | 303 | LUT  | C11-C10-C9-C19  |
| 36  | 9     | 303 | LUT  | C9-C10-C11-C12  |
| 36  | 9     | 303 | LUT  | C11-C12-C13-C14 |
| 36  | 9     | 303 | LUT  | C20-C13-C14-C15 |
| 36  | 9     | 303 | LUT  | C27-C28-C29-C39 |
| 36  | 9     | 303 | LUT  | C28-C29-C30-C31 |
| 36  | 9     | 303 | LUT  | C40-C33-C34-C35 |
| 36  | 9     | 305 | LUT  | C5-C6-C7-C8     |
| 36  | 9     | 305 | LUT  | C11-C10-C9-C19  |
| 36  | 9     | 305 | LUT  | C12-C13-C14-C15 |
| 36  | 9     | 305 | LUT  | C20-C13-C14-C15 |
| 36  | 9     | 305 | LUT  | C28-C29-C30-C31 |
| 36  | 9     | 305 | LUT  | C39-C29-C30-C31 |
| 36  | 9     | 305 | LUT  | C31-C32-C33-C34 |
| 36  | 9     | 305 | LUT  | C31-C32-C33-C40 |
| 36  | 9     | 305 | LUT  | C40-C33-C34-C35 |
| 36  | L     | 304 | LUT  | C7-C8-C9-C10    |
| 36  | L     | 304 | LUT  | C11-C10-C9-C8   |
| 36  | L     | 304 | LUT  | C9-C10-C11-C12  |
| 36  | L     | 304 | LUT  | C20-C13-C14-C15 |
| 36  | L     | 304 | LUT  | C27-C28-C29-C30 |
| 36  | L     | 304 | LUT  | C39-C29-C30-C31 |
| 36  | L     | 304 | LUT  | C31-C32-C33-C40 |
| 36  | L     | 304 | LUT  | C40-C33-C34-C35 |
| 36  | b     | 301 | LUT  | C11-C10-C9-C8   |
| 36  | b     | 301 | LUT  | C11-C10-C9-C19  |
| 36  | b     | 301 | LUT  | C12-C13-C14-C15 |
| 36  | b     | 301 | LUT  | C39-C29-C30-C31 |
| 36  | b     | 301 | LUT  | C31-C32-C33-C34 |
| 36  | b     | 301 | LUT  | C40-C33-C34-C35 |
| 36  | 2     | 301 | LUT  | C5-C6-C7-C8     |
| 36  | 2     | 301 | LUT  | C11-C10-C9-C19  |
| 36  | 2     | 301 | LUT  | C11-C12-C13-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 2     | 301 | LUT  | C20-C13-C14-C15 |
| 36  | 2     | 301 | LUT  | C27-C28-C29-C30 |
| 36  | 2     | 301 | LUT  | C39-C29-C30-C31 |
| 36  | 2     | 301 | LUT  | C40-C33-C34-C35 |
| 36  | 4     | 302 | LUT  | C5-C6-C7-C8     |
| 36  | 4     | 302 | LUT  | C7-C8-C9-C10    |
| 36  | 4     | 302 | LUT  | C7-C8-C9-C19    |
| 36  | 4     | 302 | LUT  | C11-C10-C9-C19  |
| 36  | 4     | 302 | LUT  | C11-C12-C13-C20 |
| 36  | 4     | 302 | LUT  | C20-C13-C14-C15 |
| 36  | 4     | 302 | LUT  | C27-C28-C29-C30 |
| 36  | 4     | 302 | LUT  | C27-C28-C29-C39 |
| 36  | 4     | 302 | LUT  | C39-C29-C30-C31 |
| 36  | 4     | 302 | LUT  | C40-C33-C34-C35 |
| 36  | 4     | 303 | LUT  | C11-C10-C9-C8   |
| 36  | 4     | 303 | LUT  | C11-C10-C9-C19  |
| 36  | 4     | 303 | LUT  | C11-C12-C13-C20 |
| 36  | 4     | 303 | LUT  | C20-C13-C14-C15 |
| 36  | 4     | 303 | LUT  | C27-C28-C29-C39 |
| 36  | 4     | 303 | LUT  | C28-C29-C30-C31 |
| 36  | 4     | 303 | LUT  | C40-C33-C34-C35 |
| 36  | 5     | 303 | LUT  | C5-C6-C7-C8     |
| 36  | 5     | 303 | LUT  | C7-C8-C9-C19    |
| 36  | 5     | 303 | LUT  | C11-C10-C9-C19  |
| 36  | 5     | 303 | LUT  | C11-C12-C13-C14 |
| 36  | 5     | 303 | LUT  | C20-C13-C14-C15 |
| 36  | 5     | 303 | LUT  | C27-C28-C29-C30 |
| 36  | 5     | 303 | LUT  | C39-C29-C30-C31 |
| 36  | 5     | 303 | LUT  | C40-C33-C34-C35 |
| 36  | 5     | 304 | LUT  | C5-C6-C7-C8     |
| 36  | 5     | 304 | LUT  | C7-C8-C9-C19    |
| 36  | 5     | 304 | LUT  | C11-C10-C9-C8   |
| 36  | 5     | 304 | LUT  | C11-C10-C9-C19  |
| 36  | 5     | 304 | LUT  | C9-C10-C11-C12  |
| 36  | 5     | 304 | LUT  | C11-C12-C13-C20 |
| 36  | 5     | 304 | LUT  | C12-C13-C14-C15 |
| 36  | 5     | 304 | LUT  | C27-C28-C29-C30 |
| 36  | 5     | 304 | LUT  | C39-C29-C30-C31 |
| 36  | 5     | 304 | LUT  | C40-C33-C34-C35 |
| 36  | 6     | 303 | LUT  | C5-C6-C7-C8     |
| 36  | 6     | 303 | LUT  | C7-C8-C9-C19    |
| 36  | 6     | 303 | LUT  | C11-C10-C9-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 6     | 303 | LUT  | C11-C10-C9-C19  |
| 36  | 6     | 303 | LUT  | C20-C13-C14-C15 |
| 36  | 6     | 303 | LUT  | C39-C29-C30-C31 |
| 36  | 6     | 303 | LUT  | C31-C32-C33-C40 |
| 36  | 6     | 303 | LUT  | C40-C33-C34-C35 |
| 36  | 6     | 303 | LUT  | C33-C34-C35-C15 |
| 36  | 6     | 304 | LUT  | C5-C6-C7-C8     |
| 36  | 6     | 304 | LUT  | C7-C8-C9-C19    |
| 36  | 6     | 304 | LUT  | C11-C10-C9-C19  |
| 36  | 6     | 304 | LUT  | C11-C12-C13-C14 |
| 36  | 6     | 304 | LUT  | C27-C28-C29-C39 |
| 36  | 6     | 304 | LUT  | C28-C29-C30-C31 |
| 36  | 6     | 304 | LUT  | C40-C33-C34-C35 |
| 37  | J     | 104 | LMG  | C2-C1-O1-C7     |
| 37  | J     | 104 | LMG  | O6-C1-O1-C7     |
| 37  | a     | 301 | LMG  | C2-C1-O1-C7     |
| 37  | a     | 301 | LMG  | O6-C1-O1-C7     |
| 39  | 7     | 301 | 3PH  | C1-O11-P-O13    |
| 39  | 7     | 301 | 3PH  | C1-O11-P-O14    |
| 40  | 7     | 306 | XAT  | C10-C11-C12-C13 |
| 40  | 7     | 306 | XAT  | C11-C12-C13-C14 |
| 40  | 7     | 306 | XAT  | C11-C12-C13-C20 |
| 41  | 8     | 305 | DGA  | CG1-CG2-CG3-OXT |
| 41  | 8     | 305 | DGA  | OG2-CG2-CG3-OXT |
| 42  | 4     | 304 | SQD  | O5-C5-C6-S      |
| 43  | 5     | 306 | PTY  | C11-C8-O7-C6    |
| 43  | 5     | 306 | PTY  | C3-O11-P1-O12   |
| 43  | 5     | 306 | PTY  | C3-O11-P1-O13   |
| 43  | 5     | 306 | PTY  | C3-O11-P1-O14   |
| 31  | A     | 819 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 830 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 835 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 836 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 842 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 848 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 811 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 813 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 818 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 819 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 843 | CLA  | O1D-CGD-O2D-CED |
| 31  | J     | 105 | CLA  | O1D-CGD-O2D-CED |
| 31  | K     | 206 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | a     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 319 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 317 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | L     | 306 | CLA  | O1D-CGD-O2D-CED |
| 31  | O     | 203 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 323 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 313 | CLA  | O1D-CGD-O2D-CED |
| 32  | 9     | 320 | CHL  | O1D-CGD-O2D-CED |
| 32  | 4     | 313 | CHL  | O1D-CGD-O2D-CED |
| 32  | 5     | 319 | CHL  | O1D-CGD-O2D-CED |
| 31  | A     | 823 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 828 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 833 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 844 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 854 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 855 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 857 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 822 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 824 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 825 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 827 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 828 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 838 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 839 | CLA  | O1D-CGD-O2D-CED |
| 31  | G     | 206 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | H     | 903 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 303 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 306 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 321 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 314 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 318 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 320 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 311 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 314 | CLA  | O1D-CGD-O2D-CED |
| 32  | a     | 318 | CHL  | O1D-CGD-O2D-CED |
| 32  | a     | 320 | CHL  | O1D-CGD-O2D-CED |
| 31  | A     | 819 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 823 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 828 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 830 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 841 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 846 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 847 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 848 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 854 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 855 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 857 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 818 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 820 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 824 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 825 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 827 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 828 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 835 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 838 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 839 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 843 | CLA  | CBD-CGD-O2D-CED |
| 31  | K     | 206 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 309 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | a     | 315 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 311 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 319 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 9     | 321 | CLA  | CBD-CGD-O2D-CED |
| 31  | b     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 307 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 2     | 313 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 308 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 320 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 310 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 312 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 318 | CLA  | CBD-CGD-O2D-CED |
| 31  | 5     | 320 | CLA  | CBD-CGD-O2D-CED |
| 31  | 6     | 312 | CLA  | CBD-CGD-O2D-CED |
| 32  | a     | 318 | CHL  | CBD-CGD-O2D-CED |
| 32  | 7     | 318 | CHL  | CBD-CGD-O2D-CED |
| 32  | 5     | 316 | CHL  | CBD-CGD-O2D-CED |
| 31  | A     | 818 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 827 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 834 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 841 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 845 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 846 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 815 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 820 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 821 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 826 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 834 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 835 | CLA  | O1D-CGD-O2D-CED |
| 31  | F     | 306 | CLA  | O1D-CGD-O2D-CED |
| 31  | G     | 204 | CLA  | O1D-CGD-O2D-CED |
| 31  | G     | 205 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 313 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 322 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 322 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 309 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 318 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 304 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 308 | CLA  | O1D-CGD-O2D-CED |
| 31  | 2     | 315 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 306 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 320 | CLA  | O1D-CGD-O2D-CED |
| 31  | 5     | 310 | CLA  | O1D-CGD-O2D-CED |
| 32  | 8     | 319 | CHL  | O1D-CGD-O2D-CED |
| 32  | 7     | 318 | CHL  | C4C-C3C-CAC-CBC |
| 31  | A     | 817 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 838 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 856 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 829 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 841 | CLA  | O1D-CGD-O2D-CED |
| 31  | F     | 301 | CLA  | O1D-CGD-O2D-CED |
| 31  | K     | 205 | CLA  | O1D-CGD-O2D-CED |
| 31  | a     | 319 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 318 | CLA  | O1D-CGD-O2D-CED |
| 31  | 7     | 310 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 320 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | L     | 307 | CLA  | O1D-CGD-O2D-CED |
| 31  | b     | 302 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 311 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 4     | 312 | CLA  | O1D-CGD-O2D-CED |
| 31  | 6     | 315 | CLA  | O1D-CGD-O2D-CED |
| 32  | 7     | 320 | CHL  | O1D-CGD-O2D-CED |
| 32  | 9     | 322 | CHL  | O1D-CGD-O2D-CED |
| 34  | B     | 851 | LAP  | C2-C1-O1-C13    |
| 31  | A     | 818 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 821 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 827 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 838 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 844 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 812 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 815 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 821 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 826 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 834 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 840 | CLA  | CBD-CGD-O2D-CED |
| 31  | F     | 306 | CLA  | CBD-CGD-O2D-CED |
| 31  | 3     | 314 | CLA  | CBD-CGD-O2D-CED |
| 31  | 7     | 309 | CLA  | CBD-CGD-O2D-CED |
| 32  | A     | 831 | CHL  | CBD-CGD-O2D-CED |
| 32  | 3     | 315 | CHL  | CBD-CGD-O2D-CED |
| 32  | 7     | 319 | CHL  | CBD-CGD-O2D-CED |
| 32  | 6     | 318 | CHL  | CBD-CGD-O2D-CED |
| 32  | 7     | 318 | CHL  | C2C-C3C-CAC-CBC |
| 28  | A     | 809 | LHG  | O10-C23-O8-C6   |
| 31  | A     | 857 | CLA  | O1A-CGA-O2A-C1  |
| 37  | J     | 101 | LMG  | O10-C28-O8-C9   |
| 43  | 5     | 306 | PTY  | O30-C30-O4-C1   |
| 31  | A     | 821 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 847 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 812 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 847 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 826 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 832 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 842 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 846 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 842 | CLA  | CBD-CGD-O2D-CED |
| 31  | K     | 204 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 823 | CLA  | O1D-CGD-O2D-CED |
| 31  | K     | 204 | CLA  | O1D-CGD-O2D-CED |
| 28  | 6     | 305 | LHG  | O9-C7-O7-C5     |
| 37  | J     | 104 | LMG  | O9-C10-O7-C8    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | 5     | 306 | PTY  | O10-C8-O7-C6    |
| 31  | B     | 844 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 822 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 830 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 851 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 857 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 820 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 827 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 830 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 832 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 833 | CLA  | C3-C5-C6-C7     |
| 31  | a     | 315 | CLA  | C3-C5-C6-C7     |
| 31  | 7     | 314 | CLA  | C3-C5-C6-C7     |
| 31  | 9     | 318 | CLA  | C3-C5-C6-C7     |
| 31  | 6     | 311 | CLA  | C3-C5-C6-C7     |
| 28  | A     | 809 | LHG  | C24-C23-O8-C6   |
| 31  | 7     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 37  | J     | 101 | LMG  | C29-C28-O8-C9   |
| 43  | 5     | 306 | PTY  | C31-C30-O4-C1   |
| 28  | A     | 810 | LHG  | C8-C7-O7-C5     |
| 28  | 7     | 302 | LHG  | C8-C7-O7-C5     |
| 32  | 6     | 318 | CHL  | O1D-CGD-O2D-CED |
| 31  | B     | 846 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 841 | CLA  | C4-C3-C5-C6     |
| 31  | 8     | 311 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 836 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 837 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 857 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 850 | CLA  | C2A-CAA-CBA-CGA |
| 31  | a     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 31  | a     | 316 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 32  | a     | 317 | CHL  | C2A-CAA-CBA-CGA |
| 32  | 4     | 313 | CHL  | C2A-CAA-CBA-CGA |
| 32  | 6     | 320 | CHL  | C2A-CAA-CBA-CGA |
| 34  | B     | 851 | LAP  | C5-C6-C7-C8     |
| 31  | a     | 313 | CLA  | C3-C5-C6-C7     |
| 31  | 8     | 308 | CLA  | C3-C5-C6-C7     |
| 31  | 9     | 321 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 841 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 848 | CLA  | CBA-CGA-O2A-C1  |
| 31  | a     | 313 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 3     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 8     | 308 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 825 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 831 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 836 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 840 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 841 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 850 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 3     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 7     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 8     | 308 | CLA  | O1A-CGA-O2A-C1  |
| 36  | J     | 103 | LUT  | C9-C10-C11-C12  |
| 36  | a     | 303 | LUT  | C29-C30-C31-C32 |
| 36  | 3     | 304 | LUT  | C29-C30-C31-C32 |
| 36  | 8     | 302 | LUT  | C29-C30-C31-C32 |
| 36  | 8     | 303 | LUT  | C33-C34-C35-C15 |
| 36  | 9     | 303 | LUT  | C29-C30-C31-C32 |
| 36  | 9     | 305 | LUT  | C13-C14-C15-C35 |
| 36  | 9     | 305 | LUT  | C29-C30-C31-C32 |
| 36  | L     | 304 | LUT  | C29-C30-C31-C32 |
| 36  | b     | 301 | LUT  | C33-C34-C35-C15 |
| 36  | 4     | 303 | LUT  | C13-C14-C15-C35 |
| 36  | 4     | 303 | LUT  | C29-C30-C31-C32 |
| 36  | 5     | 303 | LUT  | C33-C34-C35-C15 |
| 36  | 5     | 304 | LUT  | C13-C14-C15-C35 |
| 36  | 6     | 304 | LUT  | C29-C30-C31-C32 |
| 28  | 6     | 305 | LHG  | C23-C24-C25-C26 |
| 31  | A     | 817 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 825 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 837 | CLA  | CBD-CGD-O2D-CED |
| 31  | A     | 856 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 841 | CLA  | CBD-CGD-O2D-CED |
| 32  | 5     | 317 | CHL  | CBD-CGD-O2D-CED |
| 32  | 6     | 319 | CHL  | CBD-CGD-O2D-CED |
| 28  | 7     | 307 | LHG  | O2-C2-C3-O3     |
| 31  | A     | 821 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 836 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 823 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 834 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 845 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 857 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 850 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 8     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 41  | 8     | 305 | DGA  | CA2-CA1-OG1-CG1 |
| 31  | a     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 33  | B     | 808 | DGD  | O6E-C5E-C6E-O5E |
| 28  | 5     | 305 | LHG  | C25-C26-C27-C28 |
| 31  | A     | 845 | CLA  | O1A-CGA-O2A-C1  |
| 28  | 8     | 304 | LHG  | C23-C24-C25-C26 |
| 31  | B     | 841 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 842 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 850 | CLA  | CBA-CGA-O2A-C1  |
| 27  | A     | 807 | LMT  | O5B-C5B-C6B-O6B |
| 37  | G     | 202 | LMG  | O6-C5-C6-O5     |
| 33  | B     | 808 | DGD  | C4E-C5E-C6E-O5E |
| 31  | A     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 848 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 850 | CLA  | O1A-CGA-O2A-C1  |
| 27  | 5     | 301 | LMT  | O5B-C5B-C6B-O6B |
| 31  | A     | 848 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 855 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 314 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 830 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 848 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 855 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 314 | CLA  | C2-C3-C5-C6     |
| 31  | 8     | 311 | CLA  | C2-C3-C5-C6     |
| 31  | a     | 322 | CLA  | C2A-CAA-CBA-CGA |
| 32  | 8     | 316 | CHL  | C2A-CAA-CBA-CGA |
| 41  | 8     | 305 | DGA  | OA1-CA1-OG1-CG1 |
| 31  | O     | 203 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 5     | 323 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 4     | 317 | CHL  | C2C-C3C-CAC-CBC |
| 31  | A     | 814 | CLA  | CBD-CGD-O2D-CED |
| 31  | B     | 814 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 843 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 820 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 850 | CLA  | O1D-CGD-O2D-CED |
| 28  | A     | 809 | LHG  | C1-C2-C3-O3     |
| 27  | A     | 807 | LMT  | C4B-C5B-C6B-O6B |
| 31  | O     | 203 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 5     | 323 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | B     | 851 | LAP  | C16-C17-N8-C19  |
| 31  | B     | 849 | CLA  | O1D-CGD-O2D-CED |
| 28  | 5     | 305 | LHG  | C24-C23-O8-C6   |
| 31  | A     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 5     | 315 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 8     | 316 | CHL  | CBA-CGA-O2A-C1  |
| 27  | 5     | 301 | LMT  | O5'-C5'-C6'-O6' |
| 31  | A     | 832 | CLA  | CBD-CGD-O2D-CED |
| 31  | 4     | 316 | CLA  | CBD-CGD-O2D-CED |
| 37  | G     | 202 | LMG  | C4-C5-C6-O5     |
| 36  | F     | 304 | LUT  | C29-C30-C31-C32 |
| 36  | a     | 305 | LUT  | C13-C14-C15-C35 |
| 36  | 3     | 304 | LUT  | C33-C34-C35-C15 |
| 36  | 7     | 305 | LUT  | C29-C30-C31-C32 |
| 36  | 8     | 302 | LUT  | C33-C34-C35-C15 |
| 36  | 8     | 303 | LUT  | C29-C30-C31-C32 |
| 36  | 9     | 302 | LUT  | C13-C14-C15-C35 |
| 36  | 4     | 303 | LUT  | C9-C10-C11-C12  |
| 36  | 6     | 304 | LUT  | C13-C14-C15-C35 |
| 27  | 9     | 306 | LMT  | O5'-C5'-C6'-O6' |
| 31  | A     | 826 | CLA  | C13-C15-C16-C17 |
| 31  | 7     | 315 | CLA  | C5-C6-C7-C8     |
| 31  | 5     | 315 | CLA  | C10-C11-C12-C13 |
| 28  | A     | 809 | LHG  | O2-C2-C3-O3     |
| 28  | 7     | 302 | LHG  | O2-C2-C3-O3     |
| 31  | B     | 822 | CLA  | C2C-C3C-CAC-CBC |
| 32  | 8     | 316 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 841 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 815 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 819 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 842 | CLA  | C11-C12-C13-C14 |
| 31  | L     | 305 | CLA  | C6-C7-C8-C9     |
| 32  | 7     | 318 | CHL  | C6-C7-C8-C9     |
| 32  | 7     | 318 | CHL  | C11-C10-C8-C9   |
| 32  | 7     | 320 | CHL  | C11-C10-C8-C9   |
| 32  | 6     | 309 | CHL  | C14-C13-C15-C16 |
| 31  | A     | 816 | CLA  | O1D-CGD-O2D-CED |
| 32  | 7     | 318 | CHL  | O1D-CGD-O2D-CED |
| 31  | B     | 815 | CLA  | C5-C6-C7-C8     |
| 31  | 4     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 6     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 26  | B     | 803 | BCR  | C7-C8-C9-C34    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | B     | 803 | BCR  | C37-C22-C23-C24 |
| 26  | K     | 202 | BCR  | C37-C22-C23-C24 |
| 26  | 3     | 301 | BCR  | C7-C8-C9-C34    |
| 26  | 5     | 302 | BCR  | C37-C22-C23-C24 |
| 36  | F     | 304 | LUT  | C11-C12-C13-C20 |
| 36  | a     | 305 | LUT  | C31-C32-C33-C40 |
| 36  | 3     | 304 | LUT  | C7-C8-C9-C19    |
| 36  | 3     | 304 | LUT  | C27-C28-C29-C39 |
| 36  | 7     | 305 | LUT  | C7-C8-C9-C19    |
| 36  | 8     | 303 | LUT  | C7-C8-C9-C19    |
| 36  | 8     | 303 | LUT  | C11-C12-C13-C20 |
| 36  | 8     | 303 | LUT  | C27-C28-C29-C39 |
| 36  | 9     | 302 | LUT  | C7-C8-C9-C19    |
| 36  | 9     | 303 | LUT  | C31-C32-C33-C40 |
| 36  | 9     | 305 | LUT  | C7-C8-C9-C19    |
| 36  | 9     | 305 | LUT  | C27-C28-C29-C39 |
| 36  | L     | 304 | LUT  | C27-C28-C29-C39 |
| 36  | b     | 301 | LUT  | C7-C8-C9-C19    |
| 36  | b     | 301 | LUT  | C27-C28-C29-C39 |
| 36  | 4     | 303 | LUT  | C7-C8-C9-C19    |
| 36  | 4     | 303 | LUT  | C31-C32-C33-C40 |
| 36  | 6     | 303 | LUT  | C11-C12-C13-C20 |
| 26  | K     | 202 | BCR  | C21-C22-C23-C24 |
| 26  | 5     | 302 | BCR  | C7-C8-C9-C10    |
| 35  | 7     | 303 | QTB  | C03-C02-C09-C10 |
| 36  | F     | 304 | LUT  | C27-C28-C29-C30 |
| 36  | J     | 103 | LUT  | C31-C32-C33-C34 |
| 36  | a     | 305 | LUT  | C11-C12-C13-C14 |
| 36  | 3     | 304 | LUT  | C31-C32-C33-C34 |
| 36  | 3     | 305 | LUT  | C31-C32-C33-C34 |
| 36  | 7     | 305 | LUT  | C11-C12-C13-C14 |
| 36  | 8     | 303 | LUT  | C31-C32-C33-C34 |
| 36  | 9     | 302 | LUT  | C11-C12-C13-C14 |
| 36  | 9     | 302 | LUT  | C27-C28-C29-C30 |
| 36  | 9     | 302 | LUT  | C31-C32-C33-C34 |
| 36  | 9     | 305 | LUT  | C11-C12-C13-C14 |
| 36  | b     | 301 | LUT  | C11-C12-C13-C14 |
| 36  | 5     | 303 | LUT  | C31-C32-C33-C34 |
| 36  | 5     | 304 | LUT  | C31-C32-C33-C34 |
| 36  | 6     | 303 | LUT  | C31-C32-C33-C34 |
| 28  | 5     | 305 | LHG  | C8-C7-O7-C5     |
| 37  | J     | 104 | LMG  | C11-C10-O7-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | a     | 306 | LHG  | C32-C33-C34-C35 |
| 28  | 5     | 305 | LHG  | O10-C23-O8-C6   |
| 31  | A     | 824 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 828 | CLA  | C15-C16-C17-C18 |
| 28  | 5     | 305 | LHG  | C10-C11-C12-C13 |
| 31  | B     | 833 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 815 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 839 | CLA  | C3-C5-C6-C7     |
| 31  | a     | 312 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 827 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 814 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 820 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 840 | CLA  | C15-C16-C17-C18 |
| 31  | a     | 319 | CLA  | C10-C11-C12-C13 |
| 31  | 3     | 307 | CLA  | C8-C10-C11-C12  |
| 31  | 8     | 310 | CLA  | C13-C15-C16-C17 |
| 32  | a     | 317 | CHL  | C10-C11-C12-C13 |
| 32  | 7     | 320 | CHL  | C10-C11-C12-C13 |
| 28  | A     | 809 | LHG  | C23-C24-C25-C26 |
| 31  | A     | 829 | CLA  | C2C-C3C-CAC-CBC |
| 32  | 5     | 317 | CHL  | C2C-C3C-CAC-CBC |
| 24  | A     | 801 | PQN  | C25-C26-C27-C28 |
| 31  | A     | 836 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 832 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 833 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 840 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 307 | CLA  | C10-C11-C12-C13 |
| 31  | 3     | 311 | CLA  | C5-C6-C7-C8     |
| 31  | 7     | 314 | CLA  | C5-C6-C7-C8     |
| 31  | 9     | 318 | CLA  | C15-C16-C17-C18 |
| 31  | L     | 305 | CLA  | C5-C6-C7-C8     |
| 27  | 5     | 301 | LMT  | C4B-C5B-C6B-O6B |
| 28  | 5     | 305 | LHG  | O1-C1-C2-O2     |
| 28  | a     | 306 | LHG  | C7-C8-C9-C10    |
| 37  | J     | 101 | LMG  | C10-C11-C12-C13 |
| 37  | a     | 301 | LMG  | C10-C11-C12-C13 |
| 37  | a     | 301 | LMG  | C28-C29-C30-C31 |
| 42  | 4     | 304 | SQD  | C7-C8-C9-C10    |
| 32  | a     | 318 | CHL  | C2C-C3C-CAC-CBC |
| 31  | A     | 835 | CLA  | C5-C6-C7-C8     |
| 31  | a     | 312 | CLA  | C13-C15-C16-C17 |
| 32  | a     | 317 | CHL  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 8     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 842 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 847 | CLA  | C5-C6-C7-C8     |
| 31  | 3     | 307 | CLA  | C13-C15-C16-C17 |
| 34  | B     | 851 | LAP  | C16-C17-N8-C20  |
| 28  | 7     | 307 | LHG  | C23-C24-C25-C26 |
| 37  | J     | 101 | LMG  | C28-C29-C30-C31 |
| 31  | A     | 853 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 857 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 815 | CLA  | C11-C10-C8-C7   |
| 31  | a     | 312 | CLA  | C6-C7-C8-C10    |
| 31  | 5     | 315 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 6     | 302 | BCR  | C9-C10-C11-C12  |
| 36  | a     | 305 | LUT  | C9-C10-C11-C12  |
| 36  | a     | 305 | LUT  | C29-C30-C31-C32 |
| 36  | a     | 305 | LUT  | C33-C34-C35-C15 |
| 36  | b     | 301 | LUT  | C29-C30-C31-C32 |
| 36  | 2     | 301 | LUT  | C29-C30-C31-C32 |
| 36  | 5     | 303 | LUT  | C29-C30-C31-C32 |
| 36  | 5     | 304 | LUT  | C29-C30-C31-C32 |
| 36  | 6     | 304 | LUT  | C33-C34-C35-C15 |
| 31  | A     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 319 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 321 | CLA  | C2A-CAA-CBA-CGA |
| 32  | b     | 309 | CHL  | C2A-CAA-CBA-CGA |
| 31  | B     | 837 | CLA  | O1D-CGD-O2D-CED |
| 32  | 8     | 316 | CHL  | O1D-CGD-O2D-CED |
| 31  | a     | 315 | CLA  | C5-C6-C7-C8     |
| 31  | 8     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 28  | B     | 807 | LHG  | C23-C24-C25-C26 |
| 26  | 6     | 302 | BCR  | C10-C11-C12-C13 |
| 32  | 7     | 320 | CHL  | C3-C5-C6-C7     |
| 31  | B     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 849 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 819 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 824 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 830 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 832 | CLA  | C15-C16-C17-C18 |
| 31  | 3     | 309 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 829 | CLA  | CBD-CGD-O2D-CED |
| 31  | 8     | 312 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 837 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 837 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 842 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 825 | CLA  | C8-C10-C11-C12  |
| 31  | a     | 319 | CLA  | C8-C10-C11-C12  |
| 31  | 9     | 314 | CLA  | C10-C11-C12-C13 |
| 31  | 5     | 315 | CLA  | C8-C10-C11-C12  |
| 28  | 7     | 302 | LHG  | C3-O3-P-O6      |
| 28  | 5     | 305 | LHG  | C4-O6-P-O3      |
| 34  | B     | 851 | LAP  | C16-O6-P9-O4    |
| 28  | B     | 807 | LHG  | C24-C23-O8-C6   |
| 39  | 7     | 301 | 3PH  | C31-C32-C33-C34 |
| 28  | 5     | 305 | LHG  | O9-C7-O7-C5     |
| 32  | 6     | 320 | CHL  | C2C-C3C-CAC-CBC |
| 31  | A     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 826 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 321 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 37  | J     | 104 | LMG  | C4-C5-C6-O5     |
| 31  | A     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 851 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 6     | 321 | CHL  | C2C-C3C-CAC-CBC |
| 31  | A     | 823 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 827 | CLA  | C8-C10-C11-C12  |
| 35  | F     | 303 | QTB  | C02-C03-C04-C05 |
| 35  | a     | 302 | QTB  | C02-C03-C04-C05 |
| 35  | 9     | 304 | QTB  | C02-C03-C04-C05 |
| 36  | 3     | 305 | LUT  | C29-C30-C31-C32 |
| 36  | 7     | 305 | LUT  | C9-C10-C11-C12  |
| 36  | 9     | 302 | LUT  | C29-C30-C31-C32 |
| 36  | b     | 301 | LUT  | C13-C14-C15-C35 |
| 36  | 6     | 303 | LUT  | C29-C30-C31-C32 |
| 37  | G     | 202 | LMG  | C11-C10-O7-C8   |
| 26  | A     | 804 | BCR  | C20-C21-C22-C37 |
| 26  | B     | 803 | BCR  | C20-C21-C22-C37 |
| 26  | B     | 805 | BCR  | C20-C21-C22-C37 |
| 26  | 3     | 301 | BCR  | C16-C17-C18-C36 |
| 36  | a     | 305 | LUT  | C39-C29-C30-C31 |
| 36  | 8     | 303 | LUT  | C11-C10-C9-C19  |
| 36  | 9     | 303 | LUT  | C39-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 4     | 303 | LUT  | C39-C29-C30-C31 |
| 36  | 6     | 304 | LUT  | C20-C13-C14-C15 |
| 36  | 6     | 304 | LUT  | C39-C29-C30-C31 |
| 27  | A     | 808 | LMT  | C2-C3-C4-C5     |
| 28  | A     | 810 | LHG  | C24-C25-C26-C27 |
| 33  | 7     | 308 | DGD  | CAB-CBB-CCB-CDB |
| 33  | 7     | 308 | DGD  | CCB-CDB-CEB-CFB |
| 31  | B     | 839 | CLA  | C11-C12-C13-C14 |
| 28  | 8     | 304 | LHG  | C28-C29-C30-C31 |
| 28  | 5     | 305 | LHG  | C26-C27-C28-C29 |
| 32  | 4     | 317 | CHL  | C4C-C3C-CAC-CBC |
| 37  | J     | 101 | LMG  | C22-C23-C24-C25 |
| 31  | B     | 836 | CLA  | CBD-CGD-O2D-CED |
| 28  | 7     | 302 | LHG  | C11-C10-C9-C8   |
| 28  | 7     | 302 | LHG  | C27-C28-C29-C30 |
| 28  | 5     | 305 | LHG  | C12-C13-C14-C15 |
| 37  | G     | 202 | LMG  | C16-C17-C18-C19 |
| 33  | B     | 808 | DGD  | C7B-C8B-C9B-CAB |
| 37  | G     | 202 | LMG  | C17-C18-C19-C20 |
| 31  | A     | 845 | CLA  | C5-C6-C7-C8     |
| 31  | 8     | 308 | CLA  | C13-C15-C16-C17 |
| 26  | A     | 805 | BCR  | C20-C21-C22-C23 |
| 26  | 3     | 302 | BCR  | C12-C13-C14-C15 |
| 26  | 3     | 303 | BCR  | C11-C10-C9-C8   |
| 26  | 8     | 301 | BCR  | C20-C21-C22-C23 |
| 26  | L     | 302 | BCR  | C11-C10-C9-C8   |
| 26  | 6     | 302 | BCR  | C12-C13-C14-C15 |
| 36  | F     | 304 | LUT  | C28-C29-C30-C31 |
| 36  | J     | 103 | LUT  | C11-C10-C9-C8   |
| 36  | a     | 305 | LUT  | C11-C10-C9-C8   |
| 36  | a     | 305 | LUT  | C32-C33-C34-C35 |
| 36  | 3     | 304 | LUT  | C28-C29-C30-C31 |
| 36  | 3     | 305 | LUT  | C28-C29-C30-C31 |
| 36  | 7     | 305 | LUT  | C28-C29-C30-C31 |
| 36  | 8     | 302 | LUT  | C28-C29-C30-C31 |
| 36  | 8     | 303 | LUT  | C11-C10-C9-C8   |
| 36  | 9     | 302 | LUT  | C12-C13-C14-C15 |
| 36  | 9     | 303 | LUT  | C11-C10-C9-C8   |
| 36  | 9     | 305 | LUT  | C11-C10-C9-C8   |
| 36  | 9     | 305 | LUT  | C32-C33-C34-C35 |
| 36  | 2     | 301 | LUT  | C11-C10-C9-C8   |
| 36  | 5     | 303 | LUT  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 6     | 303 | LUT  | C12-C13-C14-C15 |
| 36  | 6     | 304 | LUT  | C12-C13-C14-C15 |
| 31  | G     | 204 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 4     | 321 | CLA  | CBA-CGA-O2A-C1  |
| 27  | A     | 808 | LMT  | C3-C4-C5-C6     |
| 28  | A     | 809 | LHG  | C27-C28-C29-C30 |
| 28  | A     | 811 | LHG  | C34-C35-C36-C37 |
| 32  | 7     | 318 | CHL  | C8-C10-C11-C12  |
| 30  | A     | 813 | CL0  | C16-C17-C18-C19 |
| 31  | A     | 851 | CLA  | O1D-CGD-O2D-CED |
| 31  | 3     | 310 | CLA  | C4-C3-C5-C6     |
| 28  | 7     | 307 | LHG  | C26-C27-C28-C29 |
| 31  | A     | 814 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 814 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 815 | CLA  | C11-C12-C13-C14 |
| 31  | a     | 312 | CLA  | C6-C7-C8-C9     |
| 31  | 5     | 318 | CLA  | C11-C10-C8-C9   |
| 28  | 6     | 301 | LHG  | C23-C24-C25-C26 |
| 28  | 7     | 307 | LHG  | C27-C28-C29-C30 |
| 37  | J     | 101 | LMG  | C29-C30-C31-C32 |
| 41  | 8     | 305 | DGA  | CA6-CA7-CA8-CA9 |
| 31  | 9     | 313 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 851 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 3     | 301 | BCR  | C37-C22-C23-C24 |
| 26  | 6     | 302 | BCR  | C11-C12-C13-C35 |
| 36  | J     | 103 | LUT  | C7-C8-C9-C19    |
| 36  | 9     | 303 | LUT  | C7-C8-C9-C19    |
| 36  | L     | 304 | LUT  | C11-C12-C13-C20 |
| 36  | 2     | 301 | LUT  | C7-C8-C9-C19    |
| 36  | 6     | 303 | LUT  | C27-C28-C29-C39 |
| 36  | 6     | 304 | LUT  | C31-C32-C33-C40 |
| 28  | A     | 810 | LHG  | C28-C29-C30-C31 |
| 28  | 8     | 304 | LHG  | C32-C33-C34-C35 |
| 33  | B     | 808 | DGD  | C7A-C8A-C9A-CAA |
| 37  | J     | 101 | LMG  | C19-C20-C21-C22 |
| 28  | A     | 810 | LHG  | O1-C1-C2-C3     |
| 28  | 6     | 301 | LHG  | O1-C1-C2-C3     |
| 28  | 6     | 305 | LHG  | O1-C1-C2-C3     |
| 26  | 3     | 302 | BCR  | C7-C8-C9-C10    |
| 36  | J     | 103 | LUT  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 7     | 305 | LUT  | C27-C28-C29-C30 |
| 36  | 7     | 305 | LUT  | C31-C32-C33-C34 |
| 36  | 8     | 302 | LUT  | C7-C8-C9-C10    |
| 36  | 2     | 301 | LUT  | C31-C32-C33-C34 |
| 36  | 4     | 302 | LUT  | C31-C32-C33-C34 |
| 36  | 4     | 303 | LUT  | C11-C12-C13-C14 |
| 36  | 6     | 303 | LUT  | C27-C28-C29-C30 |
| 31  | B     | 817 | CLA  | C3-C5-C6-C7     |
| 32  | 7     | 317 | CHL  | C3-C5-C6-C7     |
| 31  | B     | 813 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 822 | CLA  | C8-C10-C11-C12  |
| 28  | B     | 807 | LHG  | C24-C25-C26-C27 |
| 37  | a     | 301 | LMG  | C31-C32-C33-C34 |
| 28  | 5     | 305 | LHG  | C7-C8-C9-C10    |
| 28  | 5     | 305 | LHG  | C23-C24-C25-C26 |
| 27  | 5     | 301 | LMT  | C2-C3-C4-C5     |
| 28  | A     | 809 | LHG  | C11-C10-C9-C8   |
| 28  | A     | 810 | LHG  | C32-C33-C34-C35 |
| 28  | a     | 306 | LHG  | C24-C25-C26-C27 |
| 37  | a     | 301 | LMG  | C36-C37-C38-C39 |
| 31  | B     | 823 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 823 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 837 | CLA  | C8-C10-C11-C12  |
| 28  | a     | 306 | LHG  | C26-C27-C28-C29 |
| 28  | 7     | 307 | LHG  | C28-C29-C30-C31 |
| 28  | 8     | 304 | LHG  | C27-C28-C29-C30 |
| 28  | 5     | 305 | LHG  | C9-C10-C11-C12  |
| 37  | J     | 101 | LMG  | C11-C12-C13-C14 |
| 37  | a     | 301 | LMG  | C33-C34-C35-C36 |
| 28  | a     | 306 | LHG  | C11-C10-C9-C8   |
| 28  | 8     | 304 | LHG  | C11-C12-C13-C14 |
| 42  | 4     | 304 | SQD  | C9-C10-C11-C12  |
| 34  | B     | 851 | LAP  | C4-C5-C6-C7     |
| 31  | 3     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 28  | a     | 306 | LHG  | C27-C28-C29-C30 |
| 31  | B     | 817 | CLA  | O1D-CGD-O2D-CED |
| 31  | L     | 305 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 846 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 855 | CLA  | C3A-C2A-CAA-CBA |
| 31  | B     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 31  | a     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 3     | 309 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 9     | 319 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 9     | 321 | CLA  | C3A-C2A-CAA-CBA |
| 31  | L     | 307 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 302 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 4     | 305 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 4     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 37  | a     | 301 | LMG  | O6-C5-C6-O5     |
| 36  | 8     | 302 | LUT  | C13-C14-C15-C35 |
| 27  | 9     | 306 | LMT  | C2-C3-C4-C5     |
| 27  | 9     | 306 | LMT  | C7-C8-C9-C10    |
| 28  | A     | 811 | LHG  | C16-C17-C18-C19 |
| 28  | 7     | 302 | LHG  | C17-C18-C19-C20 |
| 32  | 9     | 320 | CHL  | C2C-C3C-CAC-CBC |
| 28  | a     | 306 | LHG  | C31-C32-C33-C34 |
| 28  | 8     | 304 | LHG  | C15-C16-C17-C18 |
| 28  | 8     | 304 | LHG  | C34-C35-C36-C37 |
| 31  | B     | 844 | CLA  | CBD-CGD-O2D-CED |
| 43  | 5     | 306 | PTY  | C31-C32-C33-C34 |
| 26  | 6     | 302 | BCR  | C14-C15-C16-C17 |
| 31  | A     | 855 | CLA  | C3-C5-C6-C7     |
| 37  | G     | 202 | LMG  | C11-C12-C13-C14 |
| 31  | B     | 825 | CLA  | C4-C3-C5-C6     |
| 31  | 4     | 307 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 825 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 836 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 840 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 310 | CLA  | C2-C3-C5-C6     |
| 31  | 4     | 307 | CLA  | C2-C3-C5-C6     |
| 28  | a     | 306 | LHG  | C29-C30-C31-C32 |
| 31  | A     | 856 | CLA  | C2A-CAA-CBA-CGA |
| 28  | A     | 810 | LHG  | O1-C1-C2-O2     |
| 28  | 7     | 302 | LHG  | C26-C27-C28-C29 |
| 30  | A     | 813 | CL0  | C16-C17-C18-C20 |
| 31  | B     | 822 | CLA  | C4C-C3C-CAC-CBC |
| 33  | B     | 808 | DGD  | C2B-C3B-C4B-C5B |
| 31  | 3     | 313 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 33  | B     | 808 | DGD  | C4A-C5A-C6A-C7A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 3     | 309 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 853 | CLA  | C15-C16-C17-C18 |
| 31  | B     | 830 | CLA  | C5-C6-C7-C8     |
| 35  | F     | 303 | QTB  | C03-C04-C05-C06 |
| 35  | a     | 302 | QTB  | C03-C04-C05-C06 |
| 35  | 7     | 303 | QTB  | C03-C04-C05-C06 |
| 31  | 4     | 321 | CLA  | O1A-CGA-O2A-C1  |
| 34  | B     | 851 | LAP  | C16-C17-N8-C18  |
| 26  | A     | 805 | BCR  | C23-C24-C25-C26 |
| 26  | A     | 805 | BCR  | C23-C24-C25-C30 |
| 26  | B     | 805 | BCR  | C23-C24-C25-C26 |
| 26  | G     | 203 | BCR  | C5-C6-C7-C8     |
| 26  | G     | 203 | BCR  | C23-C24-C25-C26 |
| 26  | G     | 203 | BCR  | C23-C24-C25-C30 |
| 26  | I     | 801 | BCR  | C5-C6-C7-C8     |
| 26  | J     | 102 | BCR  | C23-C24-C25-C26 |
| 26  | J     | 102 | BCR  | C23-C24-C25-C30 |
| 26  | K     | 203 | BCR  | C23-C24-C25-C26 |
| 26  | M     | 101 | BCR  | C23-C24-C25-C26 |
| 26  | 3     | 301 | BCR  | C5-C6-C7-C8     |
| 26  | 3     | 301 | BCR  | C23-C24-C25-C26 |
| 26  | 3     | 302 | BCR  | C5-C6-C7-C8     |
| 26  | 7     | 304 | BCR  | C23-C24-C25-C26 |
| 26  | 7     | 304 | BCR  | C23-C24-C25-C30 |
| 26  | 8     | 301 | BCR  | C5-C6-C7-C8     |
| 26  | 8     | 301 | BCR  | C23-C24-C25-C26 |
| 26  | L     | 302 | BCR  | C5-C6-C7-C8     |
| 26  | L     | 303 | BCR  | C23-C24-C25-C26 |
| 26  | 2     | 302 | BCR  | C1-C6-C7-C8     |
| 26  | 2     | 302 | BCR  | C5-C6-C7-C8     |
| 26  | 2     | 302 | BCR  | C23-C24-C25-C26 |
| 26  | 5     | 302 | BCR  | C23-C24-C25-C26 |
| 26  | 6     | 302 | BCR  | C5-C6-C7-C8     |
| 26  | 6     | 302 | BCR  | C23-C24-C25-C26 |
| 26  | 6     | 302 | BCR  | C23-C24-C25-C30 |
| 32  | 5     | 316 | CHL  | C3-C5-C6-C7     |
| 36  | 3     | 304 | LUT  | C1-C6-C7-C8     |
| 36  | 7     | 305 | LUT  | C1-C6-C7-C8     |
| 36  | 8     | 303 | LUT  | C5-C6-C7-C8     |
| 36  | 9     | 303 | LUT  | C1-C6-C7-C8     |
| 36  | 9     | 303 | LUT  | C5-C6-C7-C8     |
| 36  | b     | 301 | LUT  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 4     | 303 | LUT  | C1-C6-C7-C8     |
| 38  | a     | 304 | AXT  | C25-C26-C27-C28 |
| 28  | a     | 306 | LHG  | C34-C35-C36-C37 |
| 28  | 7     | 302 | LHG  | C32-C33-C34-C35 |
| 31  | B     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 31  | b     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 2     | 306 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 821 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 848 | CLA  | C15-C16-C17-C18 |
| 31  | 4     | 309 | CLA  | C5-C6-C7-C8     |
| 32  | 7     | 318 | CHL  | C15-C16-C17-C18 |
| 28  | A     | 811 | LHG  | C8-C7-O7-C5     |
| 37  | J     | 101 | LMG  | C11-C10-O7-C8   |
| 31  | G     | 204 | CLA  | O1A-CGA-O2A-C1  |
| 33  | 7     | 308 | DGD  | O1A-C1A-O1G-C1G |
| 31  | 4     | 307 | CLA  | C11-C10-C8-C9   |
| 28  | A     | 810 | LHG  | C23-C24-C25-C26 |
| 28  | A     | 811 | LHG  | C11-C10-C9-C8   |
| 28  | 7     | 302 | LHG  | C25-C26-C27-C28 |
| 28  | 7     | 307 | LHG  | C29-C30-C31-C32 |
| 31  | A     | 842 | CLA  | C13-C15-C16-C17 |
| 32  | 7     | 318 | CHL  | C13-C15-C16-C17 |
| 27  | 9     | 306 | LMT  | C3-C4-C5-C6     |
| 28  | 7     | 302 | LHG  | C28-C29-C30-C31 |
| 28  | 7     | 302 | LHG  | C29-C30-C31-C32 |
| 31  | A     | 827 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 833 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 840 | CLA  | C4-C3-C5-C6     |
| 31  | 7     | 311 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 814 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 814 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 815 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 833 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 311 | CLA  | C2-C3-C5-C6     |
| 31  | 5     | 318 | CLA  | C11-C10-C8-C7   |
| 32  | 7     | 318 | CHL  | C12-C13-C15-C16 |
| 32  | 7     | 324 | CHL  | C11-C12-C13-C15 |
| 31  | 7     | 315 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 7     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 33  | B     | 808 | DGD  | O1A-C1A-O1G-C1G |
| 31  | 8     | 310 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 5     | 304 | LUT  | C33-C34-C35-C15 |
| 28  | 7     | 307 | LHG  | O9-C7-O7-C5     |
| 33  | B     | 808 | DGD  | O1B-C1B-O2G-C2G |
| 28  | A     | 809 | LHG  | C7-C8-C9-C10    |
| 28  | A     | 811 | LHG  | C12-C13-C14-C15 |
| 31  | L     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 315 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 850 | CLA  | O1D-CGD-O2D-CED |
| 31  | 9     | 311 | CLA  | C5-C6-C7-C8     |
| 33  | 7     | 308 | DGD  | C9B-CAB-CBB-CCB |
| 41  | 8     | 305 | DGA  | CB1-CB2-CB3-CB4 |
| 37  | G     | 202 | LMG  | C15-C16-C17-C18 |
| 37  | a     | 301 | LMG  | C32-C33-C34-C35 |
| 27  | A     | 807 | LMT  | C5-C6-C7-C8     |
| 26  | A     | 805 | BCR  | C22-C23-C24-C25 |
| 37  | G     | 202 | LMG  | O10-C28-O8-C9   |
| 31  | B     | 837 | CLA  | C6-C7-C8-C10    |
| 28  | B     | 807 | LHG  | C8-C7-O7-C5     |
| 39  | 7     | 301 | 3PH  | C22-C21-O21-C2  |
| 41  | 8     | 305 | DGA  | CB2-CB1-OG2-CG2 |
| 37  | J     | 104 | LMG  | O6-C5-C6-O5     |
| 26  | L     | 303 | BCR  | C18-C19-C20-C21 |
| 28  | 7     | 307 | LHG  | C24-C25-C26-C27 |
| 31  | A     | 818 | CLA  | C5-C6-C7-C8     |
| 33  | 7     | 308 | DGD  | O1B-C1B-O2G-C2G |
| 39  | 7     | 301 | 3PH  | O22-C21-O21-C2  |
| 41  | 8     | 305 | DGA  | OB1-CB1-OG2-CG2 |
| 28  | A     | 811 | LHG  | C29-C30-C31-C32 |
| 31  | B     | 815 | CLA  | C10-C11-C12-C13 |
| 28  | 7     | 302 | LHG  | O7-C5-C6-O8     |
| 33  | B     | 808 | DGD  | O2G-C2G-C3G-O3G |
| 43  | 5     | 306 | PTY  | C32-C33-C34-C35 |
| 28  | A     | 810 | LHG  | C27-C28-C29-C30 |
| 31  | B     | 836 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 827 | CLA  | C2-C3-C5-C6     |
| 28  | 7     | 307 | LHG  | C11-C10-C9-C8   |
| 31  | A     | 837 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 853 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 857 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 819 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 824 | CLA  | C11-C10-C8-C9   |
| 31  | 7     | 312 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | 7     | 324 | CHL  | C11-C12-C13-C14 |
| 31  | A     | 853 | CLA  | O1D-CGD-O2D-CED |
| 31  | 4     | 316 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 32  | 6     | 319 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 4     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 26  | K     | 202 | BCR  | C7-C8-C9-C34    |
| 26  | L     | 302 | BCR  | C37-C22-C23-C24 |
| 36  | 9     | 302 | LUT  | C31-C32-C33-C40 |
| 36  | 9     | 303 | LUT  | C11-C12-C13-C20 |
| 31  | 3     | 310 | CLA  | C2C-C3C-CAC-CBC |
| 37  | a     | 301 | LMG  | C11-C12-C13-C14 |
| 36  | 4     | 303 | LUT  | C7-C8-C9-C10    |
| 36  | 5     | 304 | LUT  | C11-C12-C13-C14 |
| 36  | 6     | 304 | LUT  | C27-C28-C29-C30 |
| 31  | b     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 2     | 306 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 843 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 848 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 322 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 321 | CLA  | C1A-C2A-CAA-CBA |
| 31  | L     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | O     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 302 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 321 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 5     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 307 | CLA  | C1A-C2A-CAA-CBA |
| 32  | A     | 831 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 8     | 316 | CHL  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | 5     | 316 | CHL  | C1A-C2A-CAA-CBA |
| 32  | 5     | 322 | CHL  | C1A-C2A-CAA-CBA |
| 31  | A     | 841 | CLA  | C16-C17-C18-C20 |
| 31  | B     | 827 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 837 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 839 | CLA  | C11-C12-C13-C15 |
| 31  | a     | 311 | CLA  | C11-C12-C13-C14 |
| 37  | G     | 202 | LMG  | O9-C10-O7-C8    |
| 32  | 5     | 317 | CHL  | C4C-C3C-CAC-CBC |
| 37  | G     | 202 | LMG  | C31-C32-C33-C34 |
| 37  | a     | 301 | LMG  | C14-C15-C16-C17 |
| 31  | A     | 837 | CLA  | C10-C11-C12-C13 |
| 32  | 8     | 316 | CHL  | C10-C11-C12-C13 |
| 28  | A     | 809 | LHG  | C3-O3-P-O6      |
| 28  | a     | 306 | LHG  | C4-O6-P-O3      |
| 28  | 7     | 307 | LHG  | C4-O6-P-O3      |
| 28  | 6     | 301 | LHG  | C4-O6-P-O3      |
| 27  | 9     | 306 | LMT  | C4'-C5'-C6'-O6' |
| 32  | a     | 318 | CHL  | C4C-C3C-CAC-CBC |
| 31  | A     | 816 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 853 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 855 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 855 | CLA  | C8-C10-C11-C12  |
| 43  | 5     | 306 | PTY  | O14-C5-C6-C1    |
| 32  | K     | 201 | CHL  | CBA-CGA-O2A-C1  |
| 28  | a     | 306 | LHG  | C23-C24-C25-C26 |
| 31  | 6     | 312 | CLA  | C16-C17-C18-C20 |
| 28  | 8     | 304 | LHG  | C16-C17-C18-C19 |
| 31  | b     | 313 | CLA  | C2C-C3C-CAC-CBC |
| 32  | A     | 840 | CHL  | C3-C5-C6-C7     |
| 33  | B     | 808 | DGD  | C3A-C4A-C5A-C6A |
| 32  | a     | 317 | CHL  | CBA-CGA-O2A-C1  |
| 32  | 7     | 320 | CHL  | CBA-CGA-O2A-C1  |
| 28  | 7     | 307 | LHG  | C1-C2-C3-O3     |
| 31  | A     | 823 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 309 | CLA  | C2-C3-C5-C6     |
| 31  | a     | 319 | CLA  | C13-C15-C16-C17 |
| 31  | 9     | 317 | CLA  | C2-C1-O2A-CGA   |
| 37  | J     | 101 | LMG  | C18-C19-C20-C21 |
| 31  | B     | 831 | CLA  | O1D-CGD-O2D-CED |
| 31  | B     | 832 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | A     | 809 | LHG  | C18-C19-C20-C21 |
| 28  | 8     | 304 | LHG  | C4-C5-C6-O8     |
| 39  | 7     | 301 | 3PH  | C1-C2-C3-O31    |
| 31  | B     | 816 | CLA  | O1D-CGD-O2D-CED |
| 31  | A     | 857 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 852 | CLA  | O1D-CGD-O2D-CED |
| 34  | B     | 851 | LAP  | C6-C7-C8-C9     |
| 31  | A     | 849 | CLA  | CBA-CGA-O2A-C1  |
| 28  | A     | 809 | LHG  | O1-C1-C2-O2     |
| 27  | A     | 807 | LMT  | C9-C10-C11-C12  |
| 37  | G     | 202 | LMG  | C37-C38-C39-C40 |
| 37  | J     | 101 | LMG  | C16-C17-C18-C19 |
| 33  | 7     | 308 | DGD  | C1A-C2A-C3A-C4A |
| 28  | 7     | 307 | LHG  | C8-C7-O7-C5     |
| 26  | B     | 804 | BCR  | C20-C21-C22-C37 |
| 26  | F     | 302 | BCR  | C35-C13-C14-C15 |
| 26  | I     | 801 | BCR  | C20-C21-C22-C37 |
| 31  | 8     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 834 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 853 | CLA  | C4-C3-C5-C6     |
| 31  | 8     | 315 | CLA  | C4-C3-C5-C6     |
| 31  | L     | 305 | CLA  | C4-C3-C5-C6     |
| 28  | 5     | 305 | LHG  | C27-C28-C29-C30 |
| 31  | A     | 823 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 834 | CLA  | C2-C3-C5-C6     |
| 28  | 6     | 305 | LHG  | C7-C8-C9-C10    |
| 39  | 7     | 301 | 3PH  | C21-C22-C23-C24 |
| 31  | A     | 855 | CLA  | C16-C17-C18-C20 |
| 31  | O     | 203 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 316 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 833 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 28  | a     | 306 | LHG  | C9-C10-C11-C12  |
| 32  | 6     | 320 | CHL  | C4C-C3C-CAC-CBC |
| 28  | A     | 811 | LHG  | C23-C24-C25-C26 |
| 37  | G     | 202 | LMG  | C28-C29-C30-C31 |
| 31  | A     | 819 | CLA  | C3-C5-C6-C7     |
| 27  | A     | 807 | LMT  | C4-C5-C6-C7     |
| 28  | A     | 809 | LHG  | C10-C11-C12-C13 |
| 31  | 8     | 318 | CLA  | CBA-CGA-O2A-C1  |
| 39  | 7     | 301 | 3PH  | C32-C31-O31-C3  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | 6     | 301 | LHG  | O6-C4-C5-O7     |
| 31  | B     | 847 | CLA  | C16-C17-C18-C20 |
| 31  | a     | 311 | CLA  | C11-C12-C13-C15 |
| 31  | 4     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 26  | I     | 801 | BCR  | C20-C21-C22-C23 |
| 26  | K     | 202 | BCR  | C20-C21-C22-C23 |
| 26  | 7     | 304 | BCR  | C16-C17-C18-C19 |
| 26  | 6     | 302 | BCR  | C11-C10-C9-C8   |
| 36  | 7     | 305 | LUT  | C11-C10-C9-C8   |
| 36  | 5     | 304 | LUT  | C28-C29-C30-C31 |
| 36  | 6     | 303 | LUT  | C28-C29-C30-C31 |
| 28  | 6     | 301 | LHG  | O7-C5-C6-O8     |
| 37  | a     | 301 | LMG  | O1-C7-C8-O7     |
| 31  | B     | 814 | CLA  | C8-C10-C11-C12  |
| 32  | a     | 317 | CHL  | O1A-CGA-O2A-C1  |
| 31  | A     | 818 | CLA  | C4-C3-C5-C6     |
| 31  | a     | 315 | CLA  | C4-C3-C5-C6     |
| 31  | a     | 319 | CLA  | C4-C3-C5-C6     |
| 31  | 3     | 313 | CLA  | C4-C3-C5-C6     |
| 32  | a     | 317 | CHL  | C4-C3-C5-C6     |
| 31  | F     | 301 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 311 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 818 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 826 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 837 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 841 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 853 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 815 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 820 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 824 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 825 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 842 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 844 | CLA  | C12-C13-C15-C16 |
| 31  | a     | 312 | CLA  | C11-C10-C8-C7   |
| 31  | 3     | 307 | CLA  | C12-C13-C15-C16 |
| 31  | 3     | 309 | CLA  | C6-C7-C8-C10    |
| 31  | 3     | 311 | CLA  | C11-C10-C8-C7   |
| 31  | 3     | 313 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 312 | CLA  | C11-C10-C8-C7   |
| 31  | 8     | 308 | CLA  | C11-C10-C8-C7   |
| 31  | 8     | 310 | CLA  | C6-C7-C8-C10    |
| 31  | L     | 305 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | A     | 831 | CHL  | C11-C10-C8-C7   |
| 32  | 7     | 318 | CHL  | C6-C7-C8-C10    |
| 28  | 6     | 305 | LHG  | C27-C28-C29-C30 |
| 32  | 6     | 321 | CHL  | C4C-C3C-CAC-CBC |
| 37  | J     | 101 | LMG  | C24-C25-C26-C27 |
| 31  | A     | 815 | CLA  | C11-C12-C13-C14 |
| 31  | A     | 826 | CLA  | C11-C10-C8-C9   |
| 31  | A     | 838 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 841 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 820 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 824 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 825 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 840 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 844 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 844 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 848 | CLA  | C14-C13-C15-C16 |
| 31  | 7     | 311 | CLA  | C11-C10-C8-C9   |
| 31  | 7     | 311 | CLA  | C14-C13-C15-C16 |
| 31  | 8     | 308 | CLA  | C11-C10-C8-C9   |
| 31  | 8     | 310 | CLA  | C6-C7-C8-C9     |
| 31  | 9     | 314 | CLA  | C6-C7-C8-C9     |
| 31  | 9     | 321 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 855 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 312 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 9     | 318 | CLA  | CBA-CGA-O2A-C1  |
| 42  | 4     | 304 | SQD  | C24-C23-O48-C46 |
| 28  | a     | 306 | LHG  | C25-C26-C27-C28 |
| 31  | B     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 3     | 303 | BCR  | C7-C8-C9-C34    |
| 36  | b     | 301 | LUT  | C31-C32-C33-C40 |
| 36  | J     | 103 | LUT  | C11-C12-C13-C14 |
| 36  | 6     | 303 | LUT  | C11-C12-C13-C14 |
| 31  | L     | 305 | CLA  | C3-C5-C6-C7     |
| 28  | 7     | 302 | LHG  | C1-C2-C3-O3     |
| 31  | A     | 826 | CLA  | C15-C16-C17-C18 |
| 33  | 7     | 308 | DGD  | C2B-C1B-O2G-C2G |
| 37  | G     | 202 | LMG  | C13-C14-C15-C16 |
| 32  | 7     | 320 | CHL  | O1A-CGA-O2A-C1  |
| 37  | a     | 301 | LMG  | C30-C31-C32-C33 |
| 31  | B     | 847 | CLA  | C15-C16-C17-C18 |
| 31  | a     | 313 | CLA  | C5-C6-C7-C8     |
| 31  | 9     | 315 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | A     | 809 | LHG  | C28-C29-C30-C31 |
| 28  | A     | 810 | LHG  | O6-C4-C5-C6     |
| 28  | 6     | 301 | LHG  | O6-C4-C5-C6     |
| 31  | A     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 9     | 317 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 9     | 320 | CHL  | C4C-C3C-CAC-CBC |
| 31  | A     | 837 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 816 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 846 | CLA  | C4-C3-C5-C6     |
| 32  | 7     | 318 | CHL  | C4-C3-C5-C6     |
| 31  | a     | 315 | CLA  | C2-C3-C5-C6     |
| 31  | a     | 319 | CLA  | C2-C3-C5-C6     |
| 31  | 8     | 315 | CLA  | C2-C3-C5-C6     |
| 32  | a     | 317 | CHL  | C2-C3-C5-C6     |
| 31  | B     | 822 | CLA  | C10-C11-C12-C13 |
| 28  | A     | 811 | LHG  | O9-C7-O7-C5     |
| 31  | 3     | 316 | CLA  | O1A-CGA-O2A-C1  |
| 31  | B     | 818 | CLA  | C3-C5-C6-C7     |
| 32  | 8     | 316 | CHL  | C16-C17-C18-C20 |
| 28  | A     | 811 | LHG  | C10-C11-C12-C13 |
| 31  | A     | 841 | CLA  | C15-C16-C17-C18 |
| 31  | 7     | 321 | CLA  | CBA-CGA-O2A-C1  |
| 41  | 8     | 305 | DGA  | OG2-CB1-CB2-CB3 |
| 28  | 8     | 304 | LHG  | C7-C8-C9-C10    |
| 28  | A     | 809 | LHG  | C13-C14-C15-C16 |
| 31  | B     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 4     | 316 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 312 | CLA  | C3A-C2A-CAA-CBA |
| 28  | a     | 306 | LHG  | C33-C34-C35-C36 |
| 37  | a     | 301 | LMG  | C15-C16-C17-C18 |
| 31  | 3     | 312 | CLA  | C15-C16-C17-C18 |
| 28  | 7     | 302 | LHG  | C4-C5-C6-O8     |
| 33  | B     | 808 | DGD  | C1G-C2G-C3G-O3G |
| 33  | 7     | 308 | DGD  | O1G-C1G-C2G-C3G |
| 37  | J     | 101 | LMG  | C7-C8-C9-O8     |
| 37  | a     | 301 | LMG  | O1-C7-C8-C9     |
| 27  | 5     | 301 | LMT  | C6-C7-C8-C9     |
| 28  | A     | 810 | LHG  | C7-C8-C9-C10    |
| 37  | G     | 202 | LMG  | C8-C9-O8-C28    |
| 43  | 5     | 306 | PTY  | C14-C15-C16-C17 |
| 28  | A     | 810 | LHG  | C29-C30-C31-C32 |
| 31  | O     | 203 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 6     | 312 | CLA  | C16-C17-C18-C19 |
| 31  | B     | 816 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 310 | CLA  | O1D-CGD-O2D-CED |
| 27  | 9     | 306 | LMT  | C5-C6-C7-C8     |
| 28  | 7     | 307 | LHG  | C10-C11-C12-C13 |
| 31  | 3     | 310 | CLA  | C4C-C3C-CAC-CBC |
| 32  | 7     | 320 | CHL  | C2C-C3C-CAC-CBC |
| 31  | 8     | 315 | CLA  | O1D-CGD-O2D-CED |
| 32  | a     | 320 | CHL  | C3C-C2C-CMC-OMC |
| 31  | 8     | 318 | CLA  | O1A-CGA-O2A-C1  |
| 28  | 6     | 305 | LHG  | O1-C1-C2-O2     |
| 31  | 5     | 310 | CLA  | C13-C15-C16-C17 |
| 37  | G     | 202 | LMG  | C36-C37-C38-C39 |
| 42  | 4     | 304 | SQD  | C24-C25-C26-C27 |
| 28  | A     | 810 | LHG  | O6-C4-C5-O7     |
| 31  | 7     | 315 | CLA  | C3-C5-C6-C7     |
| 39  | 7     | 301 | 3PH  | O32-C31-O31-C3  |
| 42  | 4     | 304 | SQD  | O10-C23-O48-C46 |
| 31  | A     | 855 | CLA  | C16-C17-C18-C19 |
| 32  | A     | 840 | CHL  | C16-C17-C18-C19 |
| 42  | 4     | 304 | SQD  | C25-C26-C27-C28 |
| 31  | H     | 901 | CLA  | CBA-CGA-O2A-C1  |
| 28  | 8     | 304 | LHG  | O2-C2-C3-O3     |
| 31  | 3     | 312 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 9     | 318 | CLA  | O1A-CGA-O2A-C1  |
| 35  | 7     | 303 | QTB  | C04-C05-C06-O07 |
| 28  | A     | 811 | LHG  | O7-C5-C6-O8     |
| 33  | 7     | 308 | DGD  | O1G-C1G-C2G-O2G |
| 37  | J     | 101 | LMG  | O1-C7-C8-O7     |
| 31  | A     | 827 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 827 | CLA  | C11-C12-C13-C14 |
| 32  | A     | 840 | CHL  | C16-C17-C18-C20 |
| 28  | A     | 811 | LHG  | C31-C32-C33-C34 |
| 42  | 4     | 304 | SQD  | O5-C1-O6-C44    |
| 31  | B     | 827 | CLA  | C10-C11-C12-C13 |
| 34  | B     | 851 | LAP  | C13-C14-C15-O4  |
| 31  | B     | 814 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 816 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 820 | CLA  | C2-C1-O2A-CGA   |
| 32  | 6     | 309 | CHL  | C2-C1-O2A-CGA   |
| 31  | A     | 837 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 814 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 2     | 313 | CLA  | C2C-C3C-CAC-CBC |
| 31  | B     | 812 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 812 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 814 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 815 | CLA  | C11-C10-C8-C9   |
| 31  | a     | 312 | CLA  | C11-C10-C8-C9   |
| 31  | 3     | 311 | CLA  | C14-C13-C15-C16 |
| 31  | L     | 305 | CLA  | C11-C10-C8-C9   |
| 31  | b     | 313 | CLA  | C11-C10-C8-C9   |
| 32  | a     | 317 | CHL  | C11-C10-C8-C9   |
| 28  | 6     | 301 | LHG  | C5-C4-O6-P      |
| 37  | G     | 202 | LMG  | C12-C13-C14-C15 |
| 31  | 8     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 823 | CLA  | CBD-CGD-O2D-CED |
| 26  | A     | 803 | BCR  | C5-C6-C7-C8     |
| 26  | A     | 804 | BCR  | C23-C24-C25-C26 |
| 26  | A     | 805 | BCR  | C1-C6-C7-C8     |
| 26  | A     | 805 | BCR  | C5-C6-C7-C8     |
| 26  | B     | 803 | BCR  | C1-C6-C7-C8     |
| 26  | B     | 803 | BCR  | C5-C6-C7-C8     |
| 26  | B     | 804 | BCR  | C23-C24-C25-C26 |
| 26  | B     | 804 | BCR  | C23-C24-C25-C30 |
| 26  | B     | 805 | BCR  | C5-C6-C7-C8     |
| 26  | B     | 806 | BCR  | C1-C6-C7-C8     |
| 26  | B     | 806 | BCR  | C5-C6-C7-C8     |
| 26  | G     | 201 | BCR  | C5-C6-C7-C8     |
| 26  | G     | 201 | BCR  | C23-C24-C25-C26 |
| 26  | G     | 201 | BCR  | C23-C24-C25-C30 |
| 26  | K     | 202 | BCR  | C1-C6-C7-C8     |
| 26  | K     | 202 | BCR  | C5-C6-C7-C8     |
| 26  | K     | 203 | BCR  | C1-C6-C7-C8     |
| 26  | K     | 203 | BCR  | C5-C6-C7-C8     |
| 26  | M     | 101 | BCR  | C1-C6-C7-C8     |
| 26  | M     | 101 | BCR  | C5-C6-C7-C8     |
| 26  | 3     | 302 | BCR  | C23-C24-C25-C26 |
| 26  | 3     | 302 | BCR  | C23-C24-C25-C30 |
| 26  | 3     | 303 | BCR  | C5-C6-C7-C8     |
| 26  | 3     | 303 | BCR  | C23-C24-C25-C26 |
| 26  | 3     | 303 | BCR  | C23-C24-C25-C30 |
| 26  | 8     | 301 | BCR  | C1-C6-C7-C8     |
| 26  | L     | 303 | BCR  | C5-C6-C7-C8     |
| 26  | O     | 201 | BCR  | C1-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | O     | 201 | BCR  | C5-C6-C7-C8     |
| 26  | 2     | 302 | BCR  | C23-C24-C25-C30 |
| 32  | 7     | 324 | CHL  | C3-C5-C6-C7     |
| 36  | 9     | 302 | LUT  | C1-C6-C7-C8     |
| 36  | L     | 304 | LUT  | C5-C6-C7-C8     |
| 26  | 7     | 304 | BCR  | C7-C8-C9-C34    |
| 26  | L     | 303 | BCR  | C36-C18-C19-C20 |
| 33  | B     | 808 | DGD  | C8A-C9A-CAA-CBA |
| 26  | A     | 806 | BCR  | C7-C8-C9-C10    |
| 26  | F     | 302 | BCR  | C21-C22-C23-C24 |
| 26  | G     | 203 | BCR  | C17-C18-C19-C20 |
| 36  | 4     | 302 | LUT  | C11-C12-C13-C14 |
| 31  | A     | 846 | CLA  | C10-C11-C12-C13 |
| 33  | 7     | 308 | DGD  | C1B-C2B-C3B-C4B |
| 31  | B     | 840 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 9     | 314 | CLA  | C11-C12-C13-C14 |
| 35  | 7     | 303 | QTB  | C09-C10-C11-C17 |
| 31  | A     | 838 | CLA  | C8-C10-C11-C12  |
| 31  | 8     | 320 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 825 | CLA  | C10-C11-C12-C13 |
| 24  | B     | 801 | PQN  | C16-C17-C18-C20 |
| 31  | A     | 830 | CLA  | C6-C7-C8-C10    |
| 31  | A     | 838 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 812 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 812 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 814 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 817 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 840 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 844 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 846 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 848 | CLA  | C12-C13-C15-C16 |
| 31  | 7     | 311 | CLA  | C12-C13-C15-C16 |
| 31  | 9     | 314 | CLA  | C6-C7-C8-C10    |
| 31  | 9     | 321 | CLA  | C6-C7-C8-C10    |
| 31  | b     | 313 | CLA  | C11-C10-C8-C7   |
| 26  | 5     | 302 | BCR  | C19-C20-C21-C22 |
| 35  | 7     | 303 | QTB  | C02-C03-C04-C05 |
| 36  | 8     | 302 | LUT  | C9-C10-C11-C12  |
| 36  | 9     | 302 | LUT  | C33-C34-C35-C15 |
| 36  | 9     | 305 | LUT  | C9-C10-C11-C12  |
| 36  | 4     | 302 | LUT  | C33-C34-C35-C15 |
| 31  | A     | 841 | CLA  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 847 | CLA  | C16-C17-C18-C19 |
| 27  | A     | 808 | LMT  | C1-C2-C3-C4     |
| 31  | 8     | 320 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 839 | CLA  | C5-C6-C7-C8     |
| 31  | 7     | 312 | CLA  | C8-C10-C11-C12  |
| 26  | 3     | 301 | BCR  | C20-C21-C22-C37 |
| 27  | A     | 807 | LMT  | C11-C10-C9-C8   |
| 27  | A     | 808 | LMT  | O5'-C5'-C6'-O6' |
| 35  | 7     | 303 | QTB  | C01-C02-C03-C04 |
| 35  | 9     | 304 | QTB  | C01-C02-C03-C04 |
| 32  | 8     | 316 | CHL  | C16-C17-C18-C19 |
| 28  | A     | 810 | LHG  | C24-C23-O8-C6   |
| 31  | A     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 5     | 316 | CHL  | CBA-CGA-O2A-C1  |
| 37  | G     | 202 | LMG  | C29-C28-O8-C9   |
| 37  | J     | 104 | LMG  | C29-C28-O8-C9   |
| 31  | 8     | 320 | CLA  | C8-C10-C11-C12  |
| 31  | A     | 826 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 829 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 850 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 815 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 822 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 824 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 826 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 843 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 3     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 7     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 8     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 9     | 314 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 307 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 310 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 4     | 308 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 4     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 5     | 307 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 5     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 32  | A     | 831 | CHL  | CAD-CBD-CGD-O2D |
| 32  | A     | 840 | CHL  | CAD-CBD-CGD-O2D |
| 32  | a     | 317 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 8     | 319 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 4     | 313 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 6     | 318 | CHL  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | 6     | 320 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 6     | 321 | CHL  | CAD-CBD-CGD-O2D |
| 43  | 5     | 306 | PTY  | C5-C6-O7-C8     |
| 28  | 7     | 302 | LHG  | C13-C14-C15-C16 |
| 28  | 7     | 307 | LHG  | C7-C8-C9-C10    |
| 31  | 6     | 308 | CLA  | C2C-C3C-CAC-CBC |
| 31  | B     | 813 | CLA  | C4-C3-C5-C6     |
| 33  | 7     | 308 | DGD  | CBB-CCB-CDB-CEB |
| 37  | G     | 202 | LMG  | C7-C8-C9-O8     |
| 42  | 4     | 304 | SQD  | O6-C44-C45-C46  |
| 31  | B     | 845 | CLA  | CBD-CGD-O2D-CED |
| 28  | 5     | 305 | LHG  | O6-C4-C5-O7     |
| 43  | 5     | 306 | PTY  | O14-C5-C6-O7    |
| 31  | B     | 840 | CLA  | C10-C11-C12-C13 |
| 31  | B     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 26  | M     | 101 | BCR  | C14-C15-C16-C17 |
| 31  | 9     | 319 | CLA  | CBA-CGA-O2A-C1  |
| 28  | 8     | 304 | LHG  | C1-C2-C3-O3     |
| 31  | A     | 817 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 838 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 843 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 847 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 848 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 849 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 850 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 813 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 822 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 824 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 834 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 838 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 848 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 849 | CLA  | CHA-CBD-CGD-O1D |
| 31  | G     | 205 | CLA  | CHA-CBD-CGD-O1D |
| 31  | K     | 206 | CLA  | CHA-CBD-CGD-O1D |
| 31  | a     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 31  | a     | 316 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 313 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 9     | 313 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 9     | 314 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 9     | 315 | CLA  | CHA-CBD-CGD-O2D |
| 31  | L     | 306 | CLA  | CHA-CBD-CGD-O2D |
| 31  | b     | 303 | CLA  | CHA-CBD-CGD-O2D |
| 31  | b     | 313 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 304 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 304 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 2     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 4     | 308 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 4     | 319 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 4     | 320 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 4     | 320 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 5     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 5     | 323 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 313 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 322 | CLA  | CHA-CBD-CGD-O1D |
| 32  | K     | 201 | CHL  | CHA-CBD-CGD-O1D |
| 32  | K     | 201 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 7     | 324 | CHL  | CHA-CBD-CGD-O2D |
| 32  | b     | 309 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 4     | 310 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 6     | 317 | CHL  | CHA-CBD-CGD-O2D |
| 31  | 9     | 317 | CLA  | O1A-CGA-O2A-C1  |
| 26  | I     | 801 | BCR  | C16-C17-C18-C19 |
| 26  | L     | 301 | BCR  | C20-C21-C22-C23 |
| 36  | 8     | 303 | LUT  | C28-C29-C30-C31 |
| 36  | 4     | 302 | LUT  | C12-C13-C14-C15 |
| 28  | 7     | 302 | LHG  | C11-C12-C13-C14 |
| 28  | A     | 809 | LHG  | O7-C5-C6-O8     |
| 37  | G     | 202 | LMG  | O7-C8-C9-O8     |
| 37  | J     | 101 | LMG  | O7-C8-C9-O8     |
| 28  | A     | 810 | LHG  | C33-C34-C35-C36 |
| 27  | 5     | 301 | LMT  | C4'-C5'-C6'-O6' |
| 31  | 9     | 318 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 855 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 7     | 321 | CLA  | O1A-CGA-O2A-C1  |
| 31  | a     | 312 | CLA  | C16-C17-C18-C20 |
| 37  | J     | 101 | LMG  | C20-C21-C22-C23 |
| 31  | B     | 832 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 835 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 318 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 835 | CLA  | C2-C3-C5-C6     |
| 31  | 7     | 312 | CLA  | C14-C13-C15-C16 |
| 31  | 8     | 310 | CLA  | C11-C10-C8-C9   |
| 31  | 8     | 320 | CLA  | O1A-CGA-O2A-C1  |
| 32  | 5     | 316 | CHL  | O1A-CGA-O2A-C1  |
| 31  | B     | 812 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 843 | CLA  | CBD-CGD-O2D-CED |
| 28  | A     | 809 | LHG  | C16-C17-C18-C19 |
| 31  | A     | 827 | CLA  | O1A-CGA-O2A-C1  |
| 26  | 2     | 302 | BCR  | C7-C8-C9-C34    |
| 26  | 2     | 302 | BCR  | C7-C8-C9-C10    |
| 31  | A     | 835 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 847 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 847 | CLA  | C1A-C2A-CAA-CBA |
| 31  | F     | 305 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 31  | a     | 321 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 315 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 311 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 322 | CLA  | C1A-C2A-CAA-CBA |
| 24  | B     | 801 | PQN  | C26-C27-C28-C29 |
| 31  | B     | 846 | CLA  | C16-C17-C18-C20 |
| 31  | A     | 843 | CLA  | C13-C15-C16-C17 |
| 33  | B     | 808 | DGD  | C9B-CAB-CBB-CCB |
| 31  | A     | 841 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 846 | CLA  | C2-C1-O2A-CGA   |
| 31  | 5     | 323 | CLA  | C2-C1-O2A-CGA   |
| 41  | 8     | 305 | DGA  | CB3-CB4-CB5-CB6 |
| 36  | F     | 304 | LUT  | C9-C10-C11-C12  |
| 36  | 3     | 305 | LUT  | C33-C34-C35-C15 |
| 41  | 8     | 305 | DGA  | CA5-CA6-CA7-CA8 |
| 28  | A     | 809 | LHG  | C3-O3-P-O5      |
| 28  | 7     | 302 | LHG  | C3-O3-P-O5      |
| 28  | 7     | 302 | LHG  | C4-O6-P-O4      |
| 28  | 6     | 301 | LHG  | C3-O3-P-O5      |
| 28  | 6     | 301 | LHG  | C4-O6-P-O4      |
| 34  | B     | 851 | LAP  | C16-O6-P9-O5    |
| 34  | B     | 851 | LAP  | C16-O6-P9-O7    |
| 28  | 7     | 302 | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | 9     | 306 | LMT  | C11-C10-C9-C8   |
| 37  | J     | 101 | LMG  | C23-C24-C25-C26 |
| 31  | A     | 826 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 850 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 854 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 822 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 834 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 848 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 849 | CLA  | CAD-CBD-CGD-O1D |
| 31  | K     | 206 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 9     | 313 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 2     | 304 | CLA  | CAD-CBD-CGD-O1D |
| 32  | K     | 201 | CHL  | CAD-CBD-CGD-O1D |
| 31  | A     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 27  | 5     | 301 | LMT  | C3-C4-C5-C6     |
| 43  | 5     | 306 | PTY  | C33-C34-C35-C36 |
| 24  | A     | 801 | PQN  | C26-C27-C28-C30 |
| 28  | A     | 811 | LHG  | O6-C4-C5-O7     |
| 28  | 7     | 302 | LHG  | O6-C4-C5-O7     |
| 31  | A     | 821 | CLA  | C11-C10-C8-C7   |
| 31  | A     | 821 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 813 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 822 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 822 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 827 | CLA  | C6-C7-C8-C10    |
| 31  | 3     | 319 | CLA  | C11-C12-C13-C15 |
| 31  | 7     | 311 | CLA  | C11-C10-C8-C7   |
| 31  | 8     | 311 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 6     | 312 | CLA  | C11-C12-C13-C15 |
| 32  | 7     | 318 | CHL  | C11-C10-C8-C7   |
| 32  | 6     | 309 | CHL  | C11-C12-C13-C15 |
| 41  | 8     | 305 | DGA  | CB2-CB3-CB4-CB5 |
| 31  | 3     | 311 | CLA  | C3-C5-C6-C7     |
| 33  | 7     | 308 | DGD  | C6B-C7B-C8B-C9B |
| 31  | B     | 841 | CLA  | C6-C7-C8-C10    |
| 31  | 9     | 317 | CLA  | C2C-C3C-CAC-CBC |
| 32  | a     | 317 | CHL  | C1C-C2C-CMC-OMC |
| 32  | a     | 318 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 7     | 317 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 7     | 318 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 5     | 317 | CHL  | C1C-C2C-CMC-OMC |
| 32  | 6     | 321 | CHL  | C1C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | B     | 851 | LAP  | O6-C16-C17-N8   |
| 37  | J     | 101 | LMG  | O1-C7-C8-C9     |
| 28  | 8     | 304 | LHG  | O7-C5-C6-O8     |
| 39  | 7     | 301 | 3PH  | O21-C2-C3-O31   |
| 42  | 4     | 304 | SQD  | O6-C44-C45-O47  |
| 31  | 2     | 313 | CLA  | C4C-C3C-CAC-CBC |
| 32  | A     | 831 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 9     | 314 | CLA  | C11-C12-C13-C15 |
| 31  | A     | 848 | CLA  | C3-C5-C6-C7     |
| 31  | 2     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 30  | A     | 813 | CL0  | C15-C16-C17-C18 |
| 31  | B     | 820 | CLA  | C15-C16-C17-C18 |
| 31  | A     | 817 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 31  | B     | 832 | CLA  | C2-C3-C5-C6     |
| 24  | B     | 801 | PQN  | C16-C17-C18-C19 |
| 31  | A     | 830 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 851 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 827 | CLA  | C6-C7-C8-C9     |
| 31  | B     | 835 | CLA  | C6-C7-C8-C9     |
| 31  | 3     | 309 | CLA  | C14-C13-C15-C16 |
| 31  | 3     | 311 | CLA  | C11-C10-C8-C9   |
| 28  | 7     | 302 | LHG  | C14-C15-C16-C17 |
| 31  | A     | 837 | CLA  | O1D-CGD-O2D-CED |
| 31  | 8     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 36  | F     | 304 | LUT  | C10-C11-C12-C13 |
| 36  | a     | 305 | LUT  | C10-C11-C12-C13 |
| 36  | a     | 305 | LUT  | C30-C31-C32-C33 |
| 36  | 9     | 305 | LUT  | C30-C31-C32-C33 |
| 36  | L     | 304 | LUT  | C10-C11-C12-C13 |
| 32  | A     | 840 | CHL  | C8-C10-C11-C12  |
| 31  | B     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 36  | L     | 304 | LUT  | C31-C32-C33-C34 |
| 43  | 5     | 306 | PTY  | C34-C35-C36-C37 |
| 31  | 2     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 7     | 318 | CHL  | C2-C3-C5-C6     |
| 31  | B     | 820 | CLA  | C8-C10-C11-C12  |
| 39  | 7     | 301 | 3PH  | C25-C26-C27-C28 |
| 31  | A     | 849 | CLA  | O1A-CGA-O2A-C1  |
| 32  | K     | 201 | CHL  | O1A-CGA-O2A-C1  |
| 28  | 7     | 302 | LHG  | O6-C4-C5-C6     |
| 31  | B     | 832 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | b     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 317 | CLA  | C4C-C3C-CAC-CBC |
| 31  | A     | 819 | CLA  | C2-C1-O2A-CGA   |
| 31  | A     | 829 | CLA  | C2-C1-O2A-CGA   |
| 31  | 3     | 310 | CLA  | C2-C1-O2A-CGA   |
| 31  | 8     | 311 | CLA  | C2-C1-O2A-CGA   |
| 31  | O     | 203 | CLA  | C2-C1-O2A-CGA   |
| 32  | 7     | 318 | CHL  | C2-C1-O2A-CGA   |
| 32  | 7     | 320 | CHL  | C4C-C3C-CAC-CBC |
| 42  | 4     | 304 | SQD  | C11-C10-C9-C8   |
| 28  | B     | 807 | LHG  | O10-C23-O8-C6   |
| 28  | B     | 807 | LHG  | C11-C10-C9-C8   |
| 31  | 8     | 309 | CLA  | CBA-CGA-O2A-C1  |
| 33  | 7     | 308 | DGD  | C2A-C1A-O1G-C1G |
| 26  | A     | 803 | BCR  | C1-C6-C7-C8     |
| 26  | A     | 803 | BCR  | C23-C24-C25-C26 |
| 26  | A     | 803 | BCR  | C23-C24-C25-C30 |
| 26  | A     | 804 | BCR  | C23-C24-C25-C30 |
| 26  | B     | 805 | BCR  | C1-C6-C7-C8     |
| 26  | B     | 806 | BCR  | C23-C24-C25-C26 |
| 26  | B     | 806 | BCR  | C23-C24-C25-C30 |
| 26  | G     | 201 | BCR  | C1-C6-C7-C8     |
| 26  | L     | 303 | BCR  | C1-C6-C7-C8     |
| 26  | O     | 201 | BCR  | C23-C24-C25-C26 |
| 31  | 5     | 318 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 841 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 848 | CLA  | C13-C15-C16-C17 |
| 32  | 8     | 316 | CHL  | C5-C6-C7-C8     |
| 31  | 3     | 318 | CLA  | CAA-CBA-CGA-O2A |
| 32  | 4     | 310 | CHL  | C2C-C3C-CAC-CBC |
| 37  | G     | 202 | LMG  | C32-C33-C34-C35 |
| 28  | 7     | 302 | LHG  | C34-C35-C36-C37 |
| 30  | A     | 813 | CL0  | C13-C15-C16-C17 |
| 32  | 5     | 317 | CHL  | C2A-CAA-CBA-CGA |
| 32  | 6     | 309 | CHL  | C2A-CAA-CBA-CGA |
| 31  | 2     | 313 | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 804 | BCR  | C11-C10-C9-C8   |
| 36  | 3     | 304 | LUT  | C11-C10-C9-C8   |
| 36  | 4     | 302 | LUT  | C11-C10-C9-C8   |
| 37  | a     | 301 | LMG  | O7-C8-C9-O8     |
| 28  | A     | 810 | LHG  | C3-O3-P-O6      |
| 28  | A     | 811 | LHG  | C3-O3-P-O6      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | B     | 808 | DGD  | O1G-C1G-C2G-C3G |
| 37  | J     | 104 | LMG  | O1-C7-C8-C9     |
| 31  | 4     | 309 | CLA  | C4-C3-C5-C6     |
| 31  | 8     | 308 | CLA  | C8-C10-C11-C12  |
| 27  | A     | 808 | LMT  | C4'-C5'-C6'-O6' |
| 31  | B     | 835 | CLA  | C6-C7-C8-C10    |
| 31  | B     | 822 | CLA  | C11-C10-C8-C9   |
| 31  | 3     | 307 | CLA  | C14-C13-C15-C16 |
| 32  | 6     | 309 | CHL  | C11-C12-C13-C14 |
| 31  | 3     | 312 | CLA  | C13-C15-C16-C17 |
| 31  | a     | 312 | CLA  | C16-C17-C18-C19 |
| 31  | 9     | 321 | CLA  | C5-C6-C7-C8     |
| 41  | 8     | 305 | DGA  | CA4-CA5-CA6-CA7 |
| 37  | G     | 202 | LMG  | C34-C35-C36-C37 |
| 28  | 7     | 302 | LHG  | C2-C3-O3-P      |
| 28  | 7     | 302 | LHG  | C5-C4-O6-P      |
| 31  | A     | 821 | CLA  | C13-C15-C16-C17 |
| 28  | A     | 811 | LHG  | C18-C19-C20-C21 |
| 31  | 4     | 307 | CLA  | C11-C10-C8-C7   |
| 32  | A     | 840 | CHL  | C4-C3-C5-C6     |
| 28  | 6     | 301 | LHG  | O1-C1-C2-O2     |
| 31  | B     | 841 | CLA  | C6-C7-C8-C9     |
| 31  | A     | 838 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 7     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 6     | 311 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 3     | 315 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 5     | 313 | CLA  | CBD-CGD-O2D-CED |
| 28  | 5     | 305 | LHG  | C13-C14-C15-C16 |
| 26  | 3     | 302 | BCR  | C22-C23-C24-C25 |
| 31  | A     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 31  | b     | 306 | CLA  | C2A-CAA-CBA-CGA |
| 32  | 6     | 318 | CHL  | CAA-CBA-CGA-O1A |
| 33  | B     | 808 | DGD  | C2G-C1G-O1G-C1A |
| 26  | B     | 805 | BCR  | C19-C20-C21-C22 |
| 36  | 6     | 304 | LUT  | C9-C10-C11-C12  |
| 40  | 7     | 306 | XAT  | C29-C30-C31-C32 |
| 28  | 5     | 305 | LHG  | O6-C4-C5-C6     |
| 31  | A     | 820 | CLA  | O1A-CGA-O2A-C1  |
| 39  | 7     | 301 | 3PH  | C24-C25-C26-C27 |
| 41  | 8     | 305 | DGA  | CA7-CA8-CA9-CAA |
| 31  | a     | 316 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 4     | 306 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | O     | 203 | CLA  | C3-C5-C6-C7     |
| 31  | 9     | 311 | CLA  | C4-C3-C5-C6     |
| 32  | 7     | 320 | CHL  | C4-C3-C5-C6     |
| 31  | 4     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 832 | CLA  | C2-C3-C5-C6     |
| 31  | 5     | 323 | CLA  | C5-C6-C7-C8     |
| 31  | 7     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 853 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 818 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 841 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 850 | CLA  | C2-C1-O2A-CGA   |
| 31  | G     | 204 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 811 | CLA  | C15-C16-C17-C18 |
| 31  | L     | 305 | CLA  | C10-C11-C12-C13 |
| 31  | 2     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 3     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 32  | A     | 831 | CHL  | C2A-CAA-CBA-CGA |
| 37  | a     | 301 | LMG  | C35-C36-C37-C38 |
| 31  | B     | 813 | CLA  | C8-C10-C11-C12  |
| 37  | a     | 301 | LMG  | C12-C13-C14-C15 |
| 31  | A     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 32  | b     | 309 | CHL  | C3A-C2A-CAA-CBA |
| 31  | 7     | 313 | CLA  | CAA-CBA-CGA-O1A |
| 31  | L     | 307 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 4     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 5     | 318 | CLA  | CAA-CBA-CGA-O2A |
| 36  | a     | 303 | LUT  | C33-C34-C35-C15 |
| 31  | A     | 832 | CLA  | C4-C3-C5-C6     |
| 31  | 6     | 311 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 817 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 821 | CLA  | C11-C10-C8-C9   |
| 31  | B     | 822 | CLA  | C14-C13-C15-C16 |
| 31  | a     | 319 | CLA  | C11-C10-C8-C9   |
| 31  | 6     | 312 | CLA  | C11-C12-C13-C14 |
| 31  | 7     | 310 | CLA  | CAA-CBA-CGA-O2A |
| 26  | A     | 806 | BCR  | C16-C17-C18-C36 |
| 26  | B     | 803 | BCR  | C11-C10-C9-C34  |
| 26  | B     | 806 | BCR  | C20-C21-C22-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | 6     | 302 | BCR  | C20-C21-C22-C37 |
| 36  | L     | 304 | LUT  | C11-C10-C9-C19  |
| 37  | a     | 301 | LMG  | C7-C8-C9-O8     |
| 31  | 4     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 32  | 6     | 318 | CHL  | CAA-CBA-CGA-O2A |
| 31  | 5     | 309 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 33  | B     | 808 | DGD  | C2A-C1A-O1G-C1G |
| 33  | B     | 808 | DGD  | O6E-C1E-O5D-C6D |
| 26  | G     | 203 | BCR  | C36-C18-C19-C20 |
| 26  | K     | 203 | BCR  | C11-C12-C13-C35 |
| 31  | 2     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 4     | 315 | CLA  | CAA-CBA-CGA-O1A |
| 36  | 5     | 303 | LUT  | C27-C28-C29-C39 |
| 26  | M     | 101 | BCR  | C7-C8-C9-C10    |
| 28  | 7     | 302 | LHG  | C9-C10-C11-C12  |
| 31  | 3     | 312 | CLA  | C4-C3-C5-C6     |
| 31  | 9     | 315 | CLA  | C4-C3-C5-C6     |
| 32  | A     | 839 | CHL  | C4-C3-C5-C6     |
| 31  | A     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 844 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 849 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 836 | CLA  | C1A-C2A-CAA-CBA |
| 31  | B     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 3     | 318 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 309 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 7     | 312 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 9     | 317 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 2     | 310 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 314 | CLA  | C1A-C2A-CAA-CBA |
| 32  | b     | 309 | CHL  | C1A-C2A-CAA-CBA |
| 31  | A     | 815 | CLA  | C12-C13-C15-C16 |
| 31  | B     | 814 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 817 | CLA  | C11-C10-C8-C7   |
| 31  | 6     | 312 | CLA  | C6-C7-C8-C10    |
| 32  | 7     | 324 | CHL  | C11-C10-C8-C7   |
| 28  | a     | 306 | LHG  | C18-C19-C20-C21 |
| 24  | B     | 801 | PQN  | C25-C26-C27-C28 |
| 31  | 7     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 31  | L     | 307 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 313 | CLA  | O1D-CGD-O2D-CED |
| 28  | 7     | 307 | LHG  | C30-C31-C32-C33 |
| 32  | A     | 840 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 7     | 320 | CHL  | C3C-C2C-CMC-OMC |
| 32  | 3     | 315 | CHL  | CBA-CGA-O2A-C1  |
| 31  | 7     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 33  | B     | 808 | DGD  | C8B-C9B-CAB-CBB |
| 31  | 9     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 2     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 318 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 6     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 32  | 4     | 317 | CHL  | C2A-CAA-CBA-CGA |
| 31  | A     | 822 | CLA  | C5-C6-C7-C8     |
| 31  | B     | 842 | CLA  | C5-C6-C7-C8     |
| 31  | 3     | 307 | CLA  | C15-C16-C17-C18 |
| 27  | A     | 808 | LMT  | C9-C10-C11-C12  |
| 31  | b     | 304 | CLA  | CBA-CGA-O2A-C1  |
| 31  | 3     | 309 | CLA  | C8-C10-C11-C12  |
| 31  | B     | 847 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 826 | CLA  | C10-C11-C12-C13 |
| 32  | 8     | 316 | CHL  | C15-C16-C17-C18 |
| 31  | B     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 30  | A     | 813 | CL0  | C3-C5-C6-C7     |
| 31  | A     | 815 | CLA  | CBD-CGD-O2D-CED |
| 28  | B     | 807 | LHG  | O9-C7-O7-C5     |
| 26  | A     | 806 | BCR  | C11-C10-C9-C8   |
| 26  | 6     | 302 | BCR  | C20-C21-C22-C23 |
| 36  | a     | 303 | LUT  | C12-C13-C14-C15 |
| 36  | 3     | 305 | LUT  | C9-C10-C11-C12  |
| 36  | 6     | 303 | LUT  | C13-C14-C15-C35 |
| 31  | 4     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 31  | H     | 901 | CLA  | O1A-CGA-O2A-C1  |
| 31  | a     | 316 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 8     | 314 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 824 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 811 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 826 | CLA  | C2-C1-O2A-CGA   |
| 31  | 9     | 315 | CLA  | C2-C3-C5-C6     |
| 31  | 4     | 309 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 6     | 311 | CLA  | C2-C3-C5-C6     |
| 32  | A     | 839 | CHL  | C2-C3-C5-C6     |
| 32  | A     | 840 | CHL  | C2-C3-C5-C6     |
| 32  | 7     | 320 | CHL  | C2-C3-C5-C6     |
| 31  | a     | 314 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 6     | 311 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 841 | CLA  | C6-C7-C8-C9     |
| 32  | 6     | 309 | CHL  | C11-C10-C8-C9   |
| 31  | 4     | 319 | CLA  | C2C-C3C-CAC-CBC |
| 31  | 3     | 311 | CLA  | C13-C15-C16-C17 |
| 31  | B     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 28  | 6     | 305 | LHG  | C11-C10-C9-C8   |
| 31  | A     | 838 | CLA  | O1A-CGA-O2A-C1  |
| 26  | A     | 804 | BCR  | C1-C6-C7-C8     |
| 26  | B     | 802 | BCR  | C1-C6-C7-C8     |
| 26  | F     | 302 | BCR  | C1-C6-C7-C8     |
| 26  | J     | 102 | BCR  | C1-C6-C7-C8     |
| 26  | 3     | 303 | BCR  | C1-C6-C7-C8     |
| 26  | L     | 301 | BCR  | C1-C6-C7-C8     |
| 26  | L     | 301 | BCR  | C5-C6-C7-C8     |
| 26  | L     | 302 | BCR  | C23-C24-C25-C30 |
| 26  | O     | 201 | BCR  | C23-C24-C25-C30 |
| 36  | a     | 305 | LUT  | C1-C6-C7-C8     |
| 31  | B     | 848 | CLA  | CAA-CBA-CGA-O2A |
| 28  | 7     | 302 | LHG  | O1-C1-C2-C3     |
| 31  | 9     | 319 | CLA  | O1A-CGA-O2A-C1  |
| 36  | J     | 103 | LUT  | C13-C14-C15-C35 |
| 36  | 7     | 305 | LUT  | C33-C34-C35-C15 |
| 36  | 8     | 303 | LUT  | C9-C10-C11-C12  |
| 31  | 4     | 316 | CLA  | C2-C1-O2A-CGA   |
| 31  | B     | 817 | CLA  | C4-C3-C5-C6     |
| 31  | 9     | 321 | CLA  | C4-C3-C5-C6     |
| 31  | 2     | 307 | CLA  | C4-C3-C5-C6     |
| 32  | 7     | 318 | CHL  | C16-C17-C18-C19 |
| 27  | 5     | 301 | LMT  | C1-C2-C3-C4     |
| 31  | A     | 851 | CLA  | C13-C15-C16-C17 |
| 33  | B     | 808 | DGD  | C5D-C6D-O5D-C1E |
| 31  | A     | 843 | CLA  | C16-C17-C18-C19 |
| 31  | B     | 814 | CLA  | C16-C17-C18-C20 |
| 31  | B     | 850 | CLA  | C10-C11-C12-C13 |
| 31  | F     | 301 | CLA  | C15-C16-C17-C18 |
| 31  | a     | 311 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 31  | A     | 827 | CLA  | C3-C5-C6-C7     |
| 31  | 5     | 314 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 818 | CLA  | C16-C17-C18-C20 |
| 33  | B     | 808 | DGD  | C3B-C4B-C5B-C6B |
| 31  | B     | 821 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 844 | CLA  | C4-C3-C5-C6     |
| 31  | 5     | 318 | CLA  | C2C-C3C-CAC-CBC |
| 31  | A     | 851 | CLA  | C11-C10-C8-C7   |
| 31  | B     | 817 | CLA  | C11-C12-C13-C15 |
| 31  | B     | 830 | CLA  | C11-C10-C8-C7   |
| 31  | 7     | 312 | CLA  | C12-C13-C15-C16 |
| 31  | a     | 314 | CLA  | CBA-CGA-O2A-C1  |
| 43  | 5     | 306 | PTY  | N1-C2-C3-O11    |
| 28  | 8     | 304 | LHG  | C9-C10-C11-C12  |
| 28  | 7     | 302 | LHG  | O1-C1-C2-O2     |
| 36  | 4     | 302 | LUT  | C29-C30-C31-C32 |
| 38  | a     | 304 | AXT  | C29-C30-C31-C32 |
| 28  | 6     | 301 | LHG  | C7-C8-C9-C10    |
| 28  | 7     | 307 | LHG  | C5-C4-O6-P      |
| 41  | 8     | 305 | DGA  | OB1-CB1-CB2-CB3 |
| 31  | A     | 847 | CLA  | C13-C15-C16-C17 |
| 31  | 3     | 313 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 837 | CLA  | C2A-CAA-CBA-CGA |
| 31  | a     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 26  | A     | 806 | BCR  | C11-C10-C9-C34  |
| 26  | B     | 806 | BCR  | C11-C10-C9-C34  |
| 26  | 3     | 302 | BCR  | C11-C10-C9-C34  |
| 36  | F     | 304 | LUT  | C11-C10-C9-C19  |
| 31  | B     | 846 | CLA  | CAA-CBA-CGA-O2A |
| 37  | J     | 101 | LMG  | O8-C28-C29-C30  |
| 31  | A     | 822 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 856 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 829 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 837 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 842 | CLA  | C4-C3-C5-C6     |
| 31  | 6     | 312 | CLA  | C4-C3-C5-C6     |
| 32  | 7     | 324 | CHL  | C4-C3-C5-C6     |
| 37  | J     | 104 | LMG  | C10-C11-C12-C13 |
| 31  | A     | 854 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 815 | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | A     | 821 | CLA  | C14-C13-C15-C16 |
| 31  | B     | 830 | CLA  | C11-C10-C8-C9   |
| 32  | A     | 831 | CHL  | C11-C10-C8-C9   |
| 32  | 7     | 318 | CHL  | C14-C13-C15-C16 |
| 31  | 4     | 319 | CLA  | C4C-C3C-CAC-CBC |
| 39  | 7     | 301 | 3PH  | C33-C34-C35-C36 |
| 31  | B     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 31  | H     | 901 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 304 | CLA  | C3A-C2A-CAA-CBA |
| 31  | b     | 310 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 4     | 318 | CLA  | C3A-C2A-CAA-CBA |
| 28  | 7     | 307 | LHG  | O8-C23-C24-C25  |
| 31  | H     | 901 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 3     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 8     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 817 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 827 | CLA  | CAD-CBD-CGD-O2D |
| 31  | A     | 830 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 814 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 834 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 839 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 848 | CLA  | CAD-CBD-CGD-O2D |
| 31  | B     | 849 | CLA  | CAD-CBD-CGD-O2D |
| 31  | G     | 205 | CLA  | CAD-CBD-CGD-O2D |
| 31  | K     | 206 | CLA  | CAD-CBD-CGD-O2D |
| 31  | a     | 312 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 3     | 319 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 9     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 9     | 316 | CLA  | CAD-CBD-CGD-O2D |
| 31  | b     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 2     | 309 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 4     | 316 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 5     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 6     | 308 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 6     | 311 | CLA  | CAD-CBD-CGD-O2D |
| 32  | a     | 320 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 7     | 317 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 7     | 324 | CHL  | CAD-CBD-CGD-O2D |
| 32  | b     | 309 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 4     | 317 | CHL  | CAD-CBD-CGD-O2D |
| 32  | 6     | 317 | CHL  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 815 | CLA  | C8-C10-C11-C12  |
| 31  | 5     | 315 | CLA  | C15-C16-C17-C18 |
| 31  | b     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 6     | 311 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 3     | 310 | CLA  | C5-C6-C7-C8     |
| 31  | A     | 822 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 31  | b     | 307 | CLA  | CAA-CBA-CGA-O2A |
| 32  | a     | 320 | CHL  | CAA-CBA-CGA-O2A |
| 31  | A     | 821 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 839 | CLA  | C4-C3-C5-C6     |
| 31  | F     | 301 | CLA  | C4-C3-C5-C6     |
| 31  | a     | 311 | CLA  | C4-C3-C5-C6     |
| 31  | 7     | 314 | CLA  | C4-C3-C5-C6     |
| 31  | A     | 814 | CLA  | C16-C17-C18-C19 |
| 31  | 8     | 311 | CLA  | C3-C5-C6-C7     |
| 31  | A     | 822 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 838 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 847 | CLA  | C2-C3-C5-C6     |
| 31  | 3     | 312 | CLA  | C2-C3-C5-C6     |
| 31  | 9     | 321 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 826 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 833 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 838 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 8     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 6     | 306 | CLA  | CAA-CBA-CGA-O2A |
| 32  | A     | 831 | CHL  | C2C-C3C-CAC-CBC |
| 26  | 3     | 303 | BCR  | C17-C18-C19-C20 |
| 28  | A     | 809 | LHG  | C4-C5-C6-O8     |
| 28  | 6     | 301 | LHG  | C4-C5-C6-O8     |
| 39  | 7     | 301 | 3PH  | C1-O11-P-O12    |
| 31  | 3     | 317 | CLA  | O1A-CGA-O2A-C1  |
| 30  | A     | 813 | CL0  | CAA-CBA-CGA-O2A |
| 31  | G     | 205 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 9     | 315 | CLA  | CAA-CBA-CGA-O2A |
| 31  | b     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 4     | 312 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 857 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 319 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 823 | CLA  | C5-C6-C7-C8     |
| 31  | 6     | 310 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 6     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 32  | K     | 201 | CHL  | CAA-CBA-CGA-O2A |
| 37  | J     | 104 | LMG  | O8-C28-C29-C30  |
| 31  | 9     | 315 | CLA  | C3-C5-C6-C7     |
| 31  | 2     | 306 | CLA  | C3-C5-C6-C7     |
| 31  | 5     | 315 | CLA  | C3-C5-C6-C7     |
| 34  | B     | 851 | LAP  | O3-C14-C15-O4   |
| 31  | A     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 828 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 841 | CLA  | CHA-CBD-CGD-O2D |
| 31  | A     | 849 | CLA  | CHA-CBD-CGD-O1D |
| 31  | A     | 851 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 817 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 31  | B     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 841 | CLA  | CHA-CBD-CGD-O2D |
| 31  | B     | 844 | CLA  | CHA-CBD-CGD-O2D |
| 31  | K     | 204 | CLA  | CHA-CBD-CGD-O1D |
| 31  | K     | 205 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 310 | CLA  | CHA-CBD-CGD-O1D |
| 31  | a     | 311 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 314 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 316 | CLA  | CHA-CBD-CGD-O1D |
| 31  | a     | 319 | CLA  | CHA-CBD-CGD-O2D |
| 31  | a     | 322 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 317 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 3     | 319 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 7     | 309 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 7     | 312 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 7     | 316 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 7     | 321 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 8     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 9     | 321 | CLA  | CHA-CBD-CGD-O2D |
| 31  | L     | 305 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | O     | 203 | CLA  | CHA-CBD-CGD-O1D |
| 31  | b     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 31  | b     | 310 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 2     | 305 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 4     | 307 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 4     | 308 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 312 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 5     | 315 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 5     | 321 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 307 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 314 | CLA  | CHA-CBD-CGD-O2D |
| 31  | 6     | 315 | CLA  | CHA-CBD-CGD-O1D |
| 32  | A     | 840 | CHL  | CHA-CBD-CGD-O2D |
| 32  | a     | 317 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 7     | 317 | CHL  | CHA-CBD-CGD-O2D |
| 32  | 4     | 310 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 5     | 316 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 6     | 309 | CHL  | CHA-CBD-CGD-O1D |
| 32  | 6     | 309 | CHL  | CHA-CBD-CGD-O2D |
| 31  | B     | 821 | CLA  | C2-C3-C5-C6     |
| 31  | B     | 839 | CLA  | C2-C3-C5-C6     |
| 28  | A     | 811 | LHG  | C13-C14-C15-C16 |
| 37  | G     | 202 | LMG  | C30-C31-C32-C33 |
| 26  | A     | 806 | BCR  | C16-C17-C18-C19 |
| 26  | B     | 803 | BCR  | C20-C21-C22-C23 |
| 28  | 7     | 307 | LHG  | C25-C26-C27-C28 |
| 31  | 2     | 309 | CLA  | O1A-CGA-O2A-C1  |
| 28  | 7     | 302 | LHG  | O7-C7-C8-C9     |
| 31  | A     | 816 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 7     | 321 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 5     | 318 | CLA  | C4C-C3C-CAC-CBC |
| 32  | 6     | 309 | CHL  | O1A-CGA-O2A-C1  |
| 31  | 7     | 312 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 303 | CLA  | C2A-CAA-CBA-CGA |
| 31  | b     | 302 | CLA  | CAA-CBA-CGA-O2A |
| 31  | b     | 305 | CLA  | CAA-CBA-CGA-O2A |
| 31  | B     | 848 | CLA  | C4-C3-C5-C6     |
| 31  | 5     | 321 | CLA  | CBA-CGA-O2A-C1  |
| 32  | 7     | 324 | CHL  | C2-C3-C5-C6     |
| 31  | 2     | 313 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 4     | 320 | CLA  | C2C-C3C-CAC-CBC |
| 31  | B     | 814 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | B     | 817 | CLA  | C11-C10-C8-C9   |
| 31  | F     | 301 | CLA  | C11-C12-C13-C14 |
| 31  | a     | 309 | CLA  | C11-C10-C8-C9   |
| 31  | 6     | 312 | CLA  | C6-C7-C8-C9     |
| 26  | B     | 804 | BCR  | C19-C20-C21-C22 |
| 36  | F     | 304 | LUT  | C33-C34-C35-C15 |
| 31  | 4     | 320 | CLA  | C4C-C3C-CAC-CBC |
| 32  | 6     | 309 | CHL  | C10-C11-C12-C13 |
| 28  | 8     | 304 | LHG  | C25-C26-C27-C28 |
| 31  | 3     | 317 | CLA  | CBA-CGA-O2A-C1  |
| 31  | a     | 322 | CLA  | CAA-CBA-CGA-O2A |
| 37  | a     | 301 | LMG  | O7-C10-C11-C12  |
| 28  | 7     | 307 | LHG  | O10-C23-C24-C25 |
| 31  | B     | 840 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 822 | CLA  | C3-C5-C6-C7     |
| 31  | B     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 31  | B     | 839 | CLA  | C2A-CAA-CBA-CGA |
| 32  | a     | 320 | CHL  | CAA-CBA-CGA-O1A |
| 28  | A     | 811 | LHG  | O8-C23-C24-C25  |
| 31  | A     | 848 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 4     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 5     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 6     | 322 | CLA  | CAA-CBA-CGA-O2A |
| 31  | a     | 319 | CLA  | CBA-CGA-O2A-C1  |
| 36  | 2     | 301 | LUT  | C27-C28-C29-C39 |
| 32  | 7     | 318 | CHL  | C16-C17-C18-C20 |
| 31  | B     | 844 | CLA  | C2-C3-C5-C6     |
| 31  | 5     | 314 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 826 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 833 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 815 | CLA  | CAA-CBA-CGA-O1A |
| 31  | G     | 205 | CLA  | CAA-CBA-CGA-O1A |
| 26  | A     | 803 | BCR  | C21-C22-C23-C24 |
| 26  | 6     | 302 | BCR  | C21-C22-C23-C24 |
| 35  | a     | 302 | QTB  | C03-C02-C09-C10 |
| 31  | A     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 31  | A     | 856 | CLA  | C1A-C2A-CAA-CBA |
| 31  | H     | 901 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 313 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 8     | 320 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 308 | CLA  | C1A-C2A-CAA-CBA |
| 31  | b     | 310 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 2     | 306 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 4     | 318 | CLA  | C1A-C2A-CAA-CBA |
| 31  | 6     | 316 | CLA  | C1A-C2A-CAA-CBA |
| 32  | 6     | 317 | CHL  | C1A-C2A-CAA-CBA |
| 31  | B     | 812 | CLA  | C16-C17-C18-C20 |
| 31  | A     | 854 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 9     | 315 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 4     | 312 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 310 | CLA  | CAA-CBA-CGA-O1A |
| 28  | 6     | 301 | LHG  | O9-C7-C8-C9     |
| 31  | A     | 822 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 848 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 3     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 3     | 319 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 317 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 9     | 314 | CLA  | C2A-CAA-CBA-CGA |
| 31  | O     | 203 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 5     | 310 | CLA  | C2A-CAA-CBA-CGA |
| 32  | K     | 201 | CHL  | CAA-CBA-CGA-O1A |
| 31  | B     | 840 | CLA  | C13-C15-C16-C17 |
| 32  | 3     | 315 | CHL  | C5-C6-C7-C8     |
| 32  | 7     | 318 | CHL  | C5-C6-C7-C8     |
| 31  | 9     | 316 | CLA  | C2C-C3C-CAC-CBC |
| 41  | 8     | 305 | DGA  | CA9-CAA-CBA-CCA |
| 31  | A     | 847 | CLA  | C5-C6-C7-C8     |
| 28  | a     | 306 | LHG  | C10-C11-C12-C13 |
| 31  | B     | 846 | CLA  | CAA-CBA-CGA-O1A |
| 31  | b     | 307 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 304 | CLA  | O1A-CGA-O2A-C1  |
| 33  | B     | 808 | DGD  | C2E-C1E-O5D-C6D |
| 30  | A     | 813 | CL0  | C10-C11-C12-C13 |
| 31  | a     | 311 | CLA  | C8-C10-C11-C12  |
| 32  | 7     | 324 | CHL  | C5-C6-C7-C8     |
| 32  | 5     | 316 | CHL  | C2C-C3C-CAC-CBC |
| 28  | A     | 810 | LHG  | C3-O3-P-O5      |
| 28  | a     | 306 | LHG  | C4-O6-P-O5      |
| 28  | 7     | 307 | LHG  | C4-O6-P-O4      |
| 43  | 5     | 306 | PTY  | C5-O14-P1-O13   |
| 31  | 6     | 313 | CLA  | CAA-CBA-CGA-O1A |
| 26  | 3     | 303 | BCR  | C20-C21-C22-C37 |
| 26  | A     | 804 | BCR  | C5-C6-C7-C8     |
| 26  | B     | 802 | BCR  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | B     | 804 | BCR  | C5-C6-C7-C8     |
| 26  | F     | 302 | BCR  | C5-C6-C7-C8     |
| 26  | J     | 102 | BCR  | C5-C6-C7-C8     |
| 26  | 7     | 304 | BCR  | C1-C6-C7-C8     |
| 32  | 5     | 316 | CHL  | C4C-C3C-CAC-CBC |
| 31  | A     | 816 | CLA  | CAA-CBA-CGA-O1A |
| 31  | B     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 7     | 321 | CLA  | CAA-CBA-CGA-O1A |
| 31  | b     | 302 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 5     | 311 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 828 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 3     | 311 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 9     | 316 | CLA  | C4C-C3C-CAC-CBC |
| 31  | A     | 814 | CLA  | C16-C17-C18-C20 |
| 31  | 2     | 304 | CLA  | C2A-CAA-CBA-CGA |
| 31  | a     | 319 | CLA  | O1A-CGA-O2A-C1  |
| 31  | 5     | 318 | CLA  | C15-C16-C17-C18 |
| 28  | 6     | 301 | LHG  | O7-C7-C8-C9     |
| 31  | 8     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 2     | 307 | CLA  | C2-C3-C5-C6     |
| 31  | A     | 828 | CLA  | C16-C17-C18-C19 |
| 37  | J     | 101 | LMG  | C33-C34-C35-C36 |
| 31  | B     | 843 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 814 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 832 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 843 | CLA  | CAD-CBD-CGD-O1D |
| 31  | A     | 849 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 819 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 826 | CLA  | CAD-CBD-CGD-O1D |
| 31  | B     | 832 | CLA  | CAD-CBD-CGD-O1D |
| 31  | L     | 305 | CLA  | CAD-CBD-CGD-O1D |
| 31  | L     | 306 | CLA  | CAD-CBD-CGD-O1D |
| 31  | b     | 312 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 4     | 320 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 5     | 315 | CLA  | CAD-CBD-CGD-O1D |
| 31  | 6     | 308 | CLA  | CAD-CBD-CGD-O1D |
| 32  | 4     | 310 | CHL  | CAD-CBD-CGD-O1D |
| 31  | A     | 838 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 8     | 308 | CLA  | CAA-CBA-CGA-O1A |
| 31  | b     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 6     | 306 | CLA  | CAA-CBA-CGA-O1A |
| 28  | 7     | 302 | LHG  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 31  | 5     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 31  | A     | 851 | CLA  | C14-C13-C15-C16 |
| 31  | A     | 857 | CLA  | C11-C12-C13-C14 |
| 31  | B     | 817 | CLA  | C11-C12-C13-C14 |
| 31  | b     | 313 | CLA  | C4C-C3C-CAC-CBC |
| 31  | 5     | 309 | CLA  | CAA-CBA-CGA-O2A |
| 33  | 7     | 308 | DGD  | O2G-C1B-C2B-C3B |
| 31  | B     | 843 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 5     | 307 | CLA  | C2A-CAA-CBA-CGA |
| 31  | 4     | 308 | CLA  | CAA-CBA-CGA-O2A |
| 42  | 4     | 304 | SQD  | O47-C7-C8-C9    |
| 31  | B     | 811 | CLA  | C8-C10-C11-C12  |
| 31  | 3     | 310 | CLA  | C10-C11-C12-C13 |
| 39  | 7     | 301 | 3PH  | C32-C33-C34-C35 |
| 31  | 5     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 31  | A     | 843 | CLA  | C4-C3-C5-C6     |
| 31  | B     | 820 | CLA  | O1A-CGA-O2A-C1  |
| 31  | A     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 856 | CLA  | C3A-C2A-CAA-CBA |
| 31  | A     | 857 | CLA  | C11-C12-C13-C15 |
| 31  | F     | 301 | CLA  | C11-C12-C13-C15 |
| 31  | a     | 309 | CLA  | C11-C10-C8-C7   |
| 31  | 7     | 313 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 7     | 313 | CLA  | CAD-CBD-CGD-O2D |
| 31  | 8     | 320 | CLA  | C3A-C2A-CAA-CBA |
| 31  | O     | 202 | CLA  | CHA-CBD-CGD-O1D |
| 31  | 2     | 306 | CLA  | C3A-C2A-CAA-CBA |
| 31  | 5     | 315 | CLA  | C12-C13-C15-C16 |
| 32  | 4     | 310 | CHL  | C3A-C2A-CAA-CBA |
| 28  | A     | 810 | LHG  | O8-C23-C24-C25  |
| 28  | A     | 811 | LHG  | O7-C7-C8-C9     |
| 31  | A     | 834 | CLA  | CAA-CBA-CGA-O2A |
| 32  | A     | 840 | CHL  | CAA-CBA-CGA-O2A |
| 32  | 5     | 322 | CHL  | CAA-CBA-CGA-O2A |
| 41  | 8     | 305 | DGA  | OG1-CA1-CA2-CA3 |
| 31  | B     | 844 | CLA  | C5-C6-C7-C8     |
| 28  | a     | 306 | LHG  | O10-C23-C24-C25 |
| 31  | a     | 322 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 4     | 309 | CLA  | CAA-CBA-CGA-O1A |
| 31  | 5     | 313 | CLA  | CAA-CBA-CGA-O1A |
| 26  | 6     | 302 | BCR  | C13-C14-C15-C16 |
| 36  | J     | 103 | LUT  | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | 2     | 301 | LUT  | C9-C10-C11-C12  |
| 27  | 9     | 306 | LMT  | C6-C7-C8-C9     |
| 31  | A     | 853 | CLA  | C13-C15-C16-C17 |
| 31  | A     | 834 | CLA  | CAA-CBA-CGA-O1A |
| 37  | J     | 104 | LMG  | O9-C10-C11-C12  |
| 33  | B     | 808 | DGD  | C2B-C1B-O2G-C2G |
| 37  | G     | 202 | LMG  | C14-C15-C16-C17 |
| 31  | A     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 31  | a     | 313 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 8     | 320 | CLA  | CAA-CBA-CGA-O2A |
| 31  | 2     | 307 | CLA  | CAA-CBA-CGA-O2A |
| 32  | 7     | 324 | CHL  | CAA-CBA-CGA-O2A |
| 37  | a     | 301 | LMG  | O8-C28-C29-C30  |
| 41  | 8     | 305 | DGA  | OA1-CA1-CA2-CA3 |
| 31  | b     | 308 | CLA  | C2A-CAA-CBA-CGA |
| 31  | A     | 824 | CLA  | C10-C11-C12-C13 |
| 31  | 3     | 311 | CLA  | C10-C11-C12-C13 |
| 31  | 8     | 310 | CLA  | C10-C11-C12-C13 |
| 32  | 7     | 324 | CHL  | C10-C11-C12-C13 |
| 32  | 5     | 316 | CHL  | C5-C6-C7-C8     |
| 28  | A     | 811 | LHG  | O9-C7-C8-C9     |
| 31  | 2     | 313 | CLA  | CAA-CBA-CGA-O2A |

All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms                   |
|-----|-------|-----|------|-------------------------|
| 35  | F     | 303 | QTB  | C11-C12-C14-C15-C16-C17 |
| 35  | 7     | 303 | QTB  | C11-C12-C14-C15-C16-C17 |

256 monomers are involved in 557 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | 5     | 310 | CLA  | 5       | 0            |
| 31  | 9     | 311 | CLA  | 1       | 0            |
| 37  | G     | 202 | LMG  | 4       | 0            |
| 31  | A     | 837 | CLA  | 4       | 0            |
| 31  | 7     | 311 | CLA  | 3       | 0            |
| 26  | O     | 201 | BCR  | 2       | 0            |
| 31  | L     | 305 | CLA  | 7       | 0            |
| 27  | 5     | 301 | LMT  | 2       | 0            |
| 31  | A     | 828 | CLA  | 2       | 0            |
| 41  | 8     | 305 | DGA  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | 4     | 319 | CLA  | 1       | 0            |
| 32  | 5     | 319 | CHL  | 4       | 0            |
| 31  | 8     | 320 | CLA  | 1       | 0            |
| 31  | 5     | 315 | CLA  | 2       | 0            |
| 31  | 4     | 314 | CLA  | 5       | 0            |
| 31  | 4     | 311 | CLA  | 1       | 0            |
| 31  | 7     | 315 | CLA  | 6       | 0            |
| 36  | 7     | 305 | LUT  | 3       | 0            |
| 36  | L     | 304 | LUT  | 1       | 0            |
| 31  | 6     | 316 | CLA  | 1       | 0            |
| 31  | 3     | 319 | CLA  | 3       | 0            |
| 36  | 6     | 304 | LUT  | 3       | 0            |
| 26  | K     | 203 | BCR  | 4       | 0            |
| 31  | B     | 828 | CLA  | 1       | 0            |
| 31  | 5     | 321 | CLA  | 1       | 0            |
| 27  | A     | 807 | LMT  | 4       | 0            |
| 31  | A     | 846 | CLA  | 3       | 0            |
| 31  | 4     | 315 | CLA  | 2       | 0            |
| 31  | H     | 901 | CLA  | 3       | 0            |
| 31  | A     | 847 | CLA  | 1       | 0            |
| 31  | B     | 842 | CLA  | 4       | 0            |
| 26  | G     | 201 | BCR  | 2       | 0            |
| 31  | A     | 843 | CLA  | 2       | 0            |
| 31  | 9     | 315 | CLA  | 2       | 0            |
| 31  | B     | 845 | CLA  | 4       | 0            |
| 39  | 7     | 301 | 3PH  | 1       | 0            |
| 31  | 6     | 308 | CLA  | 1       | 0            |
| 31  | A     | 819 | CLA  | 3       | 0            |
| 31  | B     | 835 | CLA  | 2       | 0            |
| 31  | 4     | 318 | CLA  | 5       | 0            |
| 31  | K     | 206 | CLA  | 1       | 0            |
| 24  | B     | 801 | PQN  | 2       | 0            |
| 31  | 9     | 313 | CLA  | 1       | 0            |
| 31  | B     | 816 | CLA  | 1       | 0            |
| 36  | 3     | 305 | LUT  | 7       | 0            |
| 26  | L     | 301 | BCR  | 1       | 0            |
| 31  | 5     | 318 | CLA  | 5       | 0            |
| 31  | 7     | 313 | CLA  | 2       | 0            |
| 26  | B     | 803 | BCR  | 1       | 0            |
| 31  | B     | 849 | CLA  | 1       | 0            |
| 31  | 2     | 313 | CLA  | 2       | 0            |
| 31  | 8     | 313 | CLA  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 26  | 3     | 302 | BCR  | 5       | 0            |
| 26  | A     | 803 | BCR  | 3       | 0            |
| 31  | F     | 306 | CLA  | 1       | 0            |
| 31  | A     | 850 | CLA  | 3       | 0            |
| 31  | 8     | 311 | CLA  | 5       | 0            |
| 31  | A     | 856 | CLA  | 4       | 0            |
| 32  | 7     | 320 | CHL  | 7       | 0            |
| 31  | B     | 833 | CLA  | 2       | 0            |
| 32  | 9     | 322 | CHL  | 4       | 0            |
| 31  | B     | 831 | CLA  | 2       | 0            |
| 31  | 3     | 320 | CLA  | 1       | 0            |
| 31  | 8     | 307 | CLA  | 1       | 0            |
| 26  | 7     | 304 | BCR  | 6       | 0            |
| 33  | B     | 808 | DGD  | 4       | 0            |
| 31  | 8     | 310 | CLA  | 3       | 0            |
| 31  | 3     | 310 | CLA  | 1       | 0            |
| 26  | L     | 303 | BCR  | 3       | 0            |
| 32  | 4     | 310 | CHL  | 7       | 0            |
| 31  | 6     | 312 | CLA  | 1       | 0            |
| 31  | 8     | 315 | CLA  | 1       | 0            |
| 31  | 2     | 312 | CLA  | 1       | 0            |
| 31  | 8     | 318 | CLA  | 1       | 0            |
| 31  | B     | 811 | CLA  | 1       | 0            |
| 31  | B     | 836 | CLA  | 1       | 0            |
| 31  | B     | 843 | CLA  | 2       | 0            |
| 31  | 6     | 311 | CLA  | 1       | 0            |
| 31  | 2     | 308 | CLA  | 1       | 0            |
| 32  | 8     | 316 | CHL  | 9       | 0            |
| 32  | 6     | 309 | CHL  | 8       | 0            |
| 31  | B     | 829 | CLA  | 2       | 0            |
| 31  | A     | 829 | CLA  | 12      | 0            |
| 32  | 7     | 318 | CHL  | 9       | 0            |
| 26  | B     | 804 | BCR  | 4       | 0            |
| 31  | A     | 857 | CLA  | 3       | 0            |
| 36  | 6     | 303 | LUT  | 2       | 0            |
| 26  | F     | 302 | BCR  | 2       | 0            |
| 36  | 9     | 302 | LUT  | 2       | 0            |
| 31  | A     | 815 | CLA  | 3       | 0            |
| 32  | 5     | 316 | CHL  | 6       | 0            |
| 26  | B     | 802 | BCR  | 4       | 0            |
| 26  | L     | 302 | BCR  | 2       | 0            |
| 31  | A     | 838 | CLA  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | 5     | 303 | LUT  | 3       | 0            |
| 31  | 4     | 321 | CLA  | 1       | 0            |
| 31  | 3     | 313 | CLA  | 2       | 0            |
| 31  | A     | 816 | CLA  | 2       | 0            |
| 31  | 2     | 307 | CLA  | 2       | 0            |
| 31  | 4     | 305 | CLA  | 6       | 0            |
| 30  | A     | 813 | CL0  | 3       | 0            |
| 31  | A     | 848 | CLA  | 1       | 0            |
| 42  | 4     | 304 | SQD  | 1       | 0            |
| 31  | 5     | 313 | CLA  | 1       | 0            |
| 31  | 9     | 318 | CLA  | 1       | 0            |
| 31  | B     | 840 | CLA  | 2       | 0            |
| 31  | 6     | 313 | CLA  | 2       | 0            |
| 31  | A     | 853 | CLA  | 3       | 0            |
| 24  | A     | 801 | PQN  | 1       | 0            |
| 31  | B     | 844 | CLA  | 3       | 0            |
| 31  | 2     | 306 | CLA  | 3       | 0            |
| 31  | B     | 815 | CLA  | 1       | 0            |
| 31  | A     | 823 | CLA  | 3       | 0            |
| 32  | A     | 831 | CHL  | 3       | 0            |
| 31  | A     | 826 | CLA  | 3       | 0            |
| 31  | B     | 814 | CLA  | 4       | 0            |
| 31  | A     | 822 | CLA  | 4       | 0            |
| 31  | A     | 832 | CLA  | 2       | 0            |
| 32  | 6     | 320 | CHL  | 1       | 0            |
| 36  | 3     | 304 | LUT  | 3       | 0            |
| 26  | M     | 101 | BCR  | 3       | 0            |
| 31  | A     | 814 | CLA  | 6       | 0            |
| 32  | 6     | 318 | CHL  | 5       | 0            |
| 36  | 8     | 302 | LUT  | 5       | 0            |
| 26  | 3     | 303 | BCR  | 2       | 0            |
| 31  | 8     | 317 | CLA  | 2       | 0            |
| 32  | A     | 840 | CHL  | 5       | 0            |
| 31  | B     | 822 | CLA  | 4       | 0            |
| 31  | F     | 301 | CLA  | 4       | 0            |
| 32  | 7     | 319 | CHL  | 4       | 0            |
| 26  | 8     | 301 | BCR  | 2       | 0            |
| 31  | B     | 820 | CLA  | 4       | 0            |
| 31  | 5     | 309 | CLA  | 3       | 0            |
| 31  | A     | 852 | CLA  | 2       | 0            |
| 31  | B     | 825 | CLA  | 4       | 0            |
| 32  | 5     | 322 | CHL  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 28  | 7     | 302 | LHG  | 6       | 0            |
| 31  | A     | 836 | CLA  | 3       | 0            |
| 31  | G     | 204 | CLA  | 1       | 0            |
| 28  | A     | 809 | LHG  | 3       | 0            |
| 26  | B     | 805 | BCR  | 5       | 0            |
| 28  | 7     | 307 | LHG  | 4       | 0            |
| 31  | A     | 845 | CLA  | 4       | 0            |
| 32  | 4     | 313 | CHL  | 4       | 0            |
| 31  | A     | 824 | CLA  | 1       | 0            |
| 26  | 3     | 301 | BCR  | 2       | 0            |
| 31  | A     | 854 | CLA  | 1       | 0            |
| 36  | J     | 103 | LUT  | 3       | 0            |
| 31  | B     | 826 | CLA  | 1       | 0            |
| 31  | 5     | 312 | CLA  | 1       | 0            |
| 31  | 6     | 322 | CLA  | 3       | 0            |
| 31  | 8     | 321 | CLA  | 3       | 0            |
| 31  | A     | 849 | CLA  | 2       | 0            |
| 32  | 8     | 319 | CHL  | 1       | 0            |
| 28  | A     | 810 | LHG  | 2       | 0            |
| 31  | H     | 903 | CLA  | 3       | 0            |
| 31  | J     | 105 | CLA  | 1       | 0            |
| 31  | B     | 841 | CLA  | 4       | 0            |
| 31  | G     | 205 | CLA  | 1       | 0            |
| 32  | A     | 839 | CHL  | 4       | 0            |
| 36  | F     | 304 | LUT  | 2       | 0            |
| 31  | 5     | 314 | CLA  | 1       | 0            |
| 36  | 4     | 303 | LUT  | 4       | 0            |
| 31  | A     | 833 | CLA  | 3       | 0            |
| 31  | 5     | 307 | CLA  | 2       | 0            |
| 34  | B     | 851 | LAP  | 4       | 0            |
| 31  | A     | 830 | CLA  | 3       | 0            |
| 31  | B     | 839 | CLA  | 2       | 0            |
| 31  | B     | 850 | CLA  | 3       | 0            |
| 31  | 2     | 304 | CLA  | 6       | 0            |
| 31  | 3     | 308 | CLA  | 2       | 0            |
| 32  | 3     | 315 | CHL  | 2       | 0            |
| 31  | 3     | 314 | CLA  | 2       | 0            |
| 37  | J     | 101 | LMG  | 4       | 0            |
| 31  | 6     | 314 | CLA  | 2       | 0            |
| 31  | 6     | 306 | CLA  | 5       | 0            |
| 32  | 5     | 317 | CHL  | 4       | 0            |
| 32  | 6     | 317 | CHL  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | 5     | 311 | CLA  | 1       | 0            |
| 31  | B     | 832 | CLA  | 3       | 0            |
| 31  | B     | 837 | CLA  | 5       | 0            |
| 26  | B     | 806 | BCR  | 2       | 0            |
| 31  | B     | 846 | CLA  | 3       | 0            |
| 36  | 4     | 302 | LUT  | 8       | 0            |
| 32  | 6     | 321 | CHL  | 2       | 0            |
| 31  | A     | 820 | CLA  | 2       | 0            |
| 43  | 5     | 306 | PTY  | 1       | 0            |
| 31  | 7     | 322 | CLA  | 1       | 0            |
| 31  | B     | 838 | CLA  | 1       | 0            |
| 32  | 6     | 319 | CHL  | 2       | 0            |
| 31  | B     | 812 | CLA  | 2       | 0            |
| 31  | A     | 827 | CLA  | 3       | 0            |
| 26  | 6     | 302 | BCR  | 2       | 0            |
| 31  | B     | 848 | CLA  | 4       | 0            |
| 26  | 2     | 302 | BCR  | 3       | 0            |
| 31  | 2     | 315 | CLA  | 1       | 0            |
| 31  | B     | 818 | CLA  | 2       | 0            |
| 31  | A     | 835 | CLA  | 3       | 0            |
| 32  | 7     | 317 | CHL  | 8       | 0            |
| 31  | A     | 821 | CLA  | 2       | 0            |
| 26  | J     | 102 | BCR  | 1       | 0            |
| 26  | A     | 805 | BCR  | 3       | 0            |
| 36  | 8     | 303 | LUT  | 2       | 0            |
| 31  | A     | 842 | CLA  | 1       | 0            |
| 31  | 4     | 308 | CLA  | 1       | 0            |
| 28  | 5     | 305 | LHG  | 2       | 0            |
| 31  | B     | 813 | CLA  | 6       | 0            |
| 36  | 5     | 304 | LUT  | 6       | 0            |
| 31  | 8     | 309 | CLA  | 1       | 0            |
| 31  | 4     | 312 | CLA  | 1       | 0            |
| 31  | 2     | 314 | CLA  | 3       | 0            |
| 31  | 6     | 307 | CLA  | 2       | 0            |
| 31  | G     | 206 | CLA  | 4       | 0            |
| 31  | 4     | 316 | CLA  | 4       | 0            |
| 33  | 7     | 308 | DGD  | 1       | 0            |
| 32  | 9     | 320 | CHL  | 3       | 0            |
| 31  | 5     | 320 | CLA  | 1       | 0            |
| 31  | 8     | 314 | CLA  | 1       | 0            |
| 26  | K     | 202 | BCR  | 4       | 0            |
| 26  | A     | 804 | BCR  | 2       | 0            |

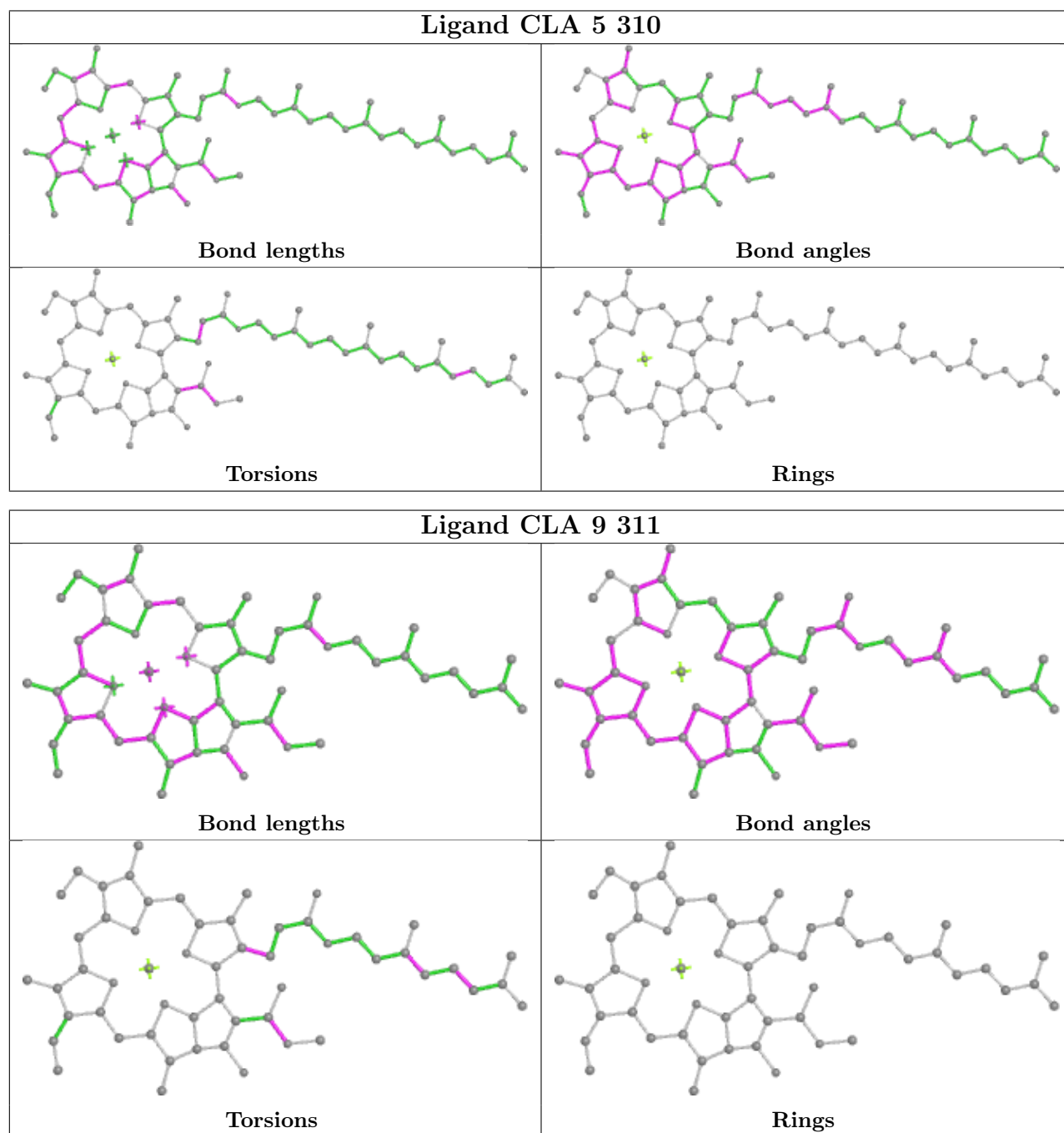
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | B     | 830 | CLA  | 1       | 0            |
| 31  | 3     | 311 | CLA  | 2       | 0            |
| 31  | 7     | 321 | CLA  | 2       | 0            |
| 31  | B     | 817 | CLA  | 1       | 0            |
| 31  | B     | 823 | CLA  | 1       | 0            |
| 31  | A     | 855 | CLA  | 3       | 0            |
| 36  | 9     | 303 | LUT  | 6       | 0            |
| 26  | 5     | 302 | BCR  | 2       | 0            |
| 31  | B     | 819 | CLA  | 2       | 0            |
| 31  | A     | 834 | CLA  | 7       | 0            |
| 32  | K     | 201 | CHL  | 2       | 0            |
| 28  | 6     | 301 | LHG  | 3       | 0            |
| 31  | A     | 818 | CLA  | 4       | 0            |
| 31  | 4     | 307 | CLA  | 1       | 0            |
| 28  | A     | 811 | LHG  | 3       | 0            |
| 32  | 7     | 324 | CHL  | 5       | 0            |
| 36  | 9     | 305 | LUT  | 1       | 0            |
| 31  | 7     | 309 | CLA  | 2       | 0            |
| 31  | 3     | 309 | CLA  | 7       | 0            |
| 31  | B     | 834 | CLA  | 3       | 0            |
| 31  | 5     | 308 | CLA  | 1       | 0            |
| 31  | H     | 902 | CLA  | 6       | 0            |
| 31  | 9     | 314 | CLA  | 2       | 0            |
| 32  | 4     | 317 | CHL  | 10      | 0            |
| 31  | B     | 847 | CLA  | 2       | 0            |
| 31  | 2     | 311 | CLA  | 1       | 0            |
| 31  | A     | 841 | CLA  | 8       | 0            |
| 31  | A     | 851 | CLA  | 5       | 0            |
| 31  | 5     | 323 | CLA  | 3       | 0            |
| 36  | 2     | 301 | LUT  | 4       | 0            |
| 26  | A     | 806 | BCR  | 4       | 0            |
| 28  | 6     | 305 | LHG  | 1       | 0            |
| 31  | 6     | 315 | CLA  | 1       | 0            |
| 26  | I     | 801 | BCR  | 1       | 0            |
| 31  | A     | 825 | CLA  | 3       | 0            |
| 31  | 8     | 308 | CLA  | 6       | 0            |

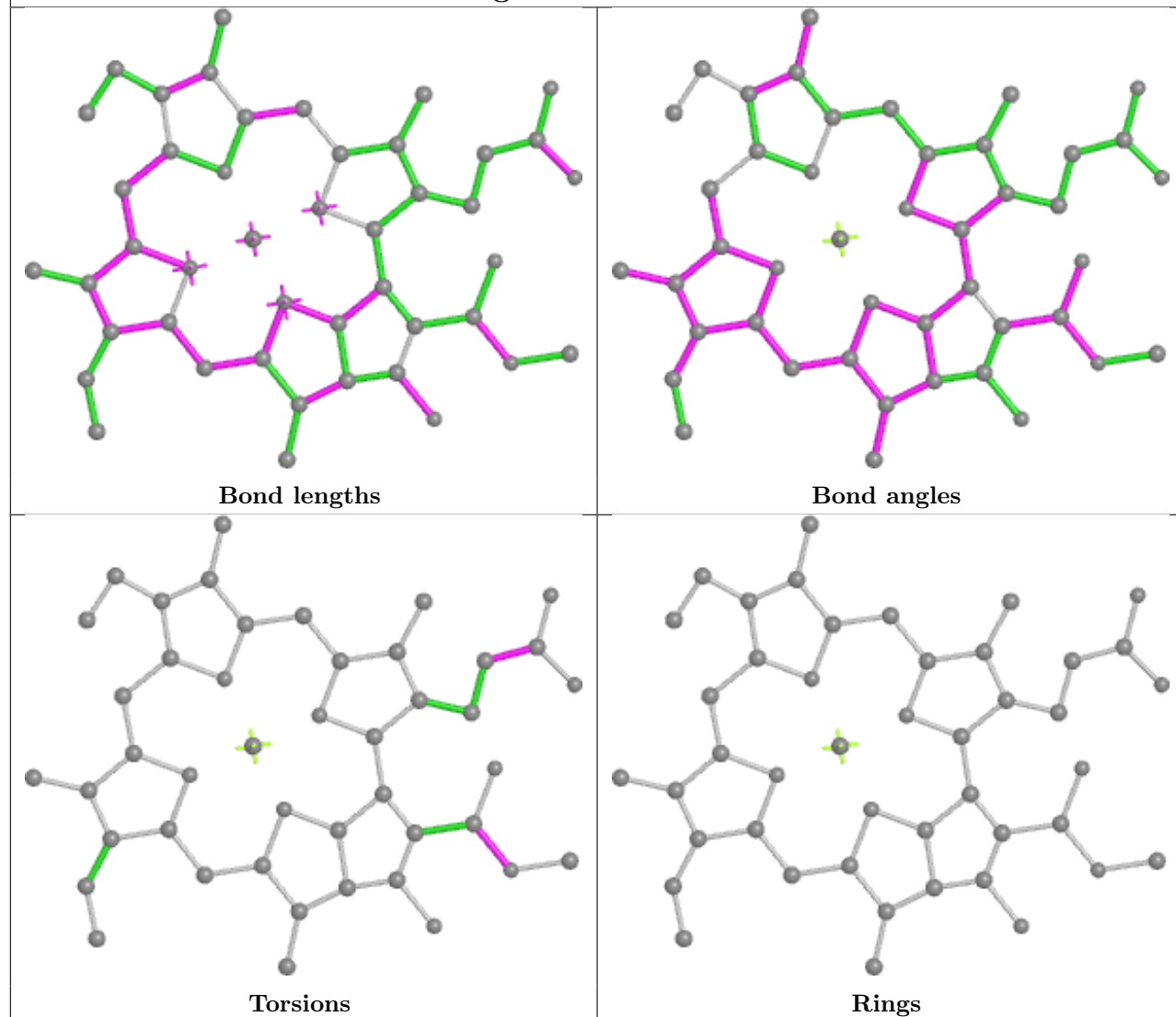
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

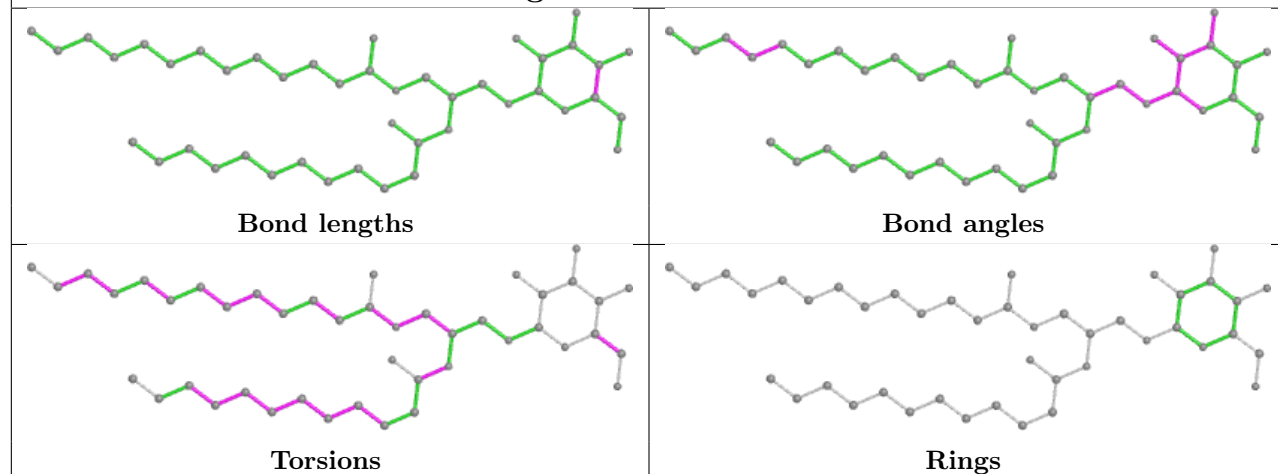


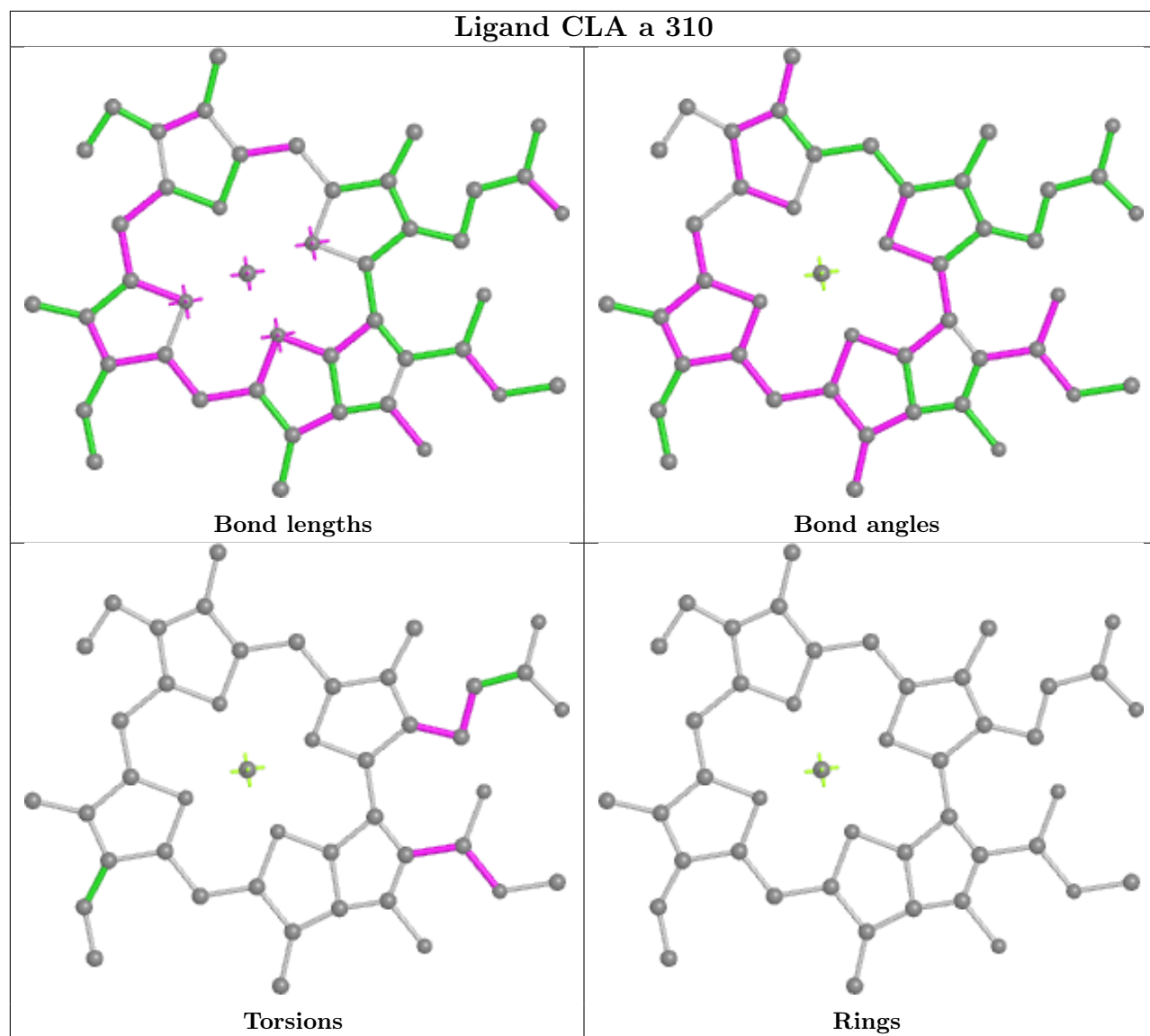
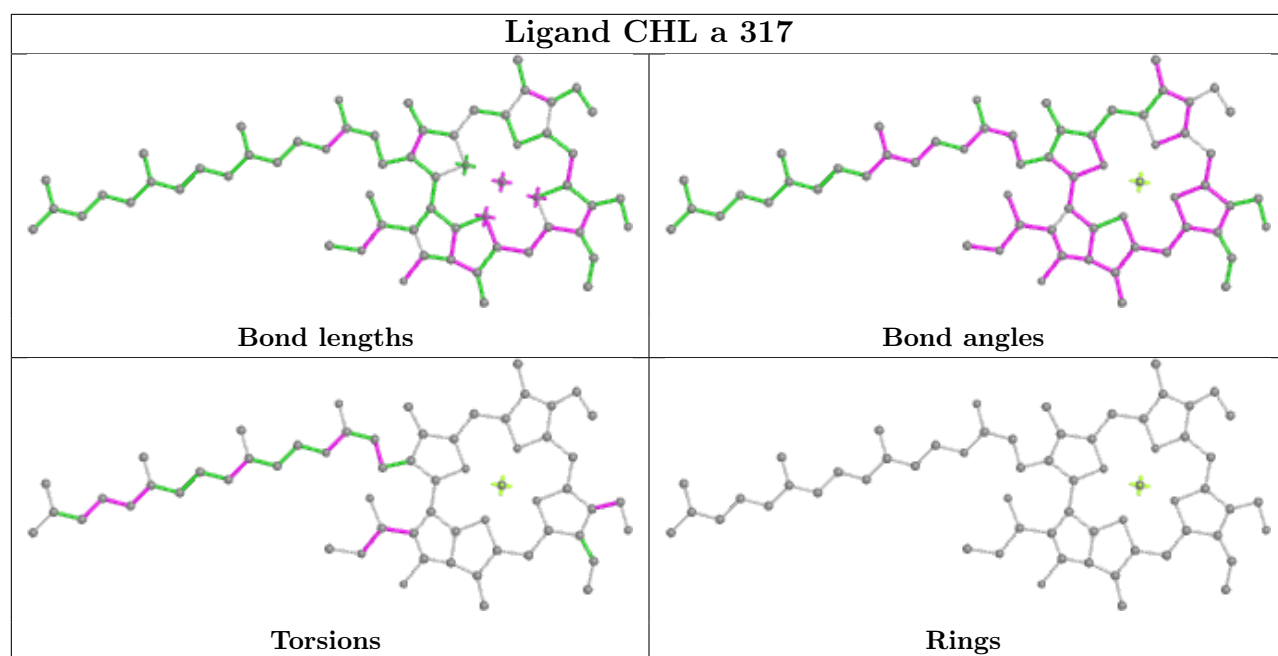


## Ligand CLA 4 306

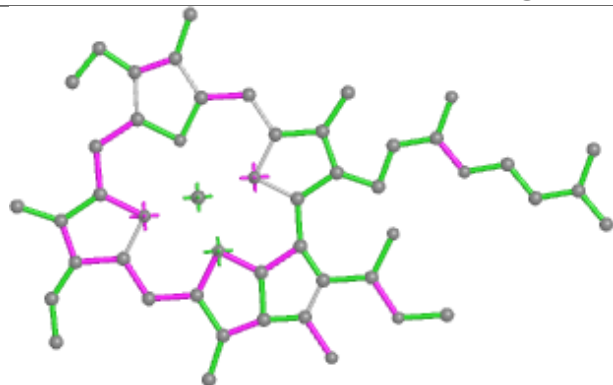


## Ligand LMG G 202

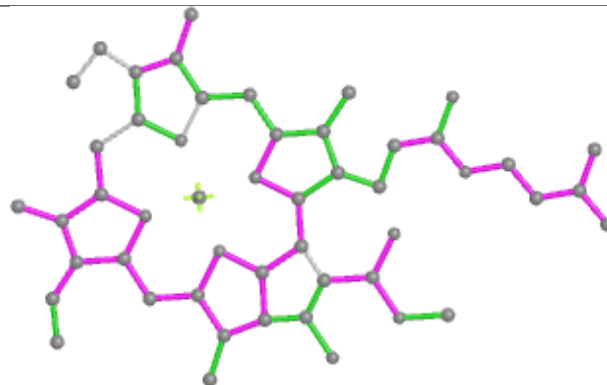




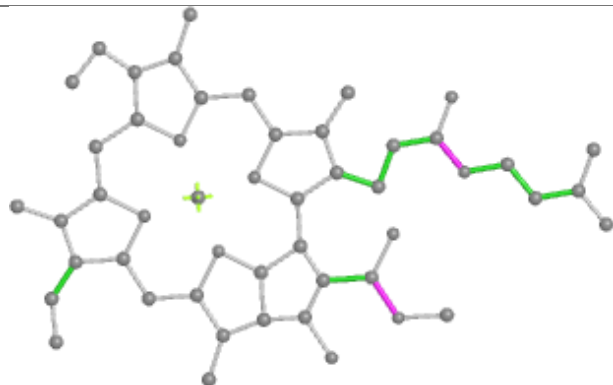
## Ligand CLA 8 312



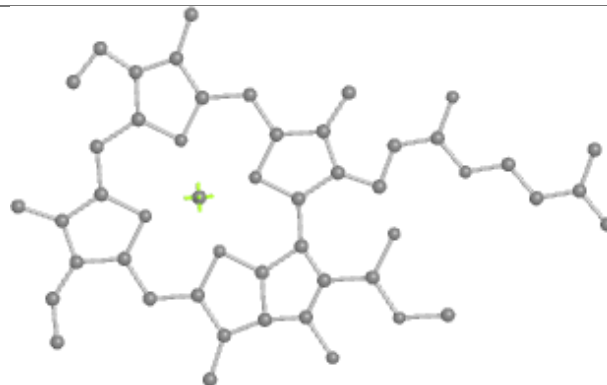
Bond lengths



Bond angles

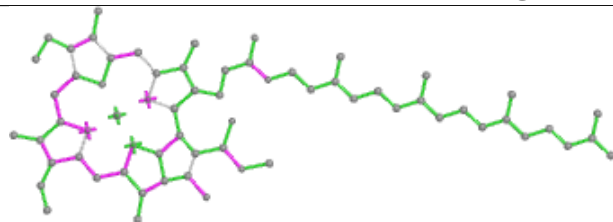


Torsions

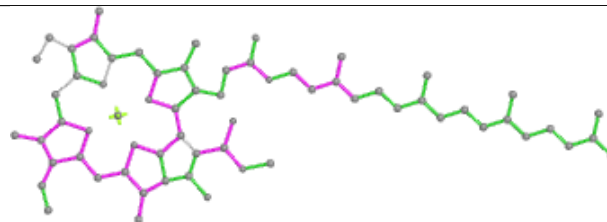


Rings

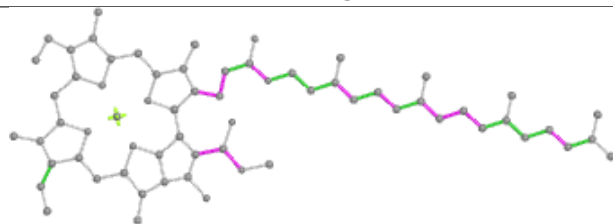
## Ligand CLA A 837



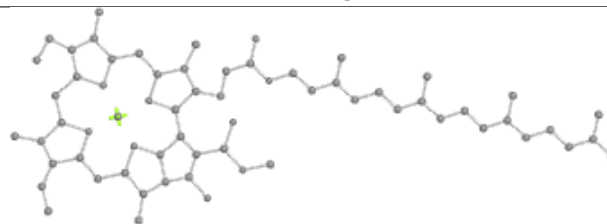
Bond lengths



Bond angles

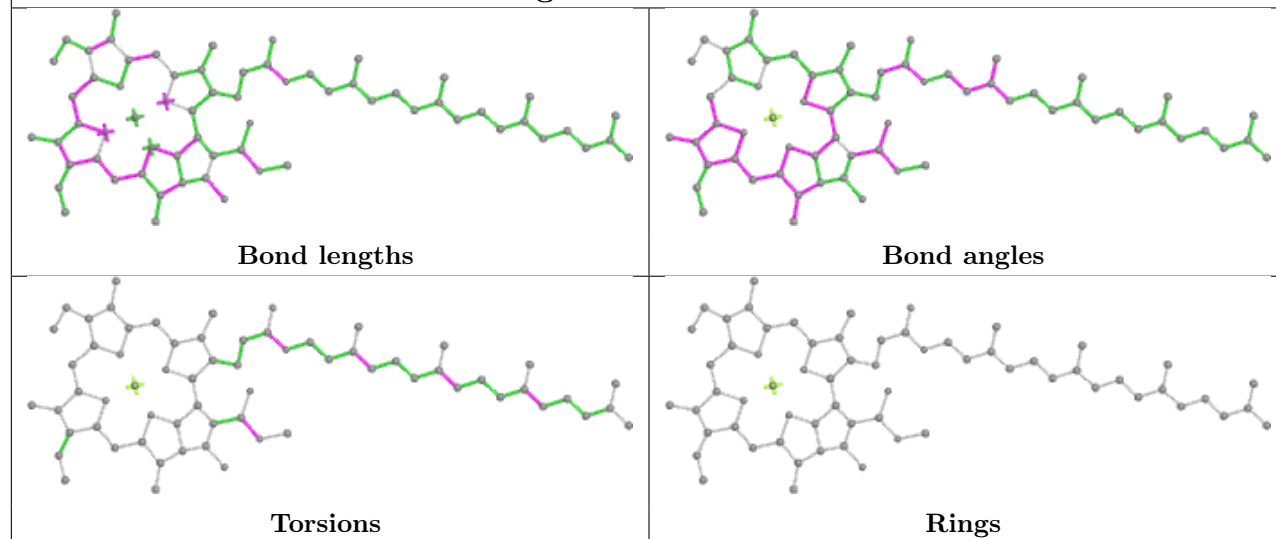


Torsions

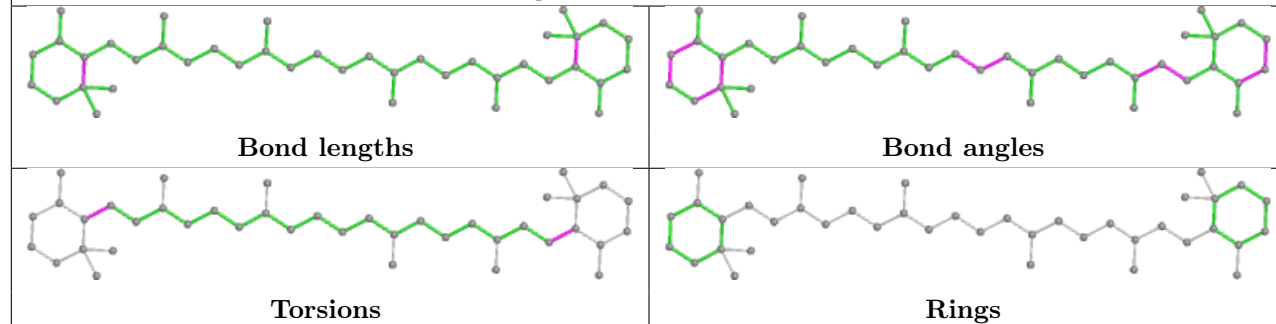


Rings

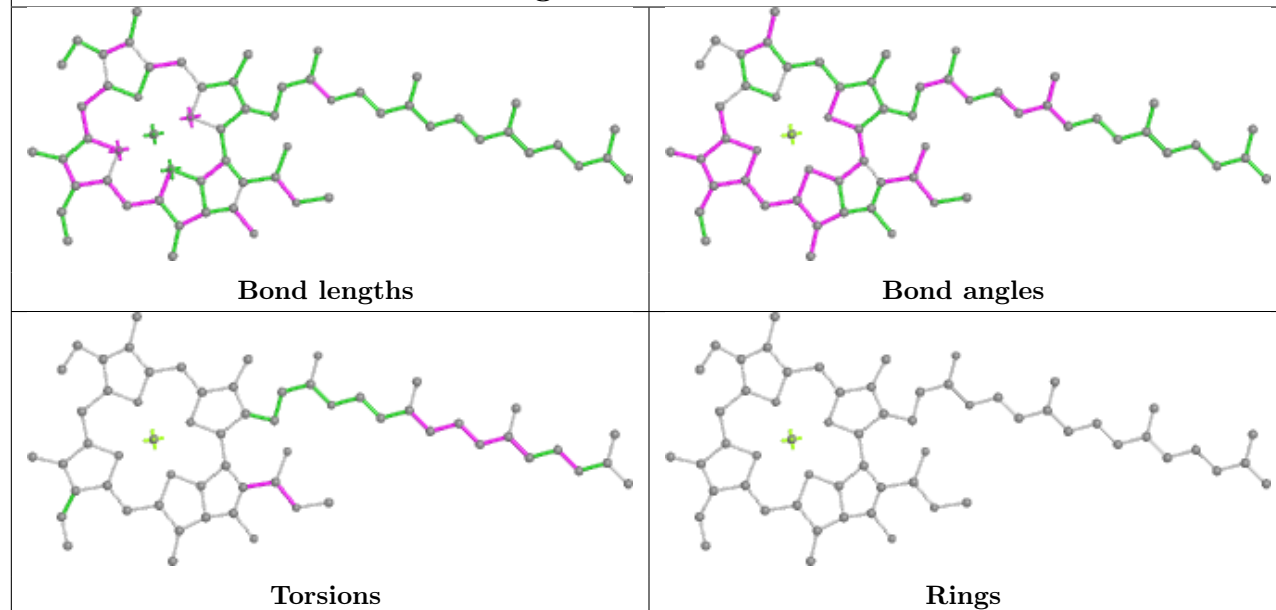
## Ligand CLA 7 311

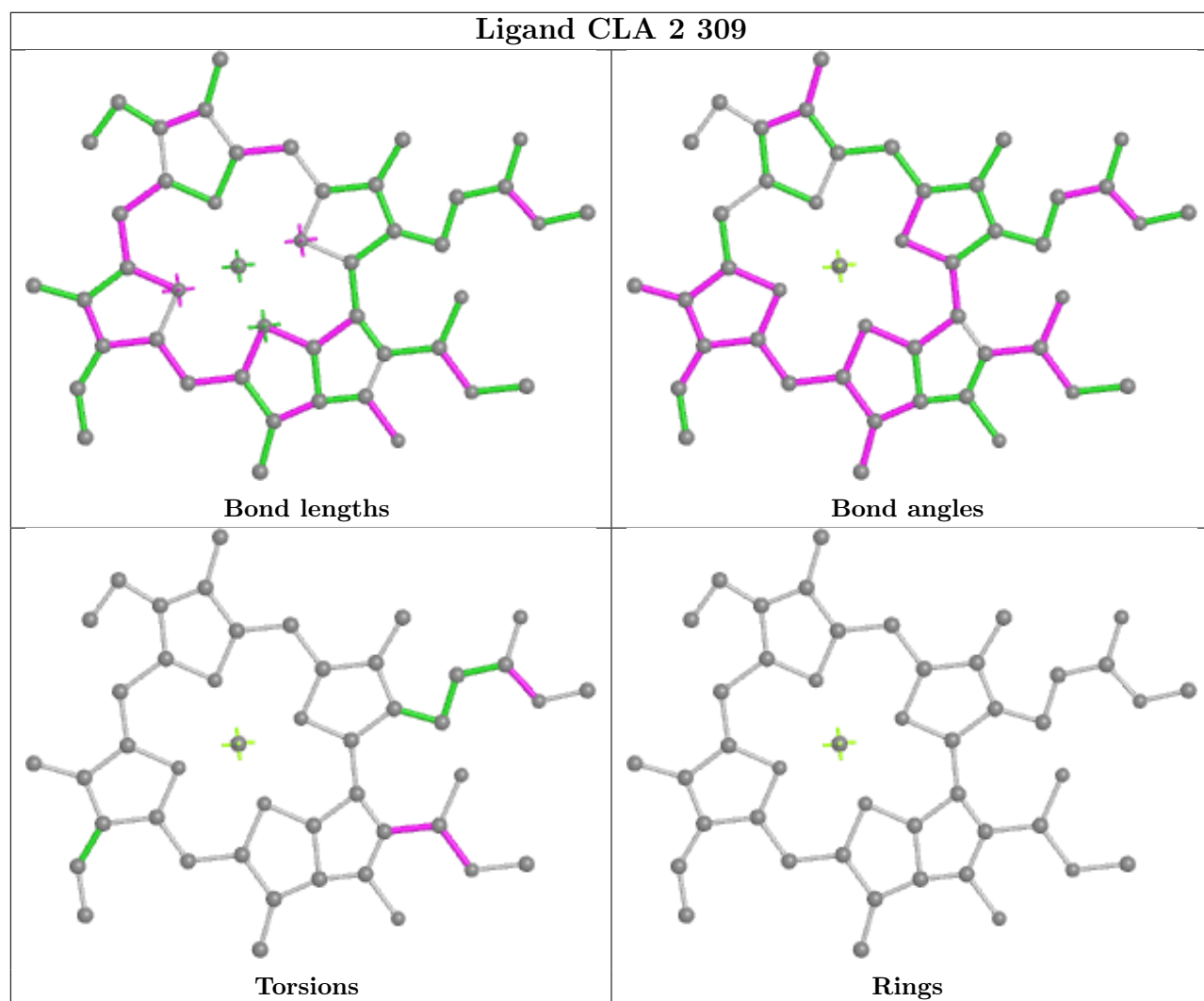
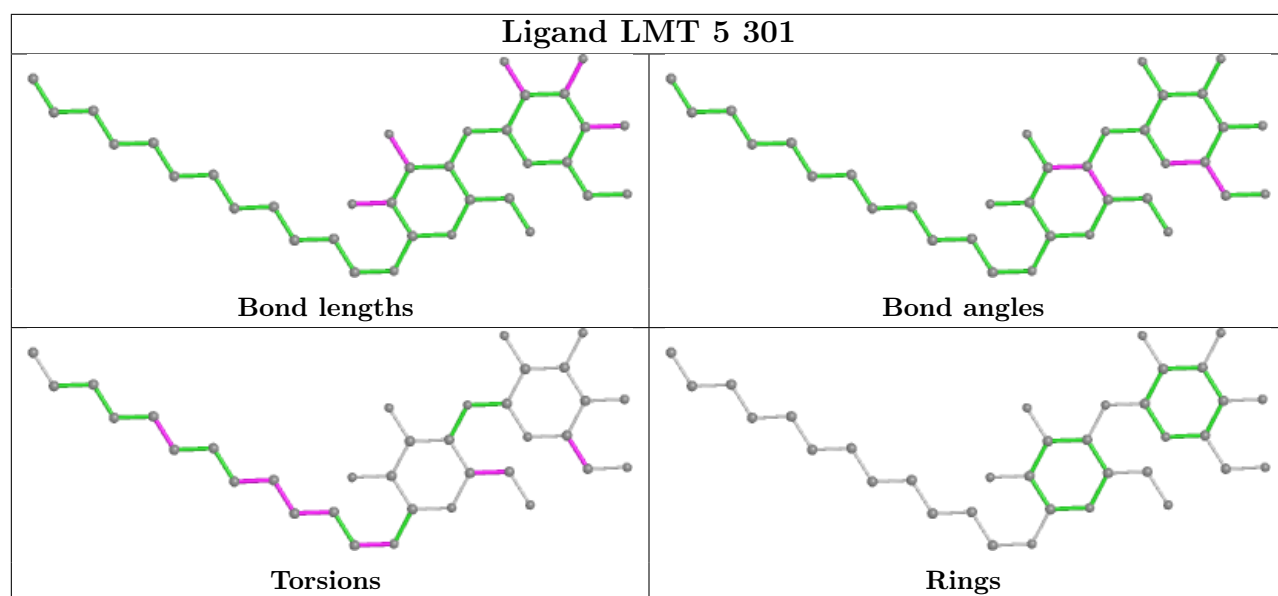


## Ligand BCR O 201

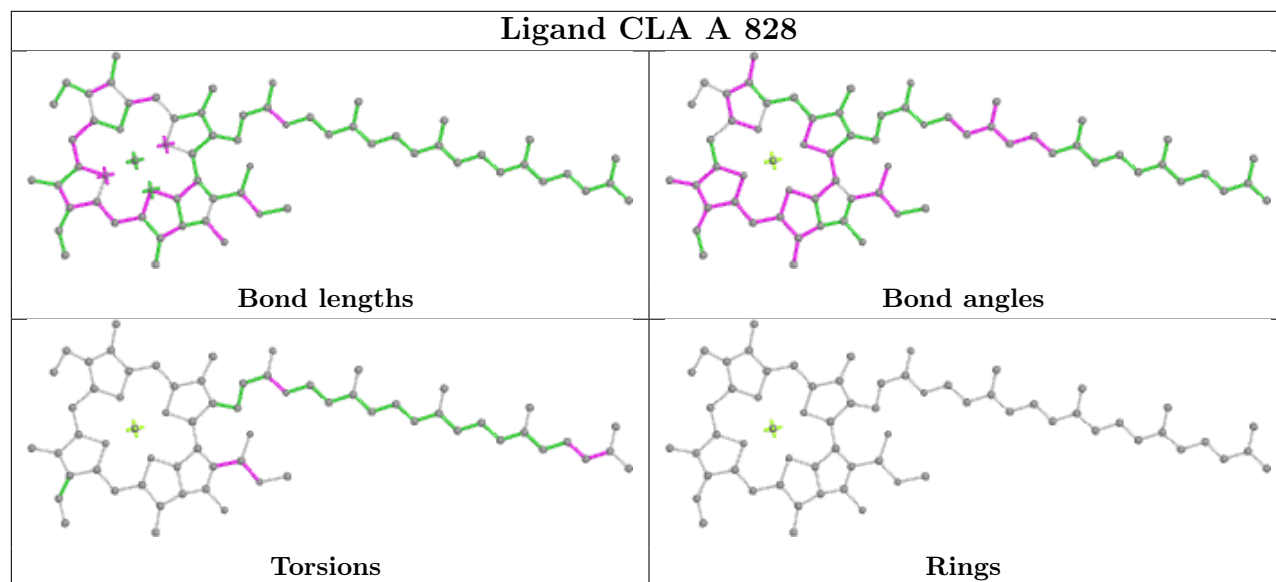


## Ligand CLA L 305

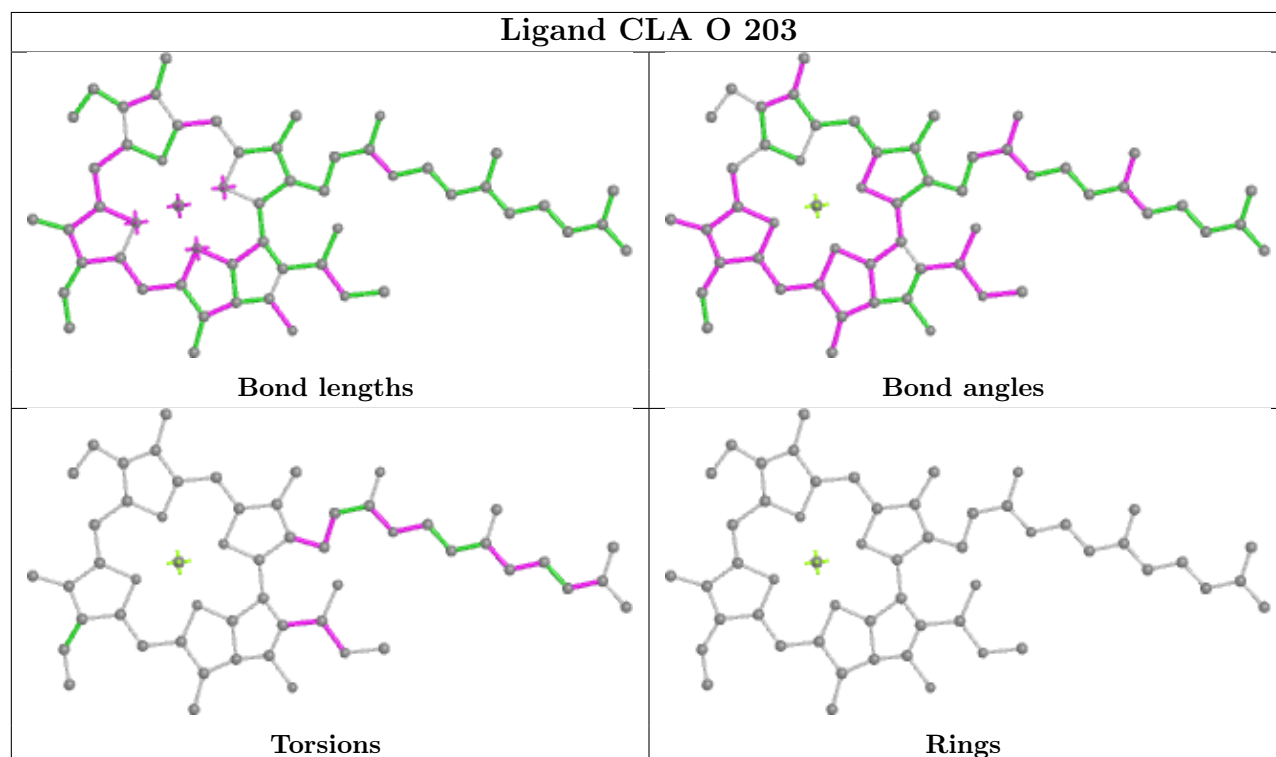




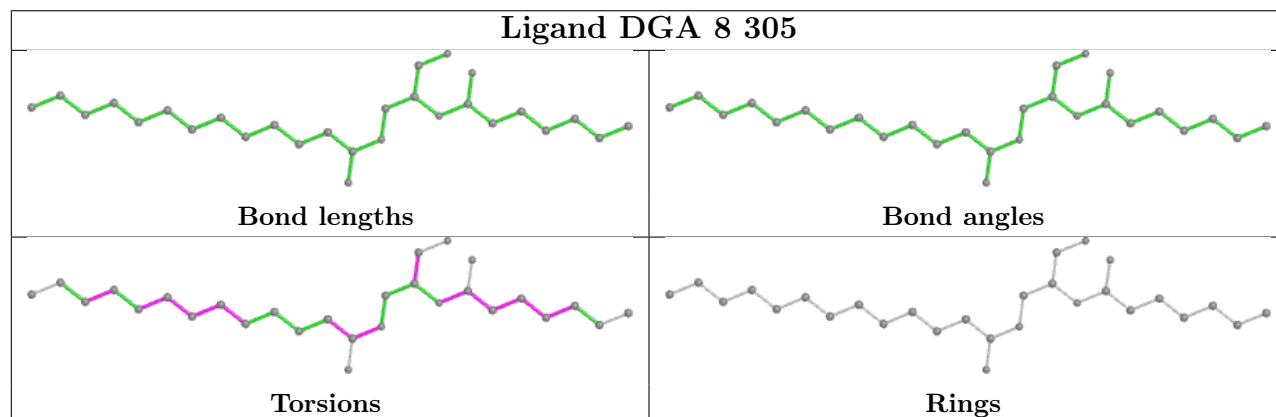
## Ligand CLA A 828



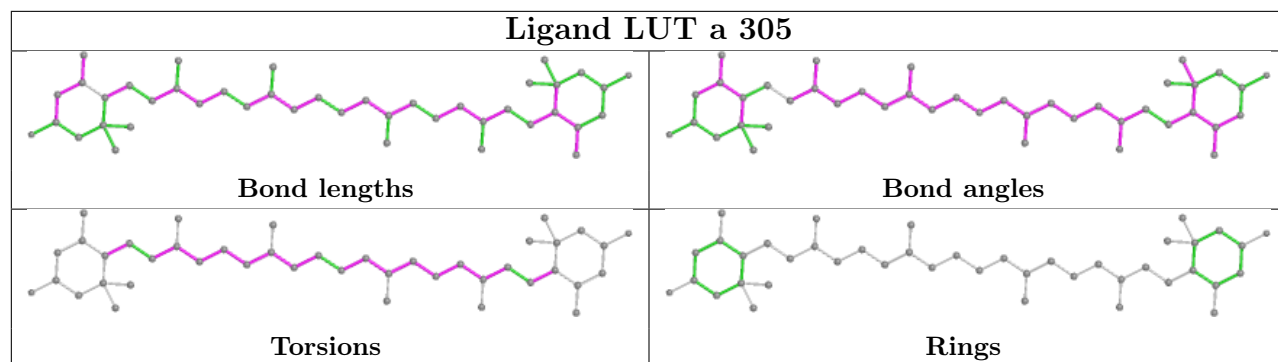
## Ligand CLA O 203



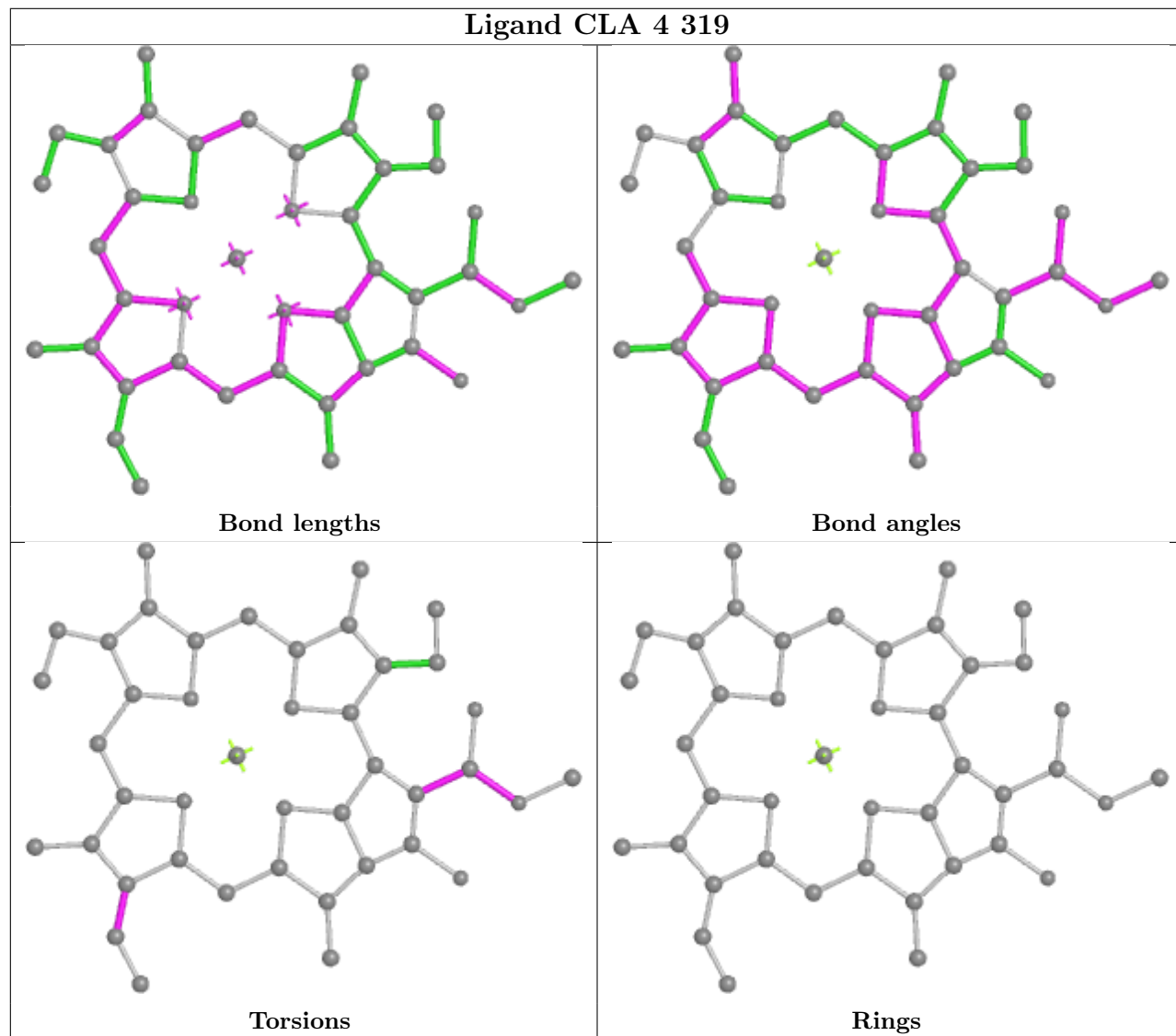
## Ligand DGA 8 305



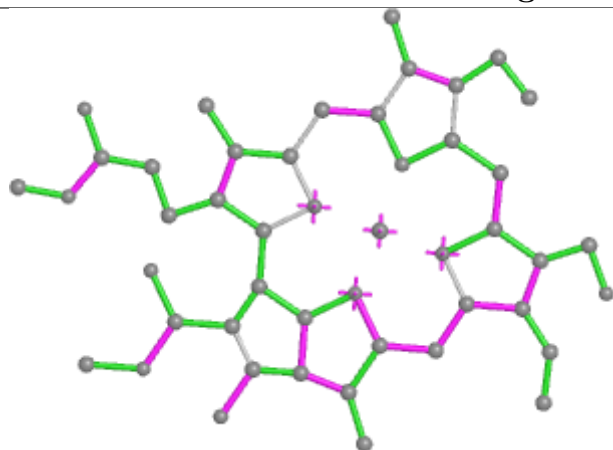
## Ligand LUT a 305



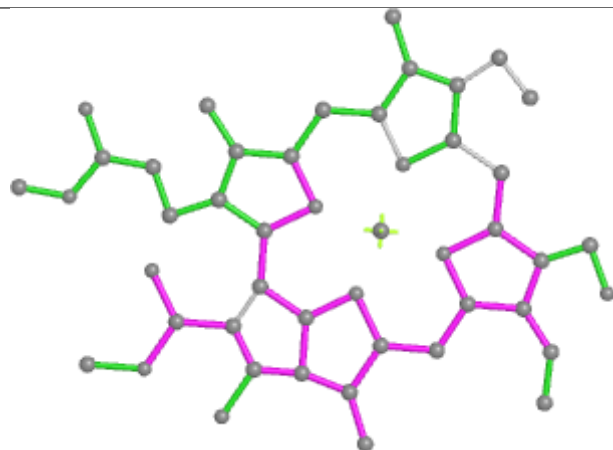
## Ligand CLA 4 319



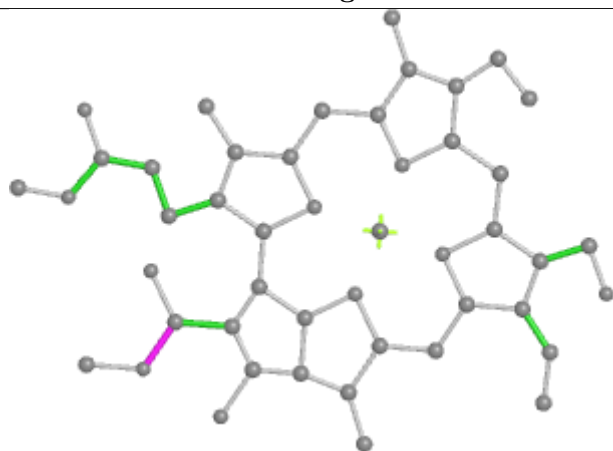
## Ligand CHL 5 319



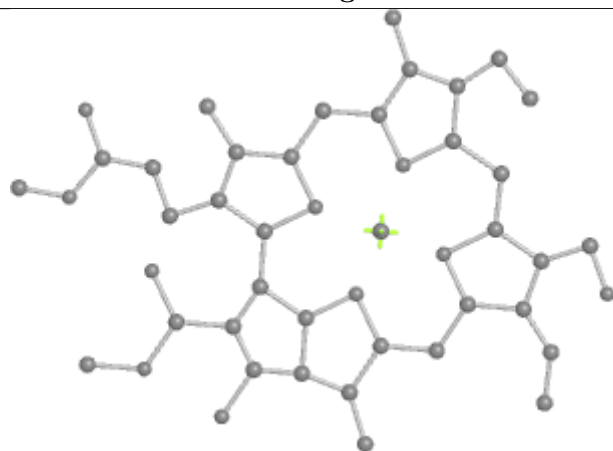
Bond lengths



Bond angles

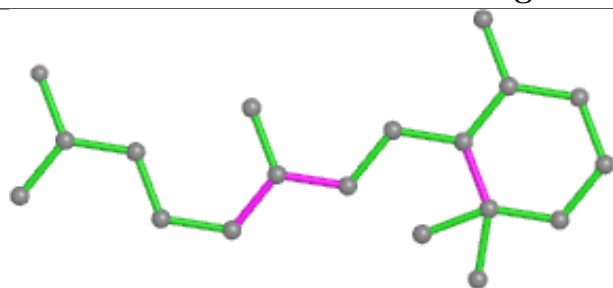


Torsions

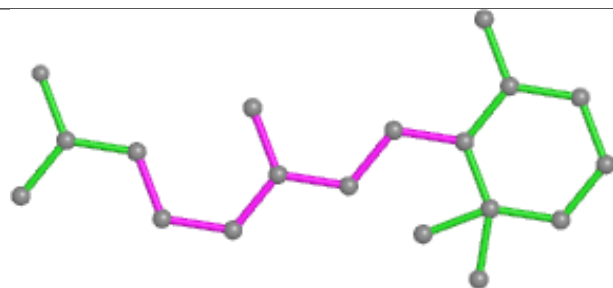


Rings

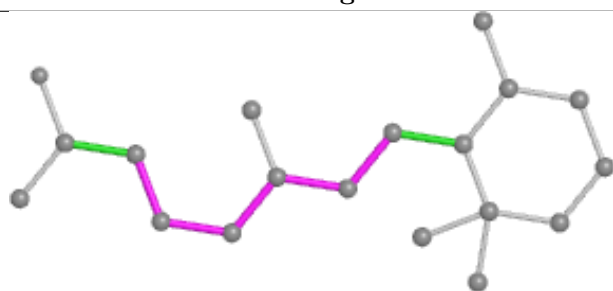
## Ligand QTB F 303



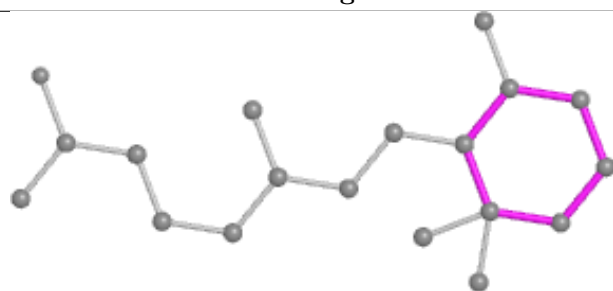
Bond lengths



Bond angles

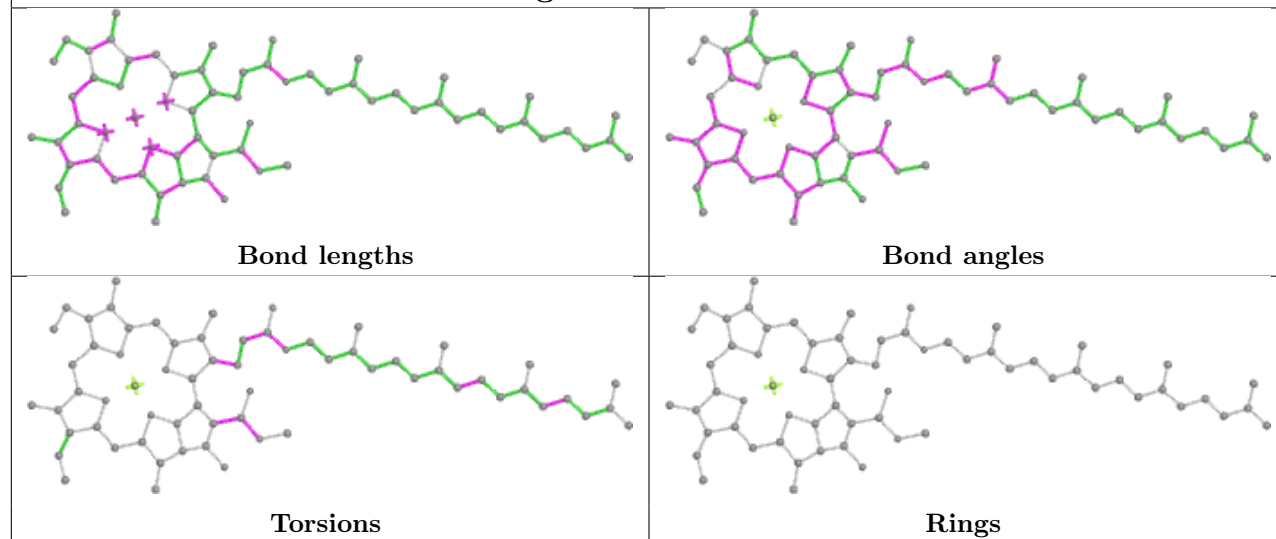
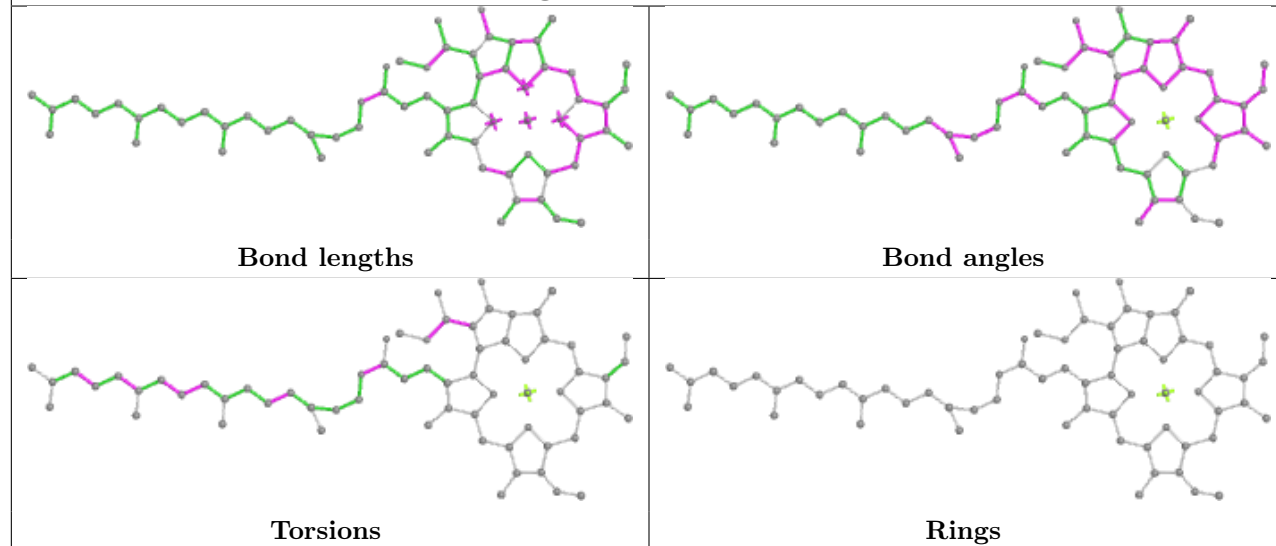


Torsions

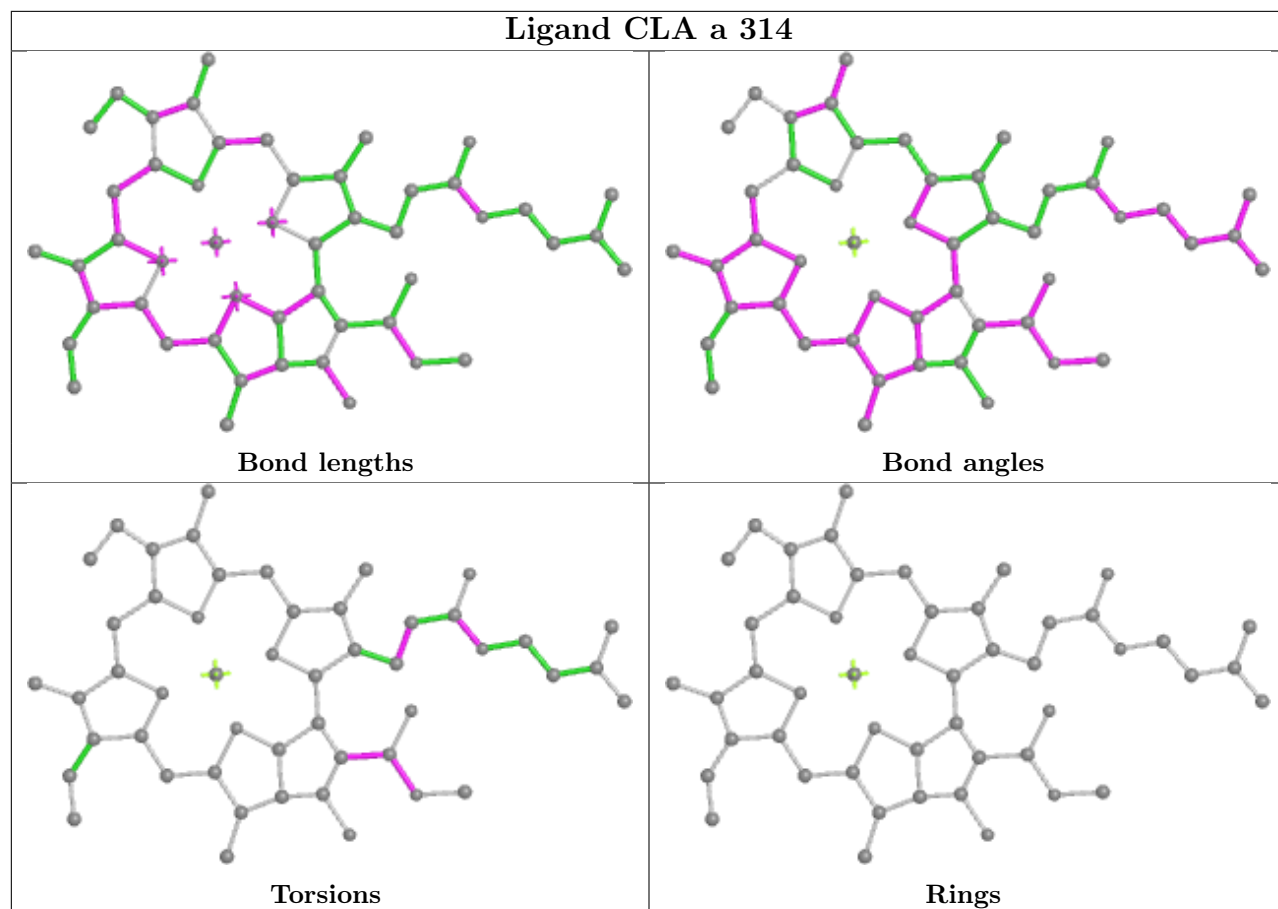


Rings

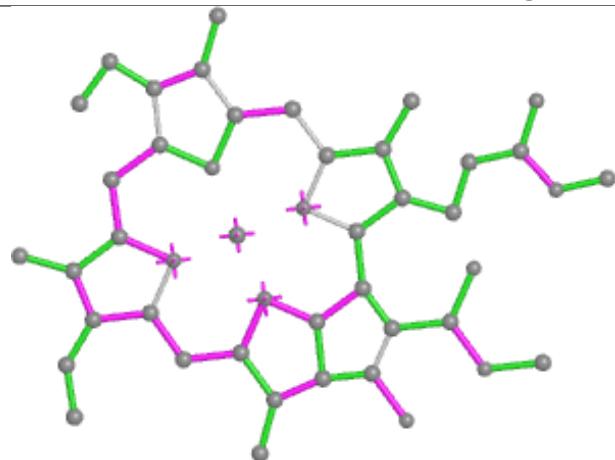


**Ligand CLA 8 320****Ligand CLA 5 315**

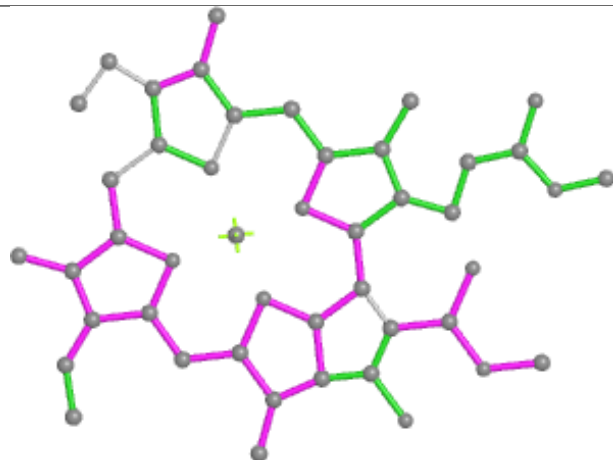
## Ligand CLA a 314



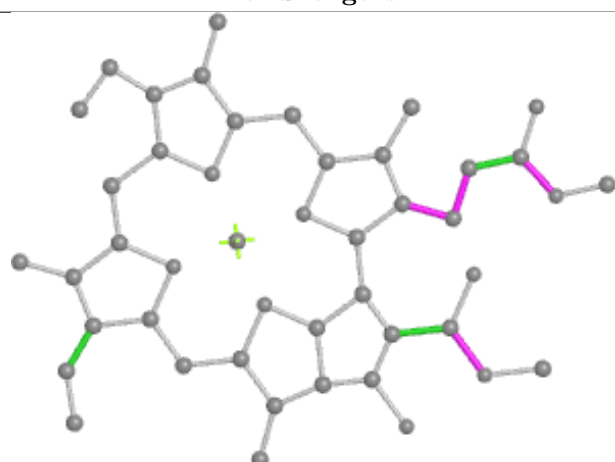
## Ligand CLA 9 319



Bond lengths



Bond angles

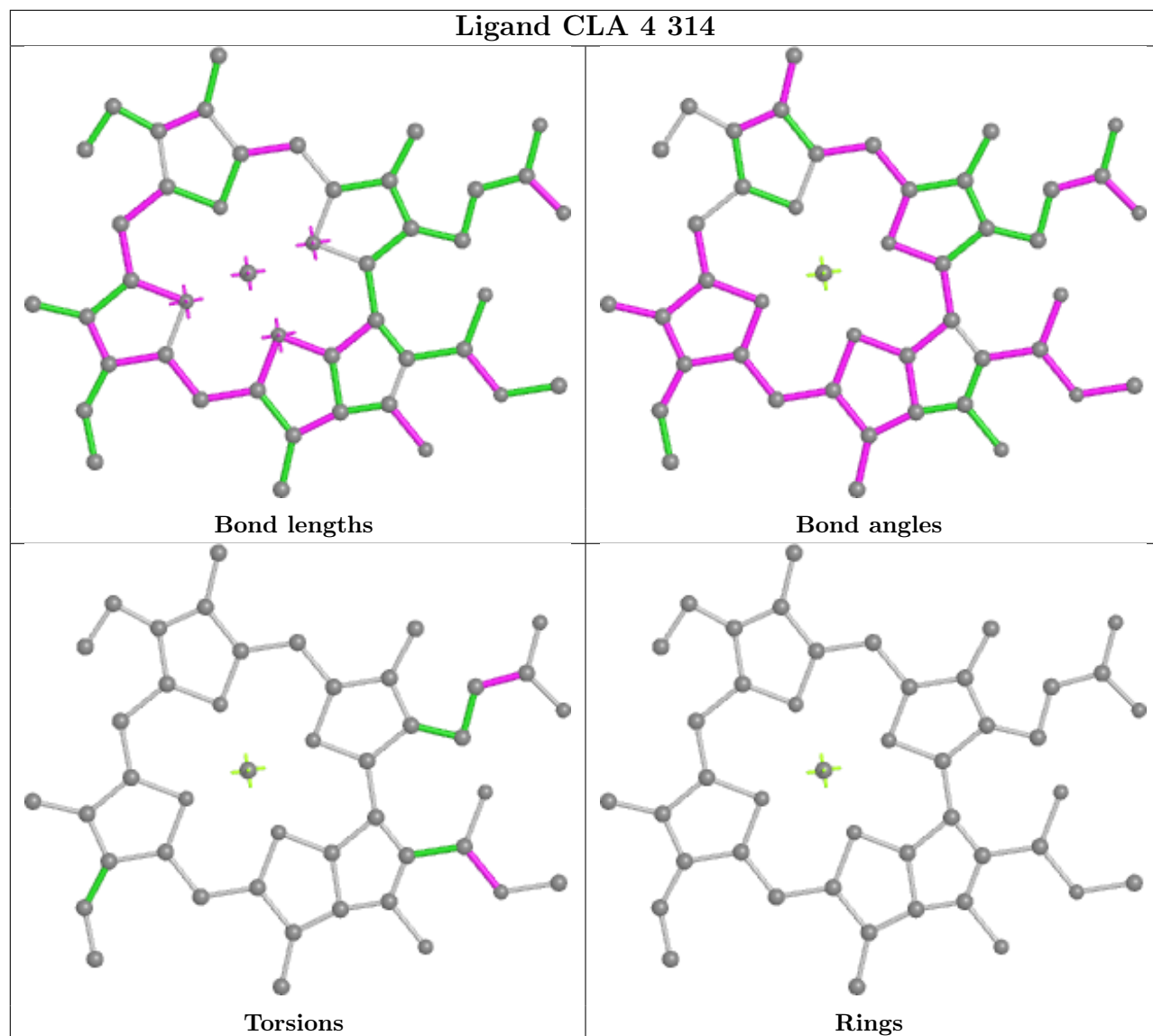


Torsions

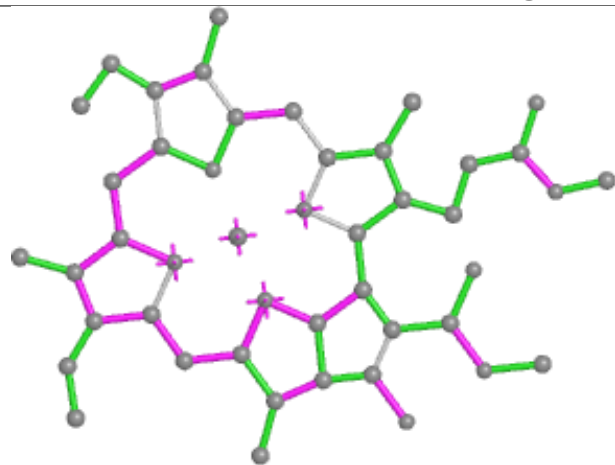


Rings

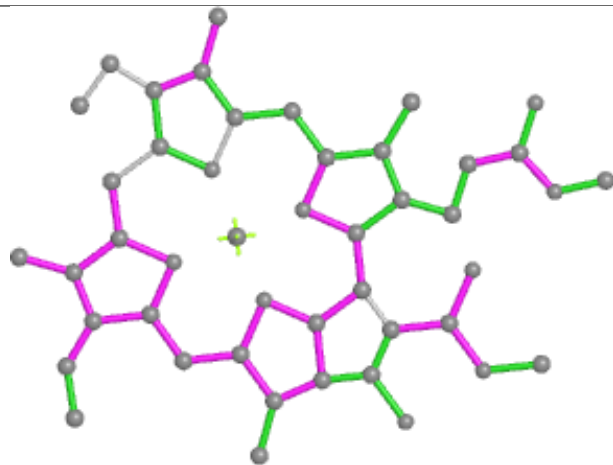
## Ligand CLA 4 314



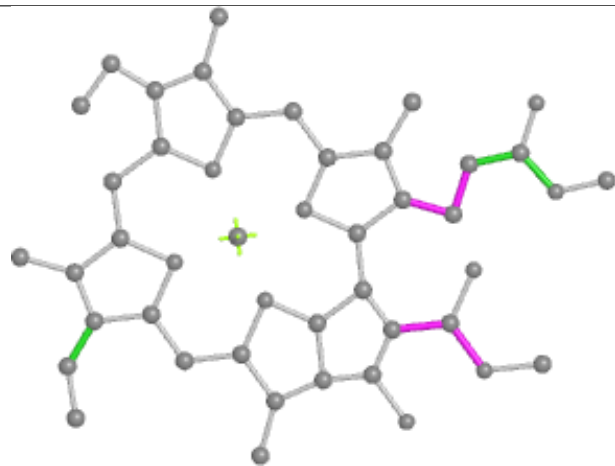
## Ligand CLA 4 311



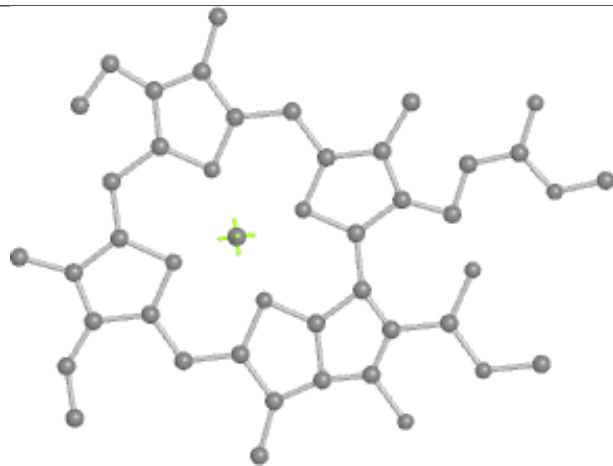
Bond lengths



Bond angles

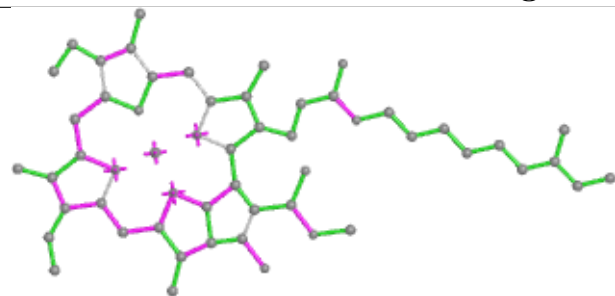


Torsions

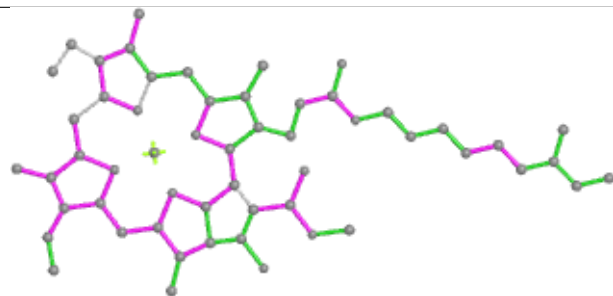


Rings

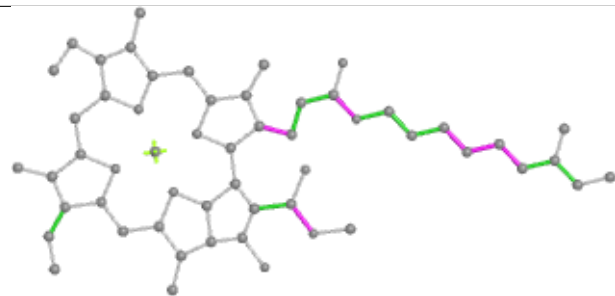
## Ligand CLA 7 315



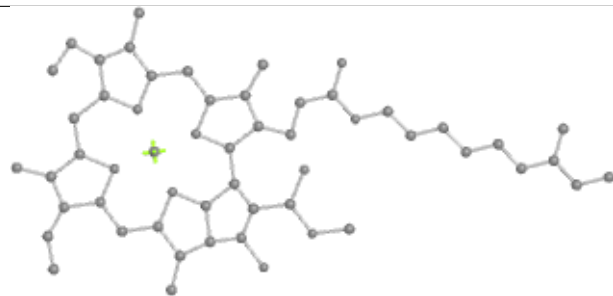
Bond lengths



Bond angles

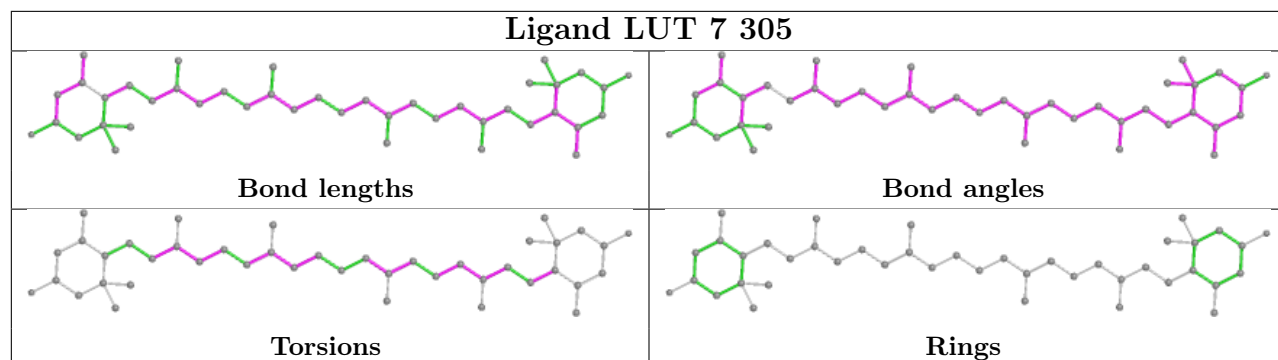


Torsions

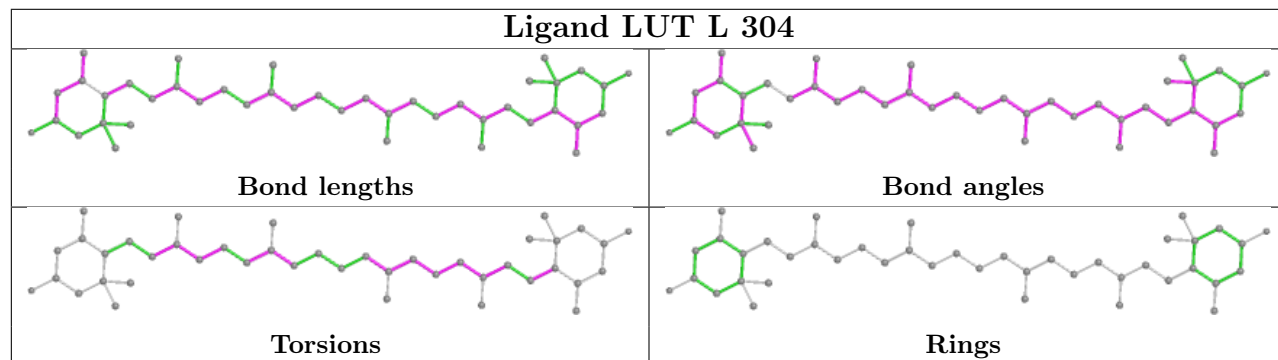


Rings

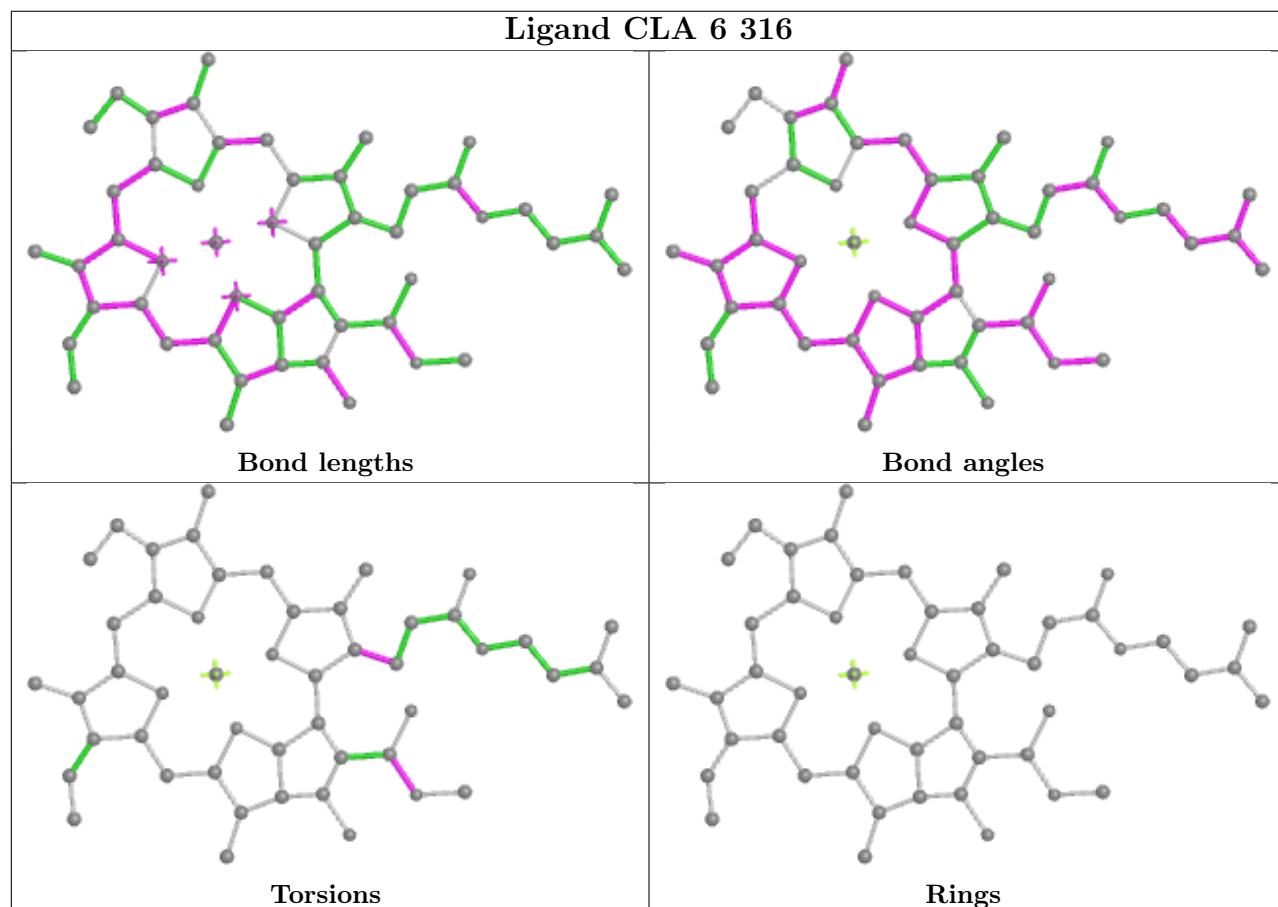
## Ligand LUT 7 305

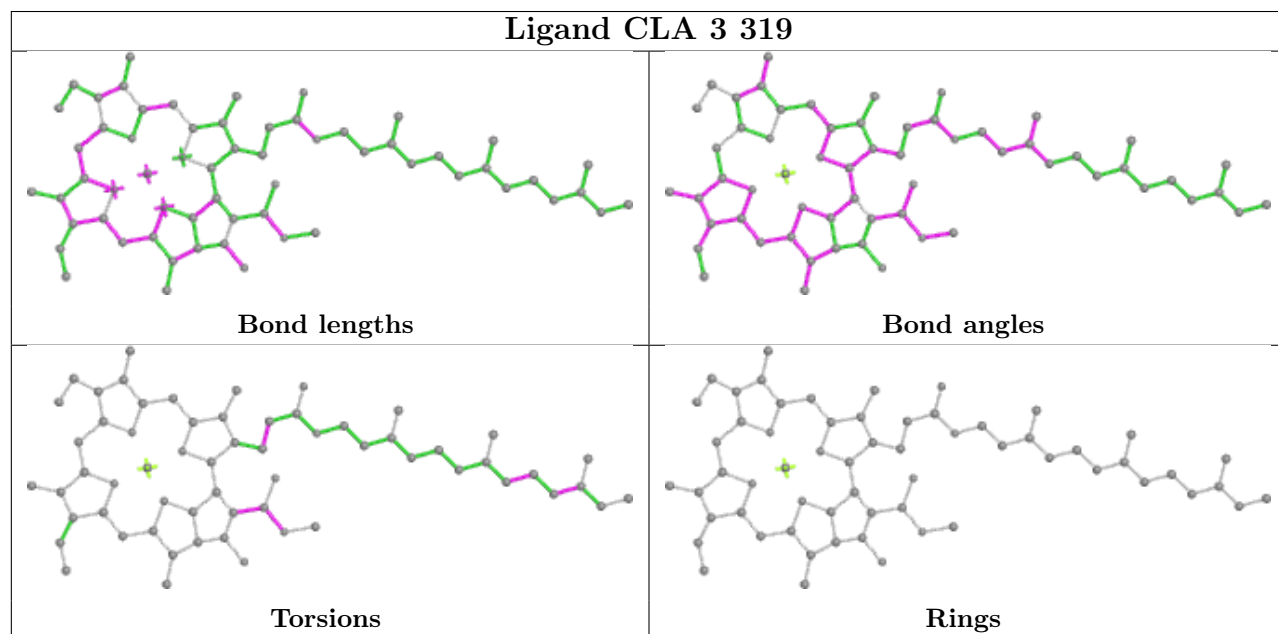
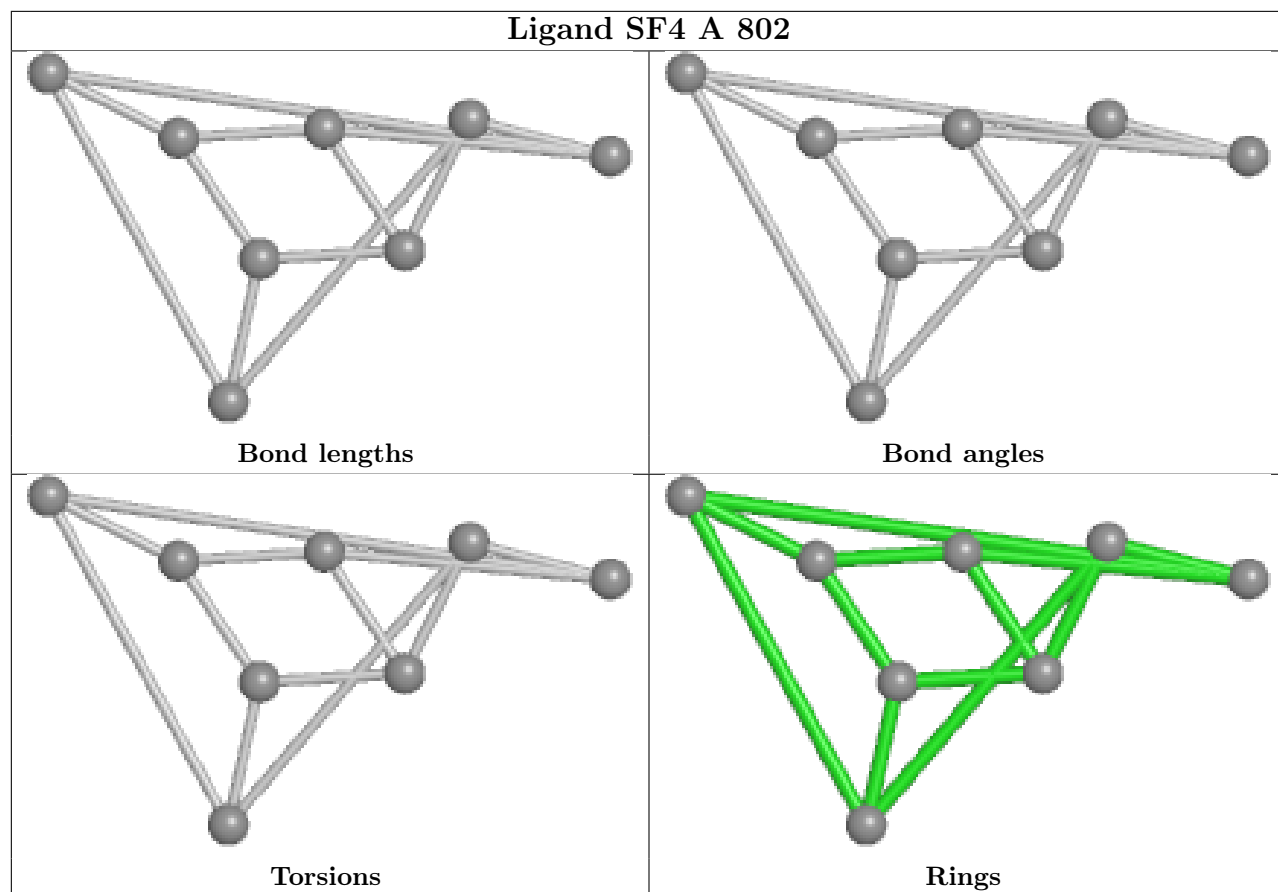


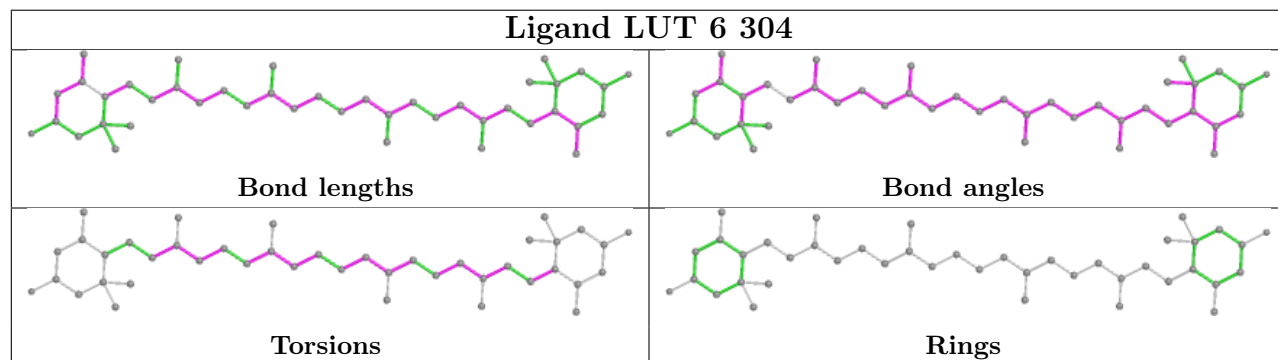
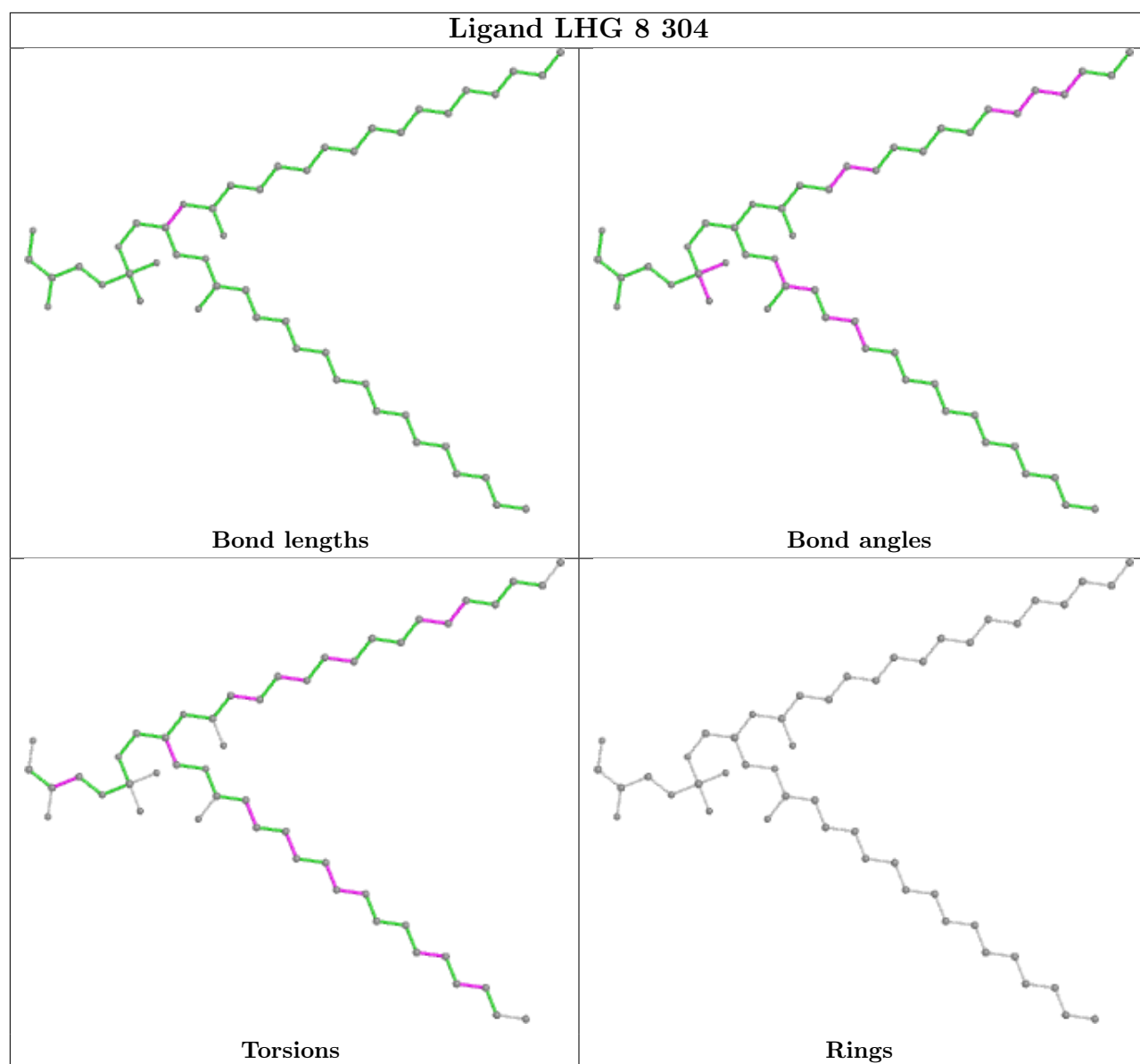
## Ligand LUT L 304



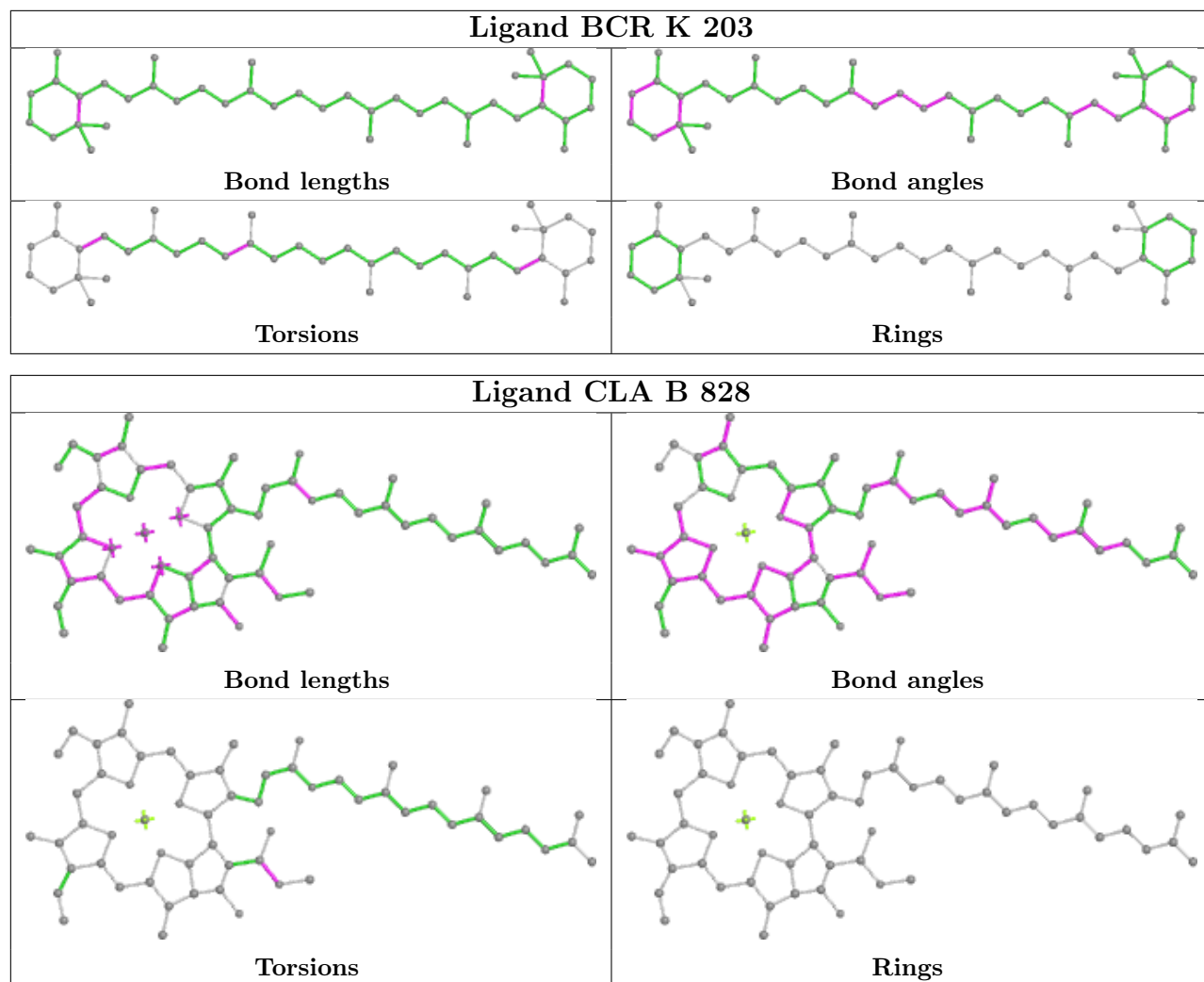
## Ligand CLA 6 316



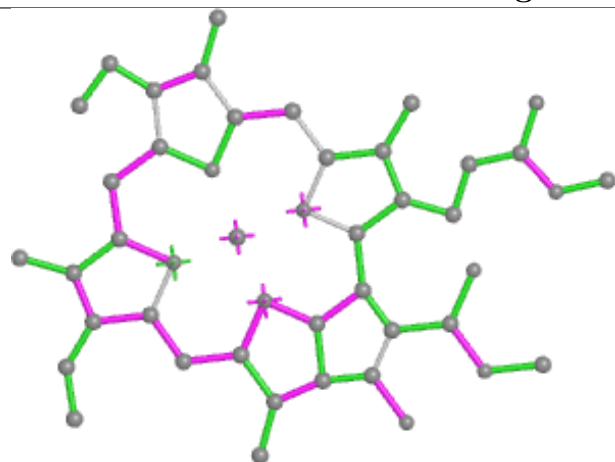




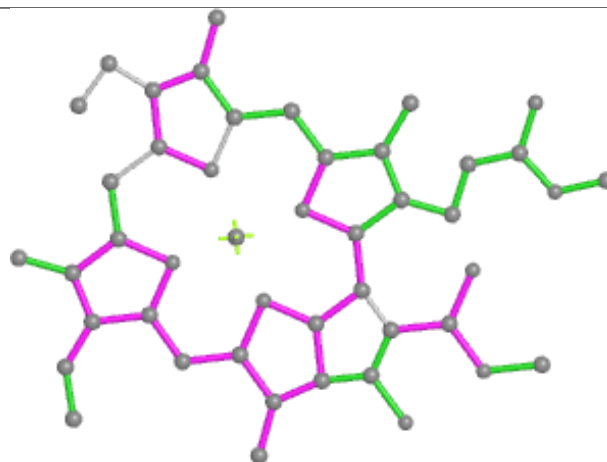




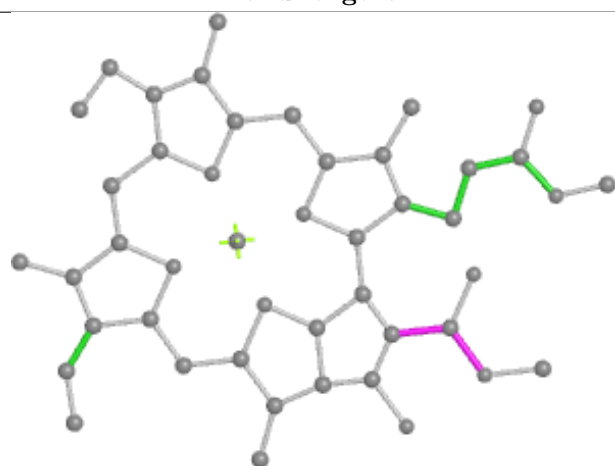
## Ligand CLA K 205



Bond lengths



Bond angles

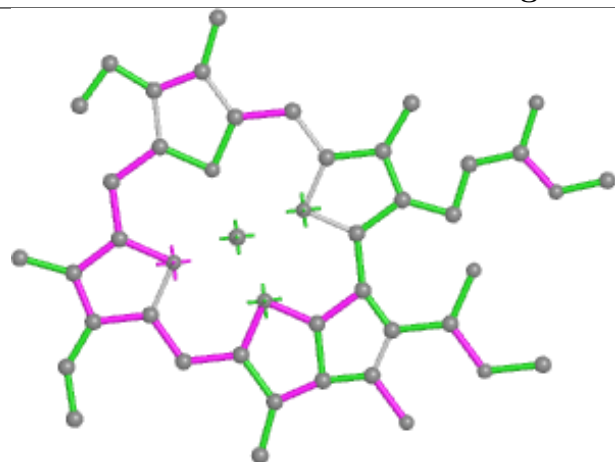


Torsions

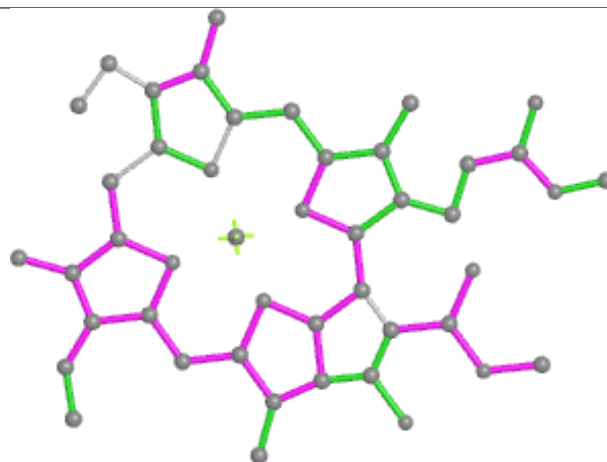


Rings

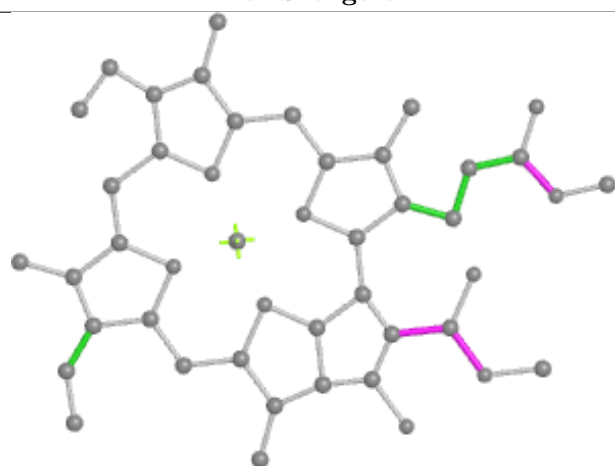
## Ligand CLA 5 321



Bond lengths



Bond angles

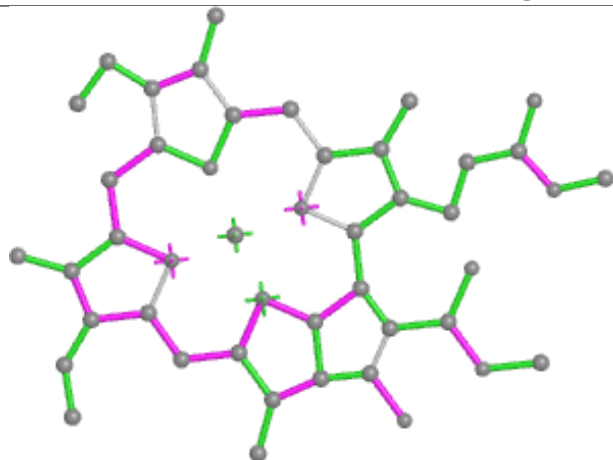


Torsions

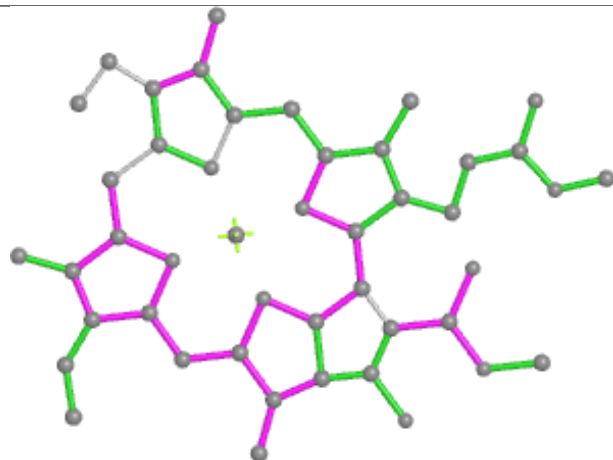


Rings

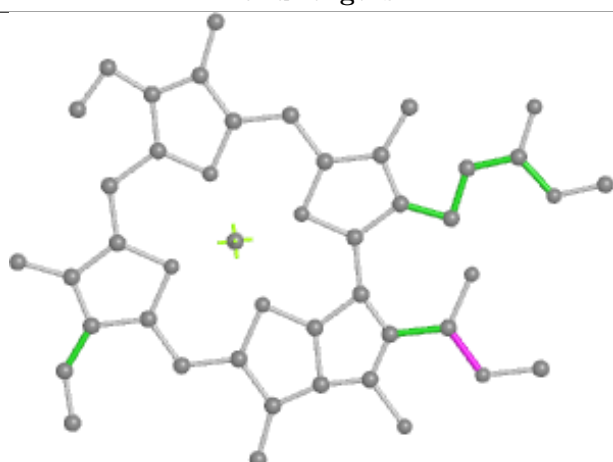
## Ligand CLA 9 312



Bond lengths



Bond angles

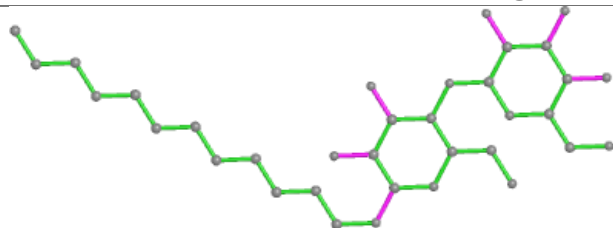


Torsions

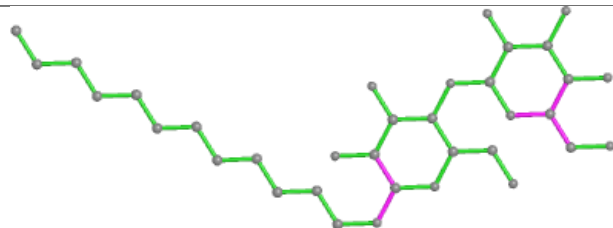


Rings

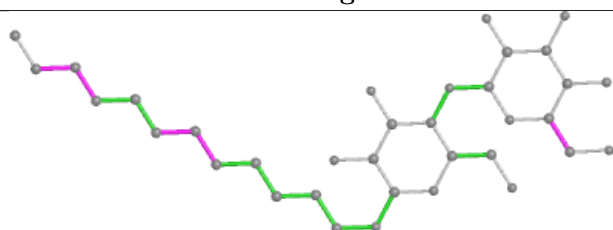
## Ligand LMT A 807



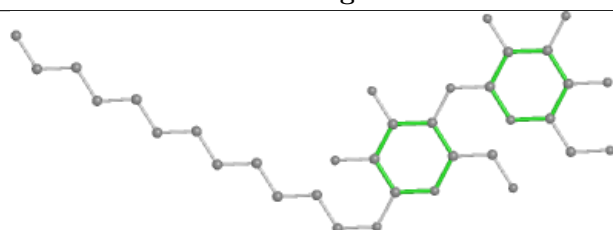
Bond lengths



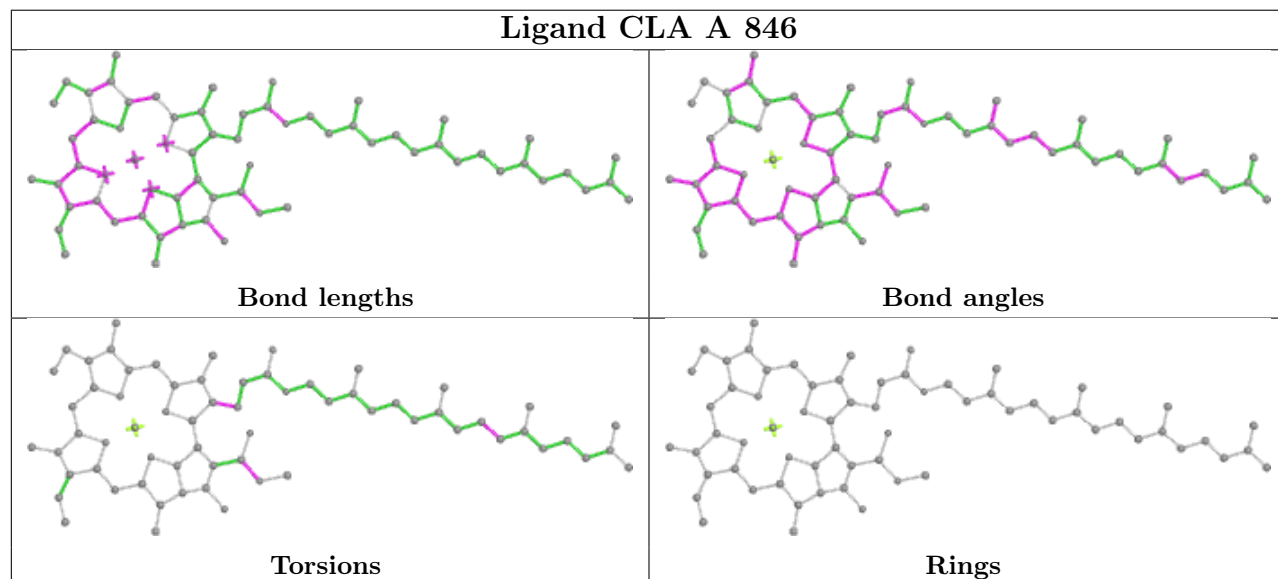
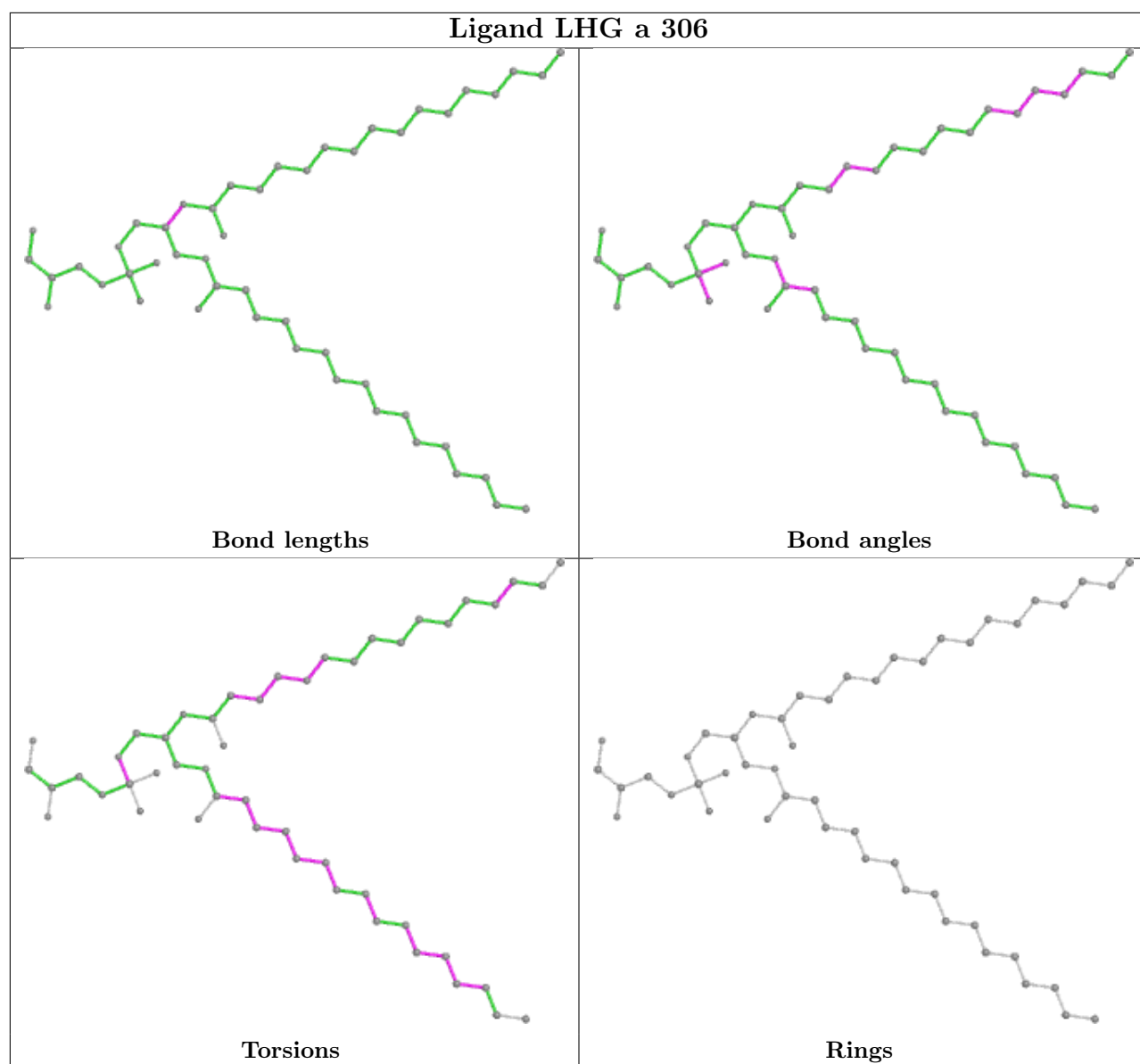
Bond angles



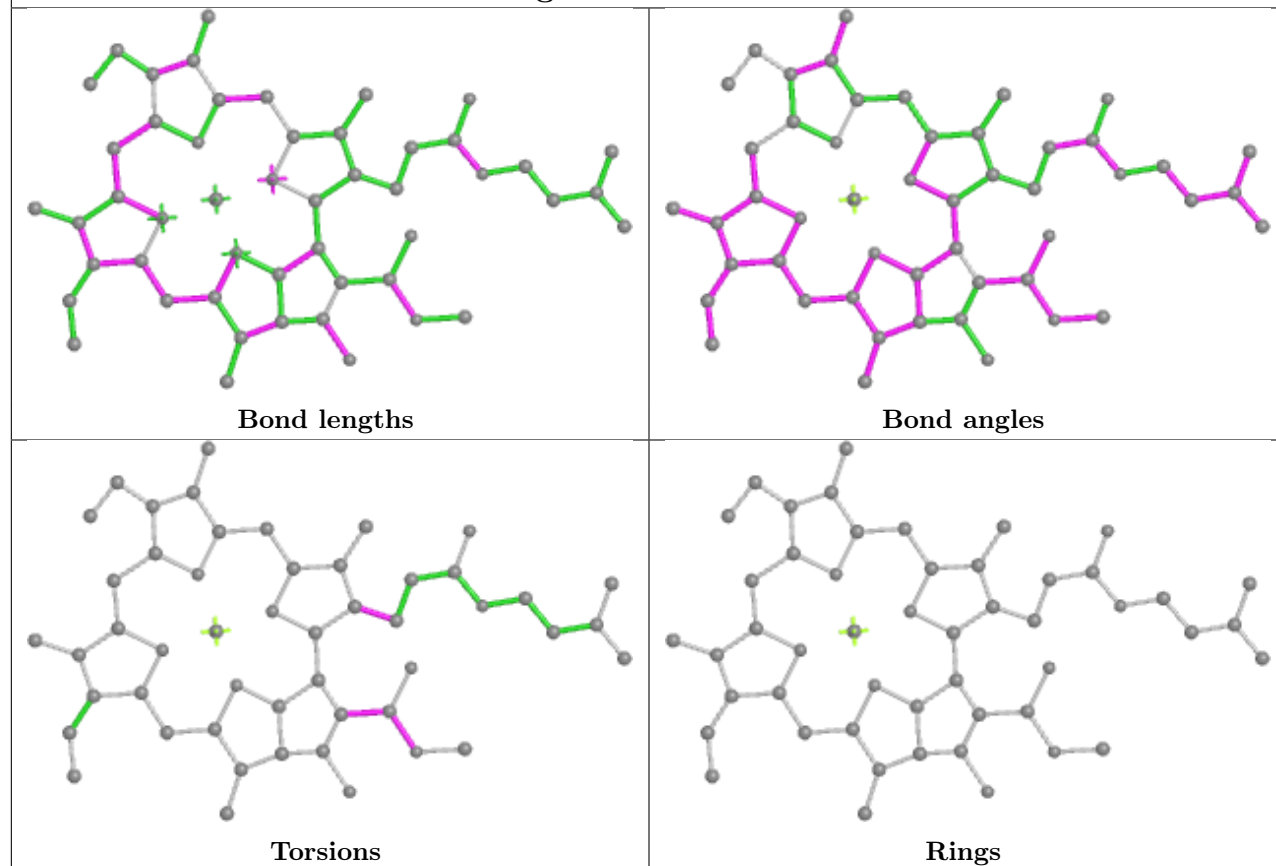
Torsions



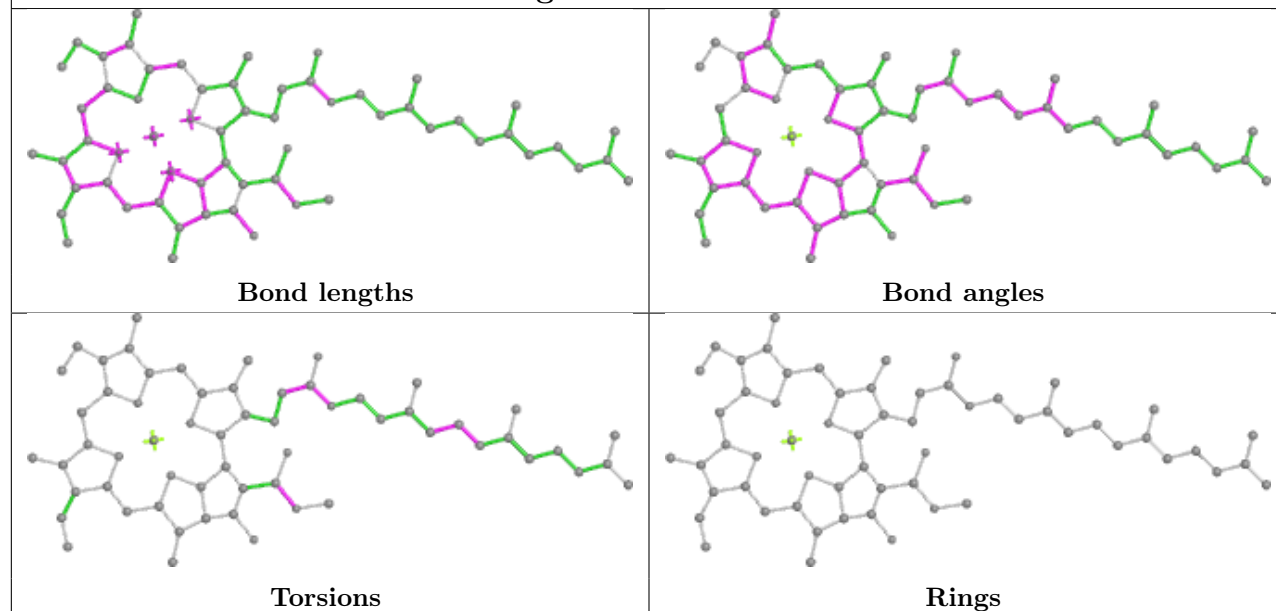
Rings



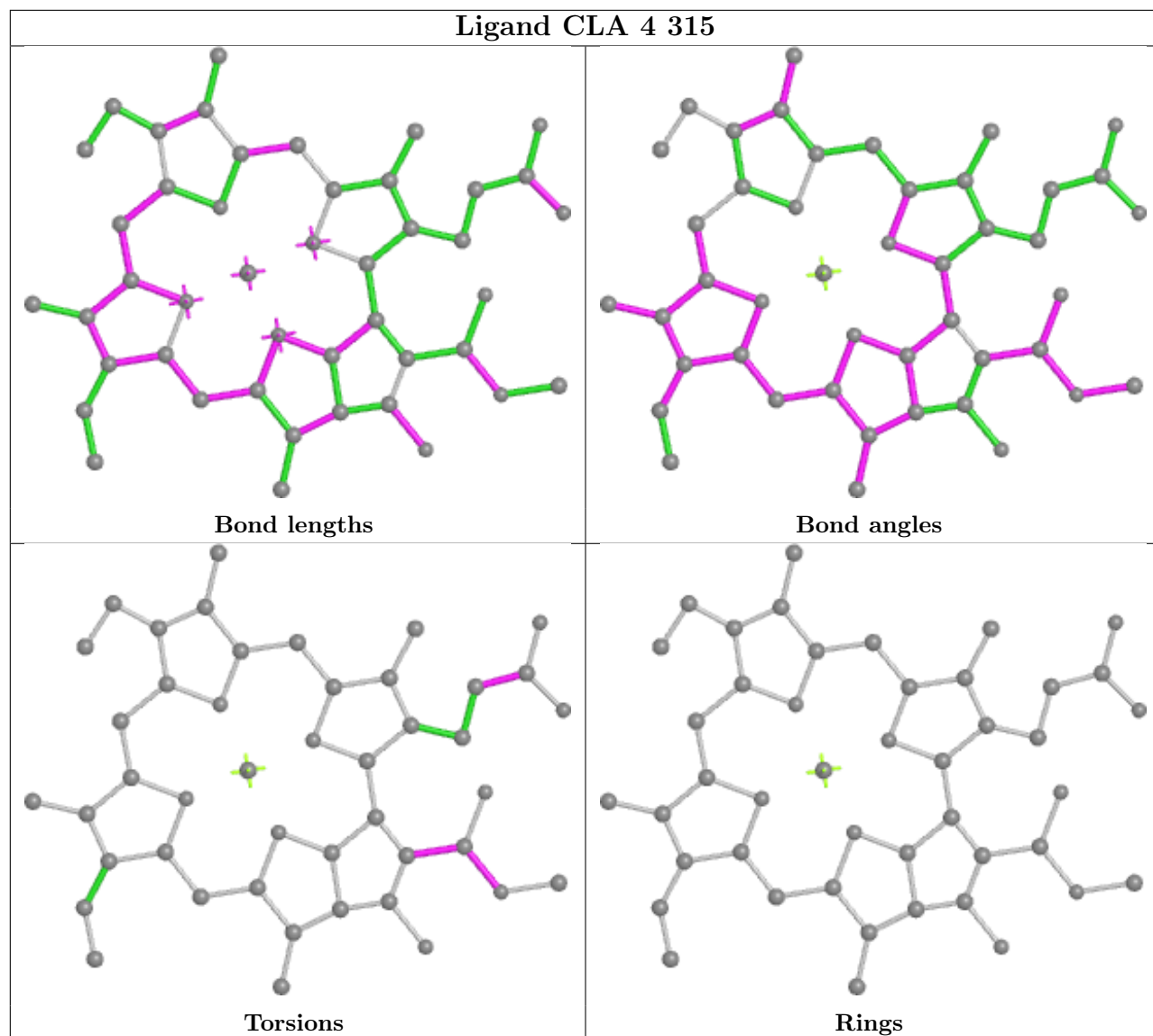
## Ligand CLA a 321



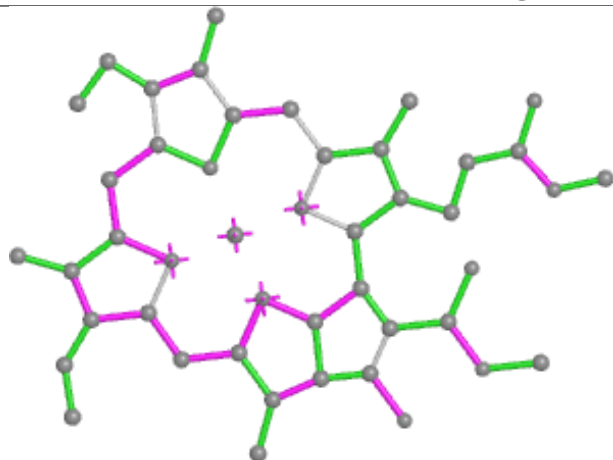
## Ligand CLA a 313



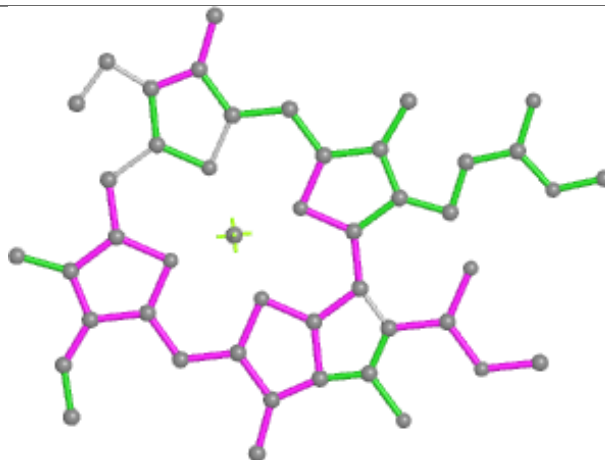
## Ligand CLA 4 315



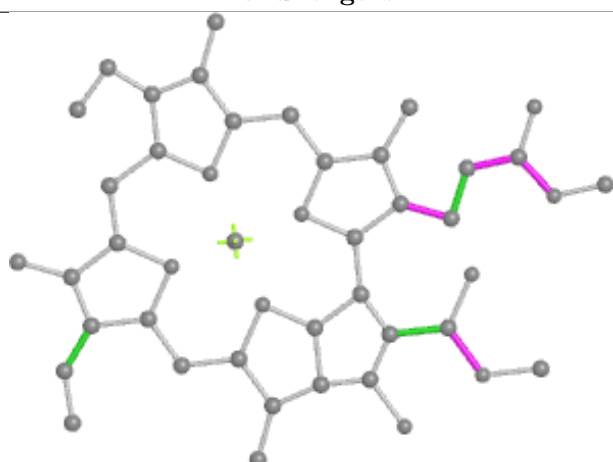
## Ligand CLA H 901



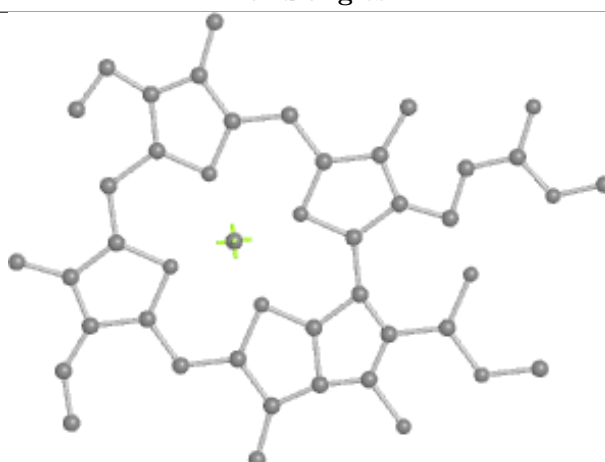
Bond lengths



Bond angles

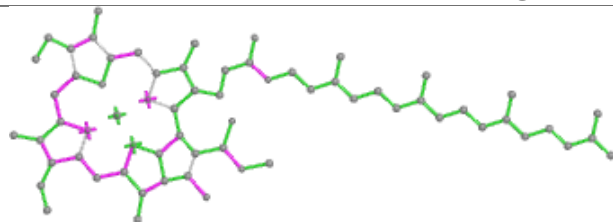


Torsions

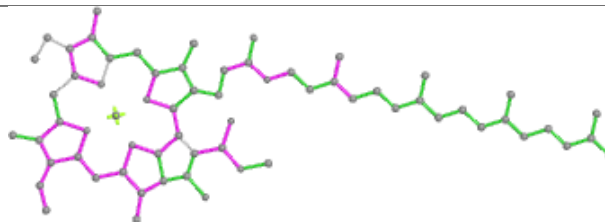


Rings

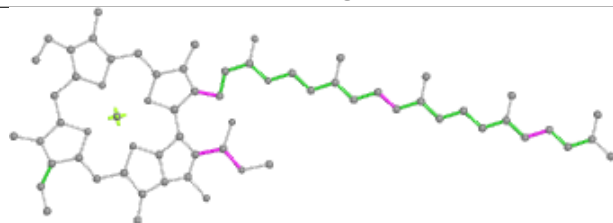
## Ligand CLA A 847



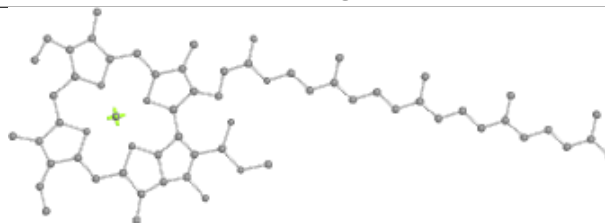
Bond lengths



Bond angles

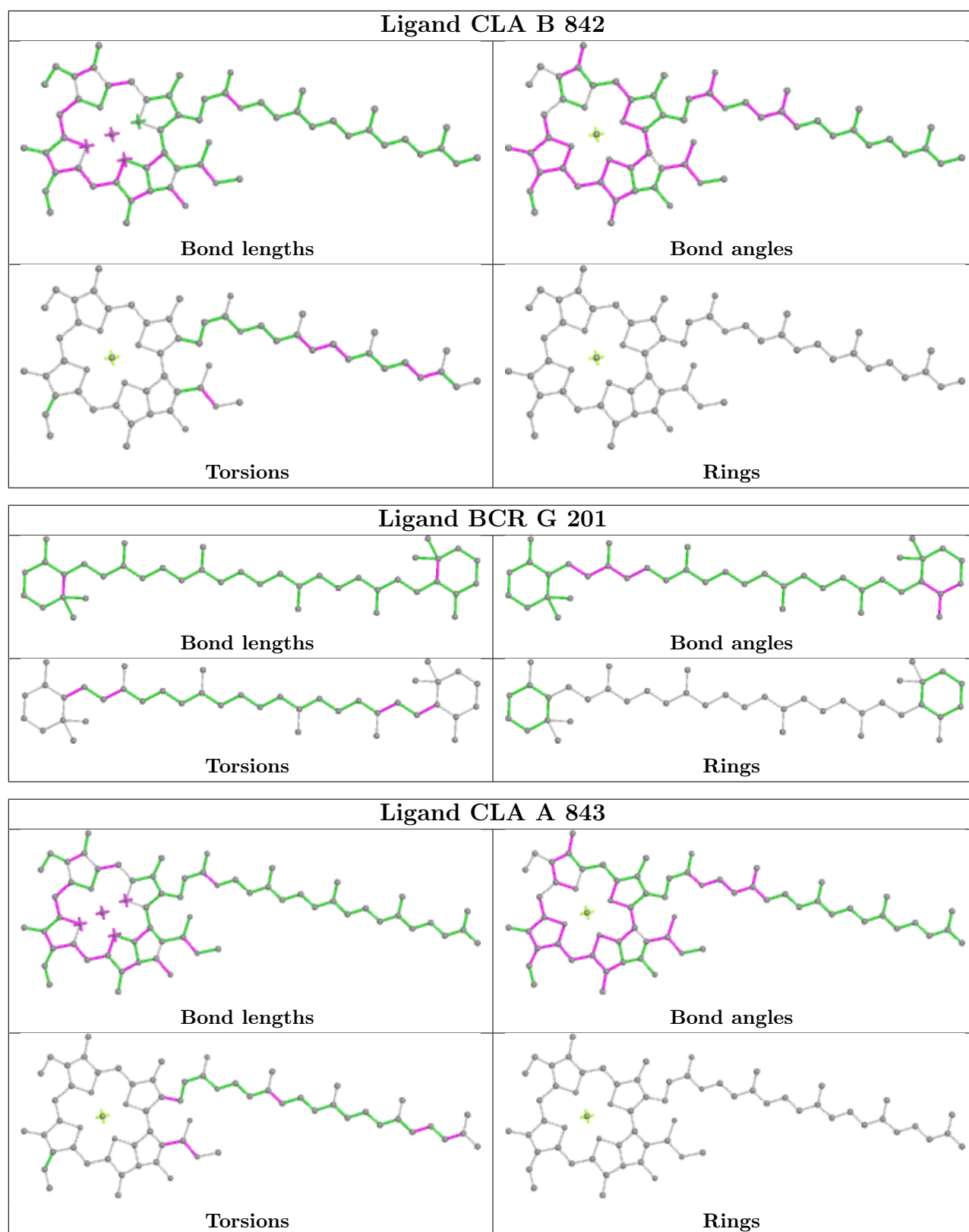


Torsions

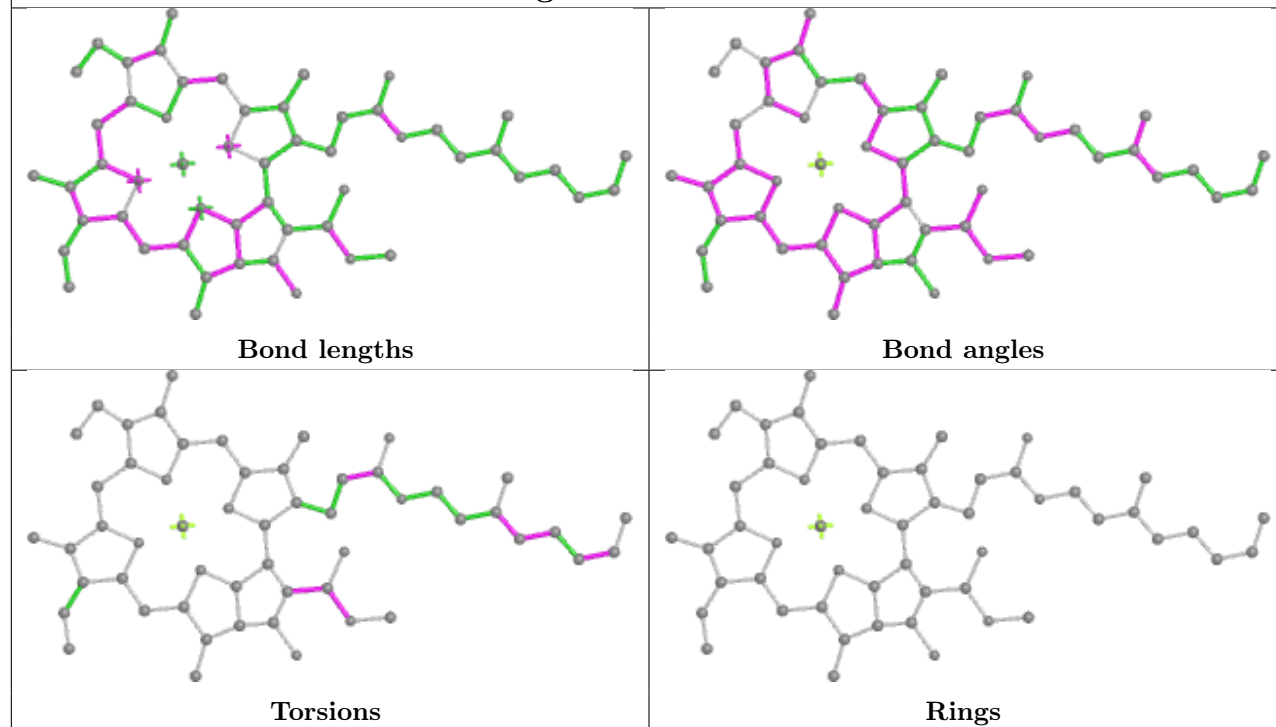


Rings

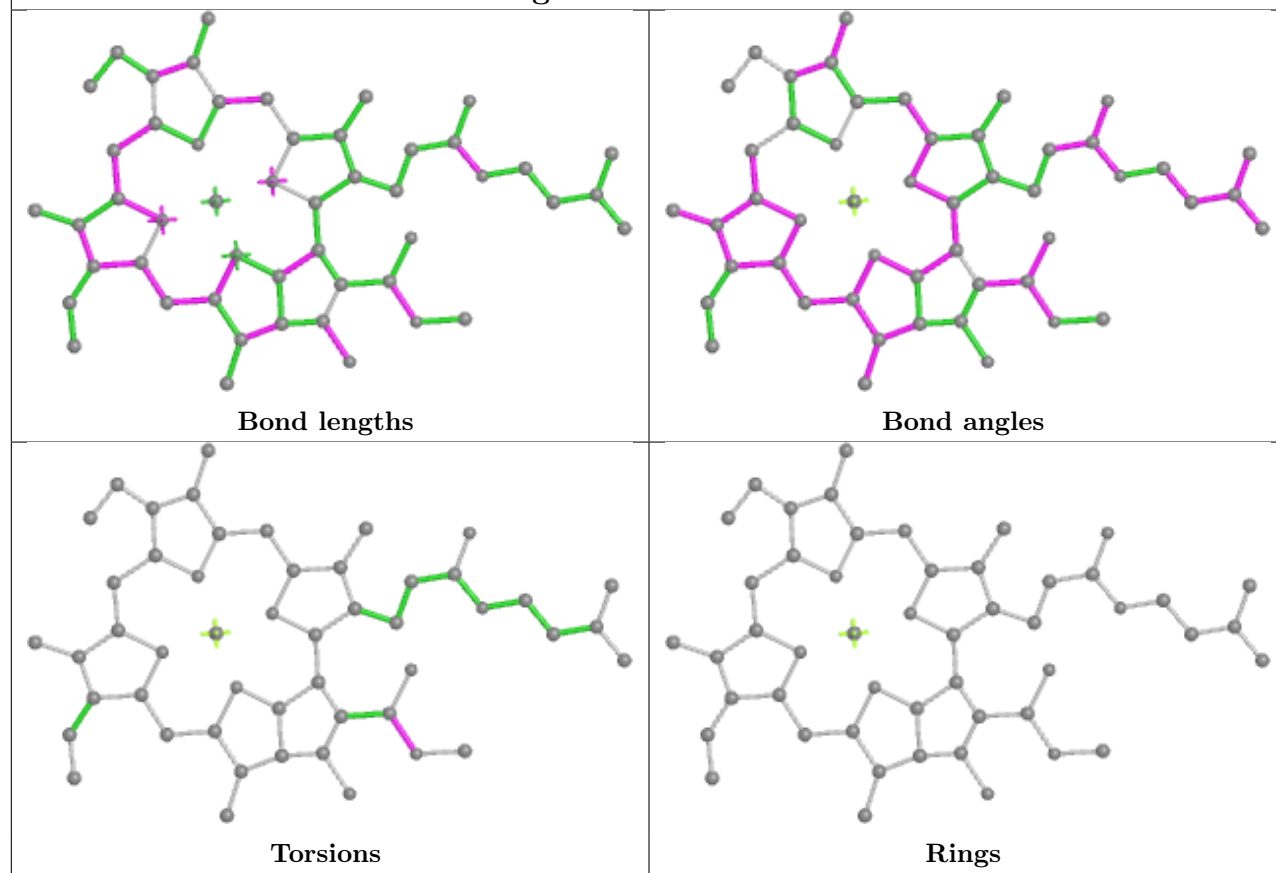




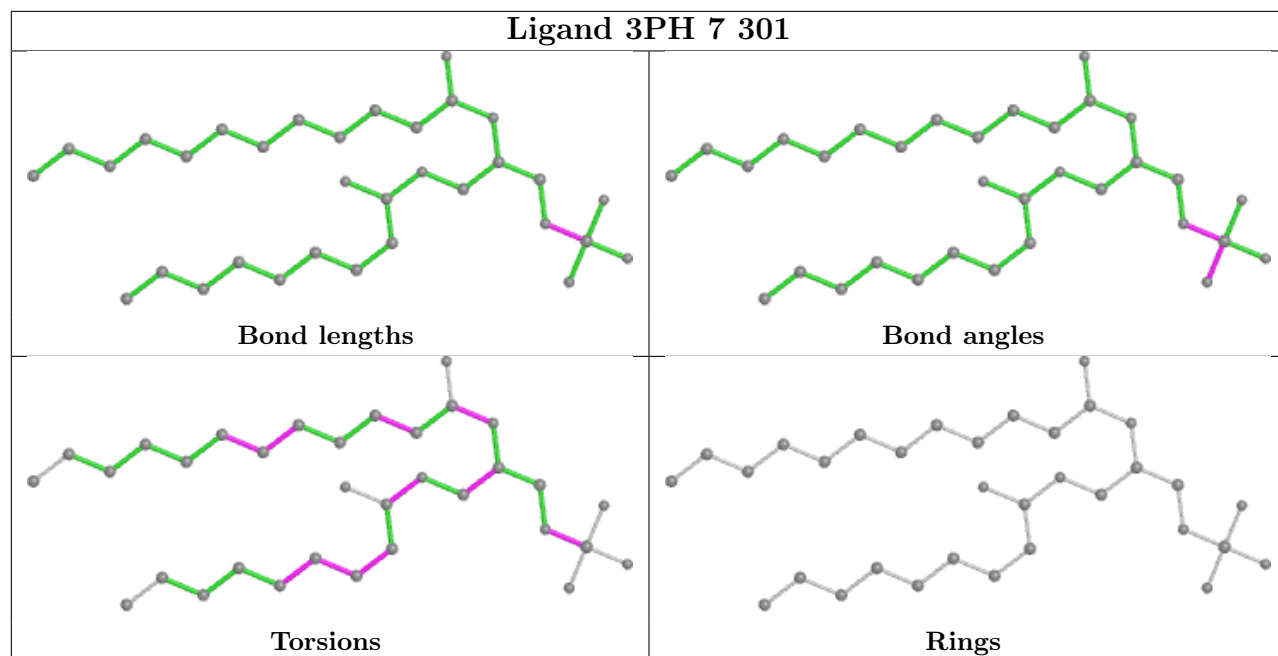
## Ligand CLA 9 315



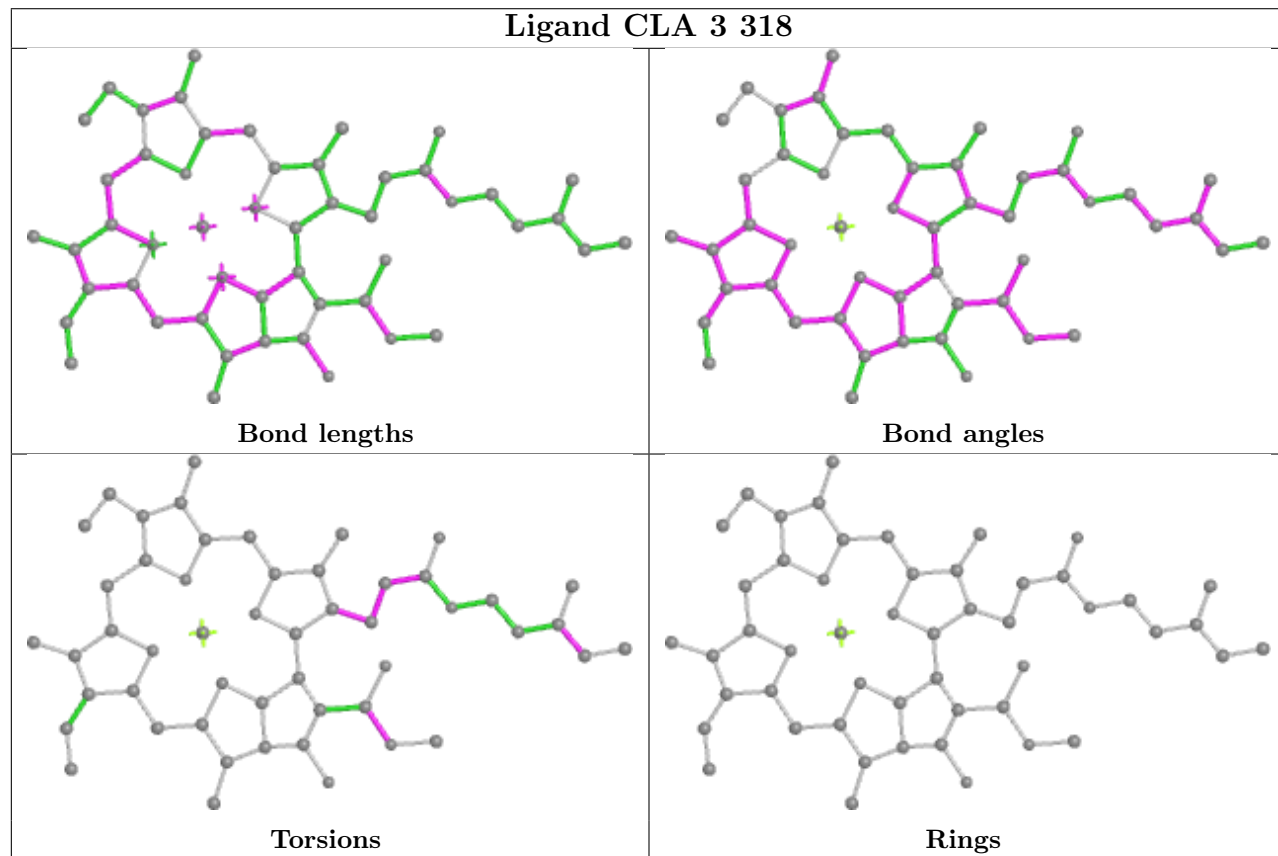
## Ligand CLA B 845



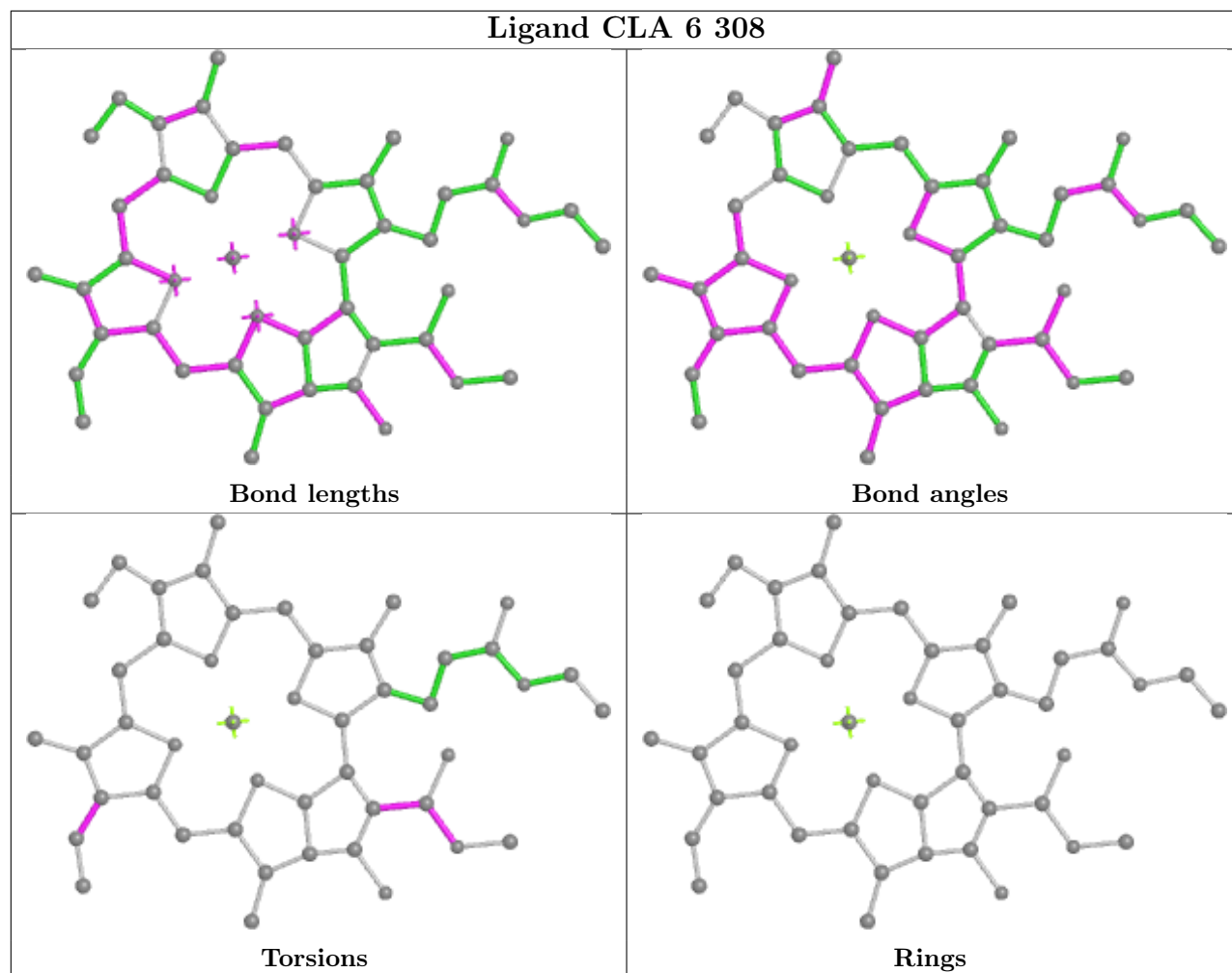
## Ligand 3PH 7 301

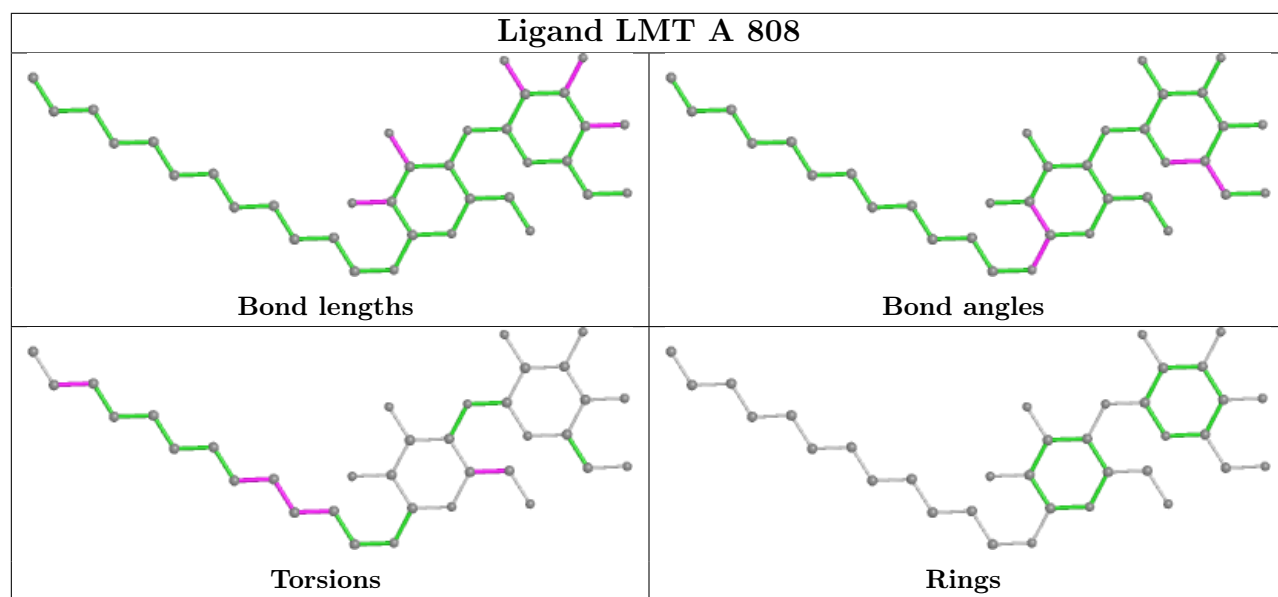
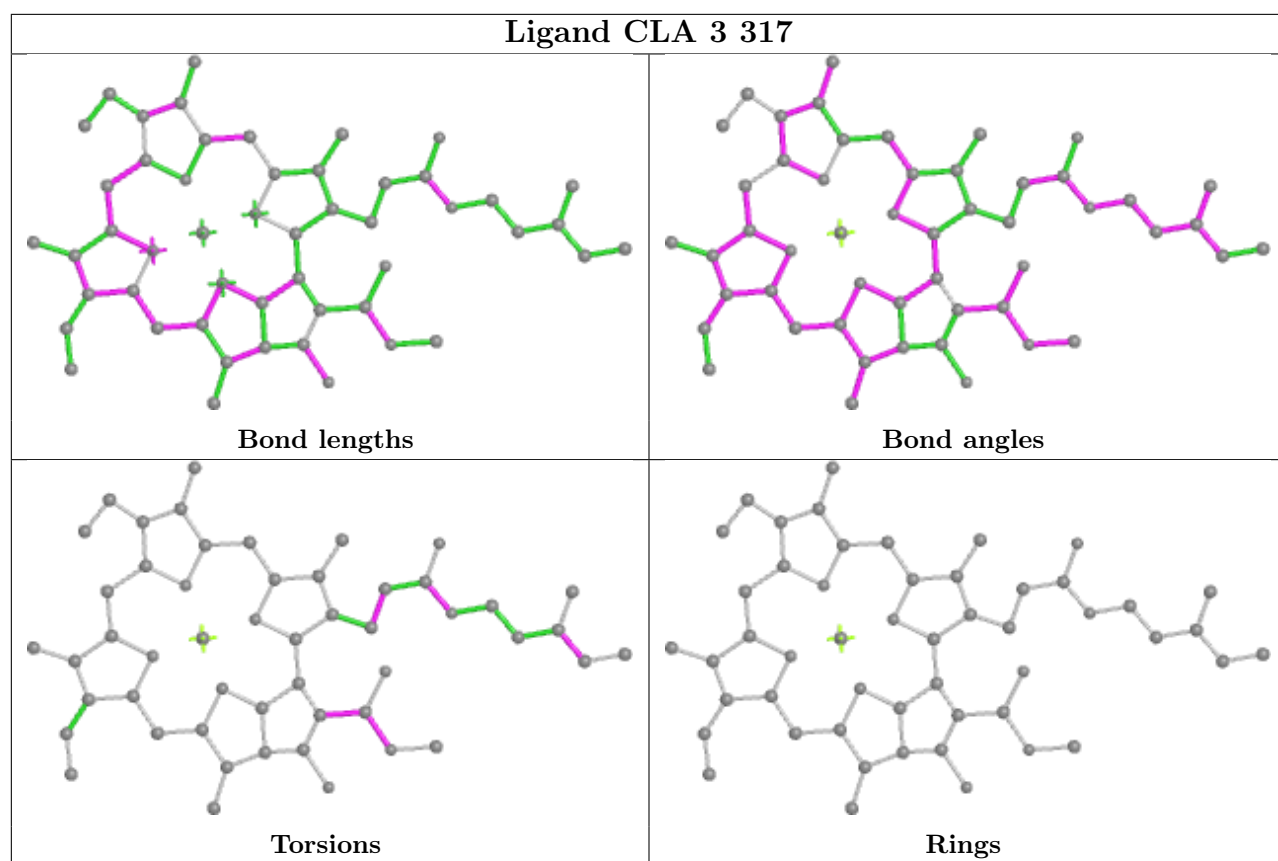


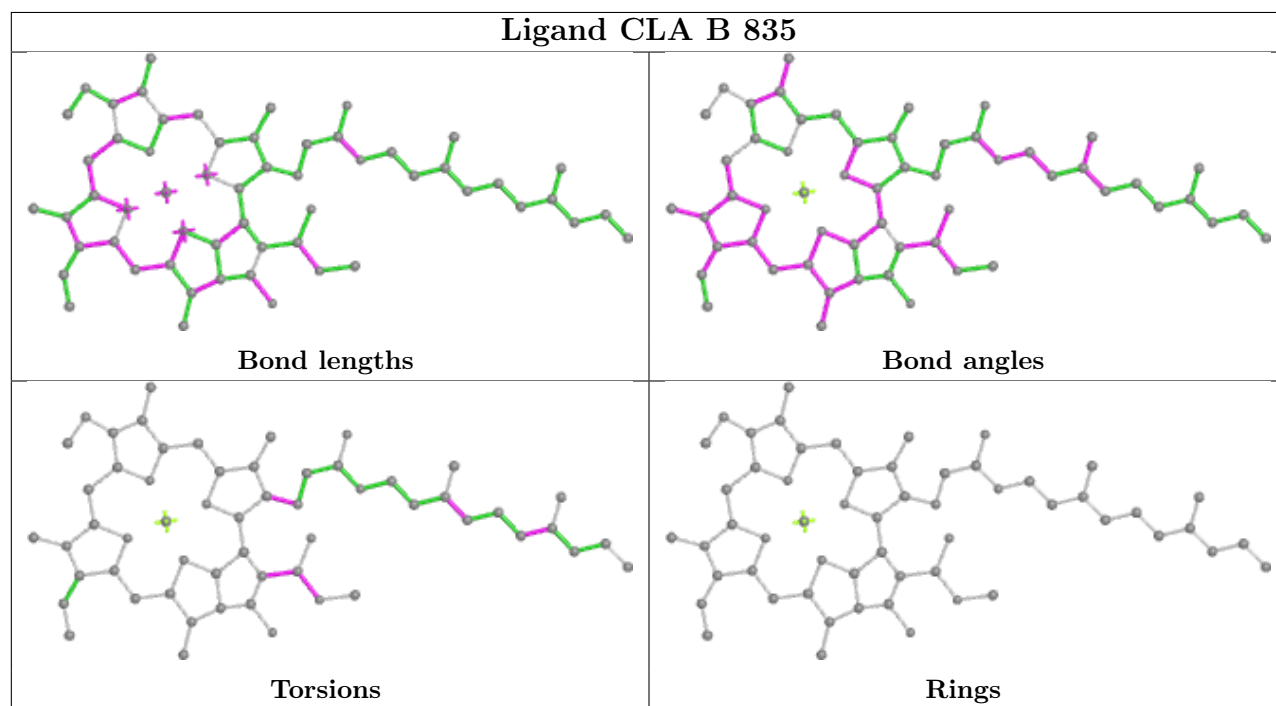
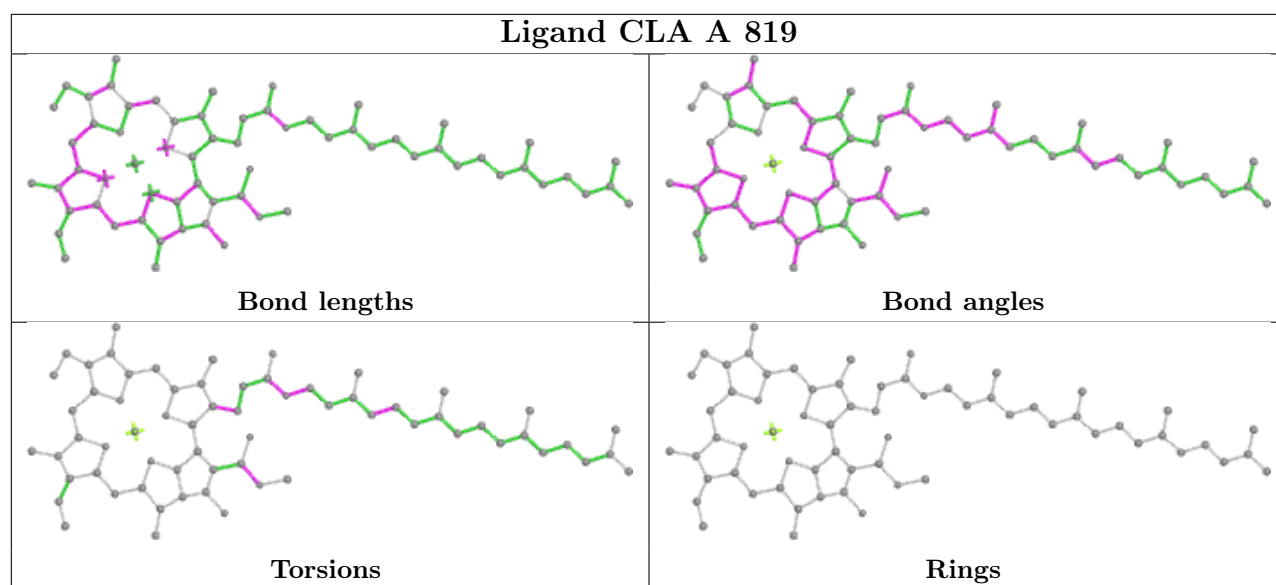
## Ligand CLA 3 318



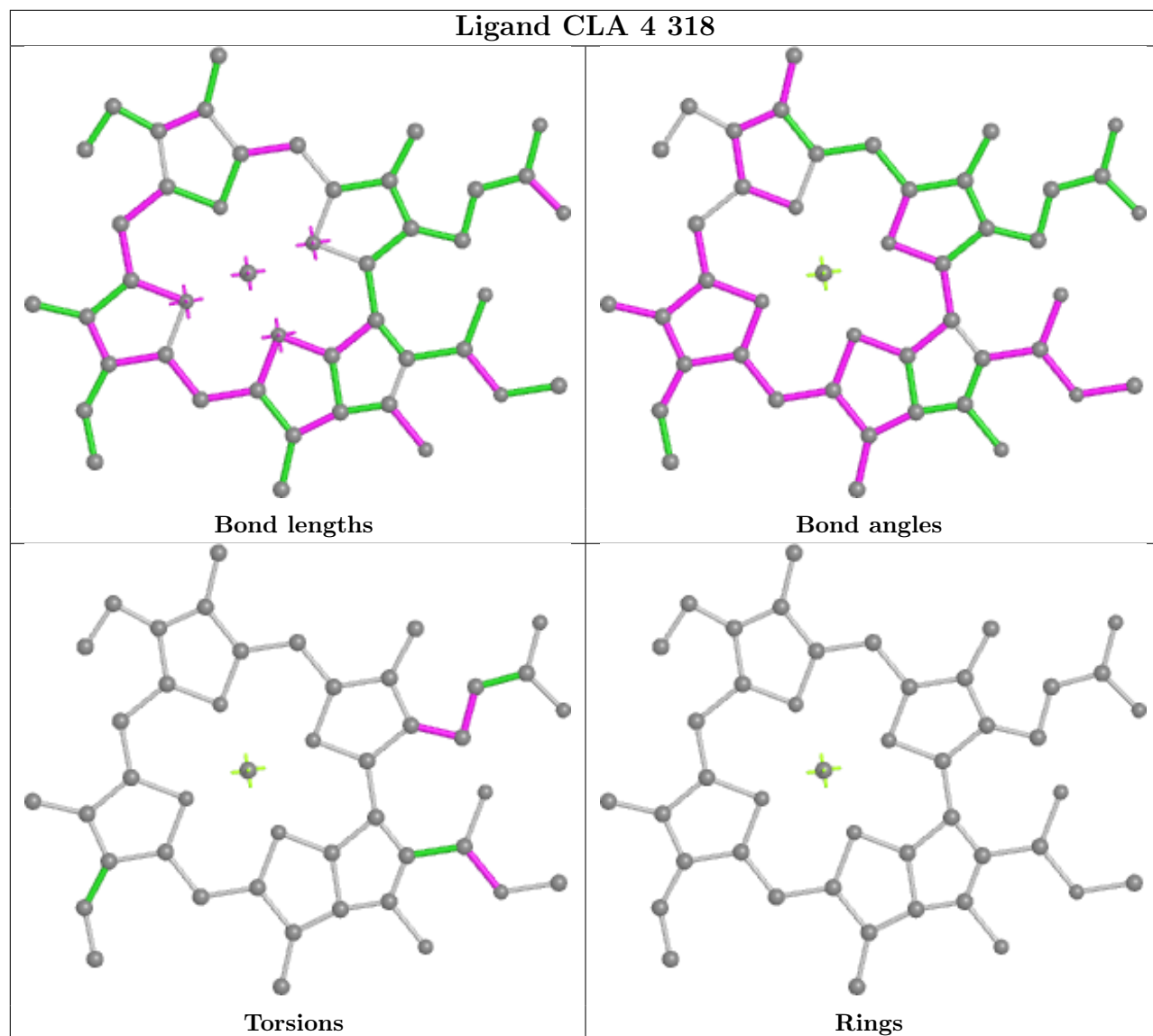
## Ligand CLA 6 308



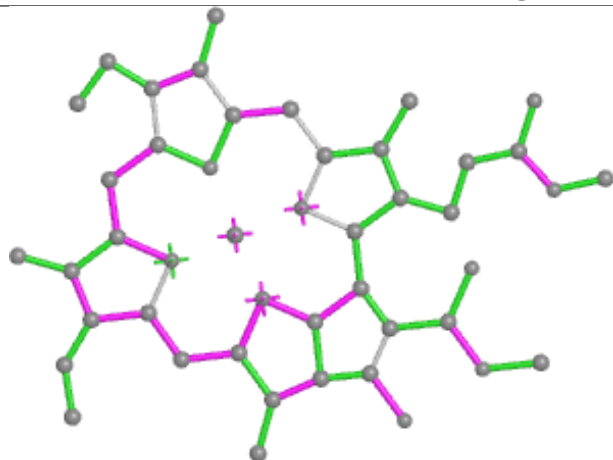




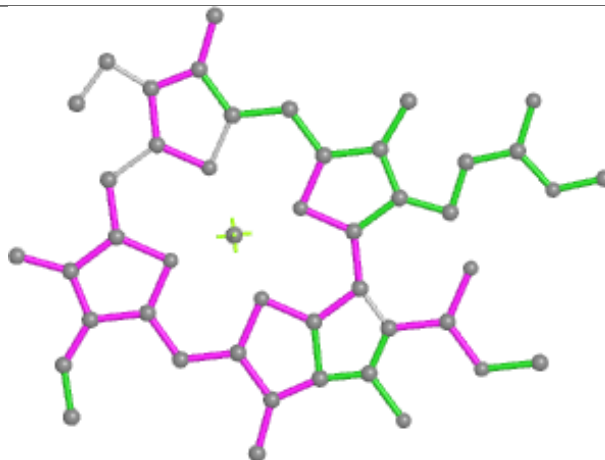
## Ligand CLA 4 318



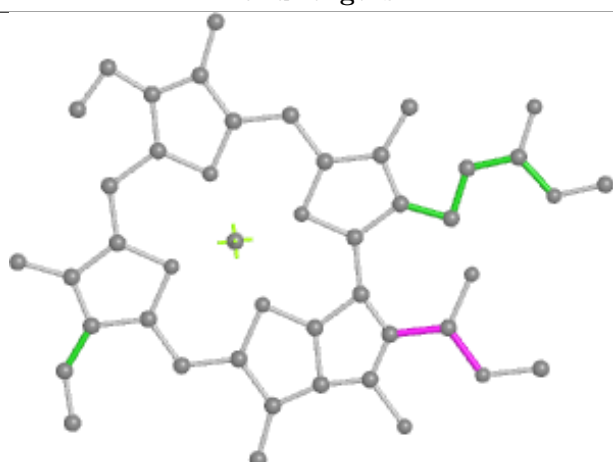
## Ligand CLA K 206



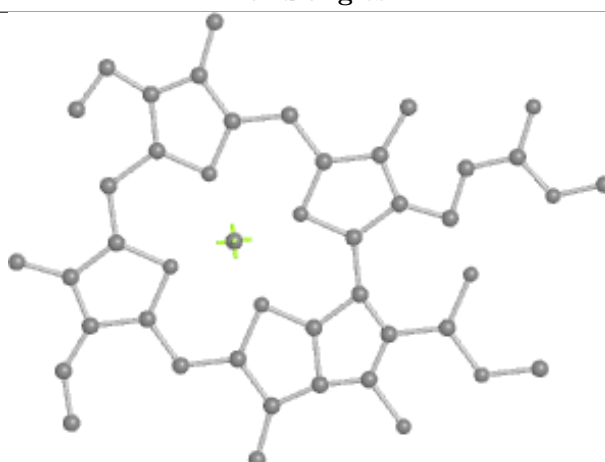
Bond lengths



Bond angles



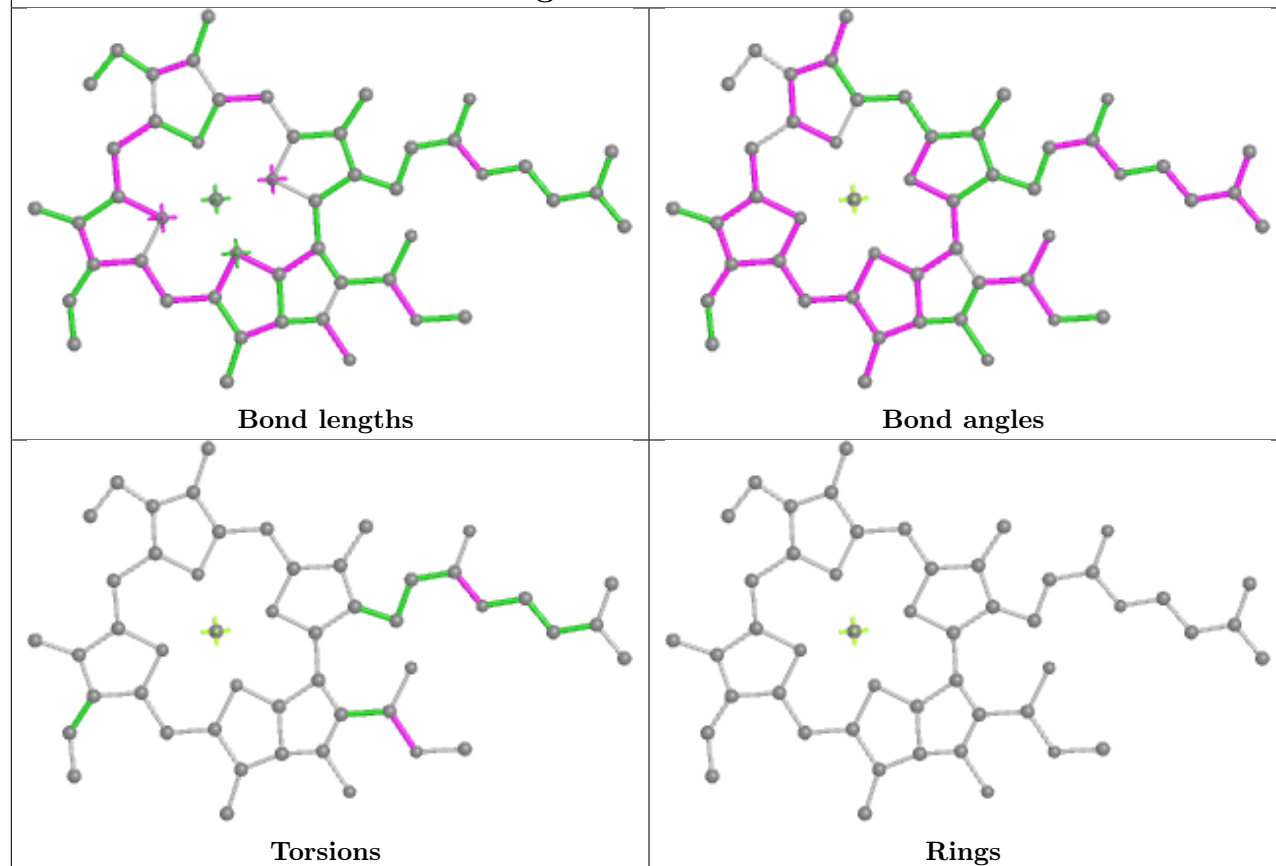
Torsions



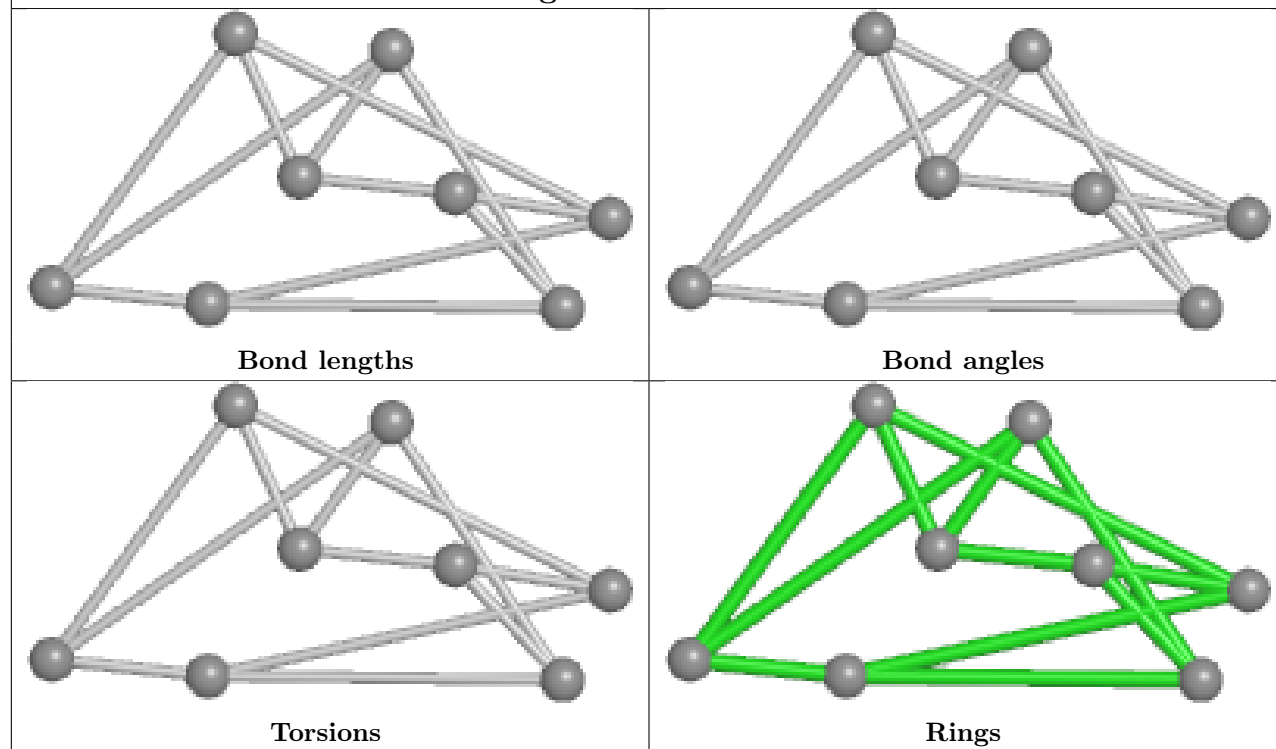
Rings

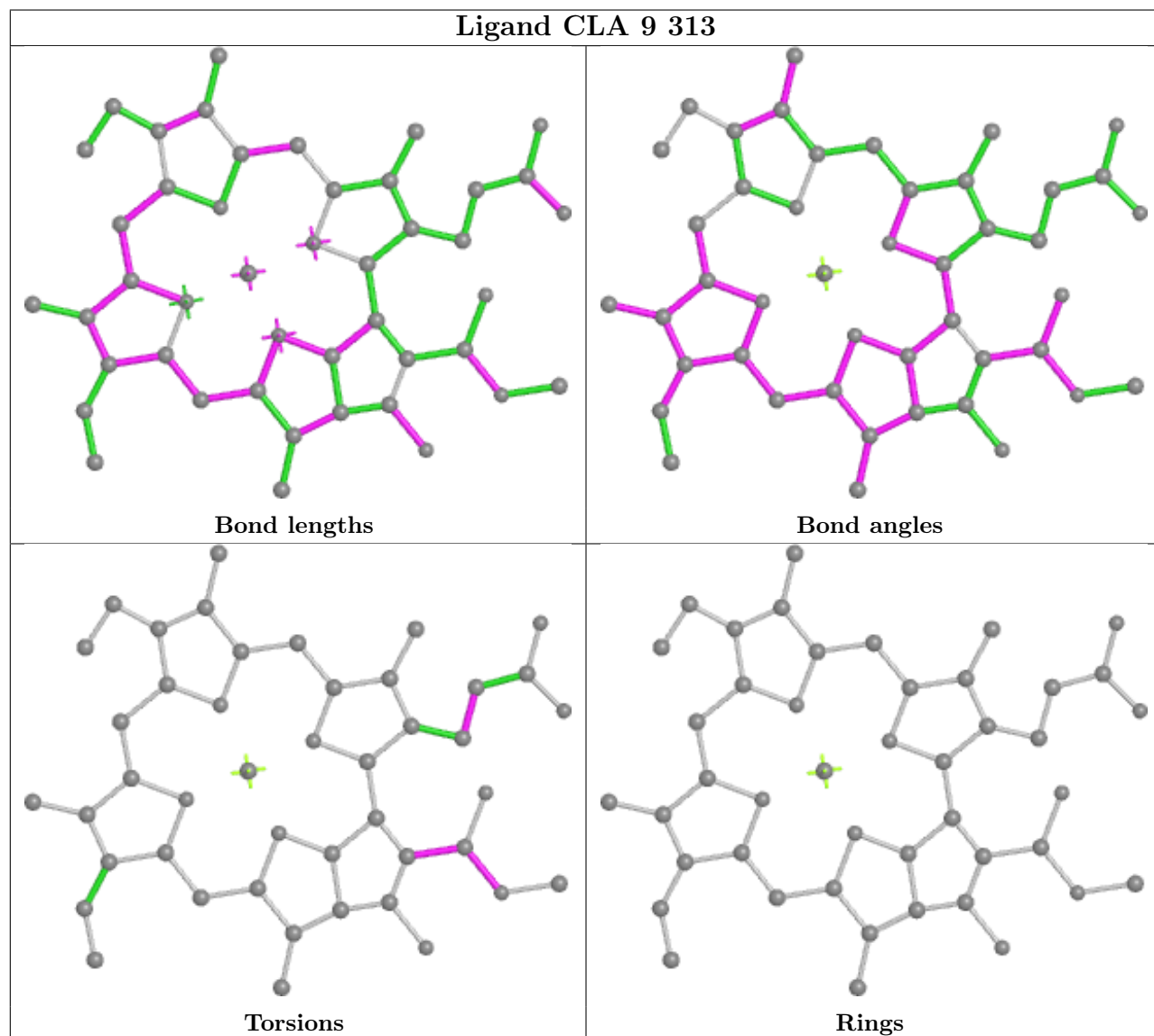
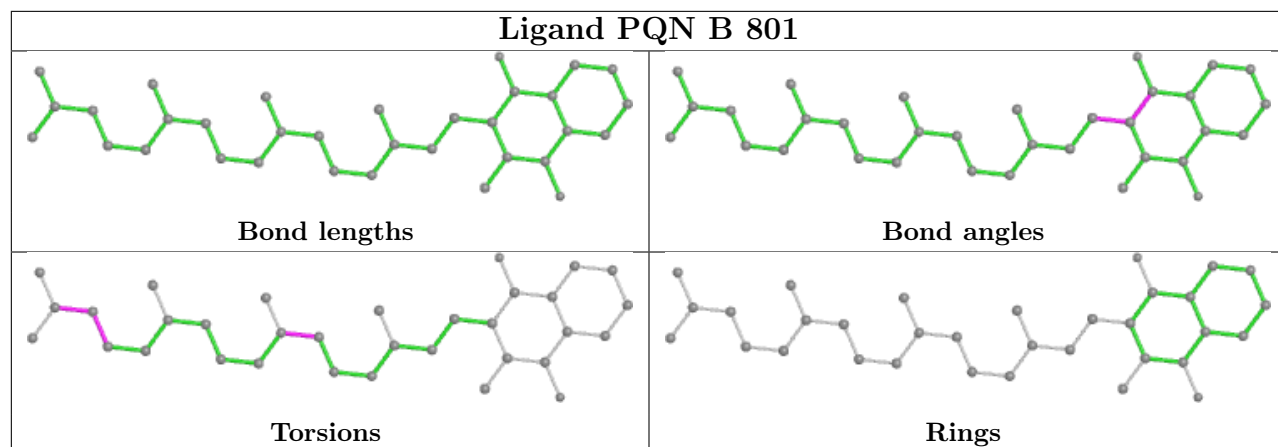


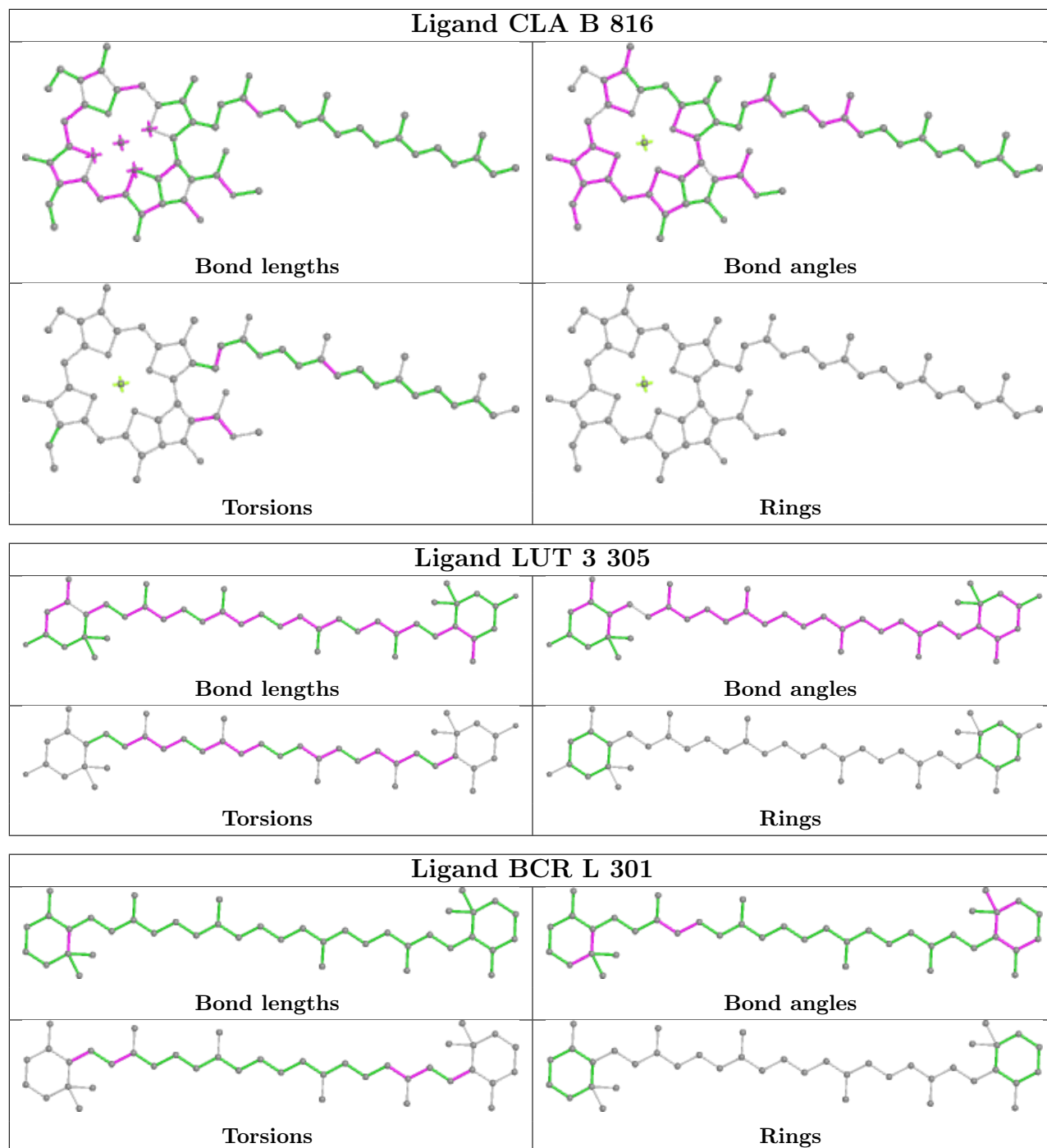
## Ligand CLA 3 316



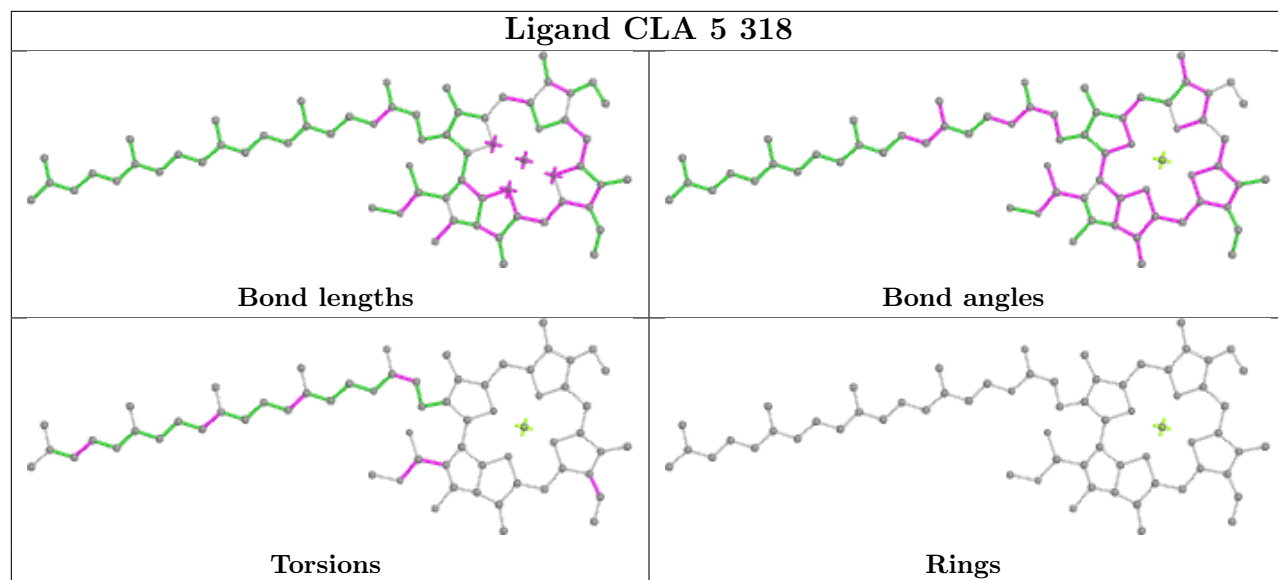
## Ligand SF4 C 102



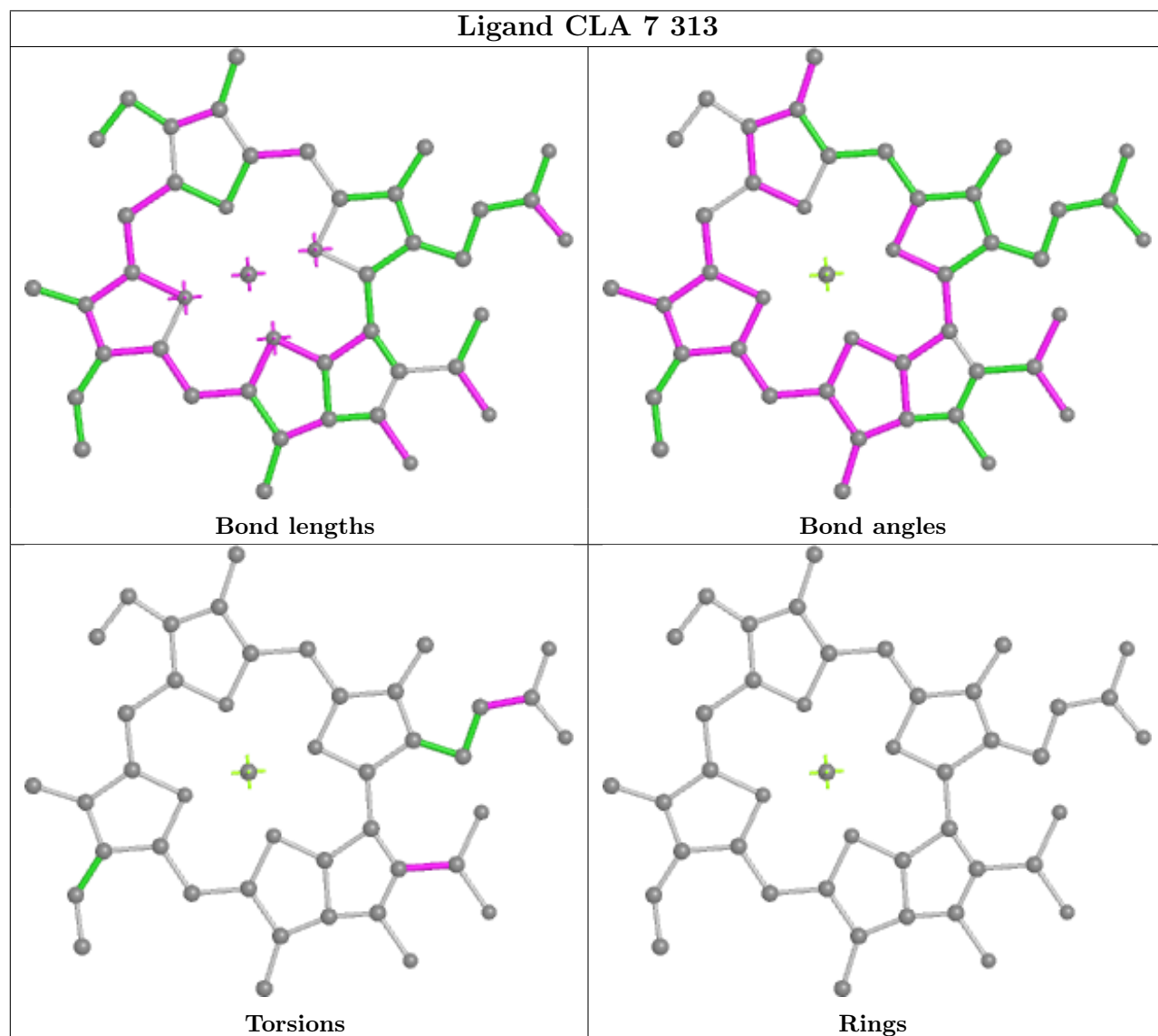


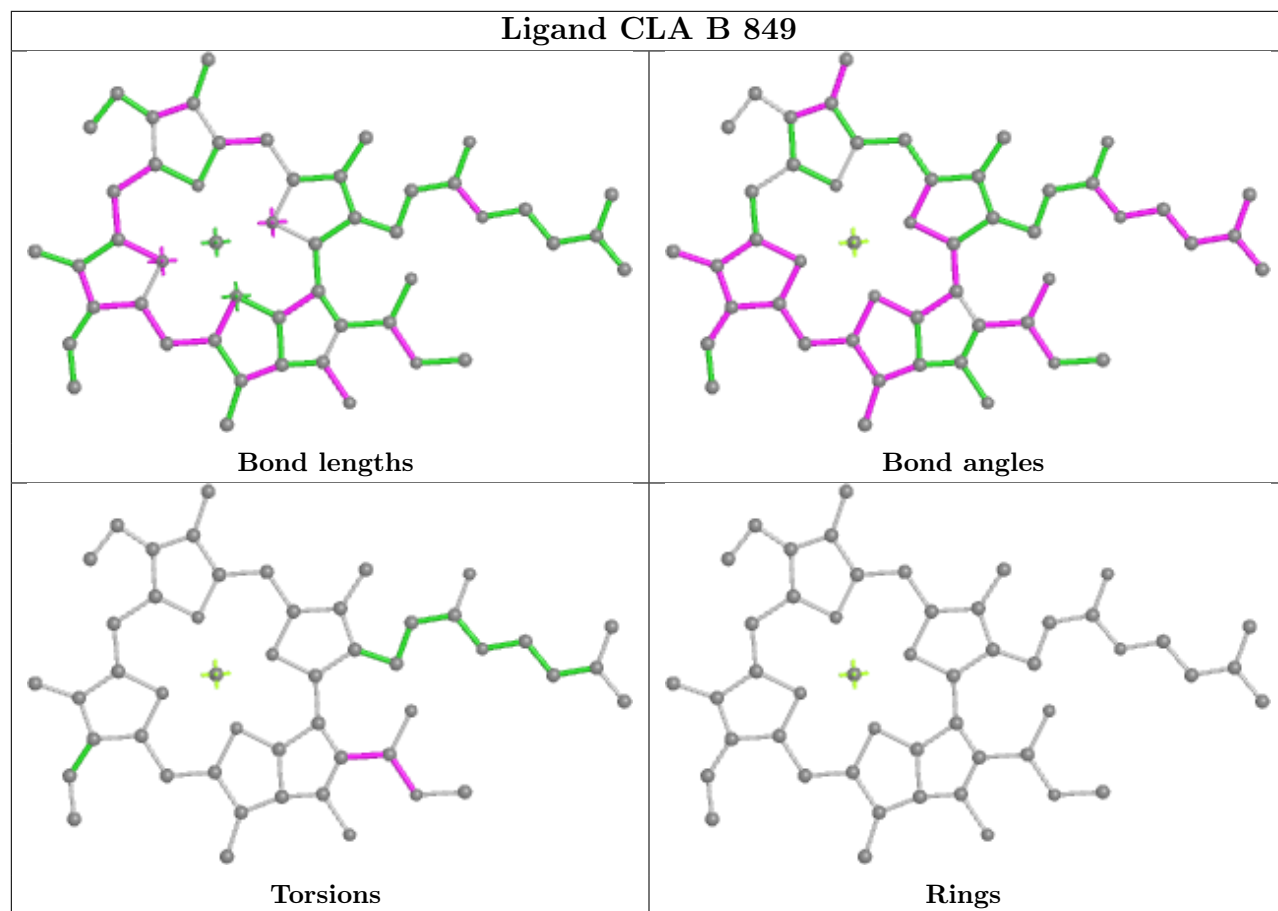
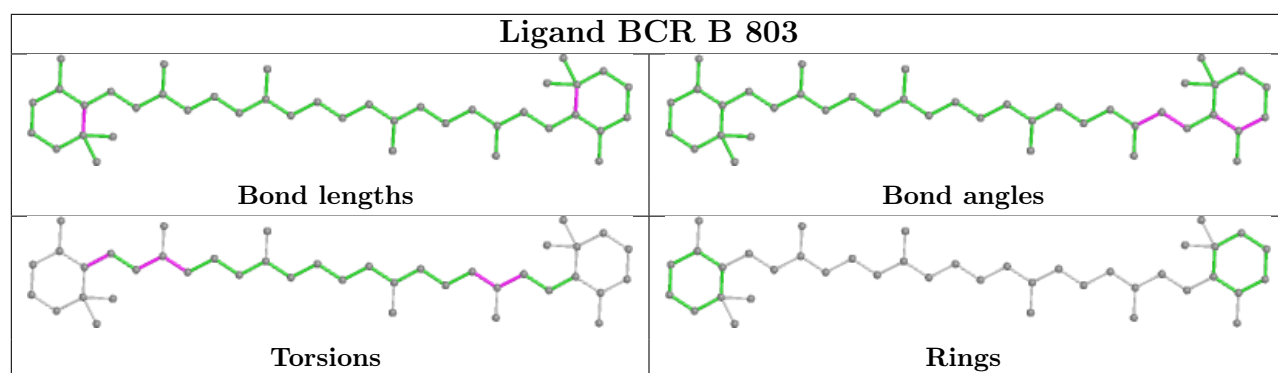


## Ligand CLA 5 318

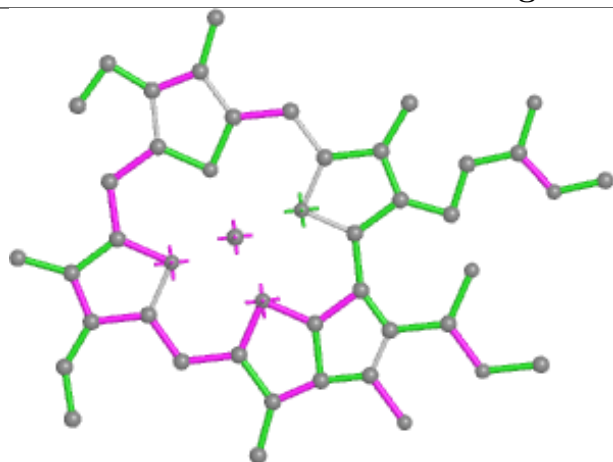


## Ligand CLA 7 313

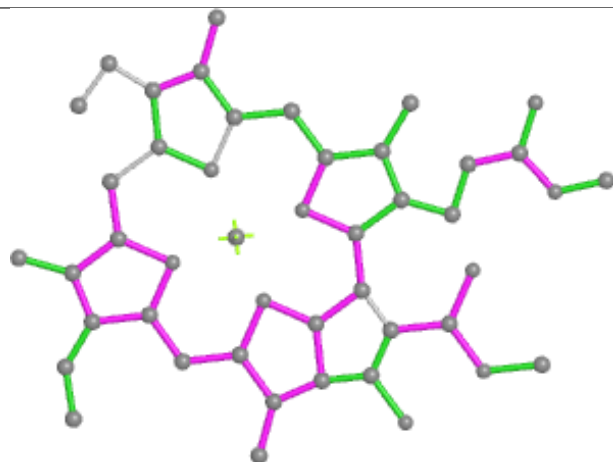




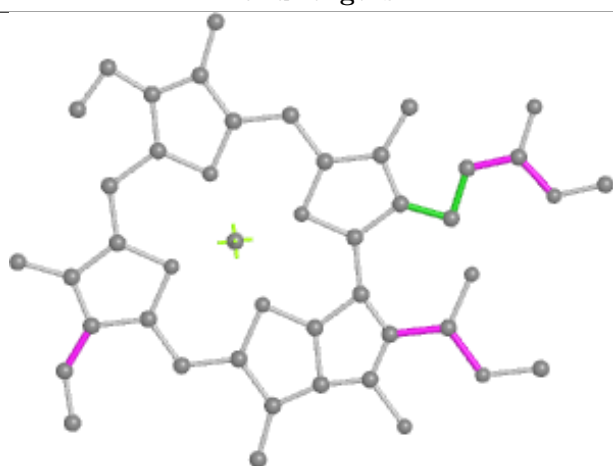
## Ligand CLA 2 313



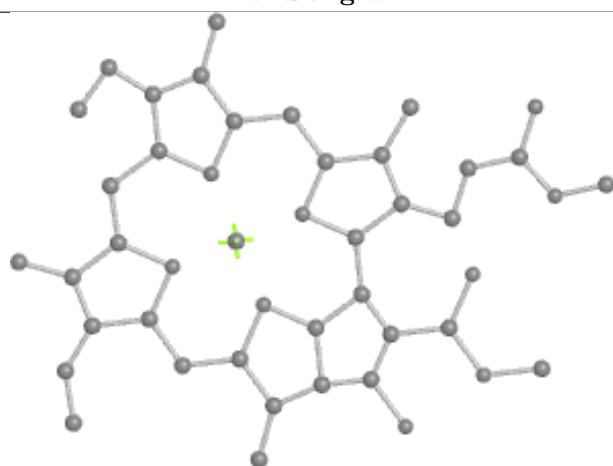
Bond lengths



Bond angles

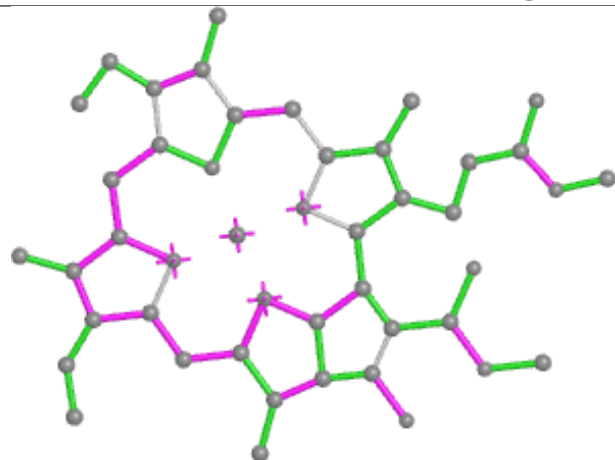


Torsions

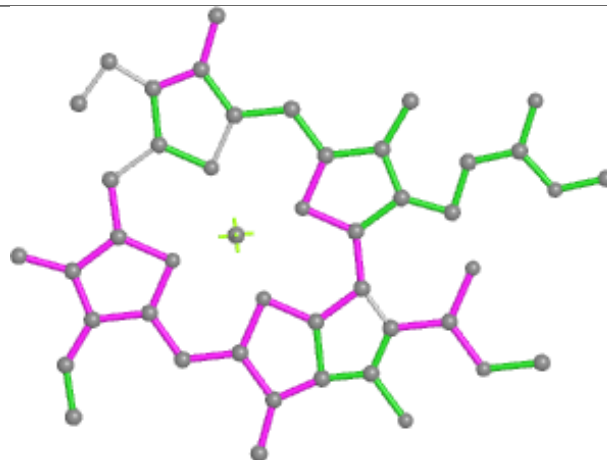


Rings

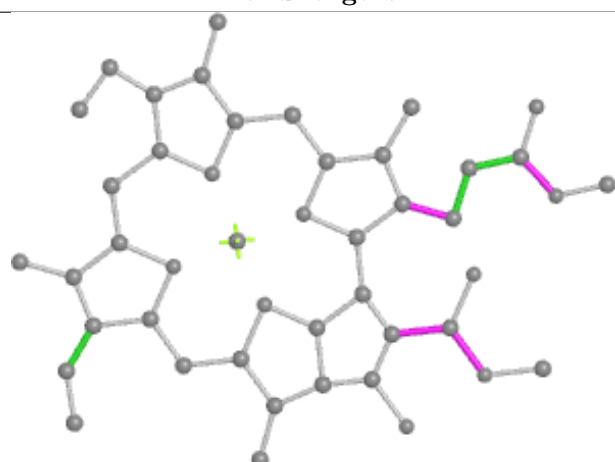
## Ligand CLA 8 313



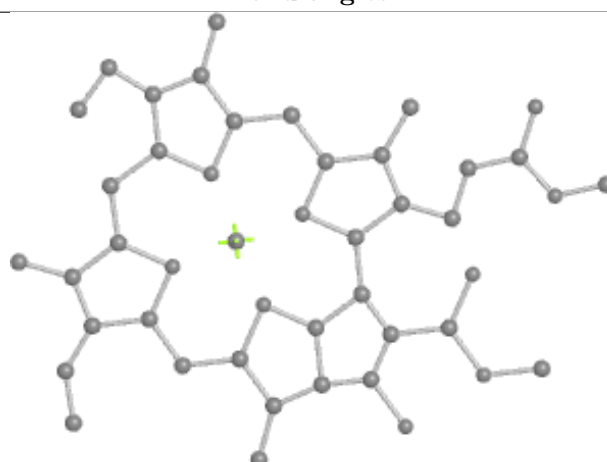
Bond lengths



Bond angles

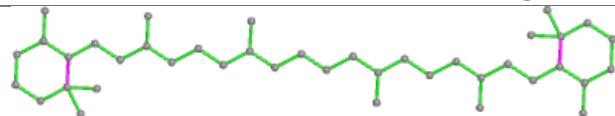


Torsions

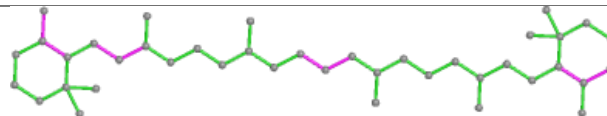


Rings

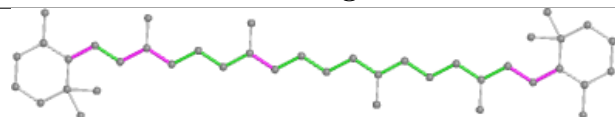
## Ligand BCR 3 302



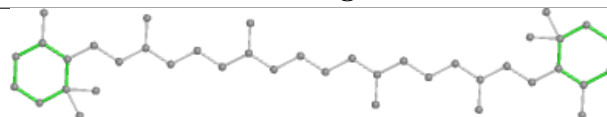
Bond lengths



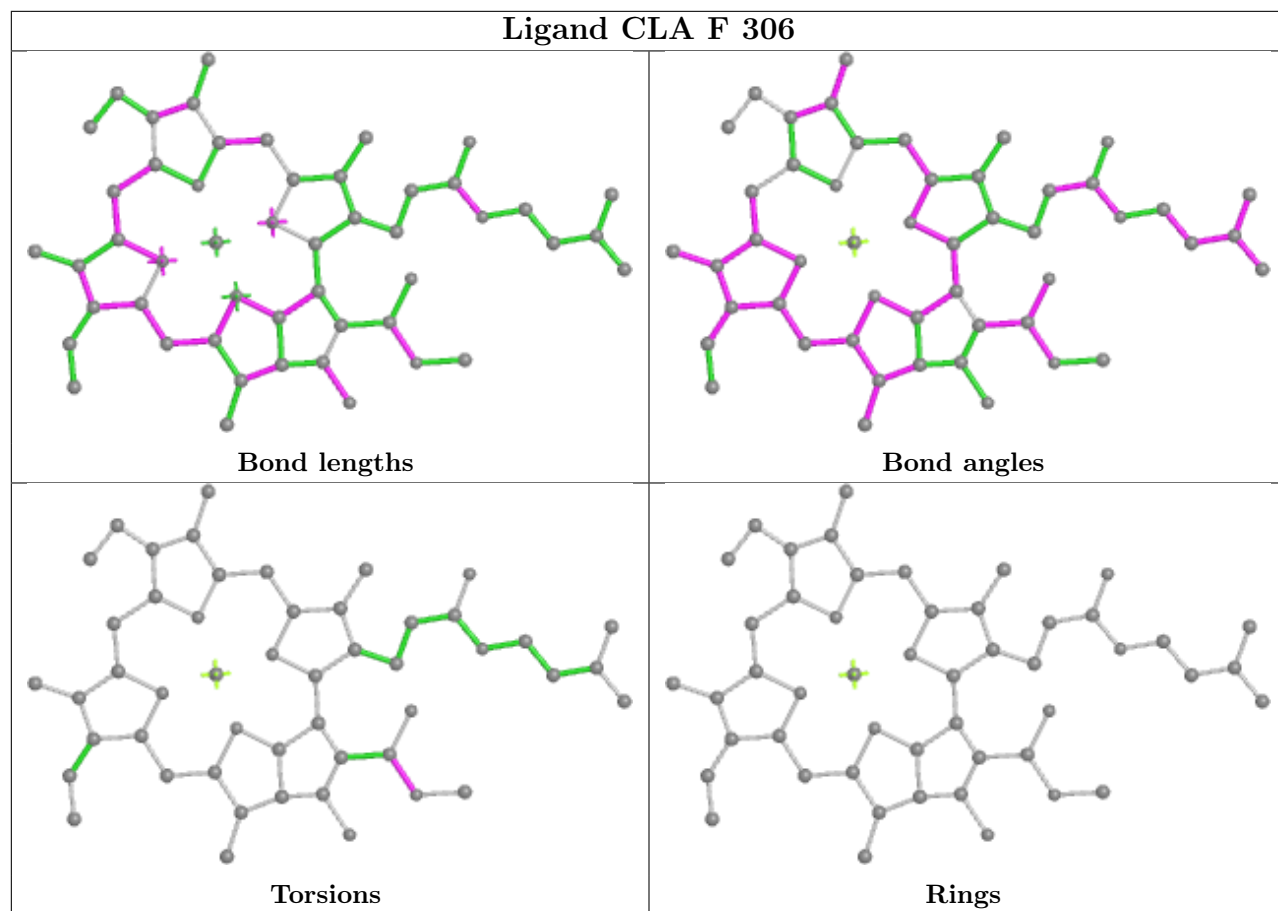
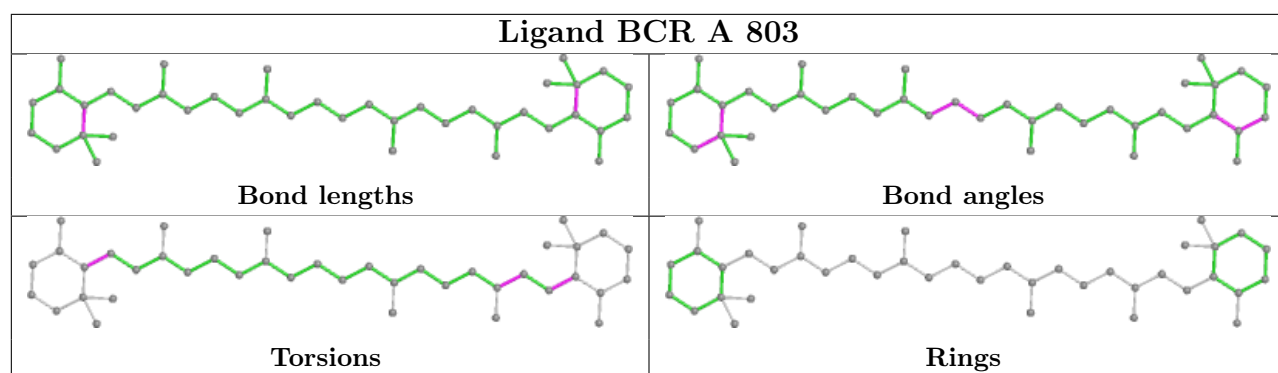
Bond angles



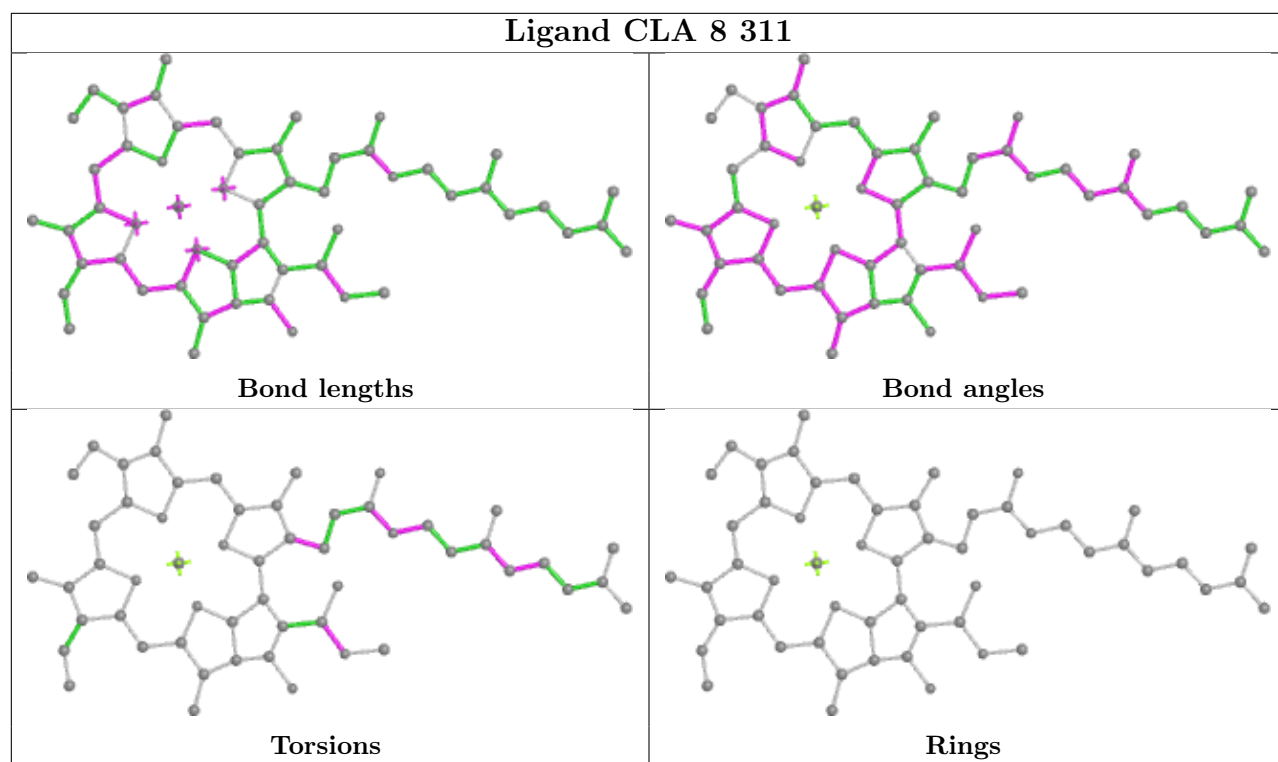
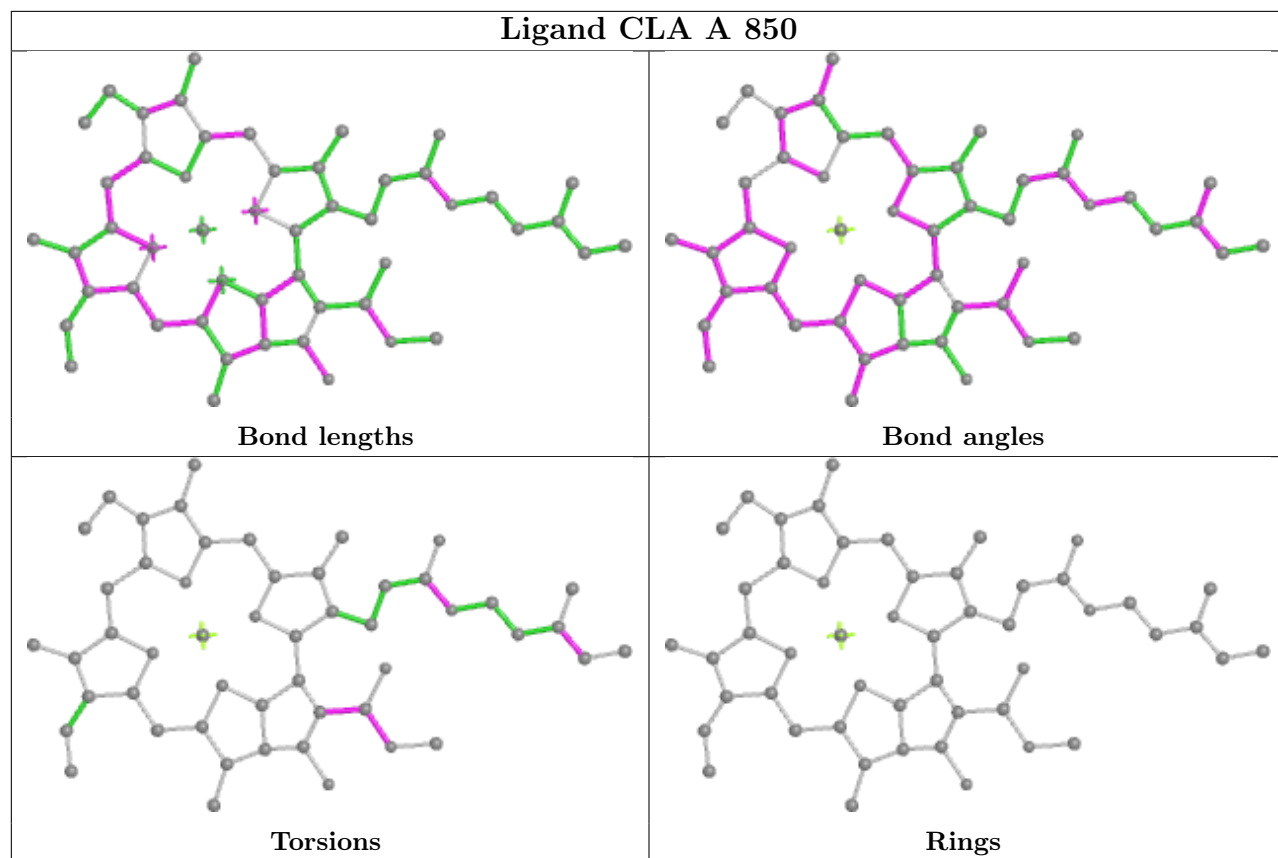
Torsions



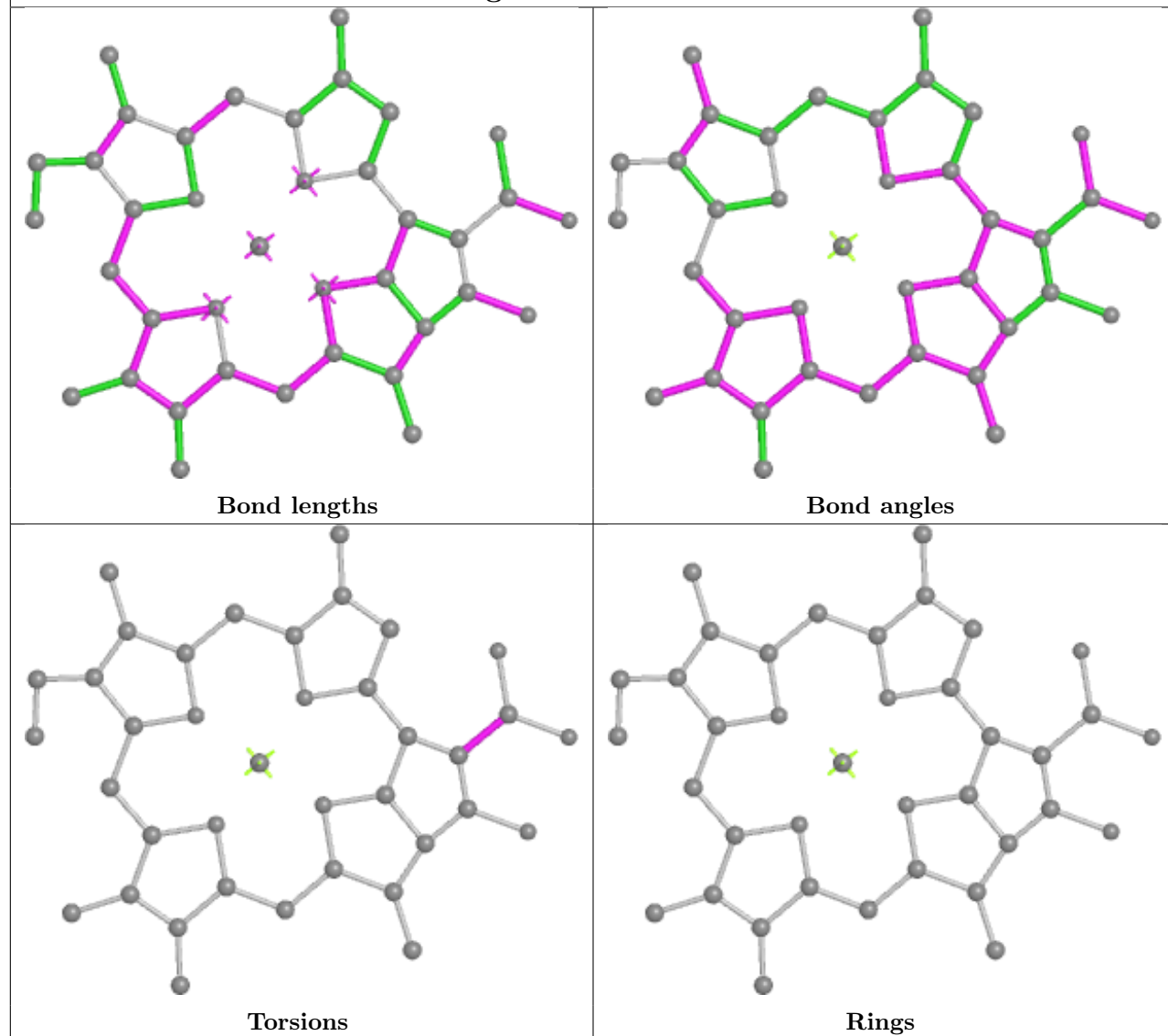
Rings



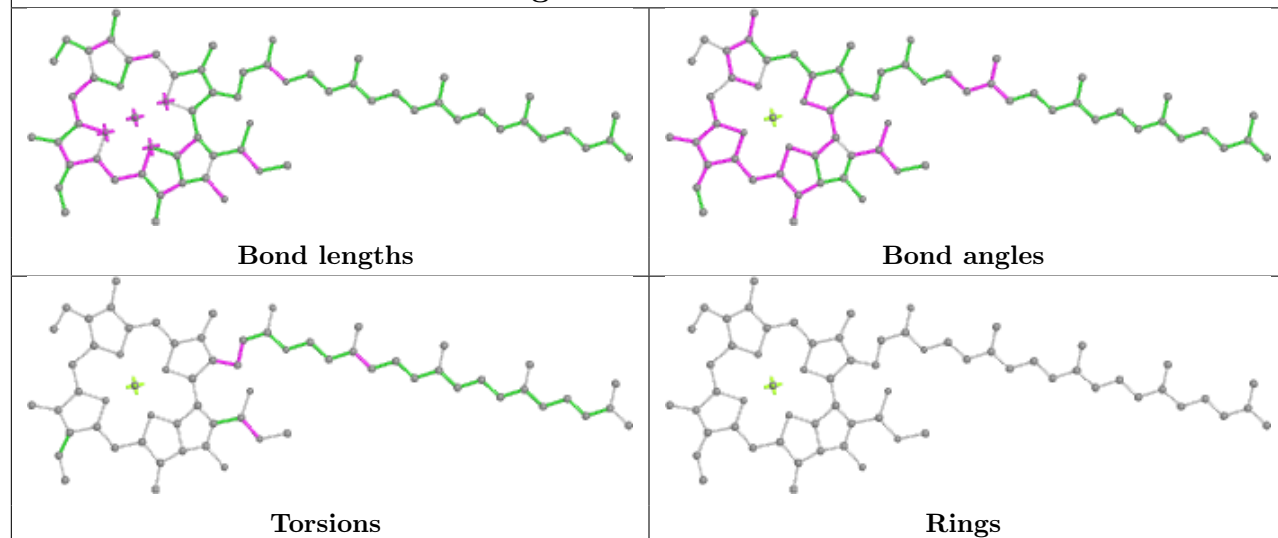


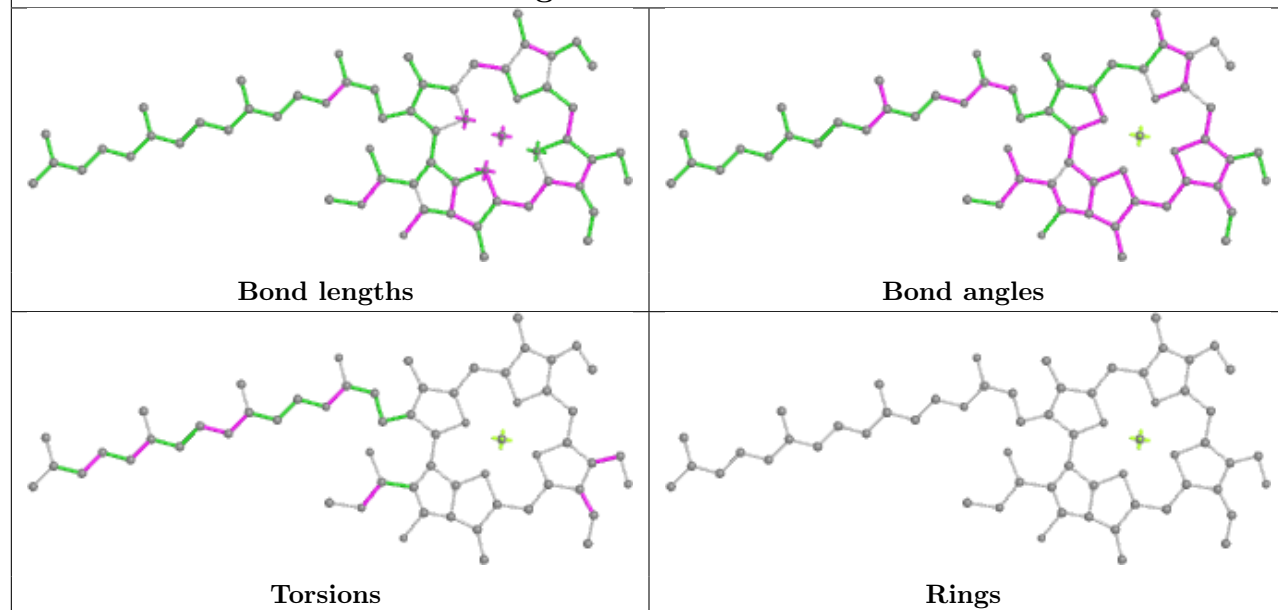
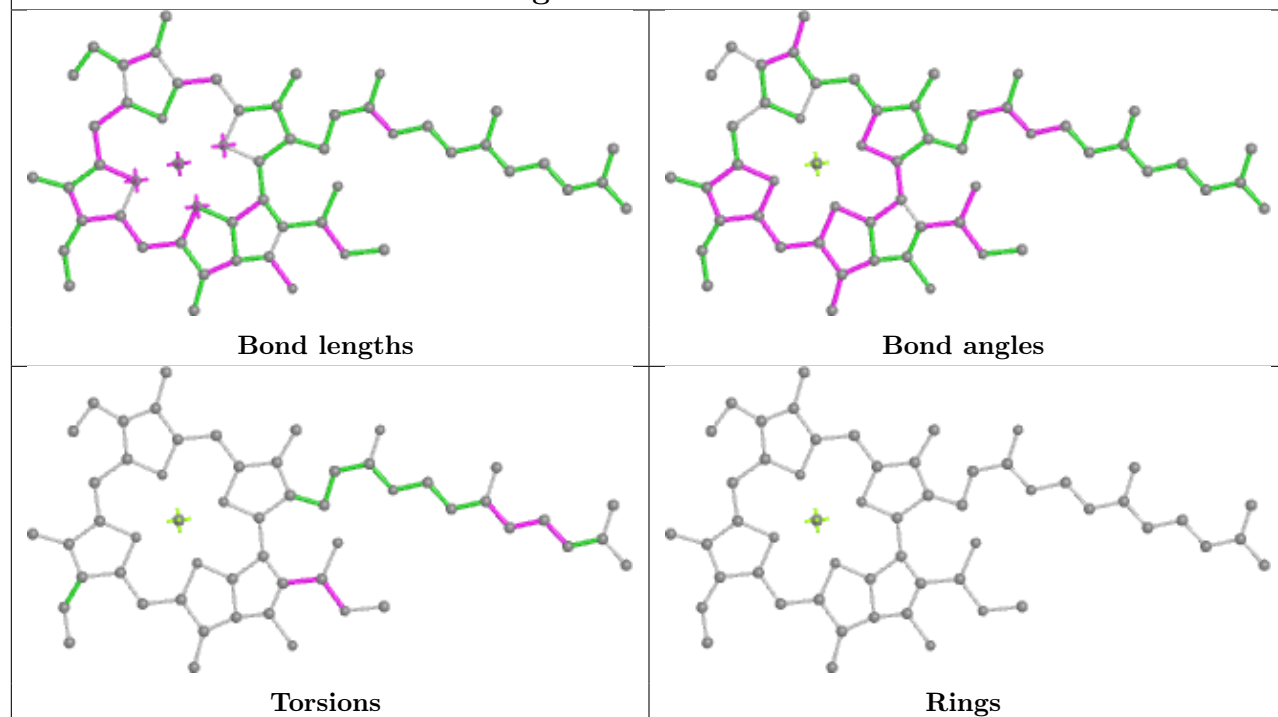


## Ligand CLA O 202

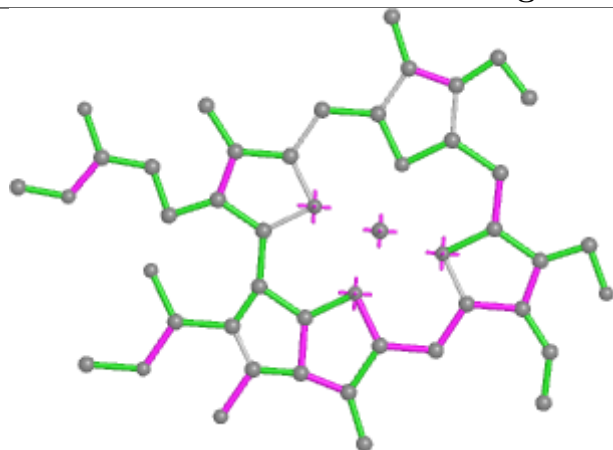


## Ligand CLA A 856

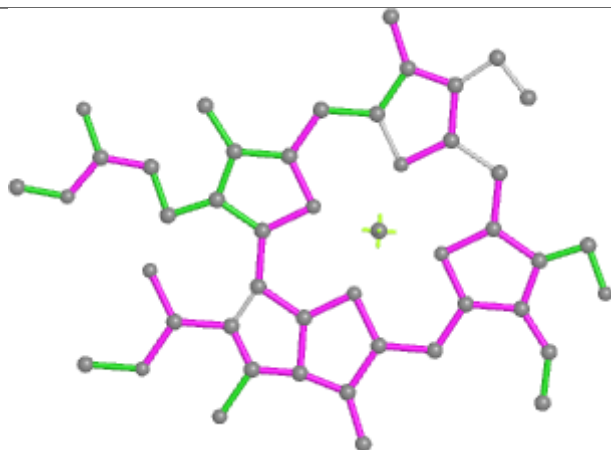


**Ligand CHL 7 320****Ligand CLA B 833**

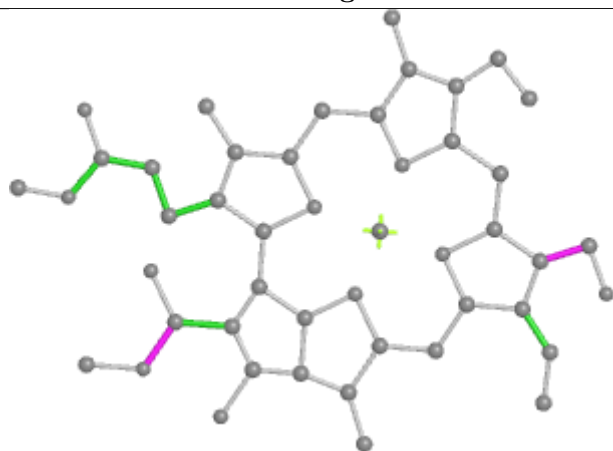
## Ligand CHL 9 322



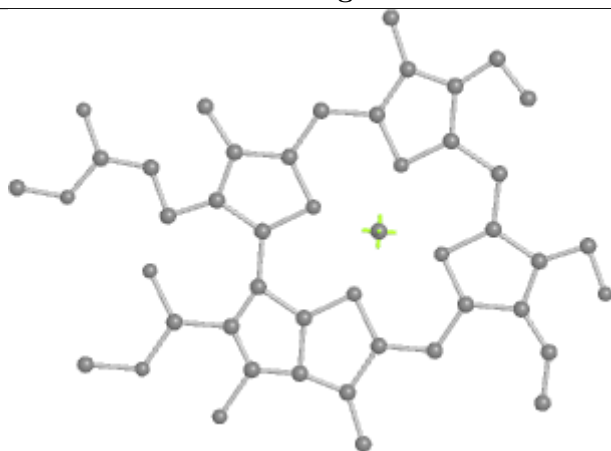
Bond lengths



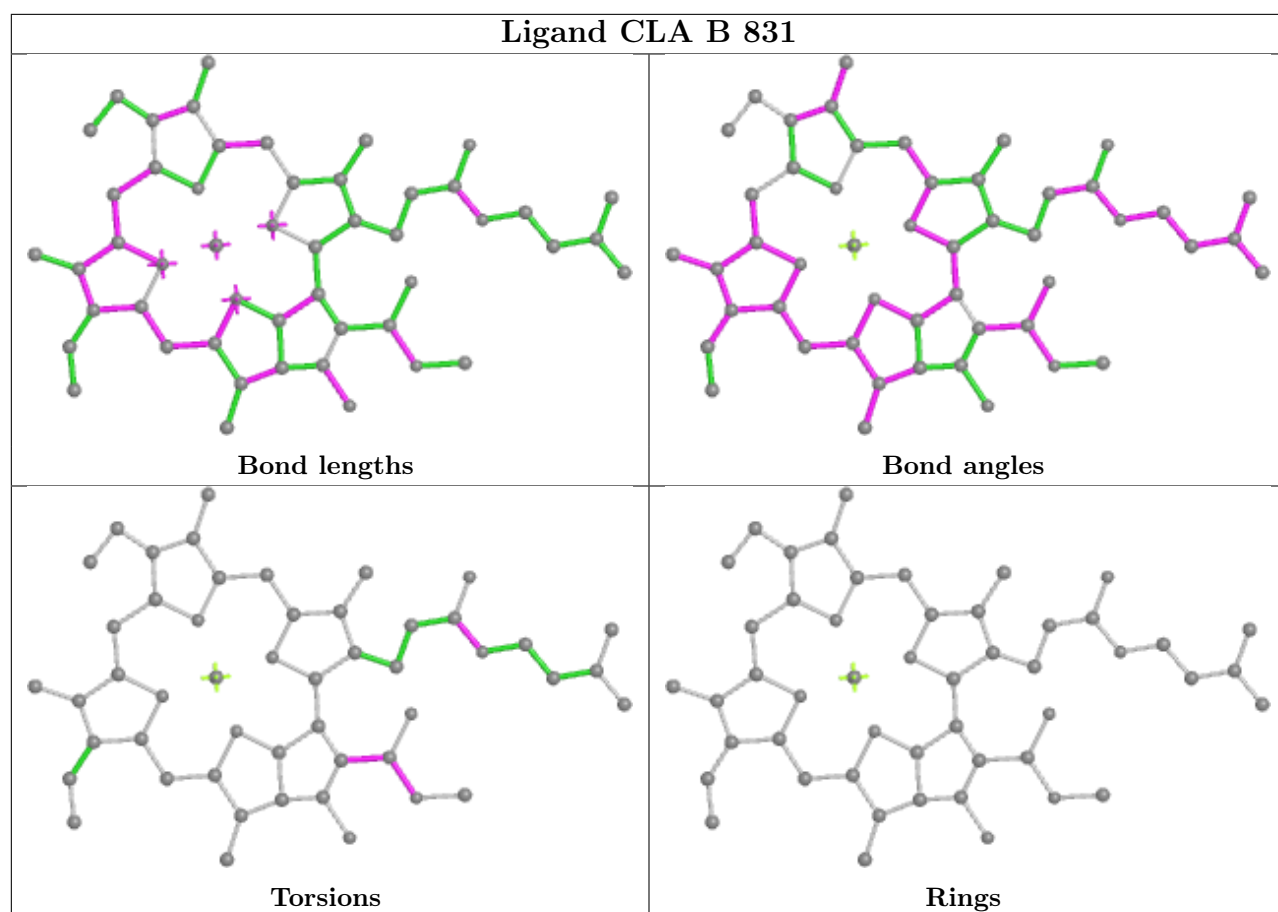
Bond angles



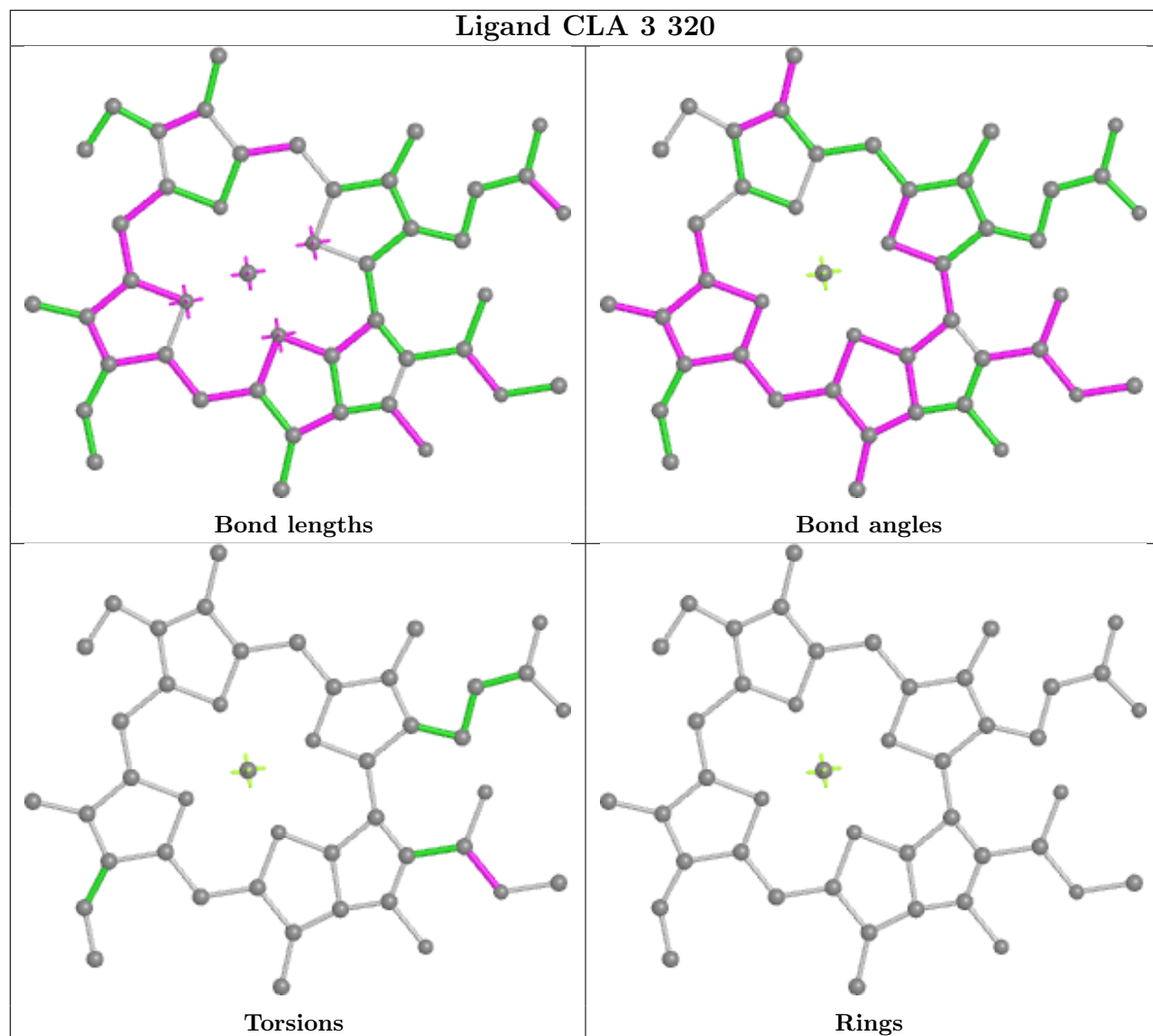
Torsions



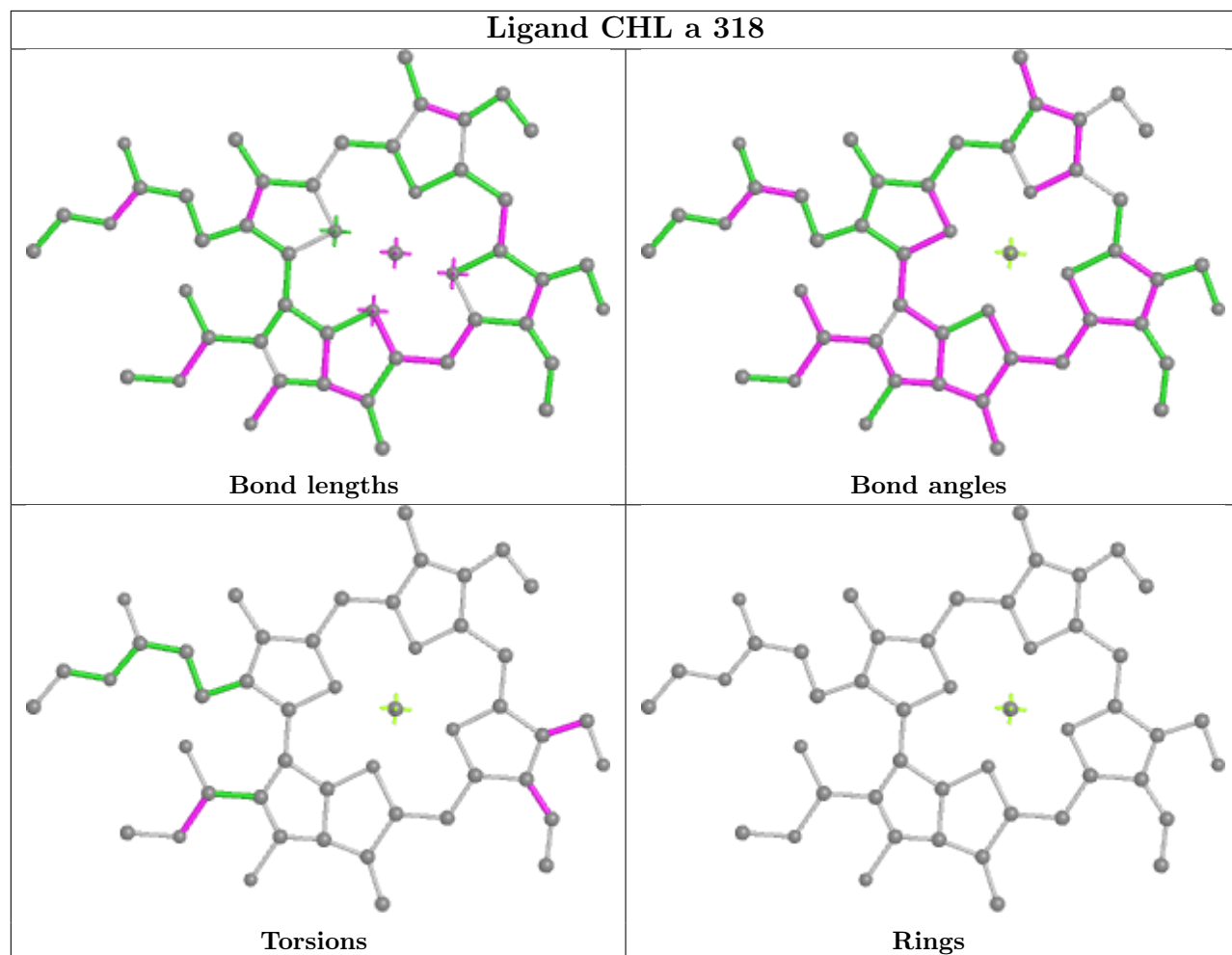
Rings



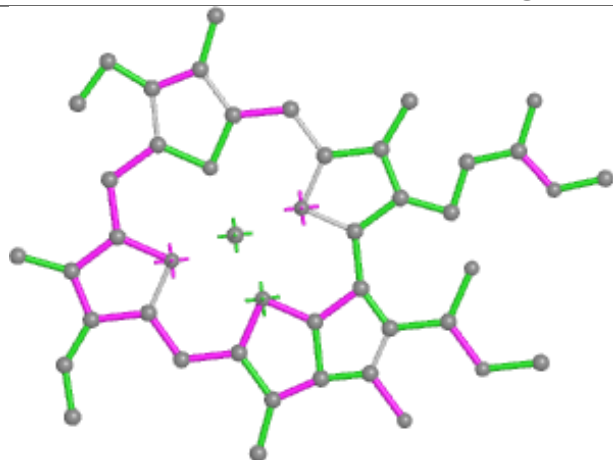
## Ligand CLA 3 320



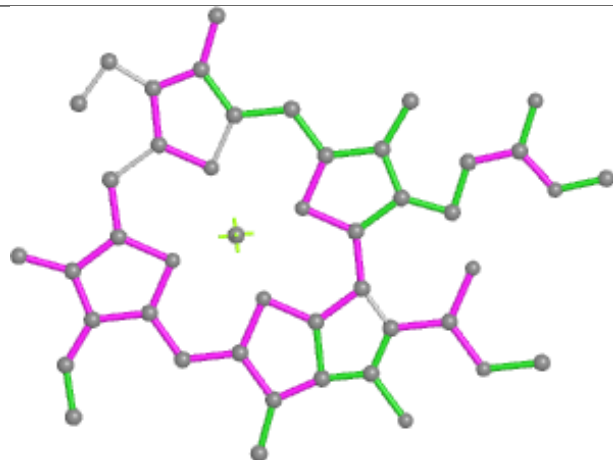
## Ligand CHL a 318



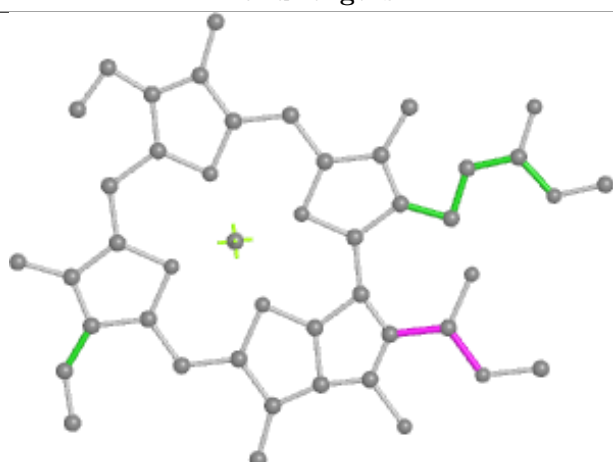
## Ligand CLA 8 307



Bond lengths



Bond angles

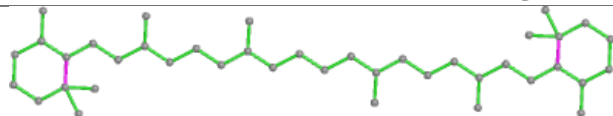


Torsions

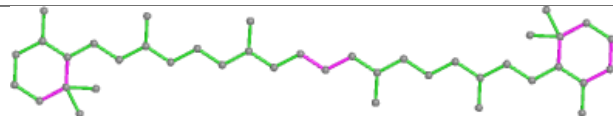


Rings

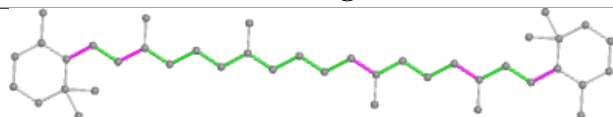
## Ligand BCR 7 304



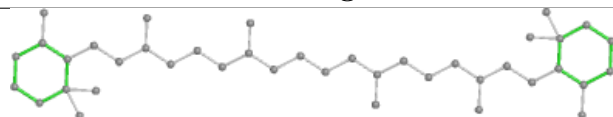
Bond lengths



Bond angles

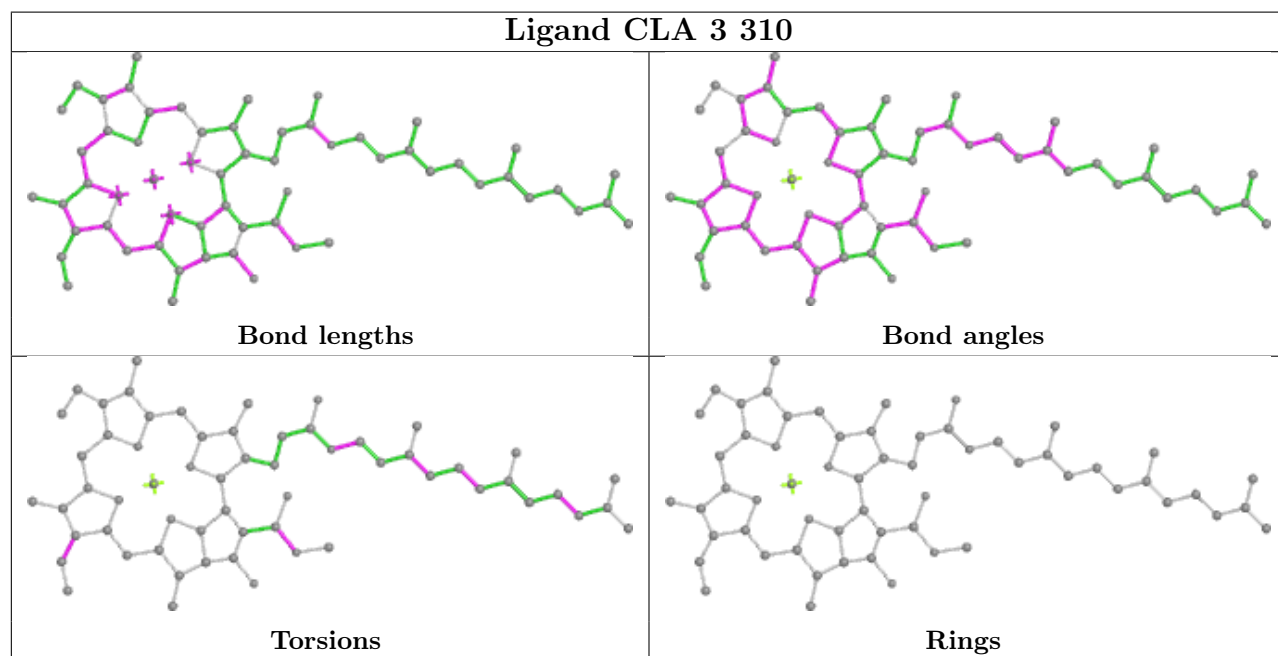
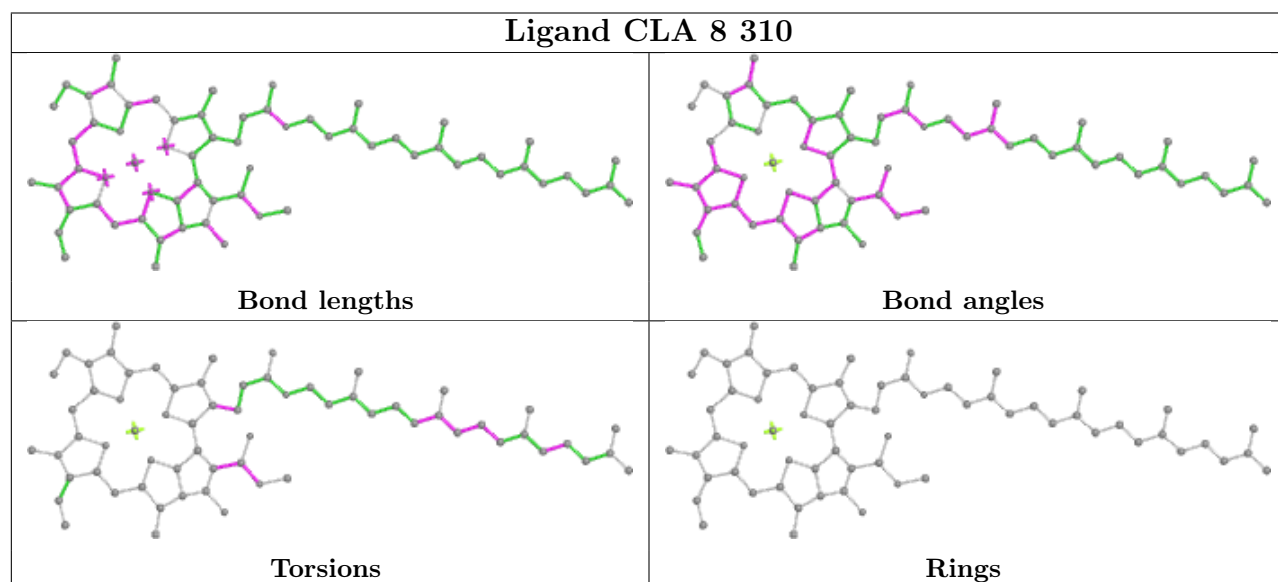
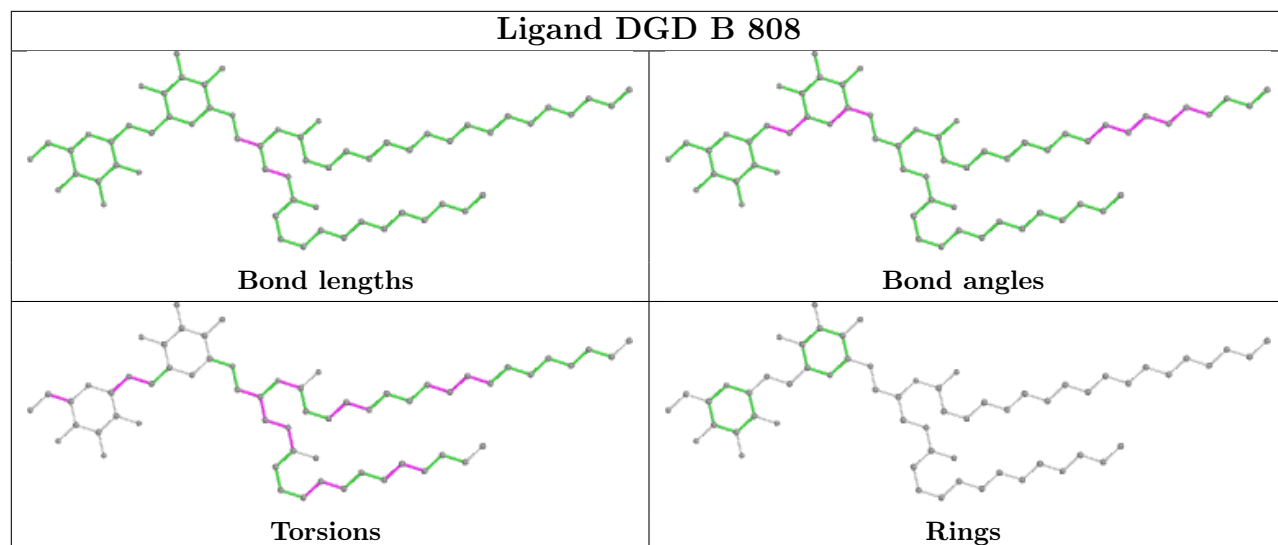


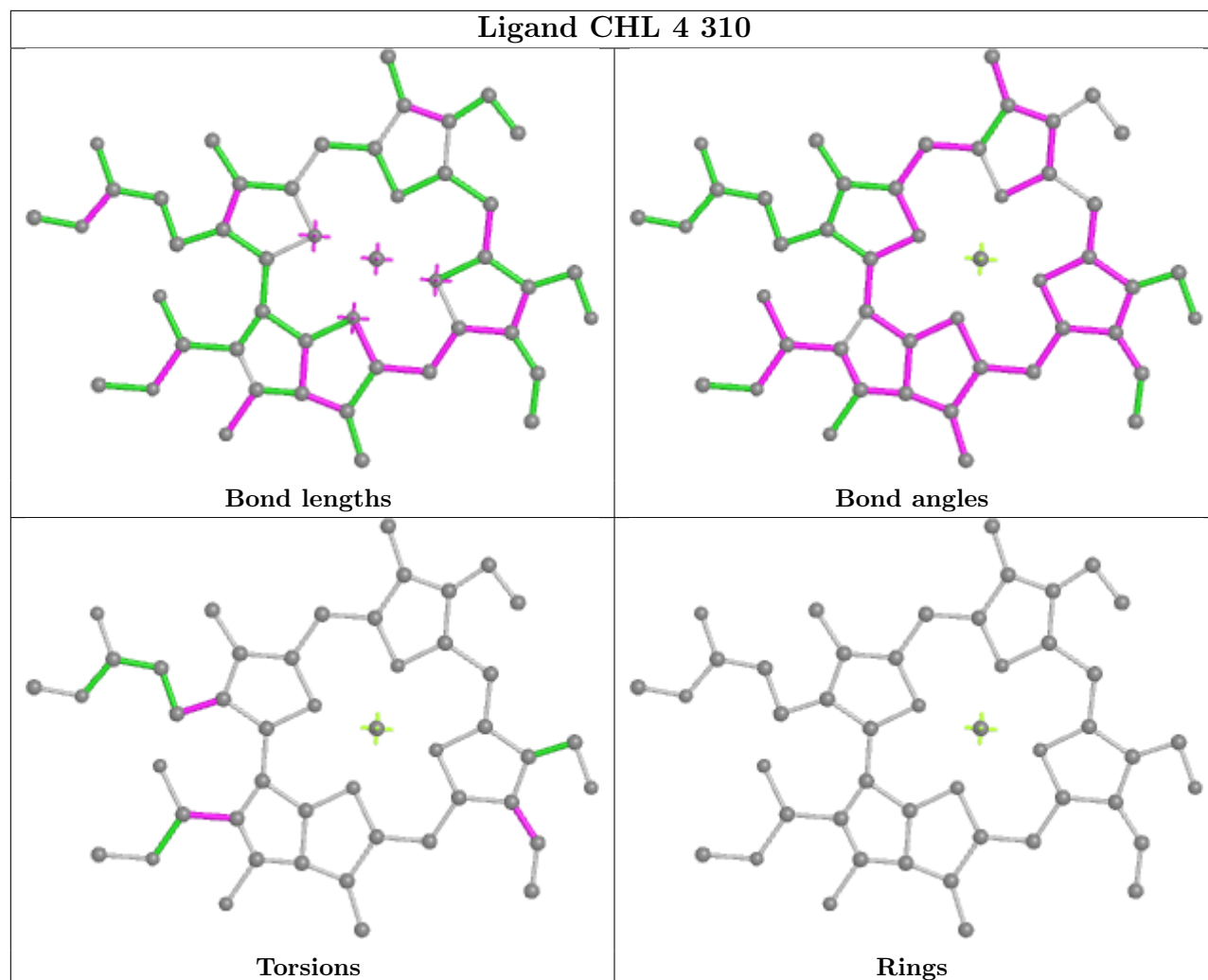
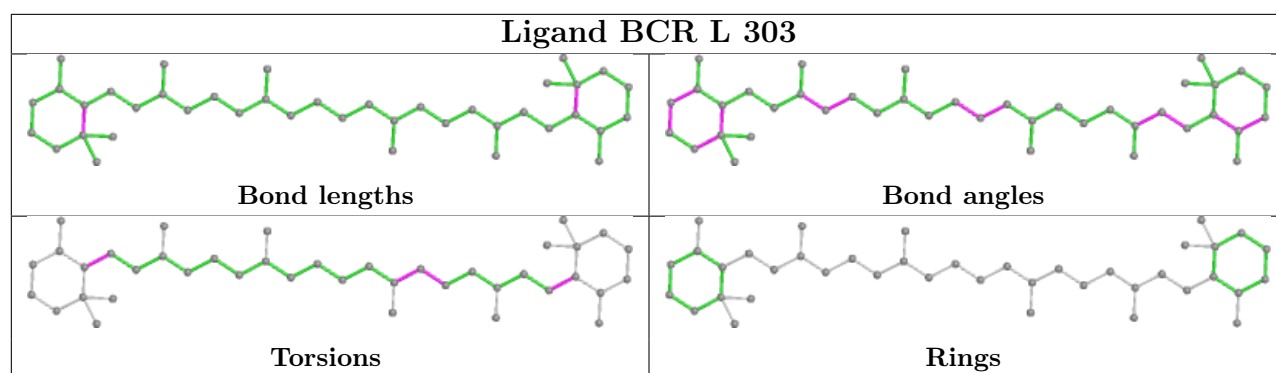
Torsions



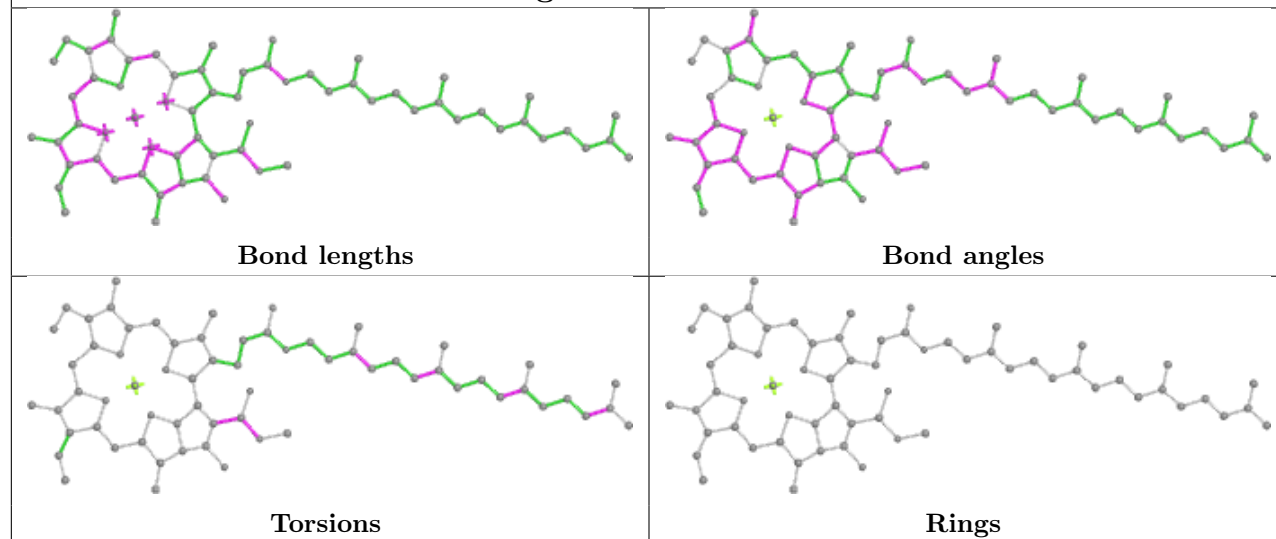
Rings



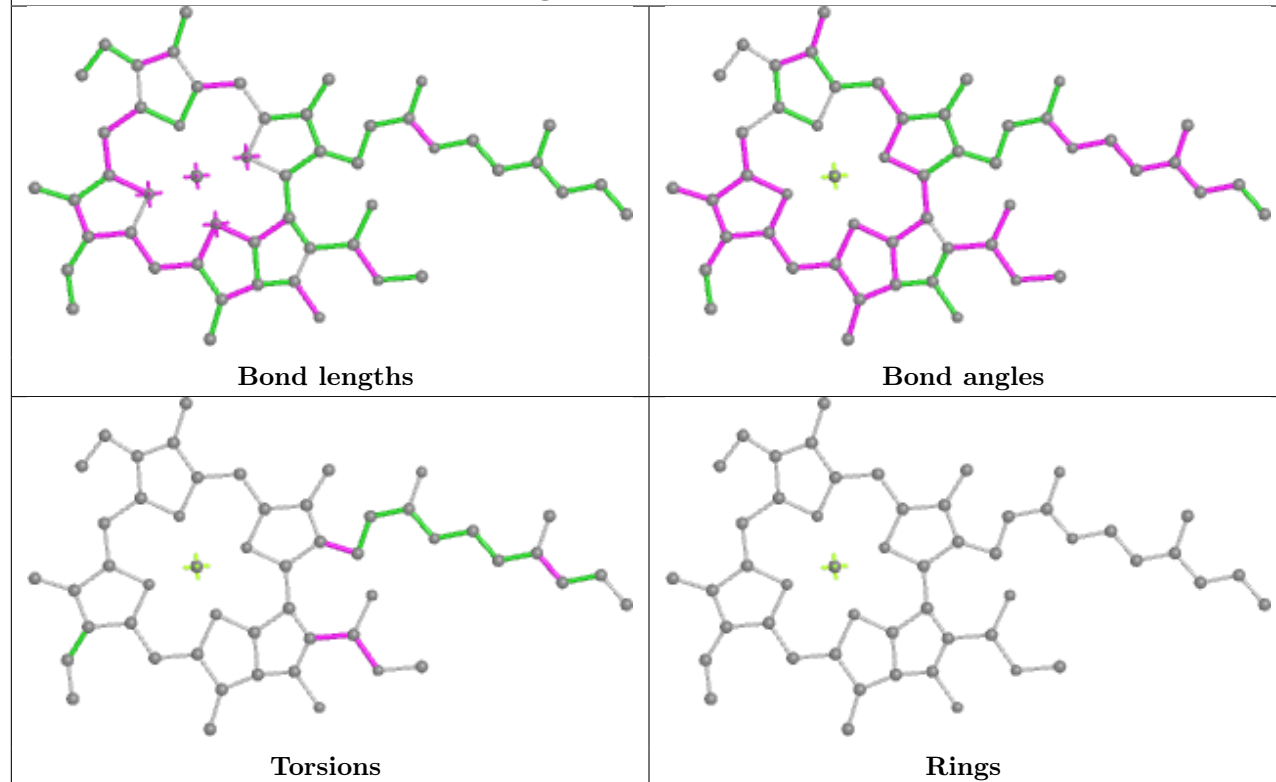




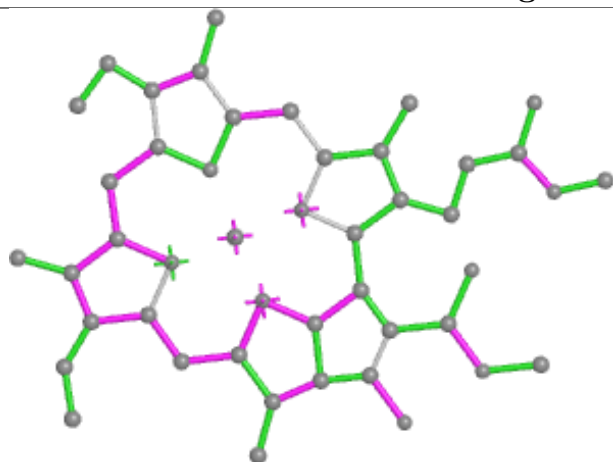
## Ligand CLA 6 312



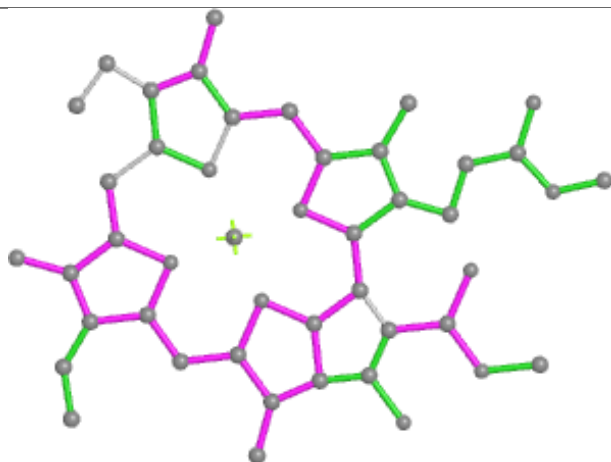
## Ligand CLA 8 315



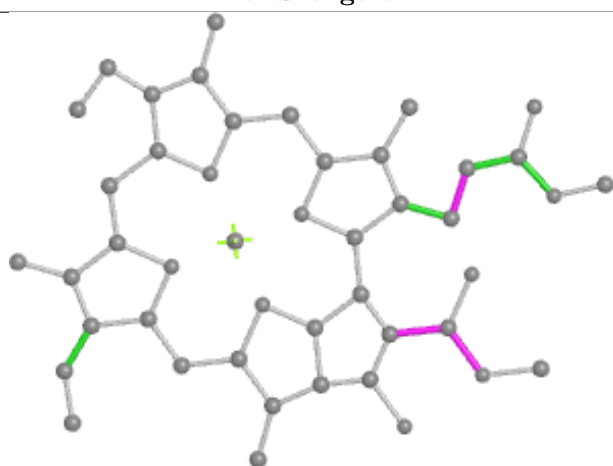
## Ligand CLA 2 312



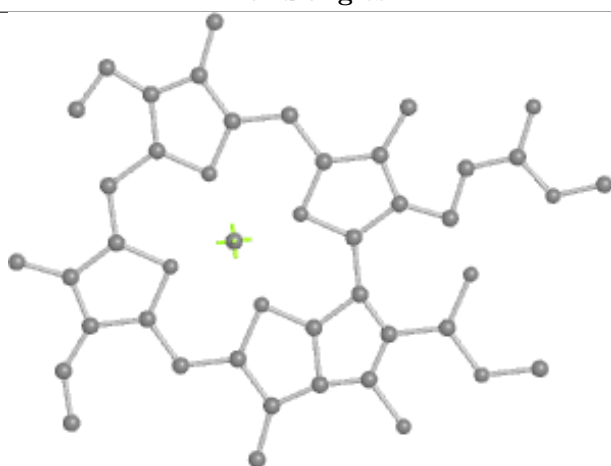
Bond lengths



Bond angles

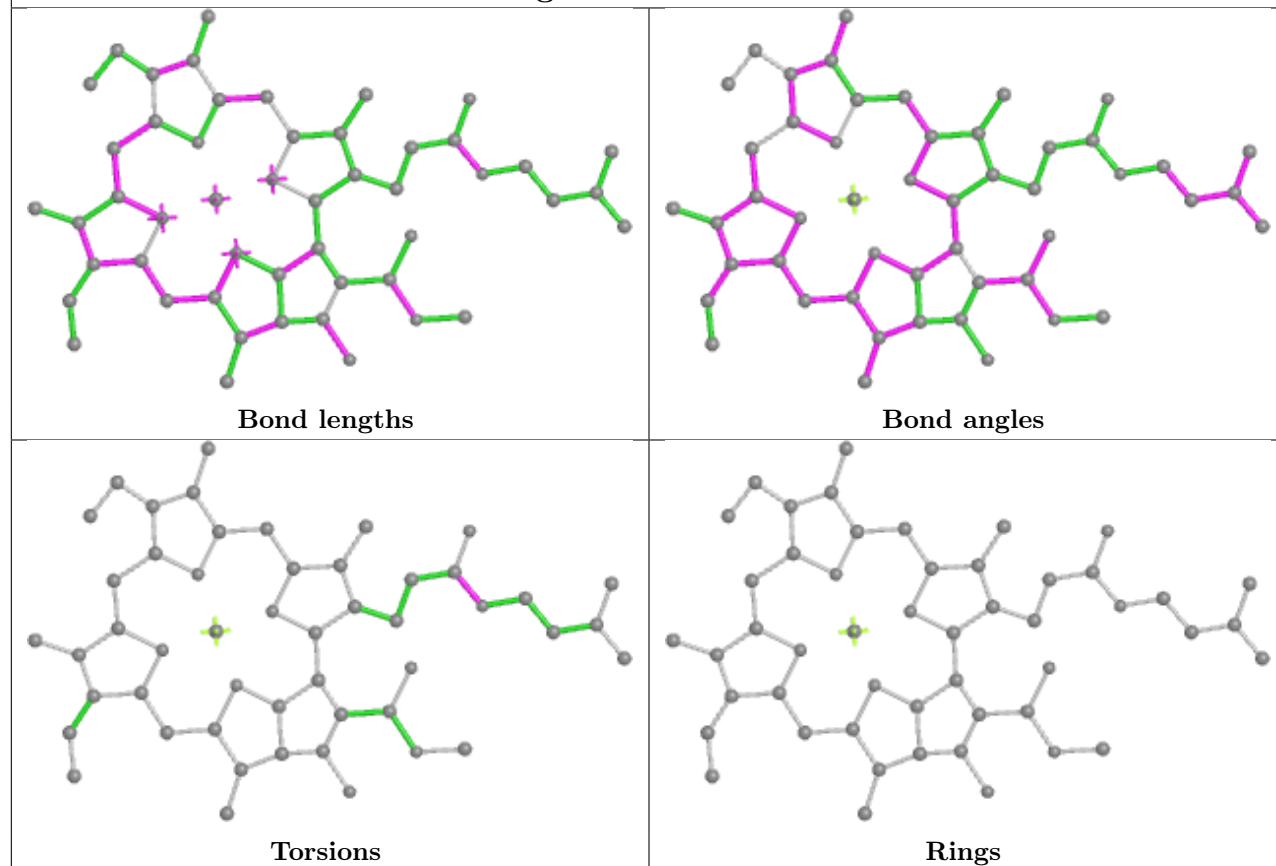


Torsions

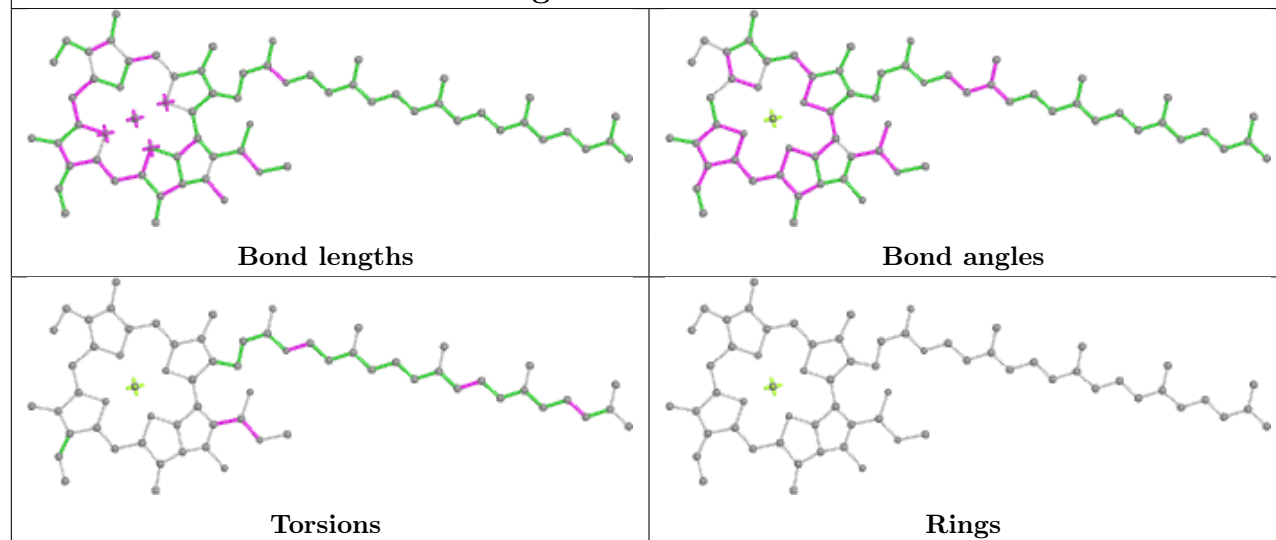


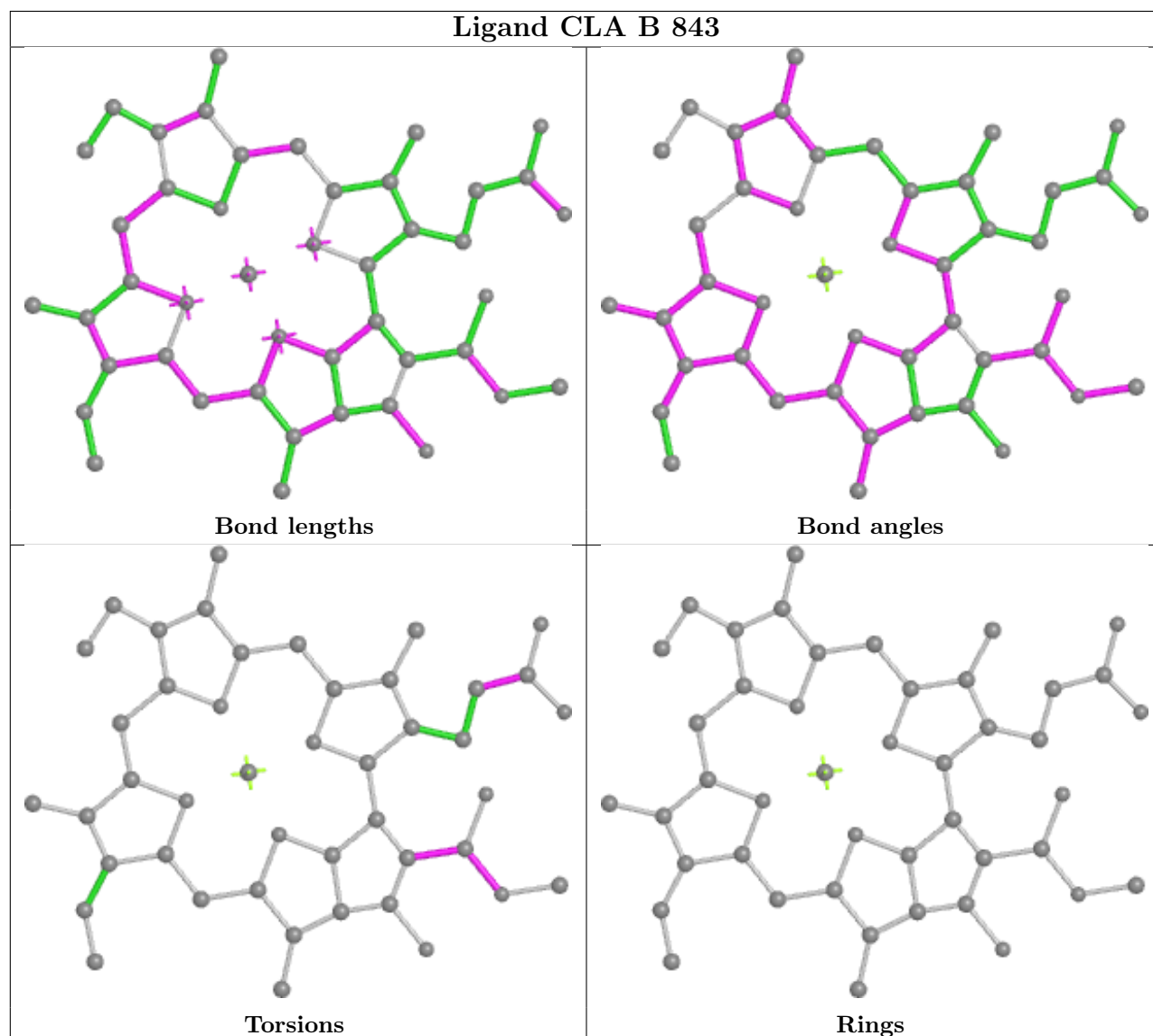
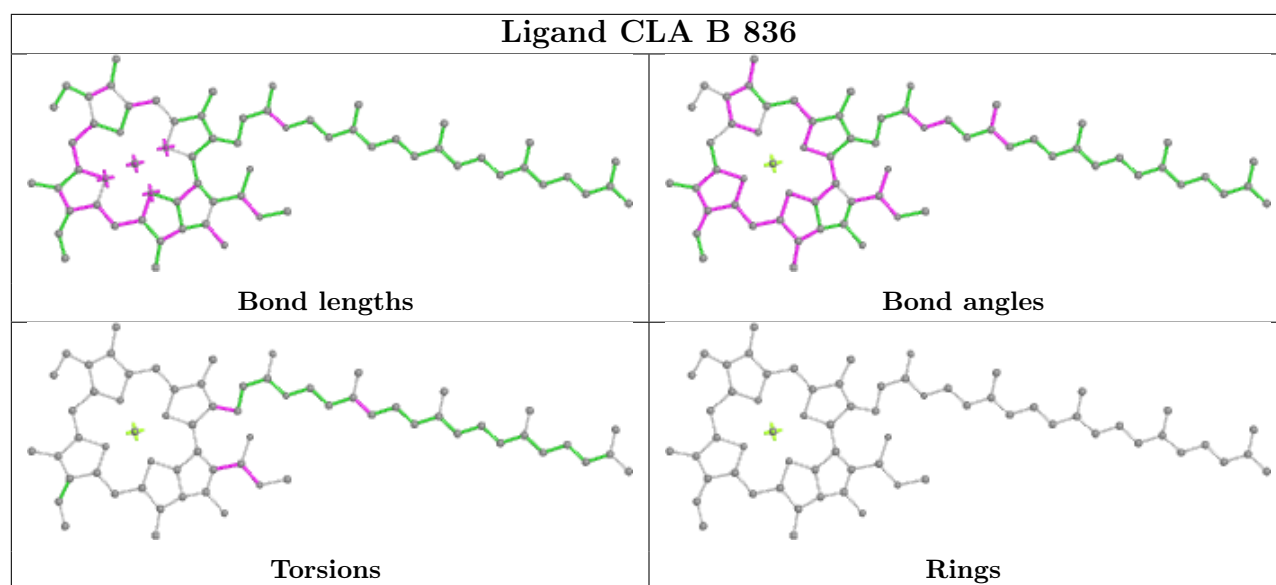
Rings

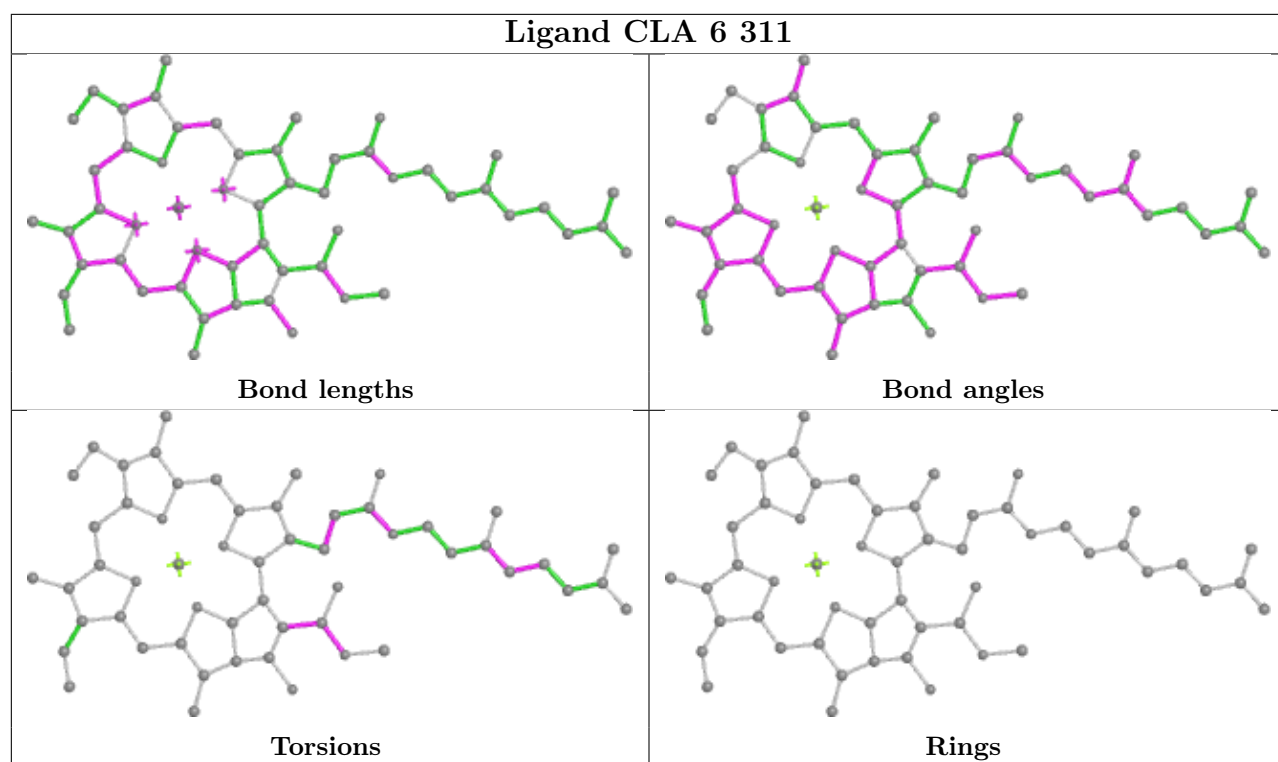
## Ligand CLA 8 318



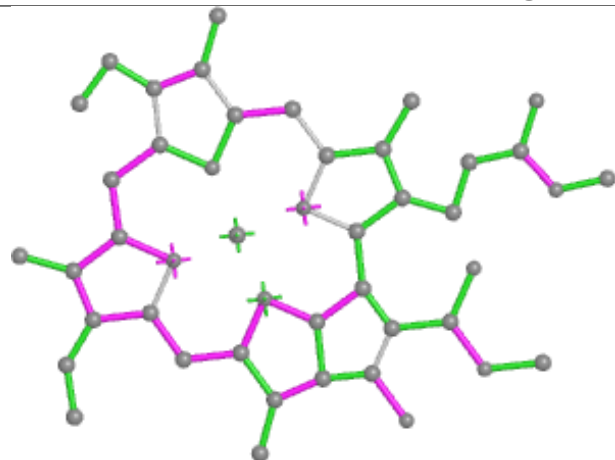
## Ligand CLA B 811



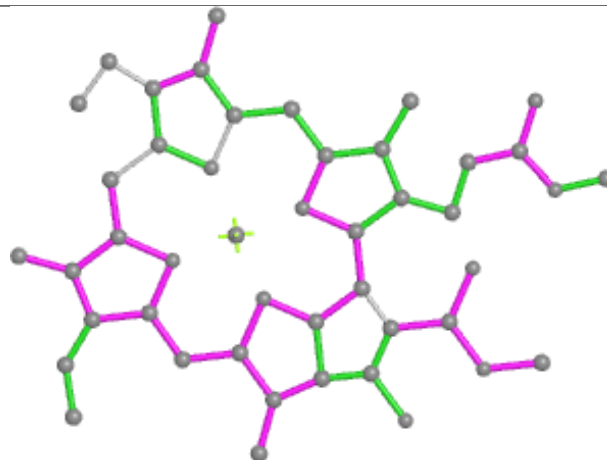




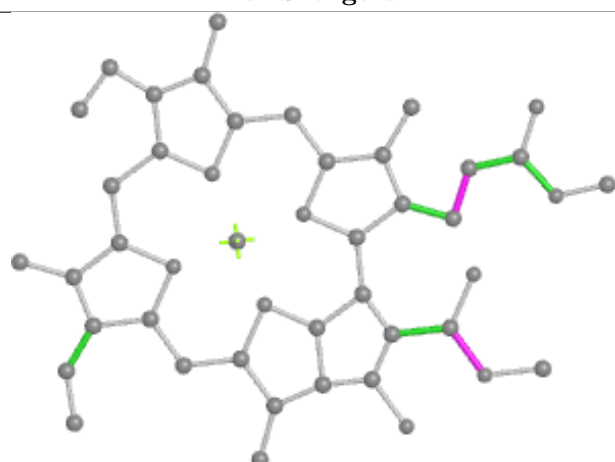
## Ligand CLA 2 308



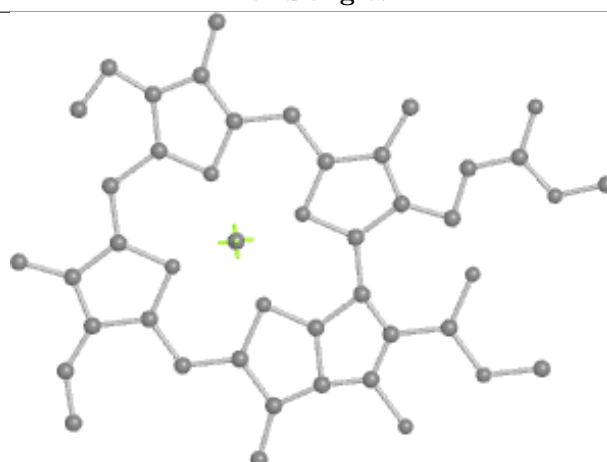
Bond lengths



Bond angles

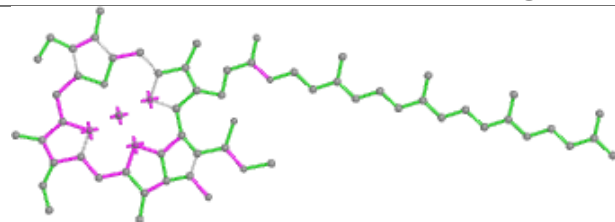


Torsions

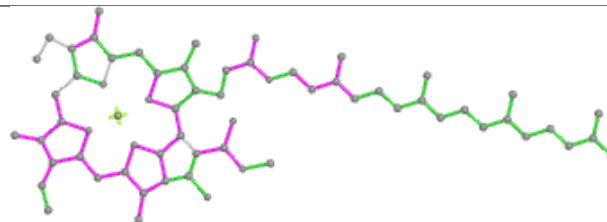


Rings

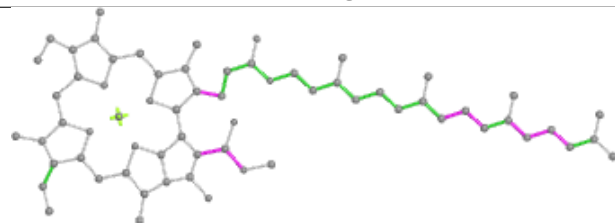
## Ligand CLA 3 307



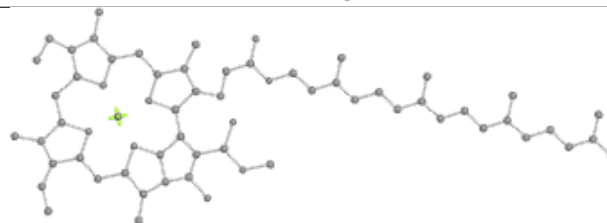
Bond lengths



Bond angles

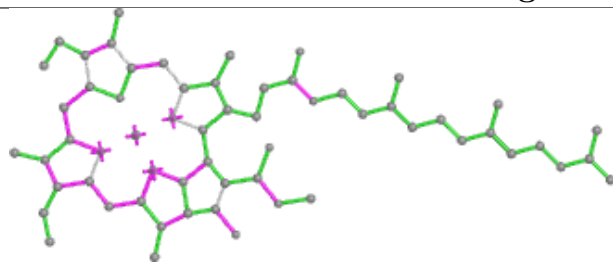


Torsions

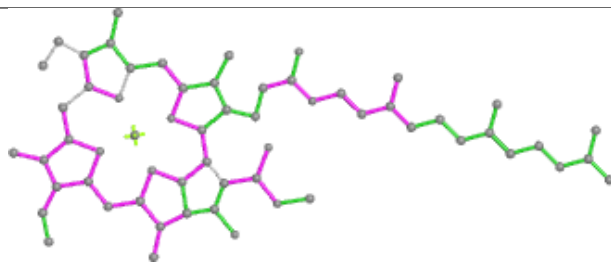


Rings

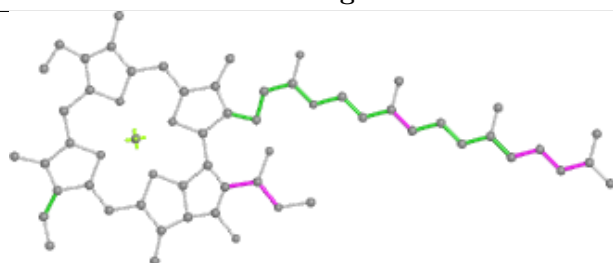


**Ligand CLA a 311**

Bond lengths



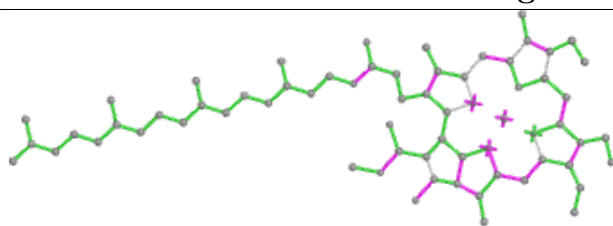
Bond angles



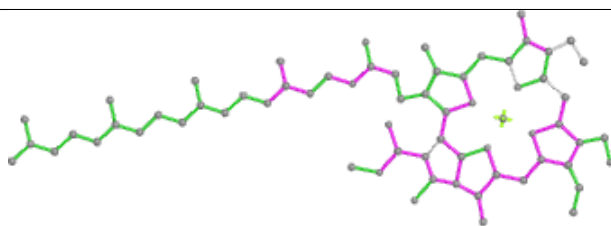
Torsions



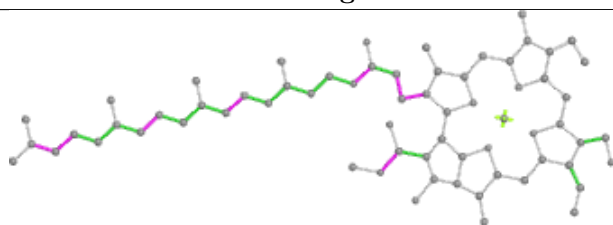
Rings

**Ligand CHL 8 316**

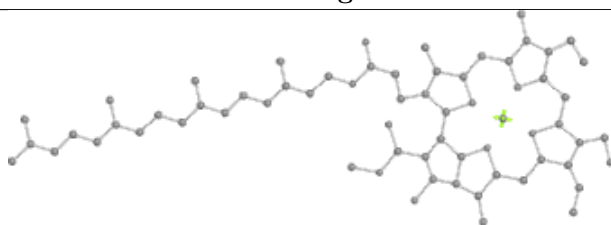
Bond lengths



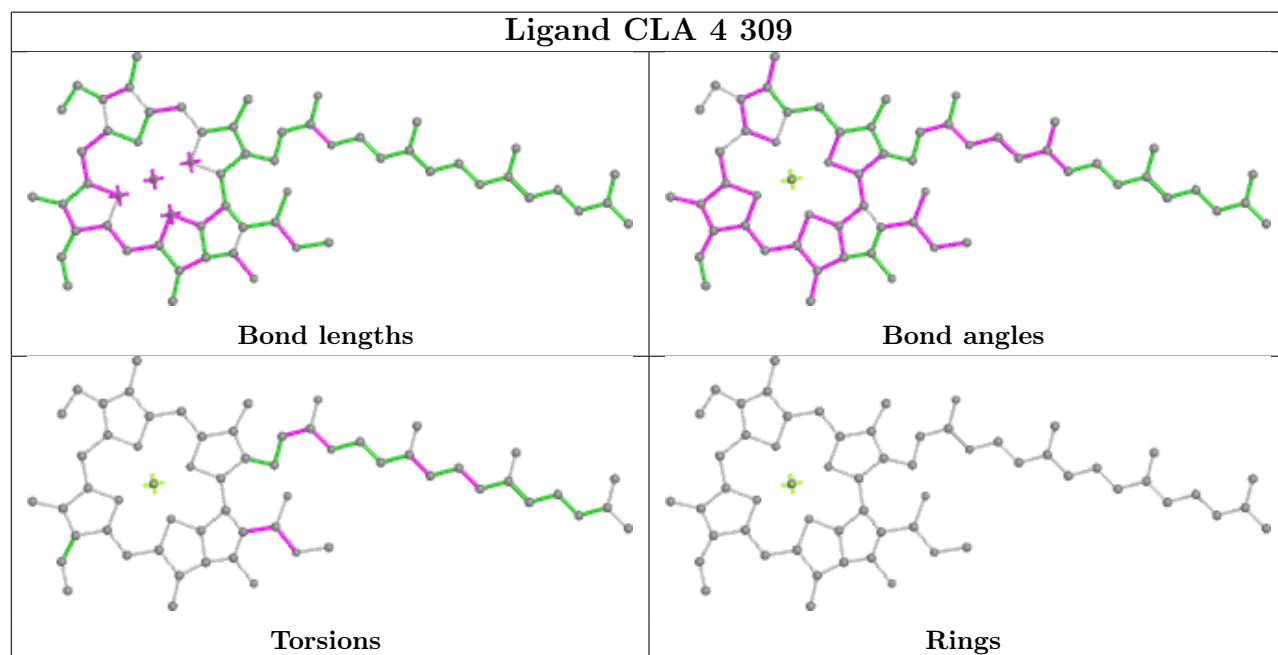
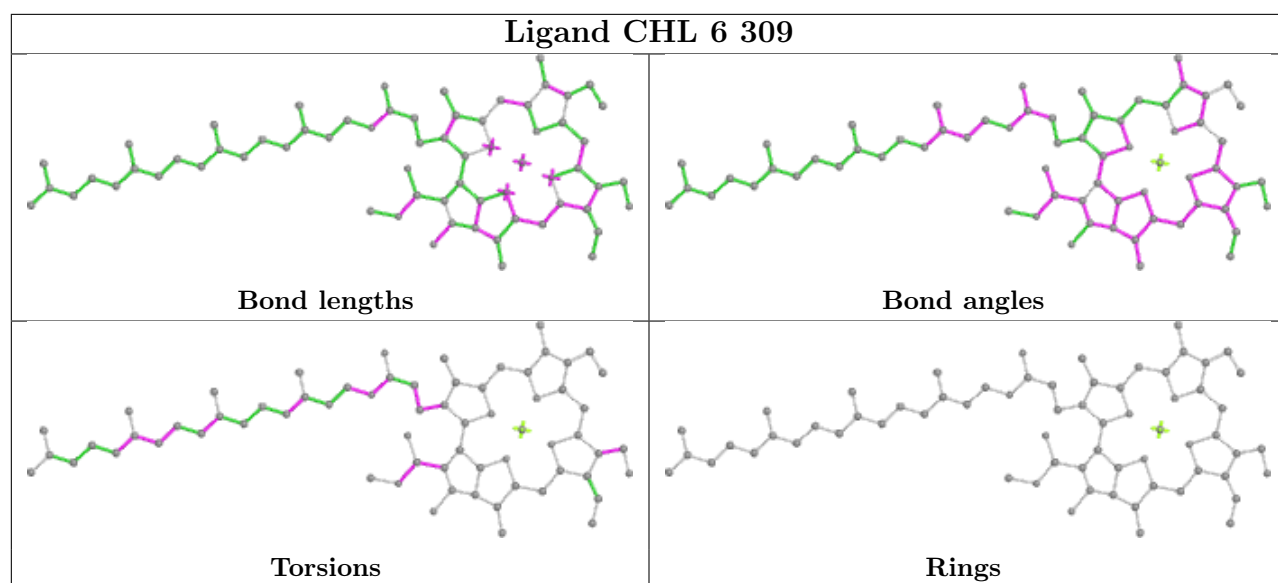
Bond angles



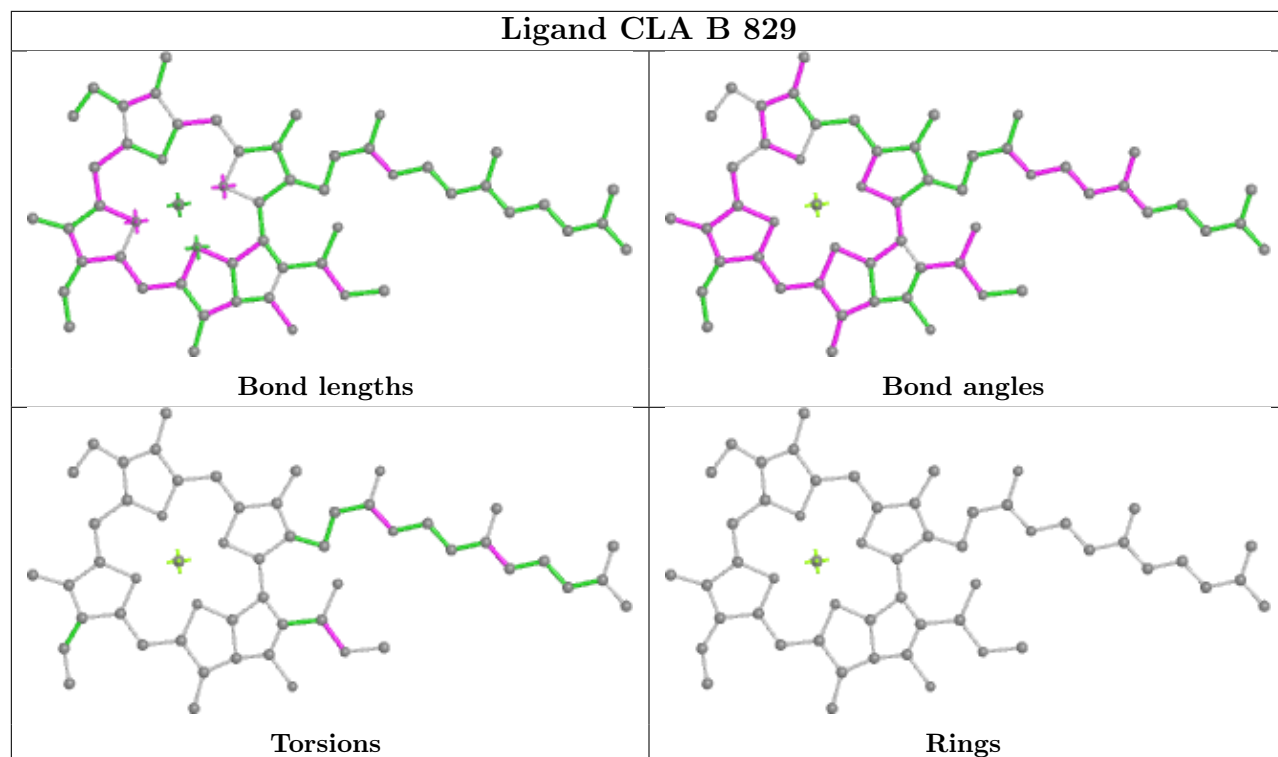
Torsions



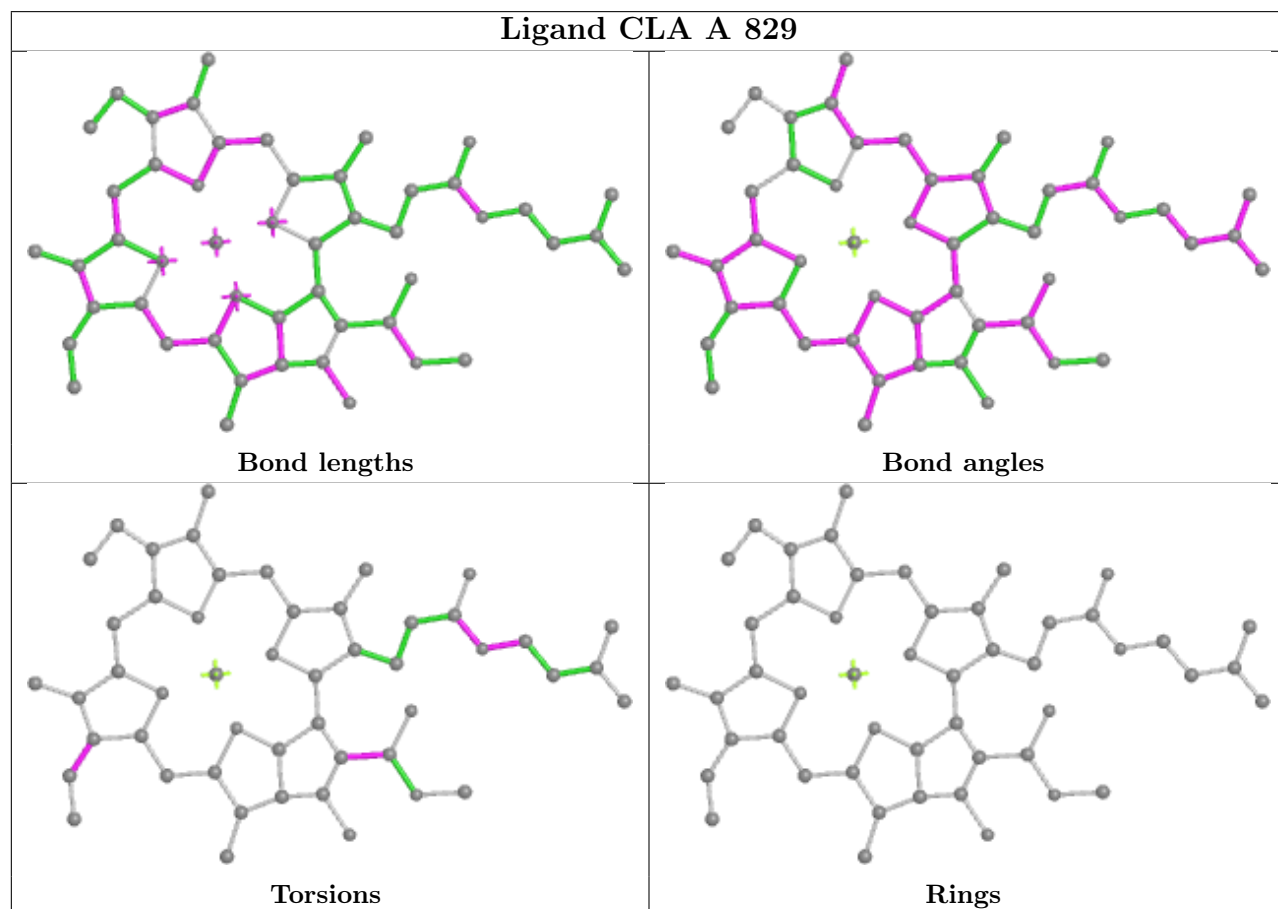
Rings

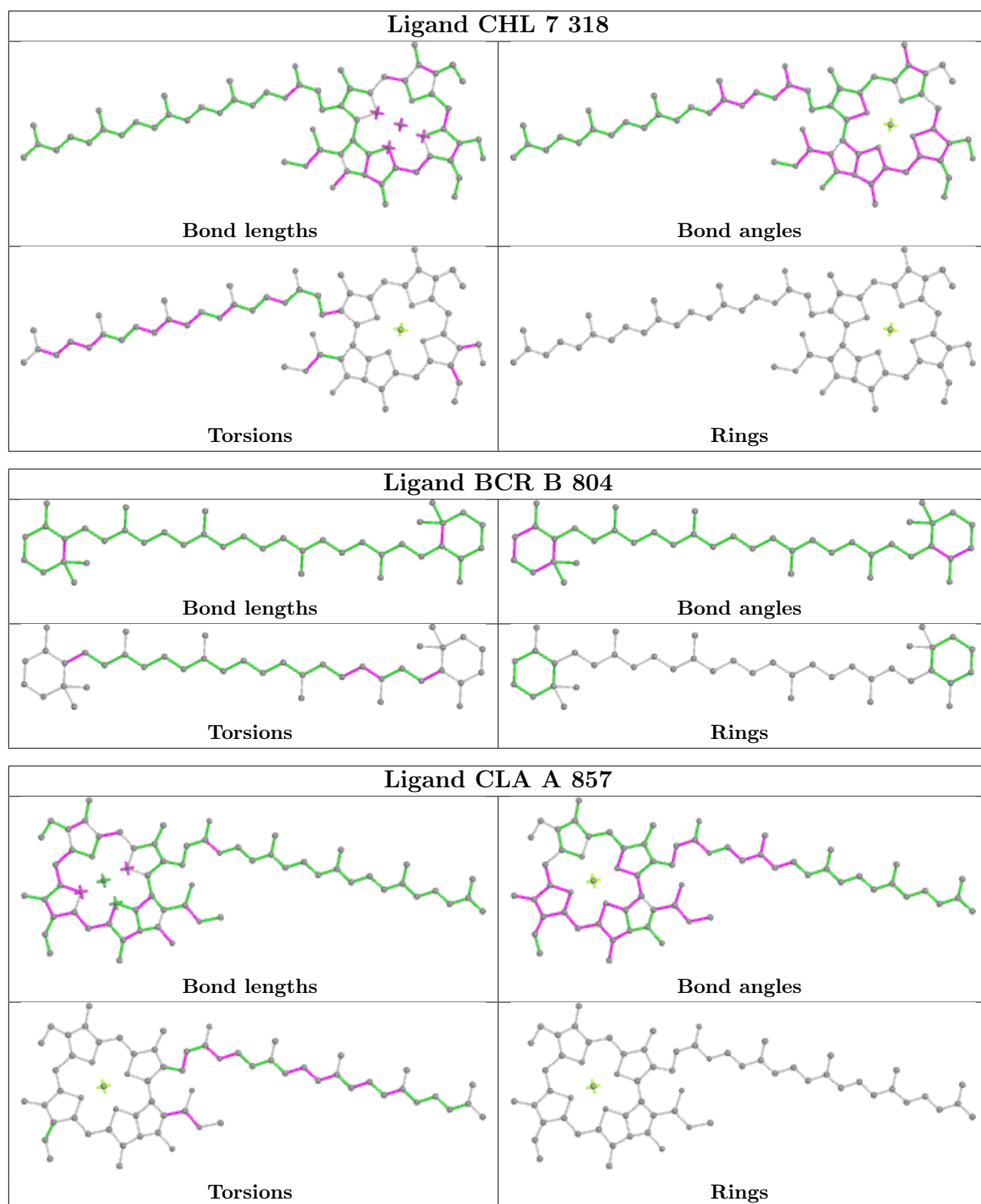


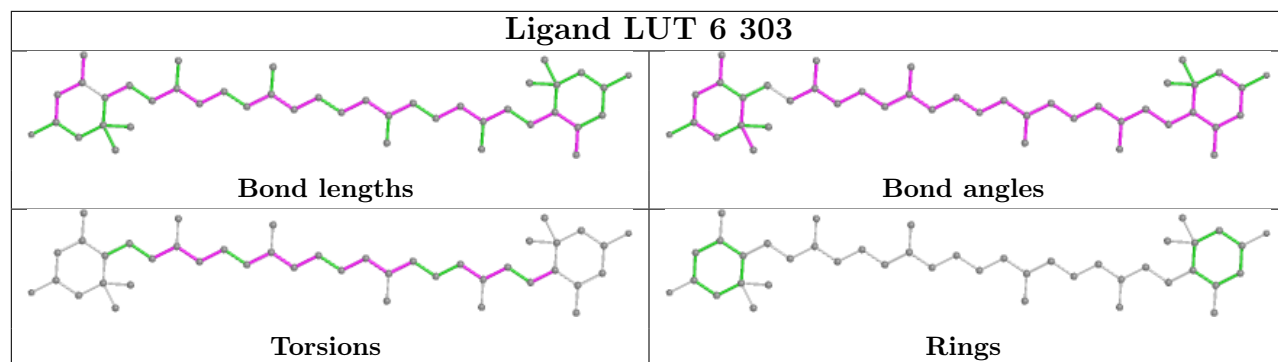
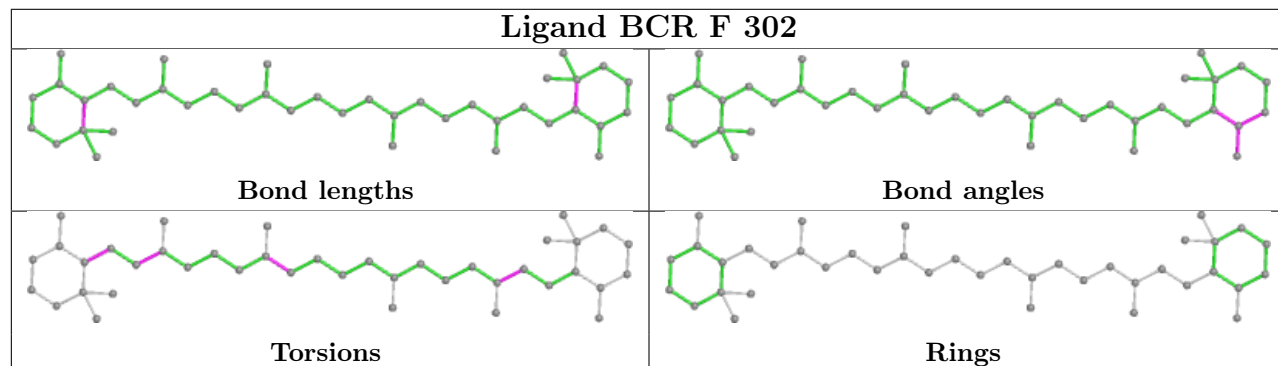
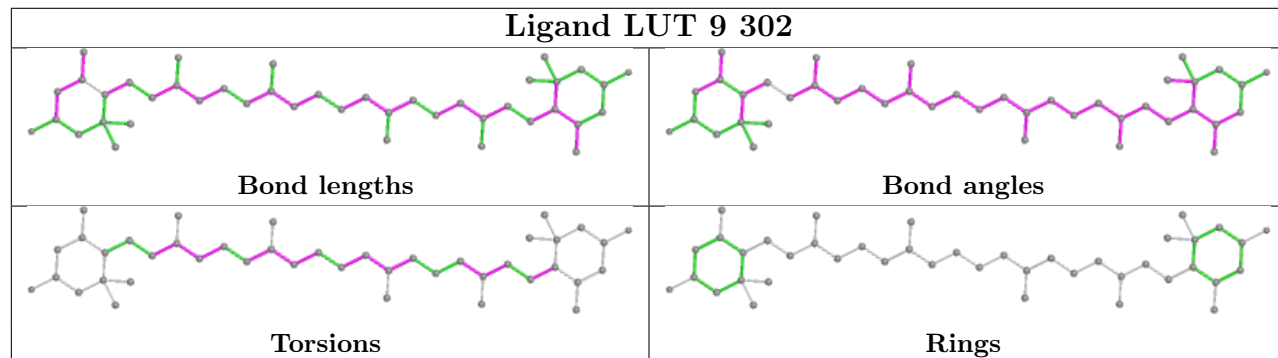
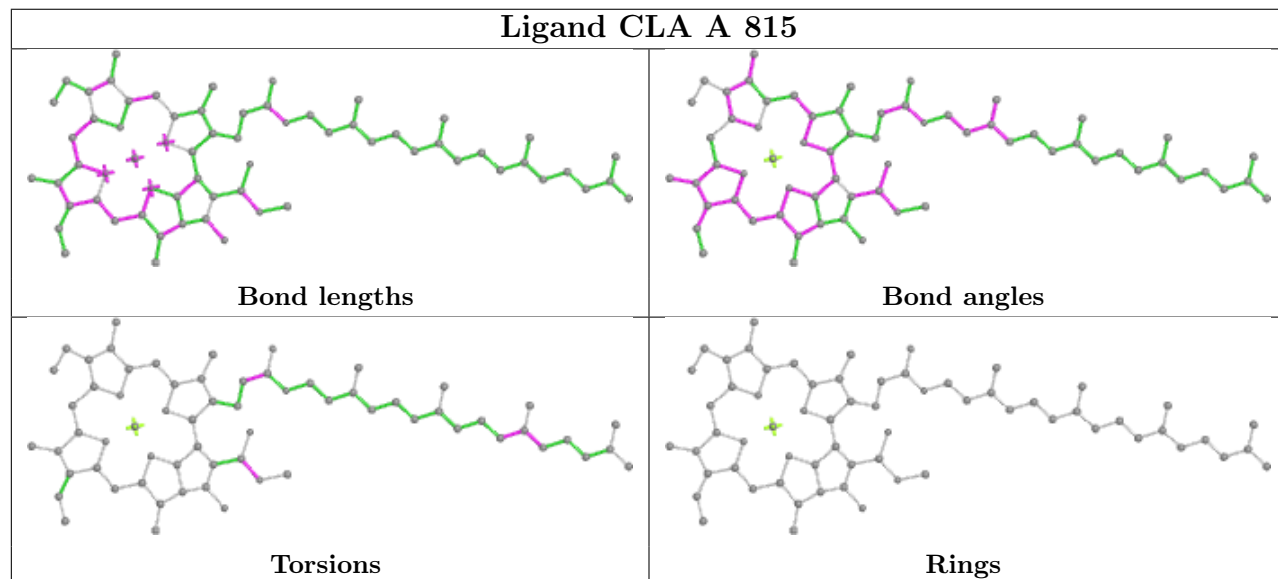
## Ligand CLA B 829

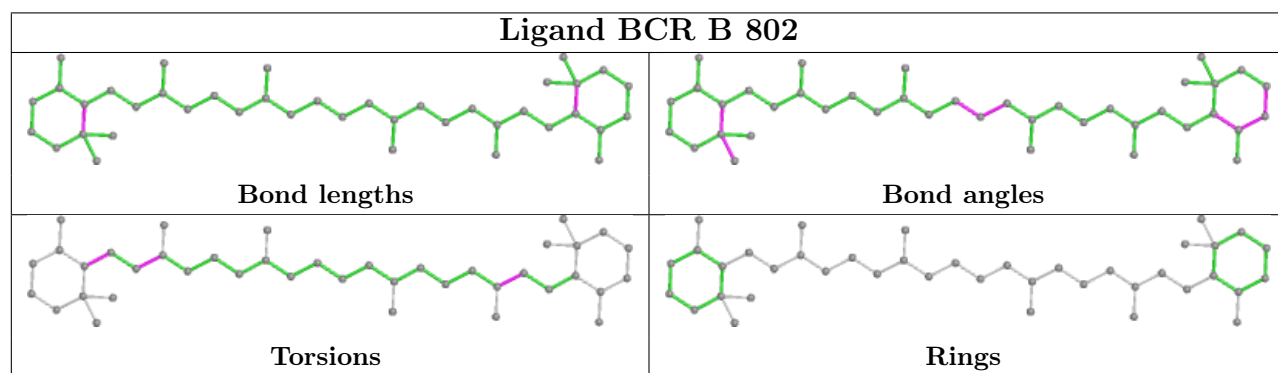
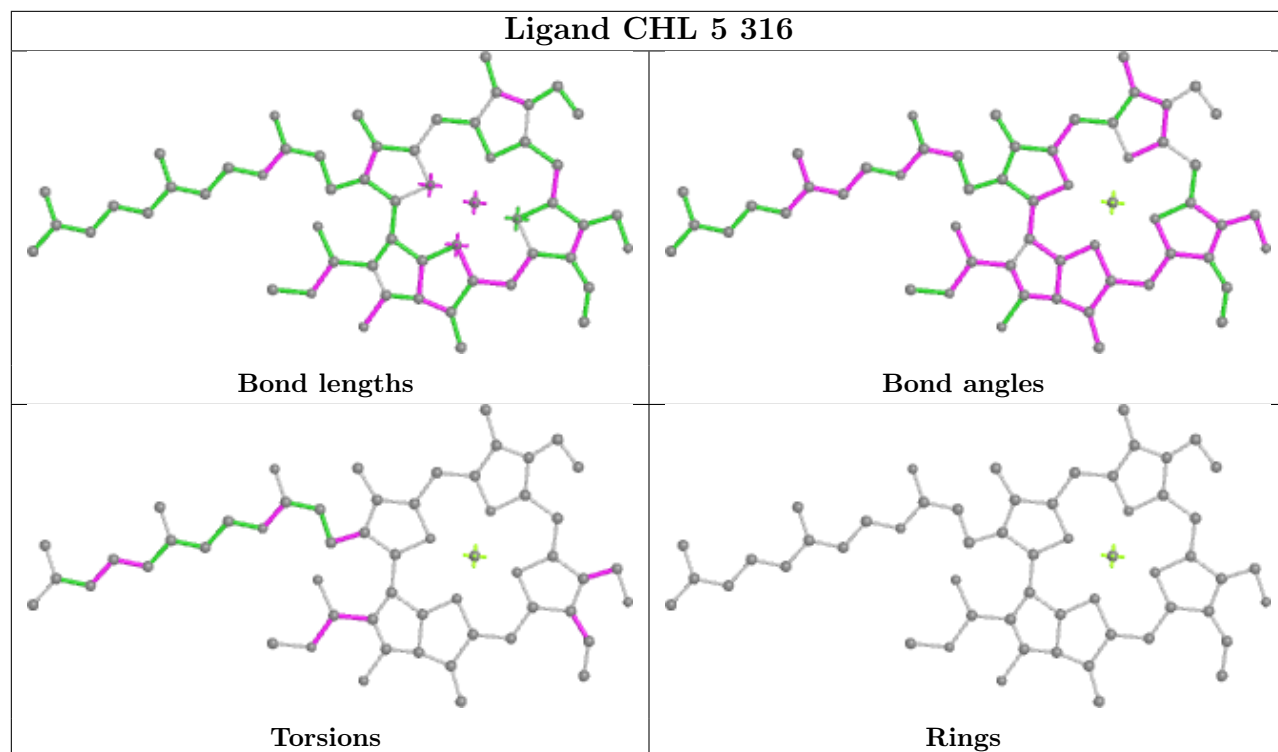
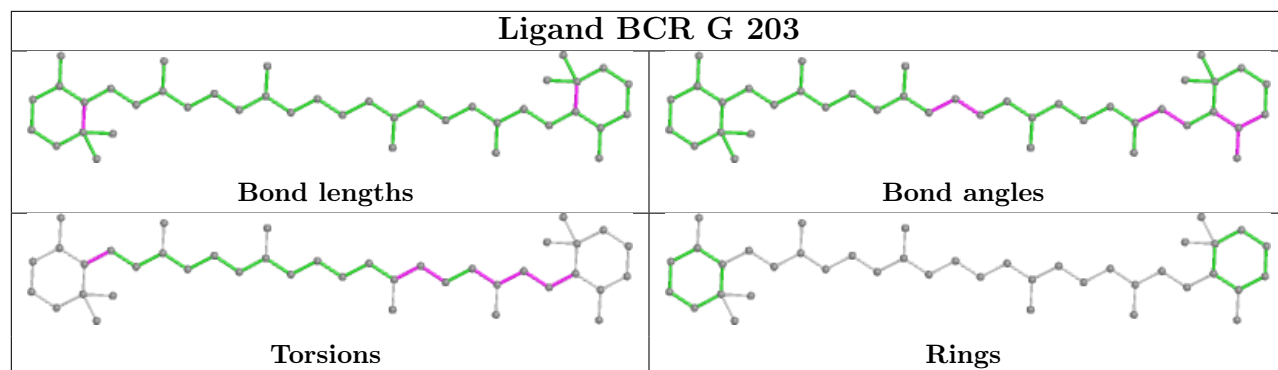


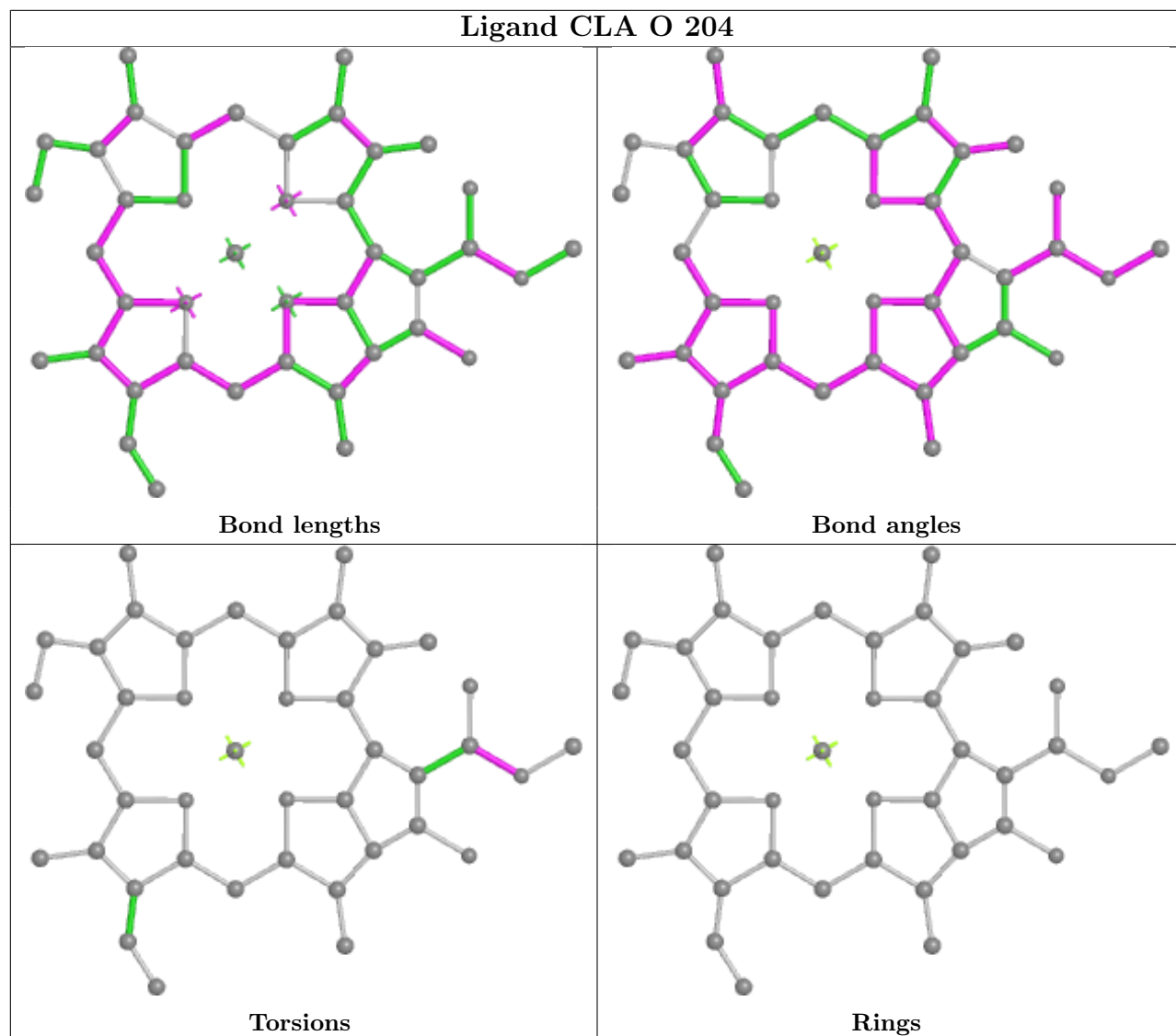
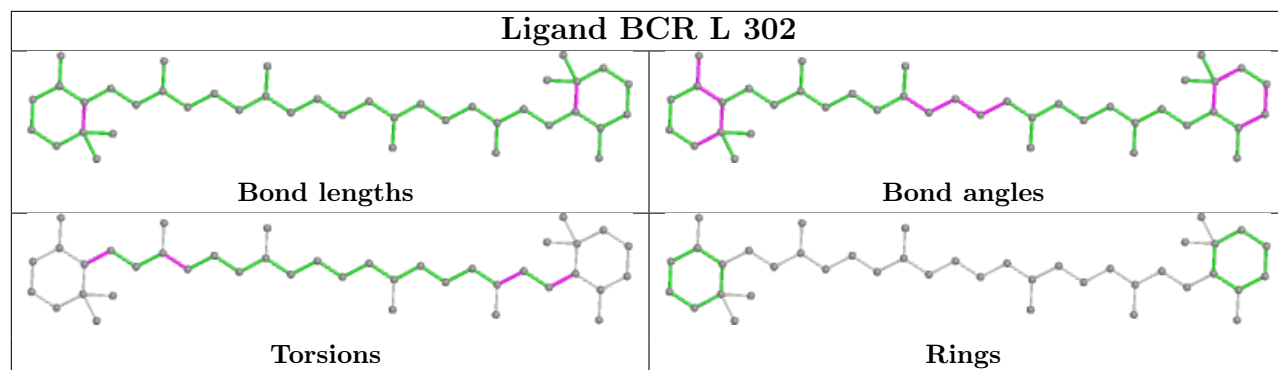
## Ligand CLA A 829



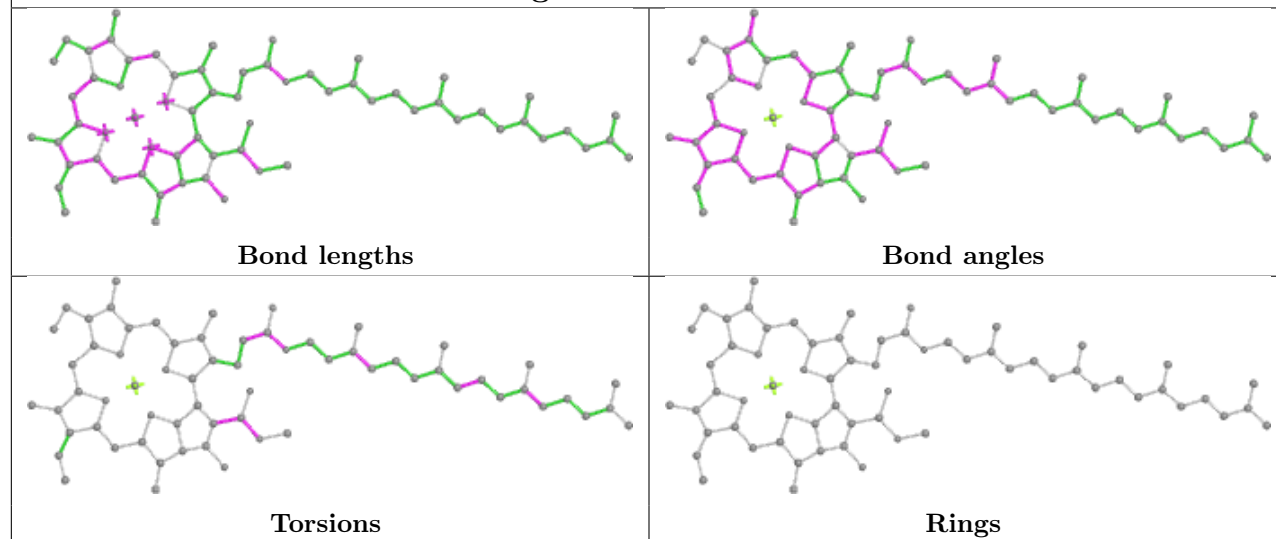


**Ligand LUT 6 303****Ligand BCR F 302****Ligand LUT 9 302****Ligand CLA A 815**

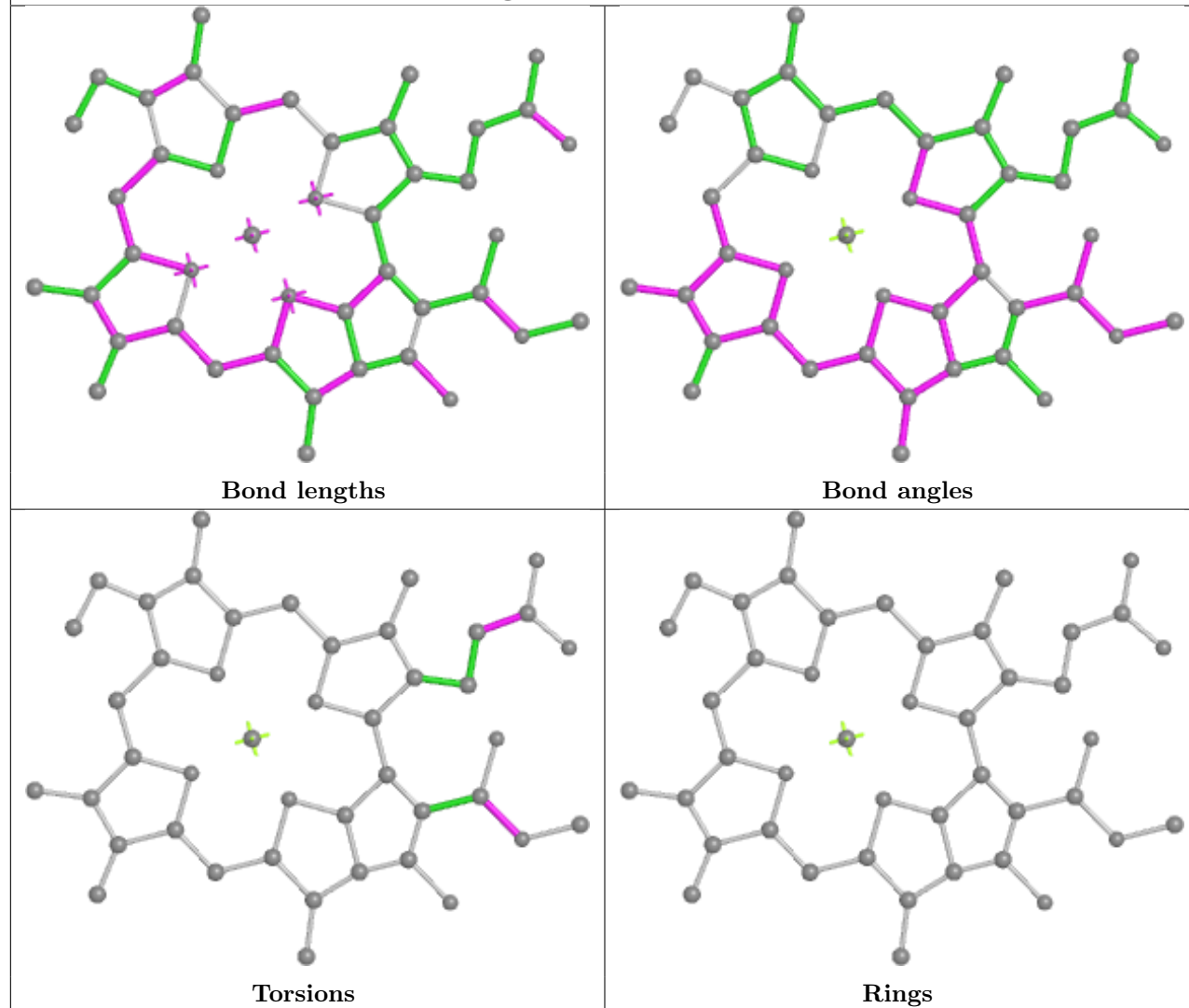




## Ligand CLA A 838

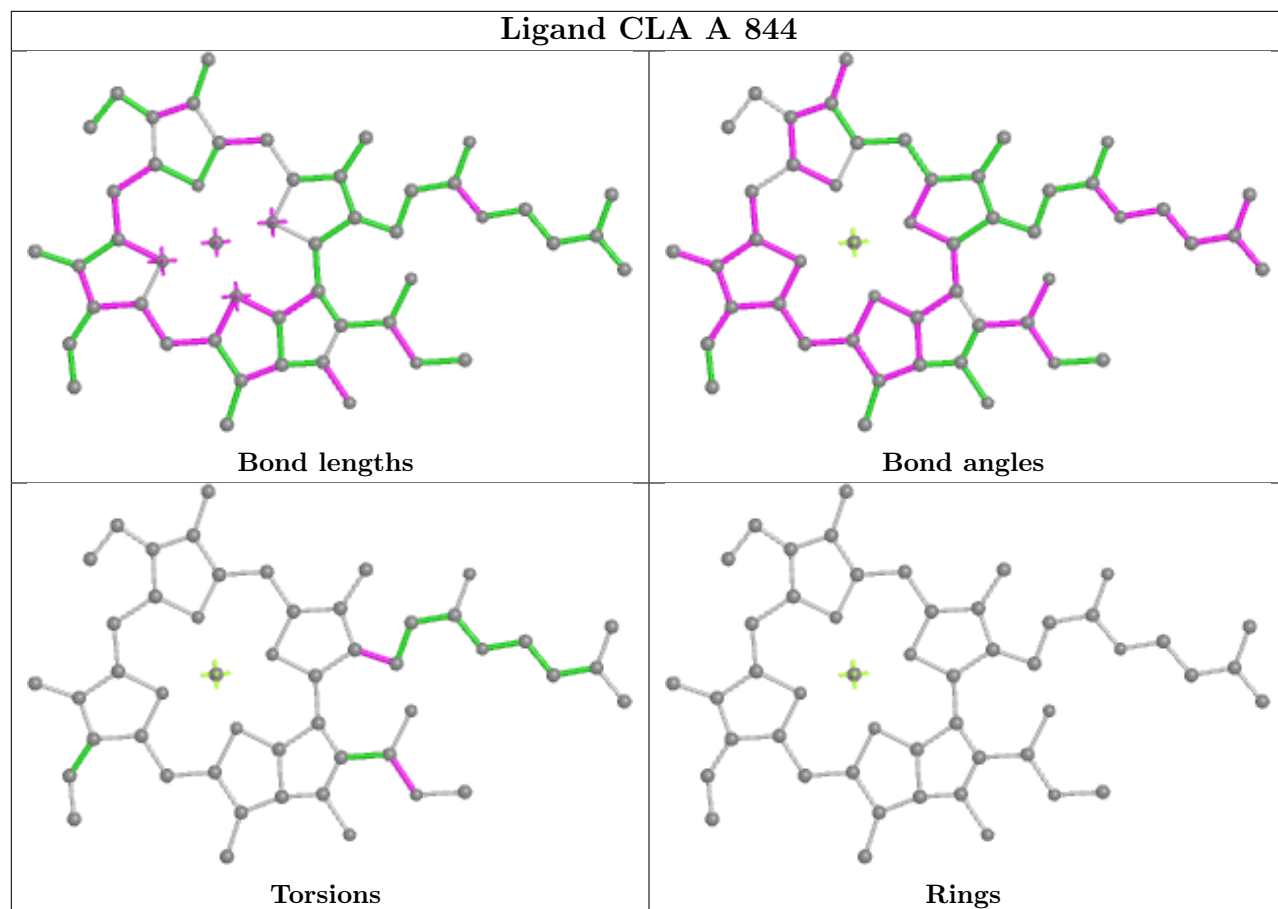


## Ligand CLA 7 310

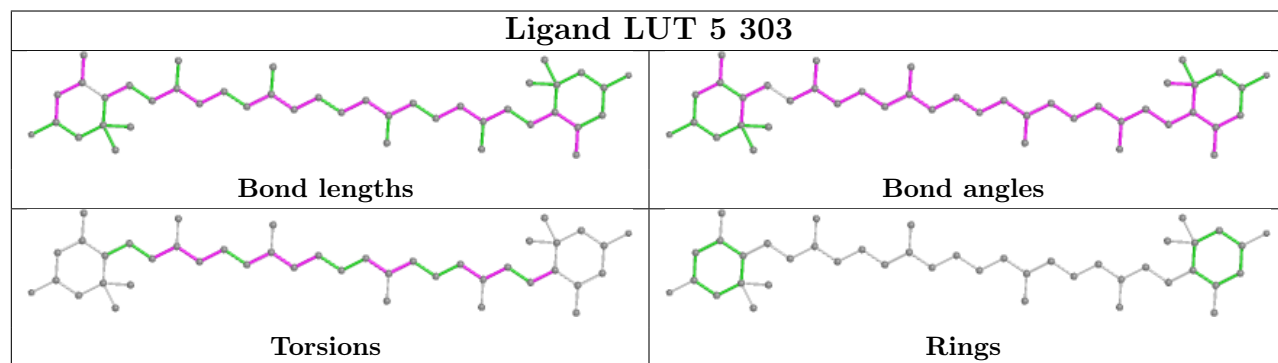




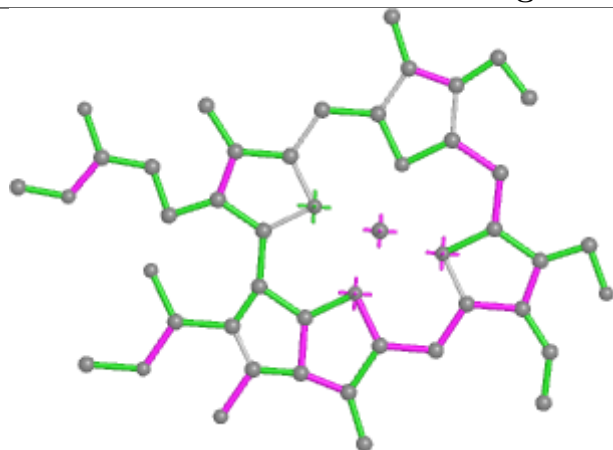
## Ligand CLA A 844



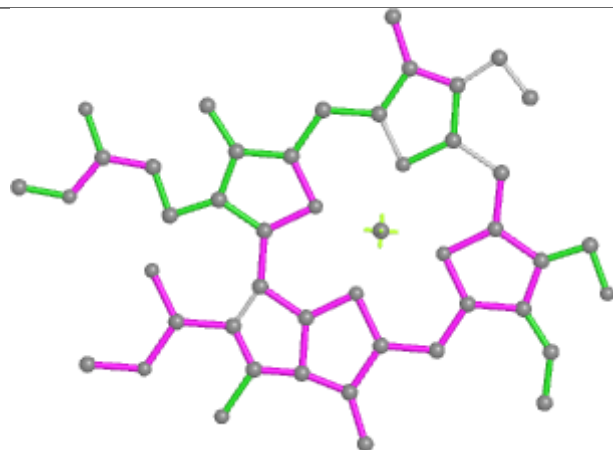
## Ligand LUT 5 303



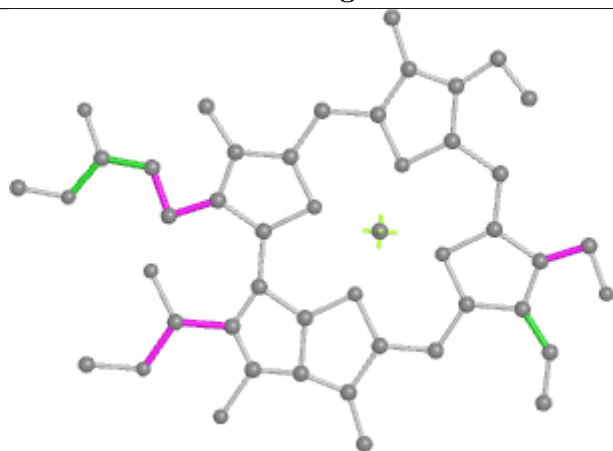
## Ligand CHL b 309



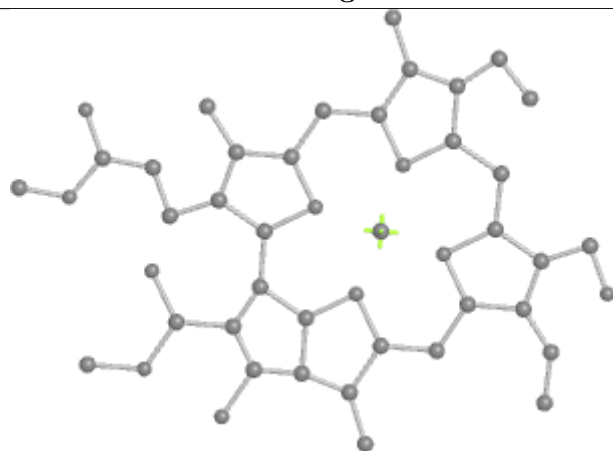
Bond lengths



Bond angles

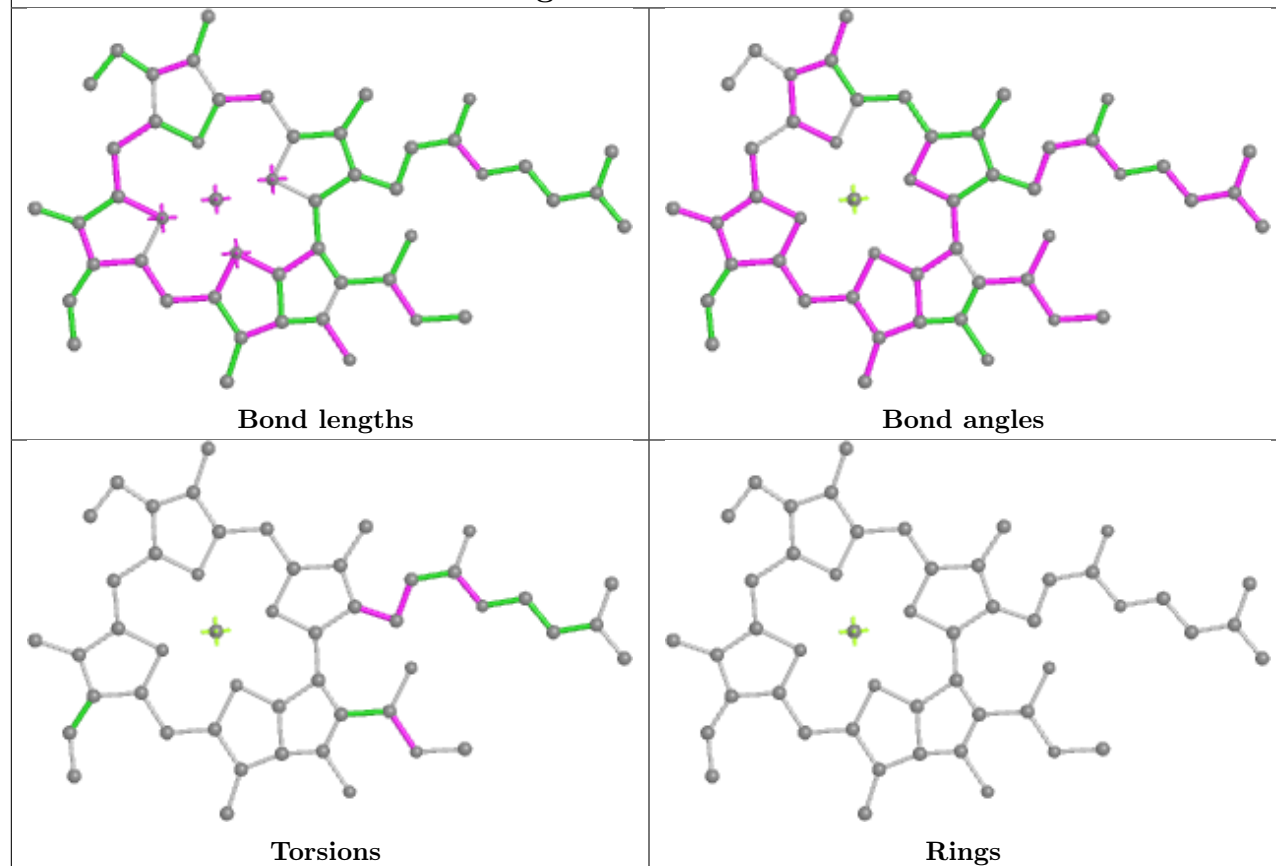


Torsions

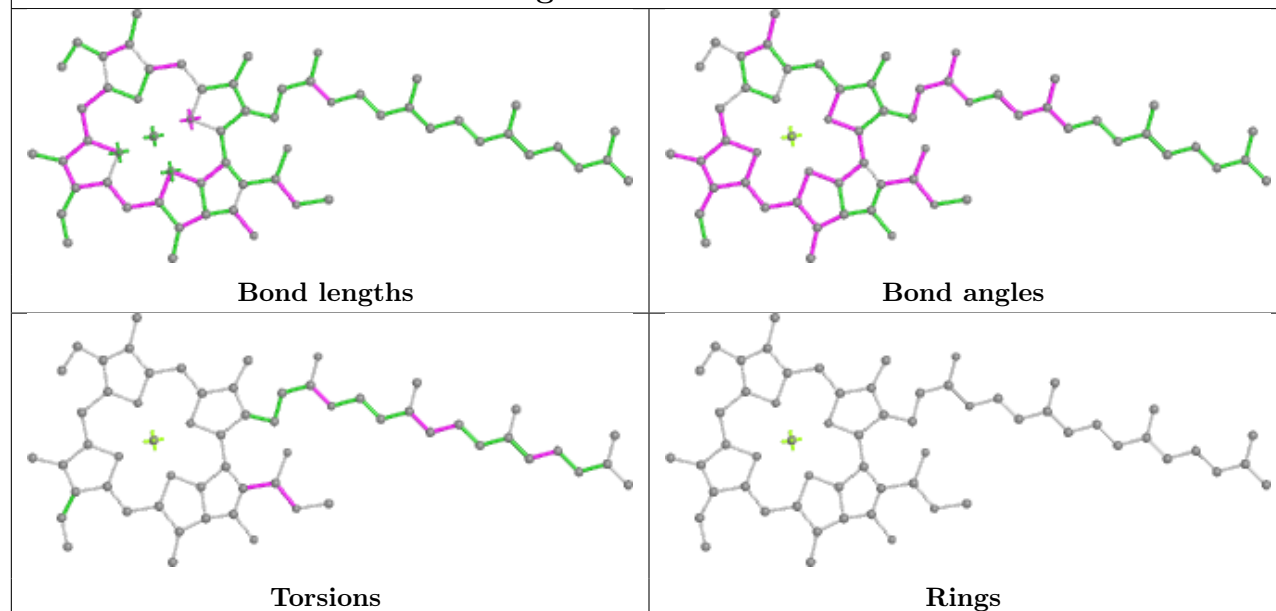


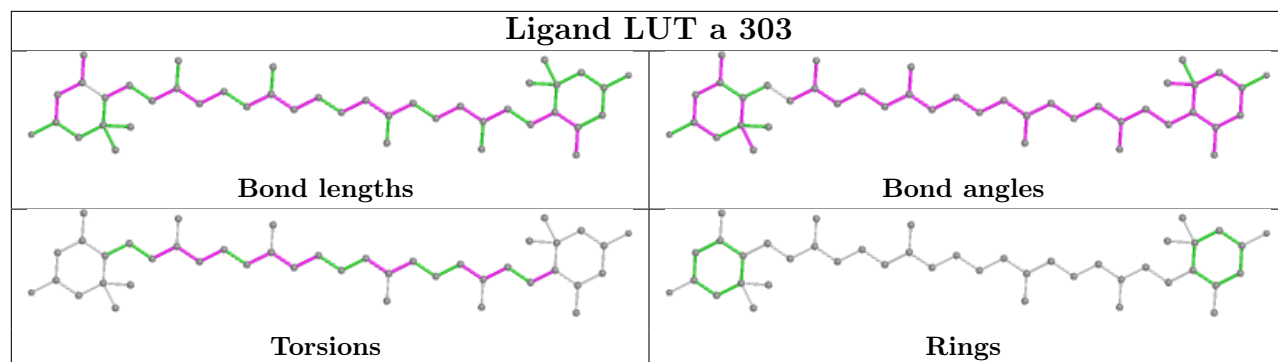
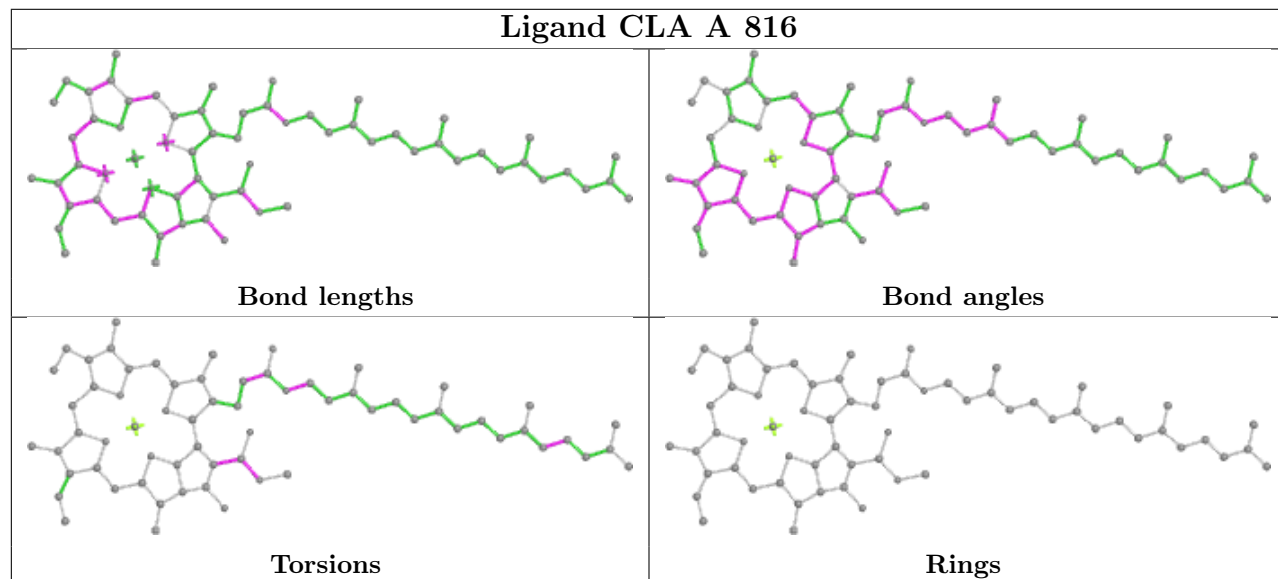
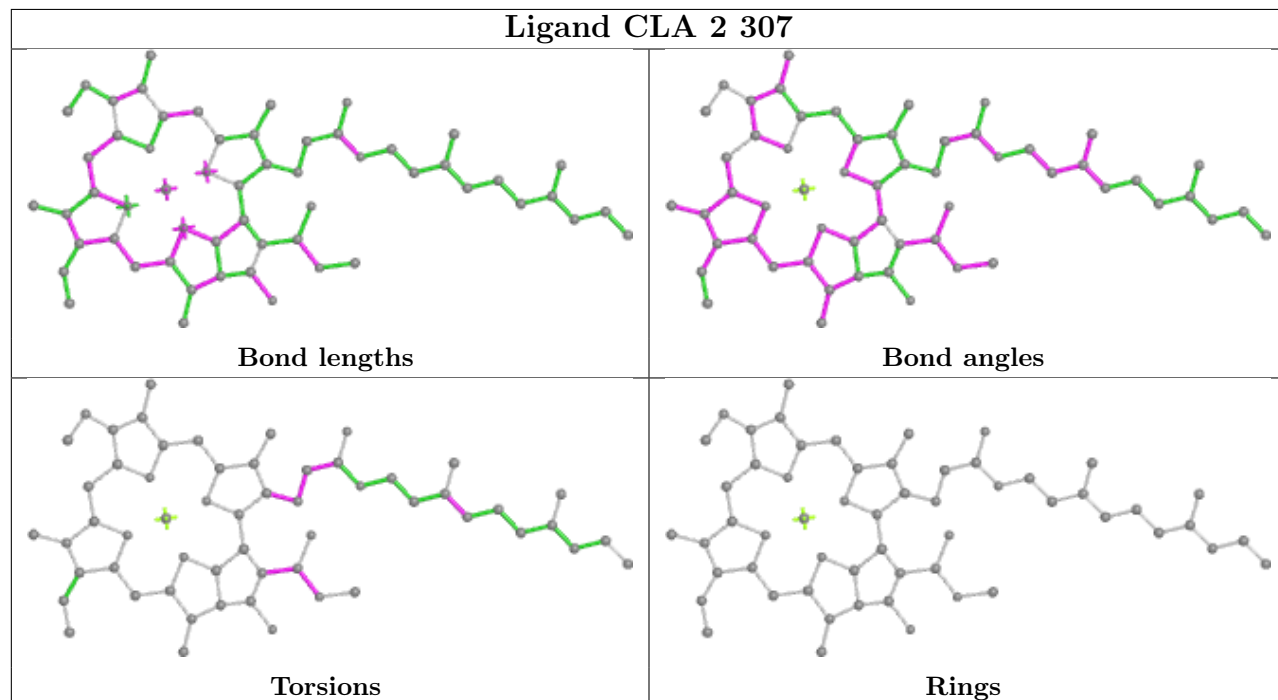
Rings

## Ligand CLA 4 321

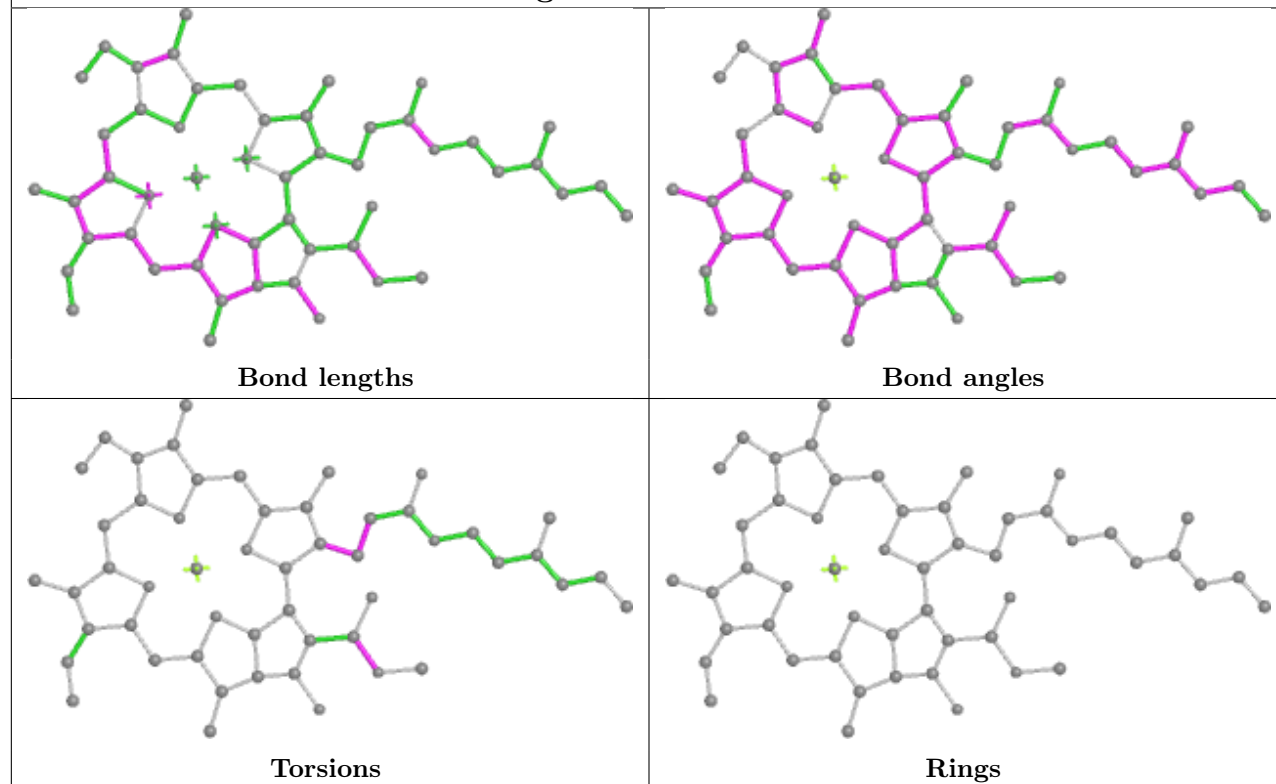


## Ligand CLA 3 313

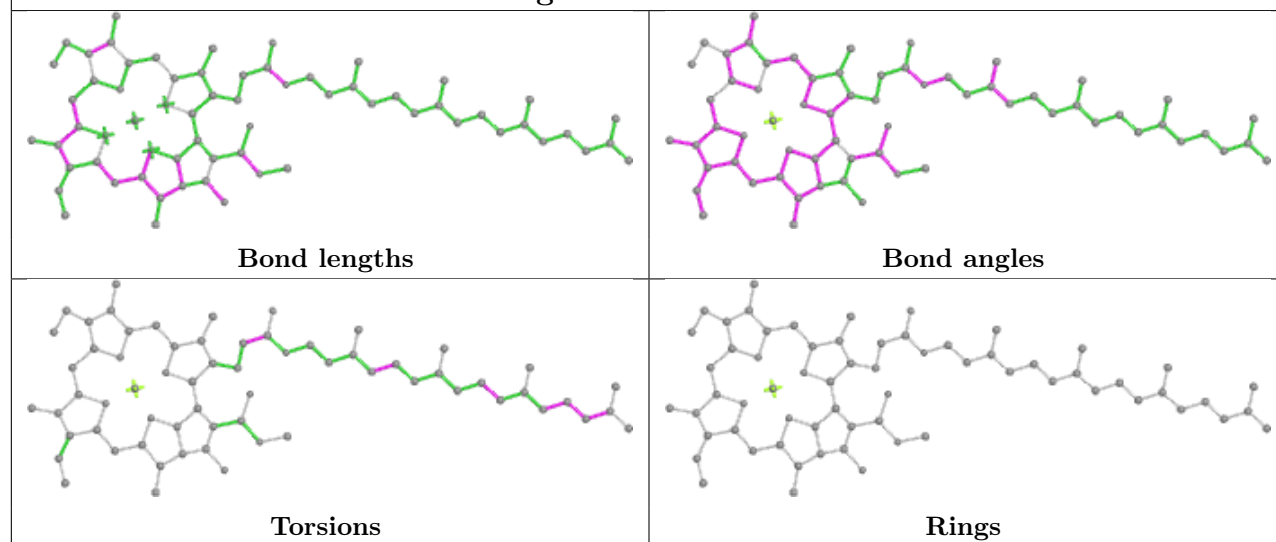


**Ligand LUT a 303****Ligand CLA A 816****Ligand CLA 2 307**

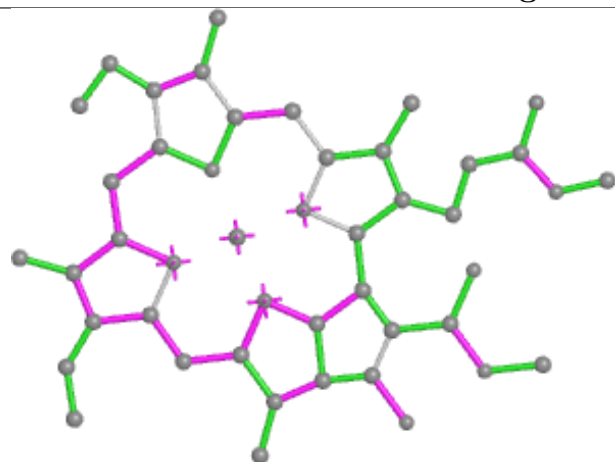
## Ligand CLA 4 305



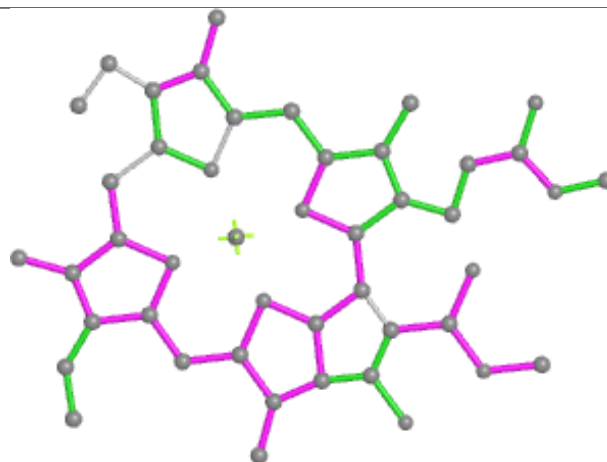
## Ligand CL0 A 813



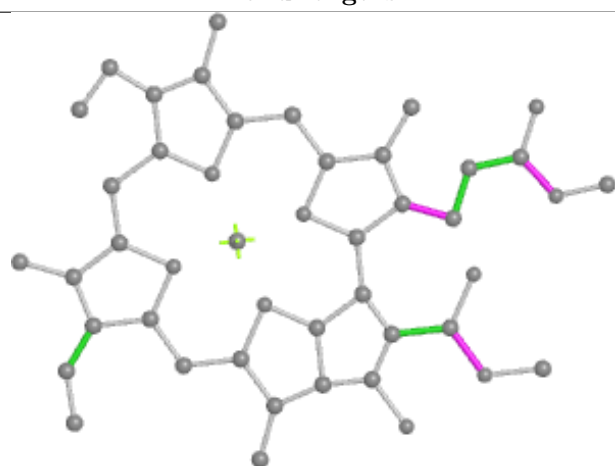
## Ligand CLA b 304



Bond lengths



Bond angles

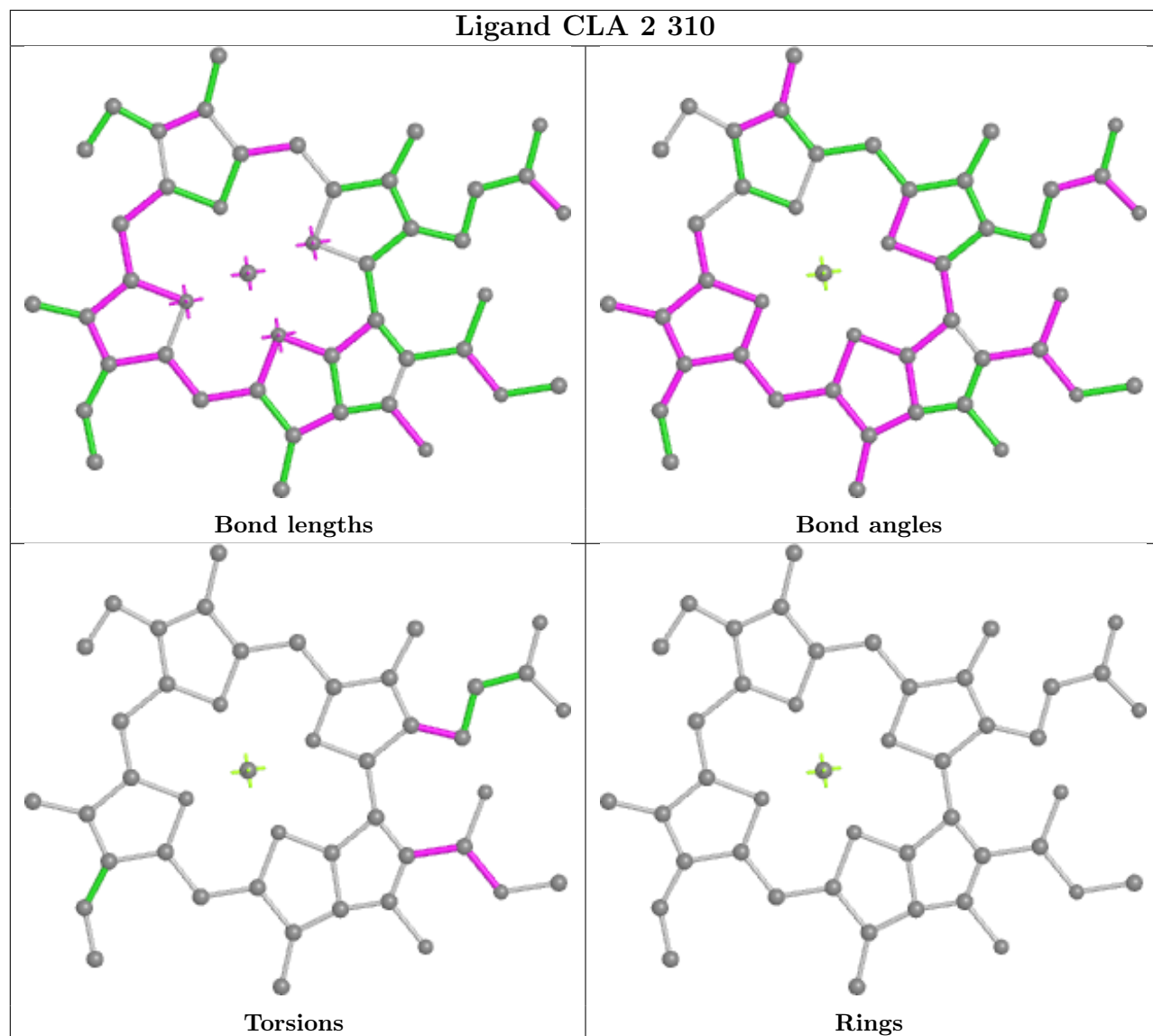


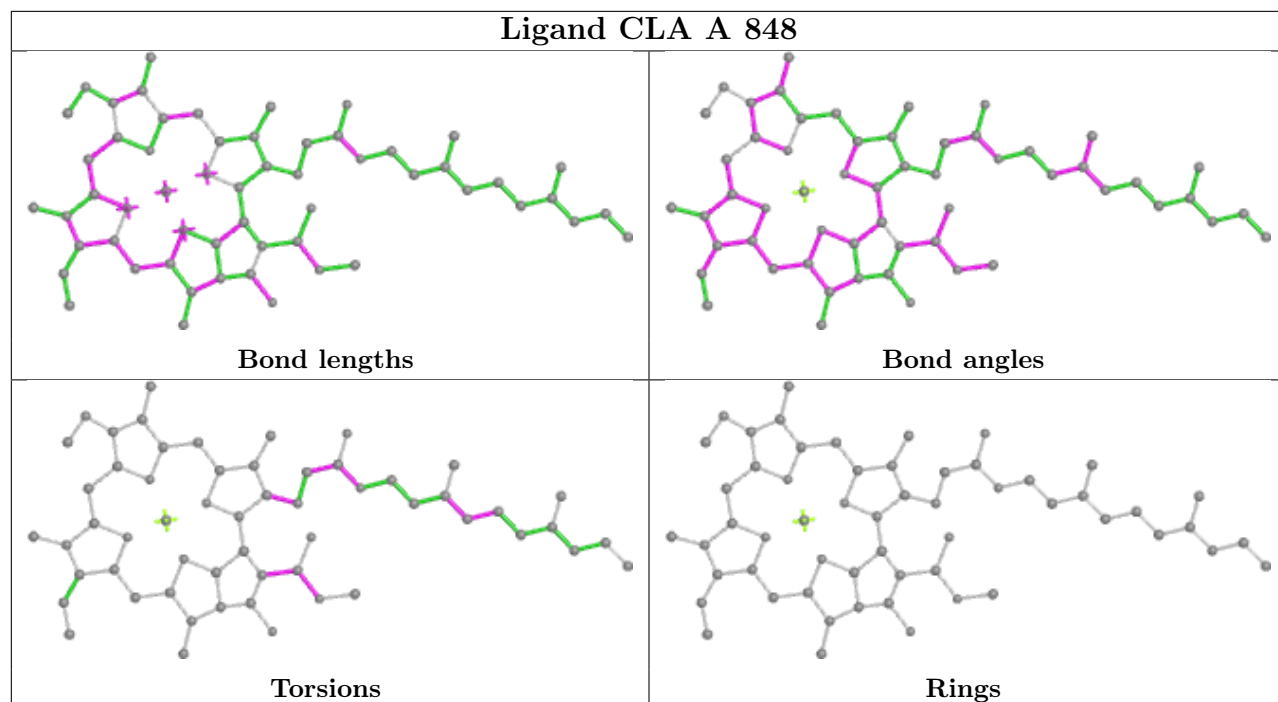
Torsions



Rings

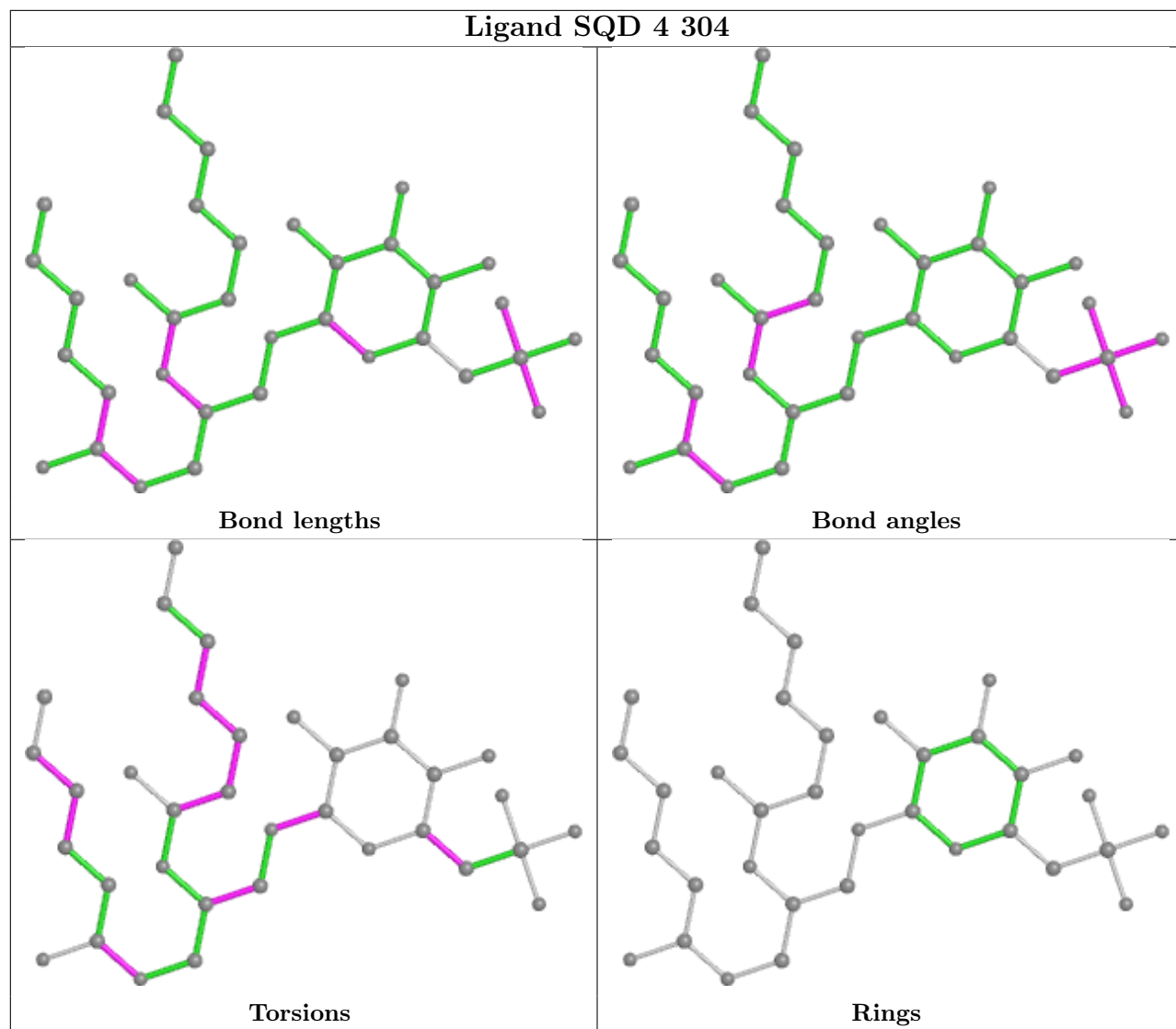
## Ligand CLA 2 310



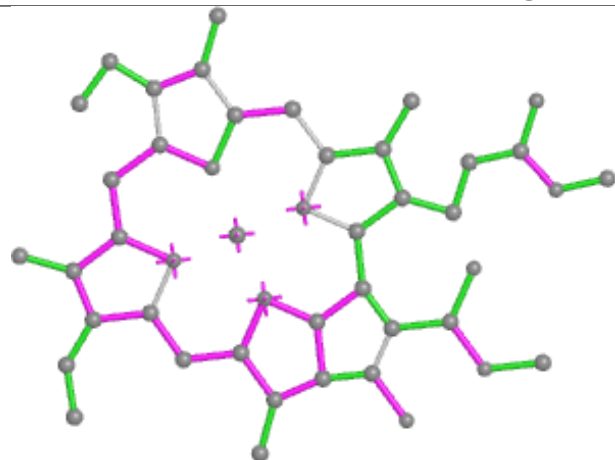




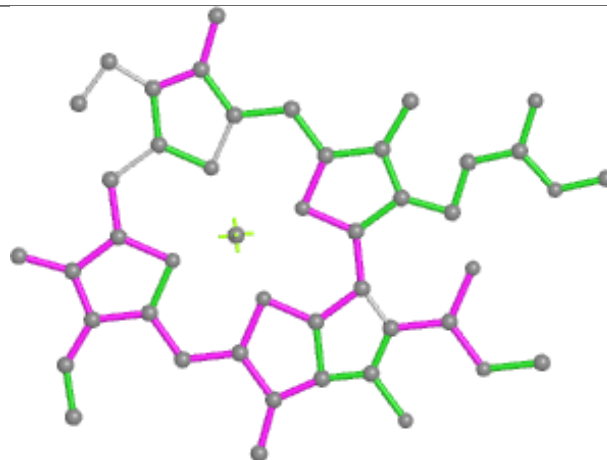
## Ligand SQD 4 304



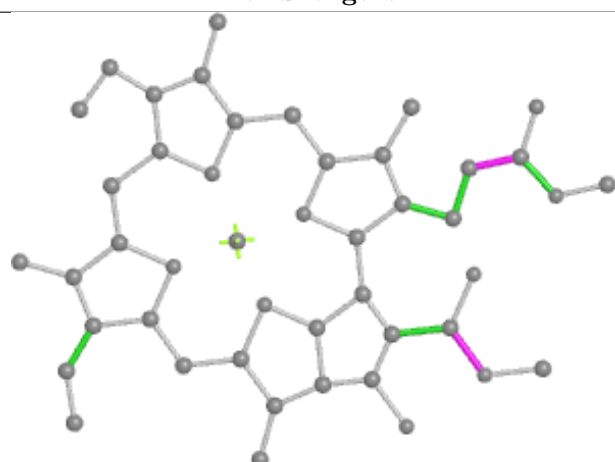
## Ligand CLA 5 313



Bond lengths



Bond angles

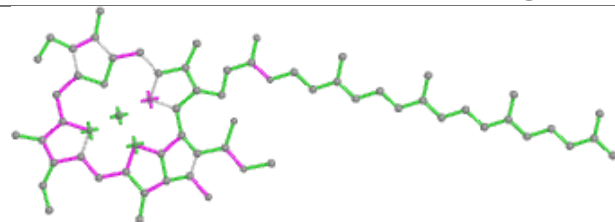


Torsions

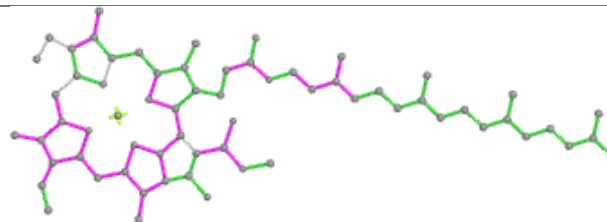


Rings

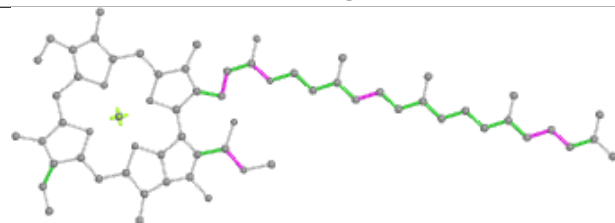
## Ligand CLA 9 318



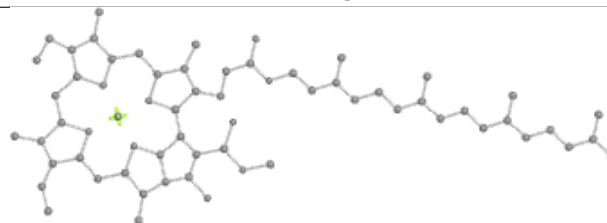
Bond lengths



Bond angles

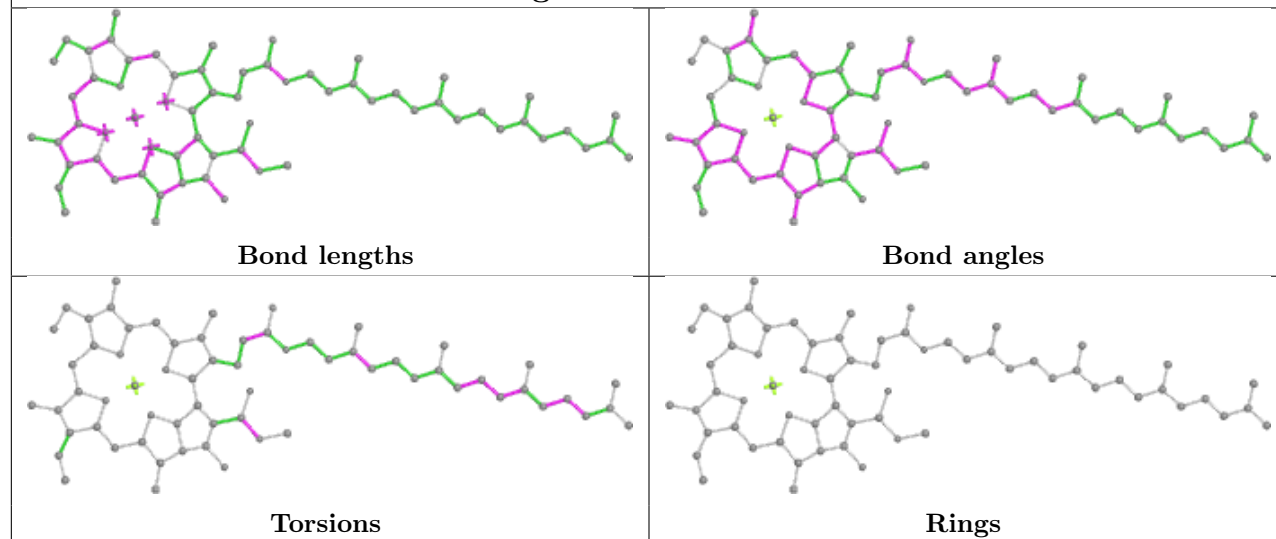


Torsions

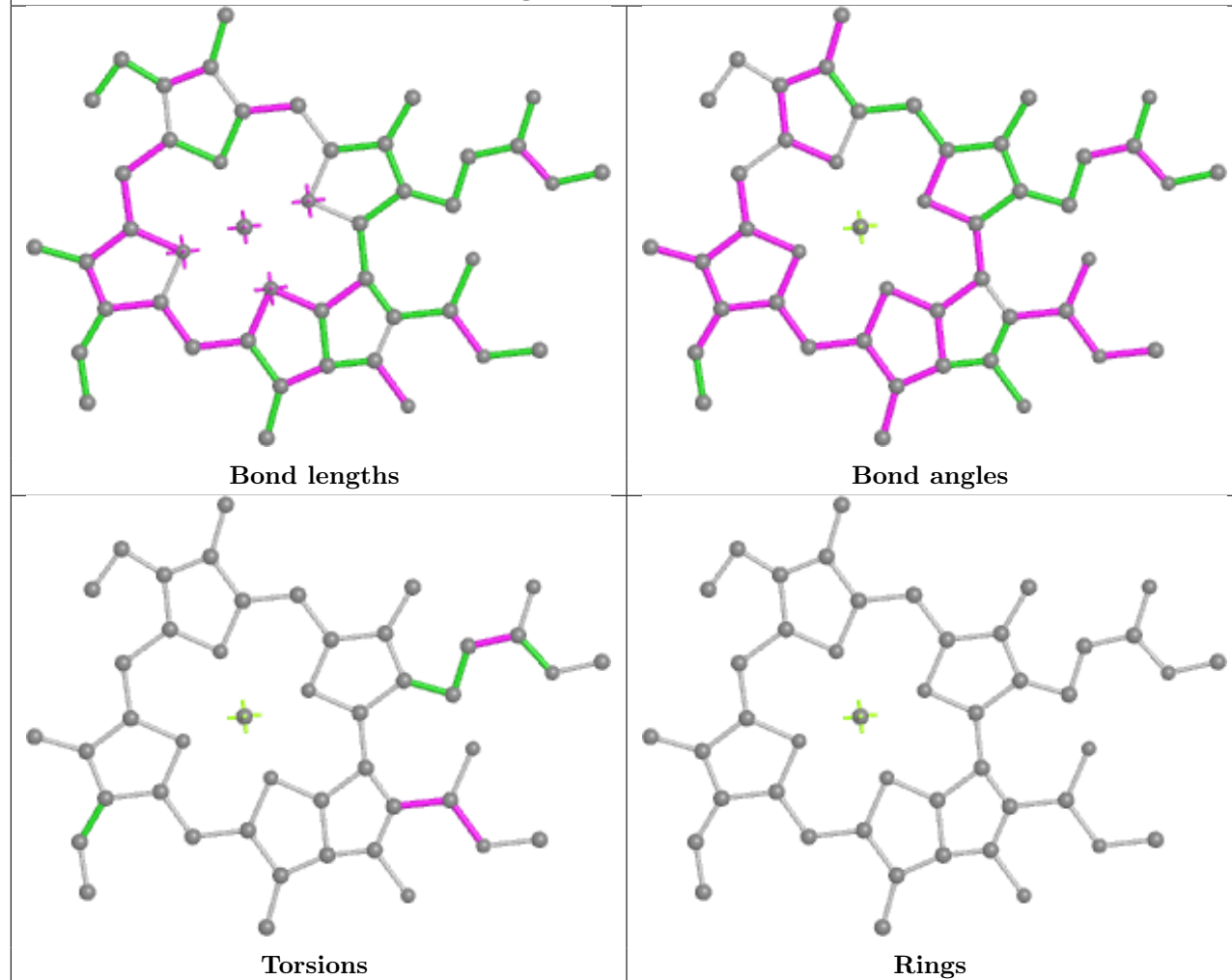


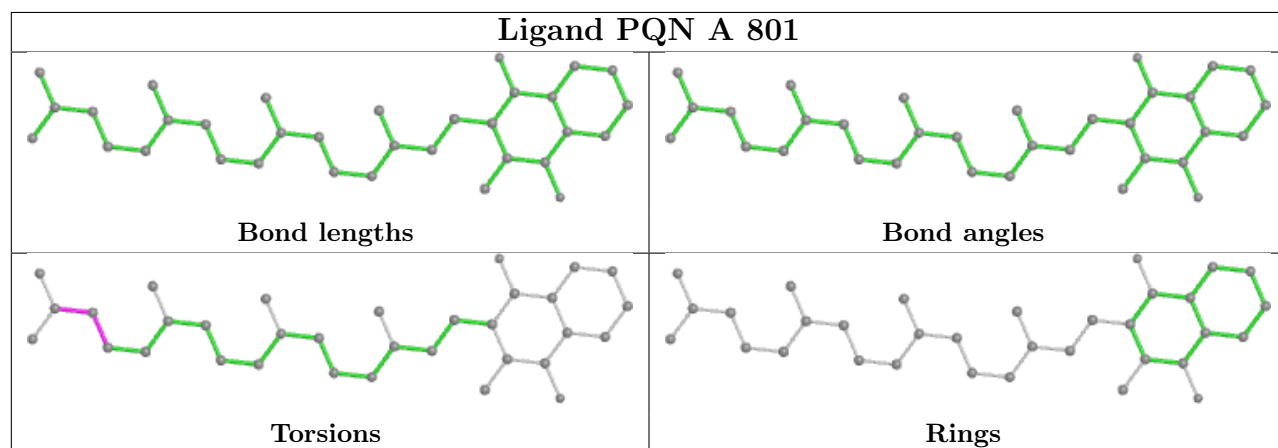
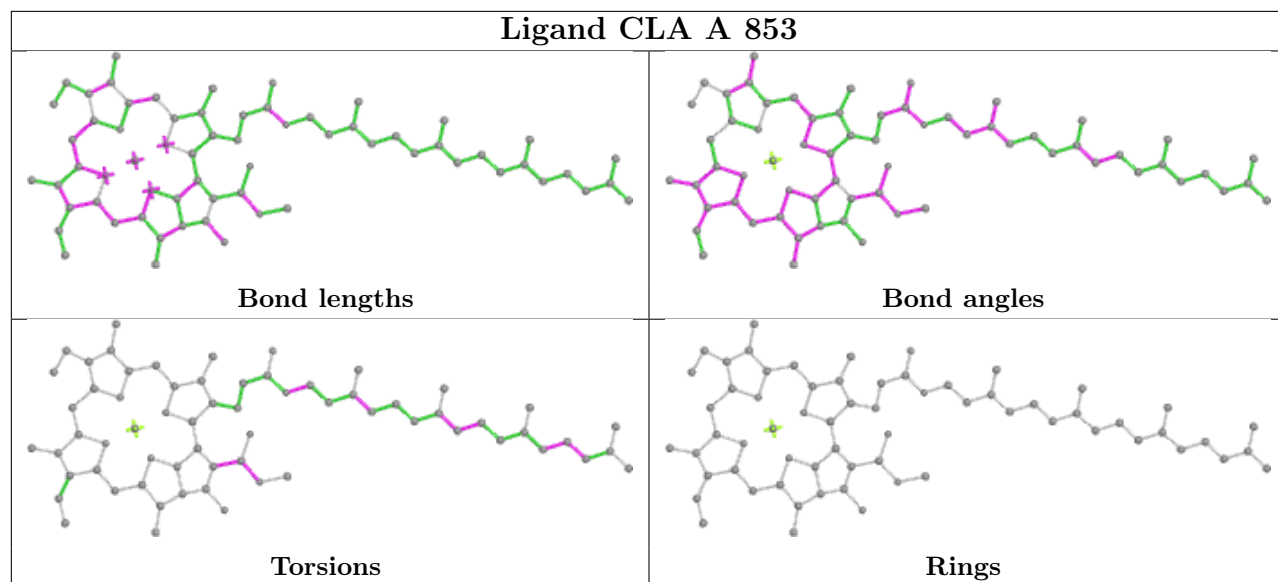
Rings

## Ligand CLA B 840

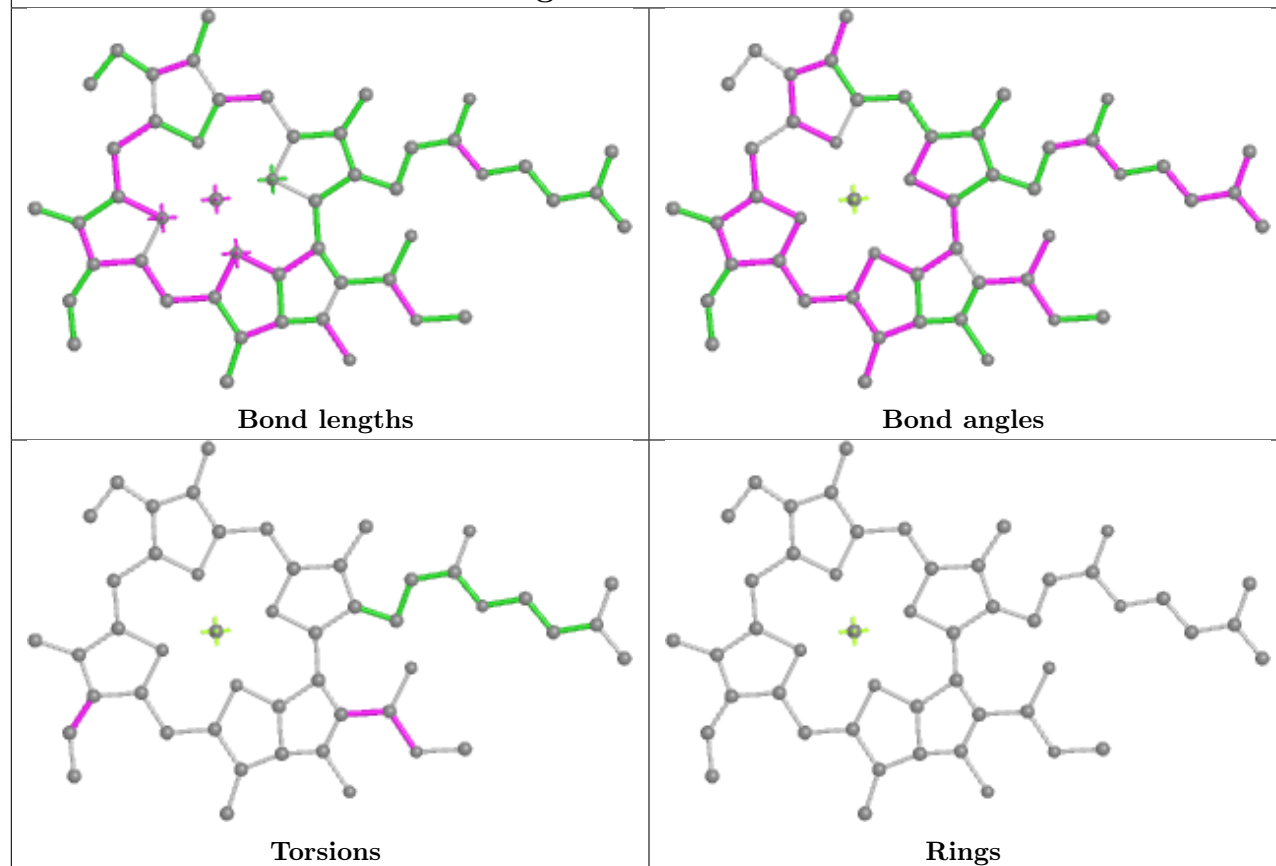


## Ligand CLA 6 313

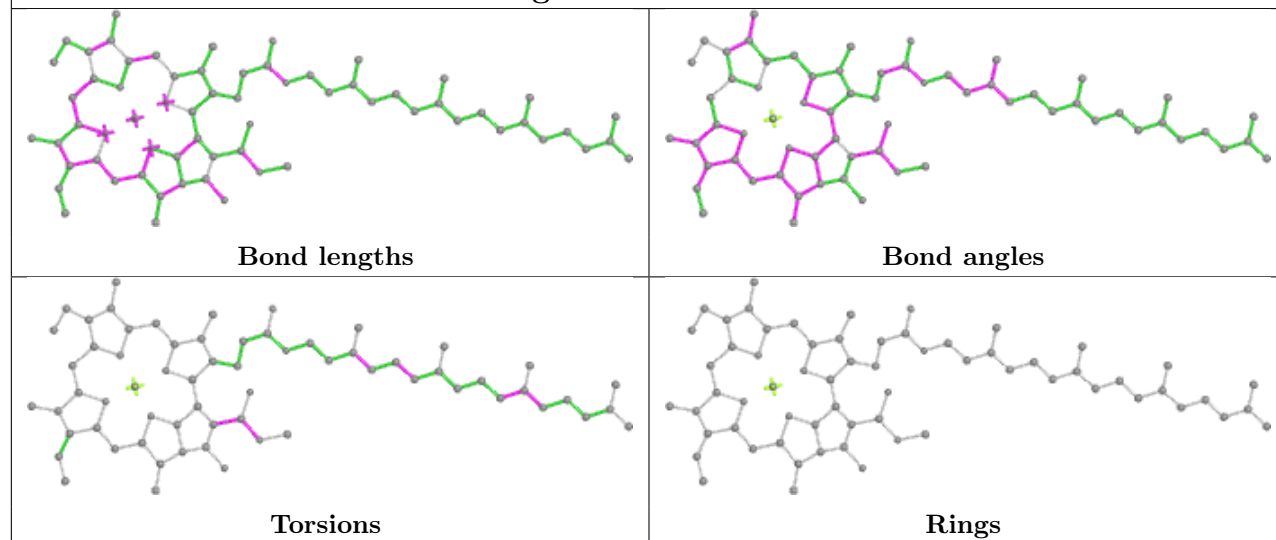




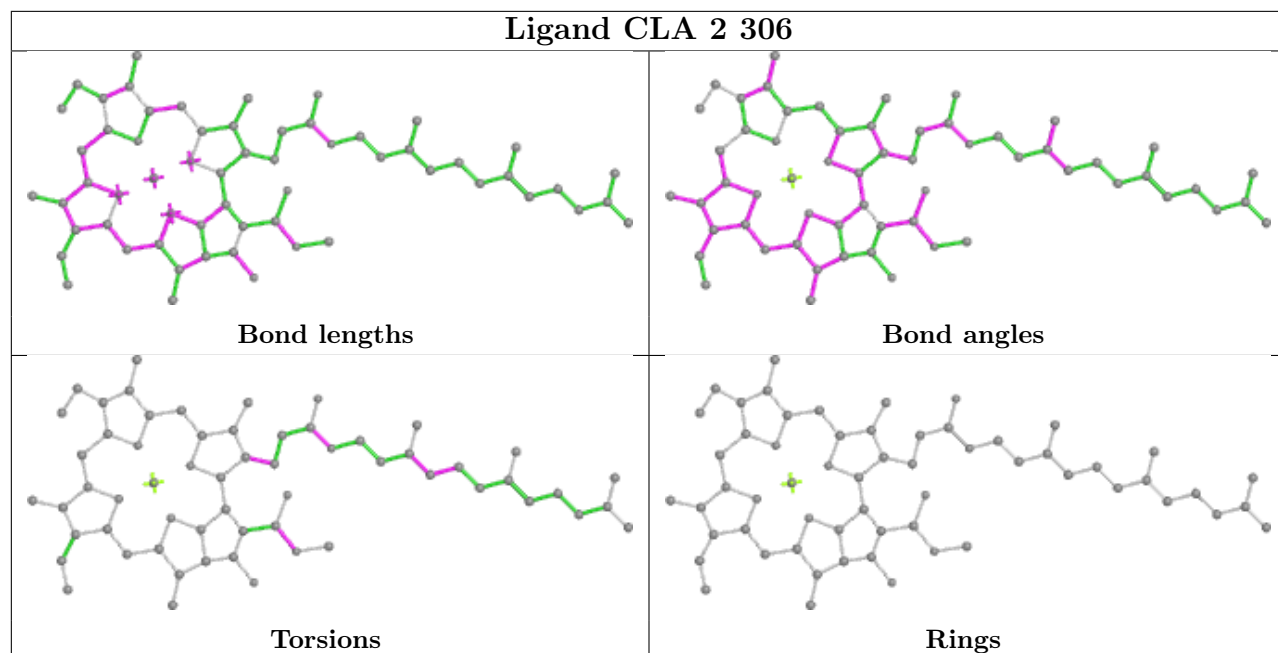
## Ligand CLA 9 316



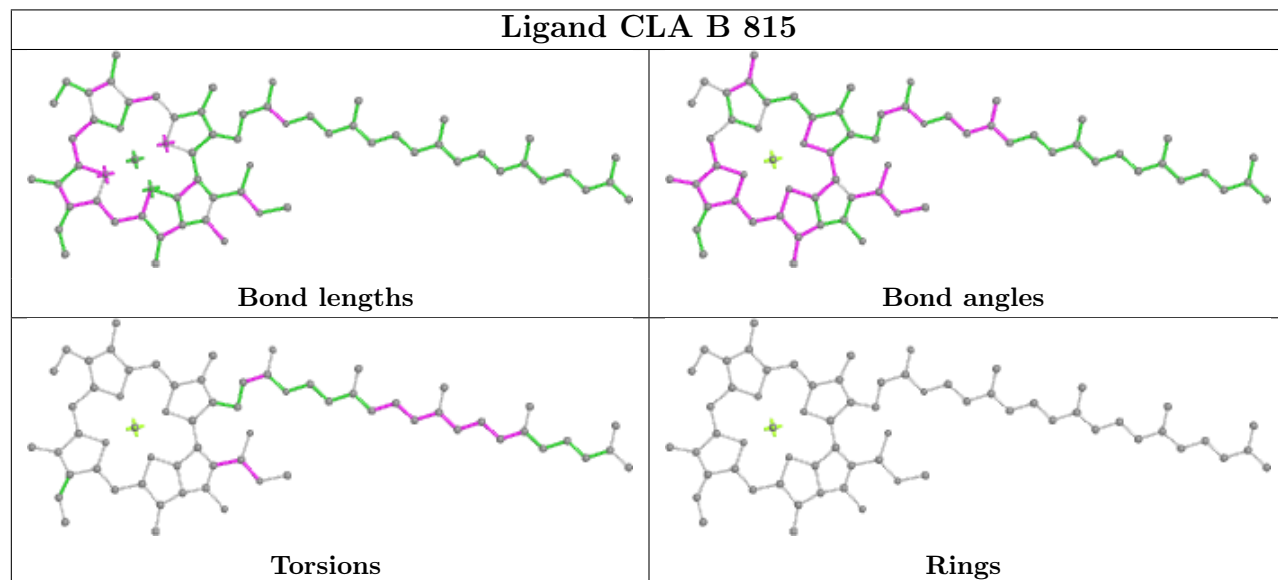
## Ligand CLA B 844



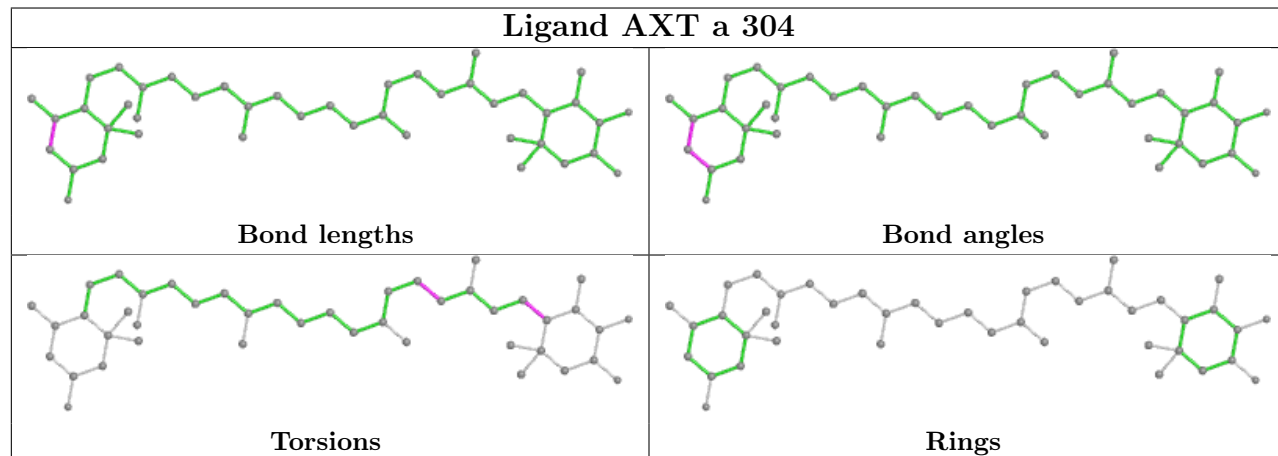
## Ligand CLA 2 306



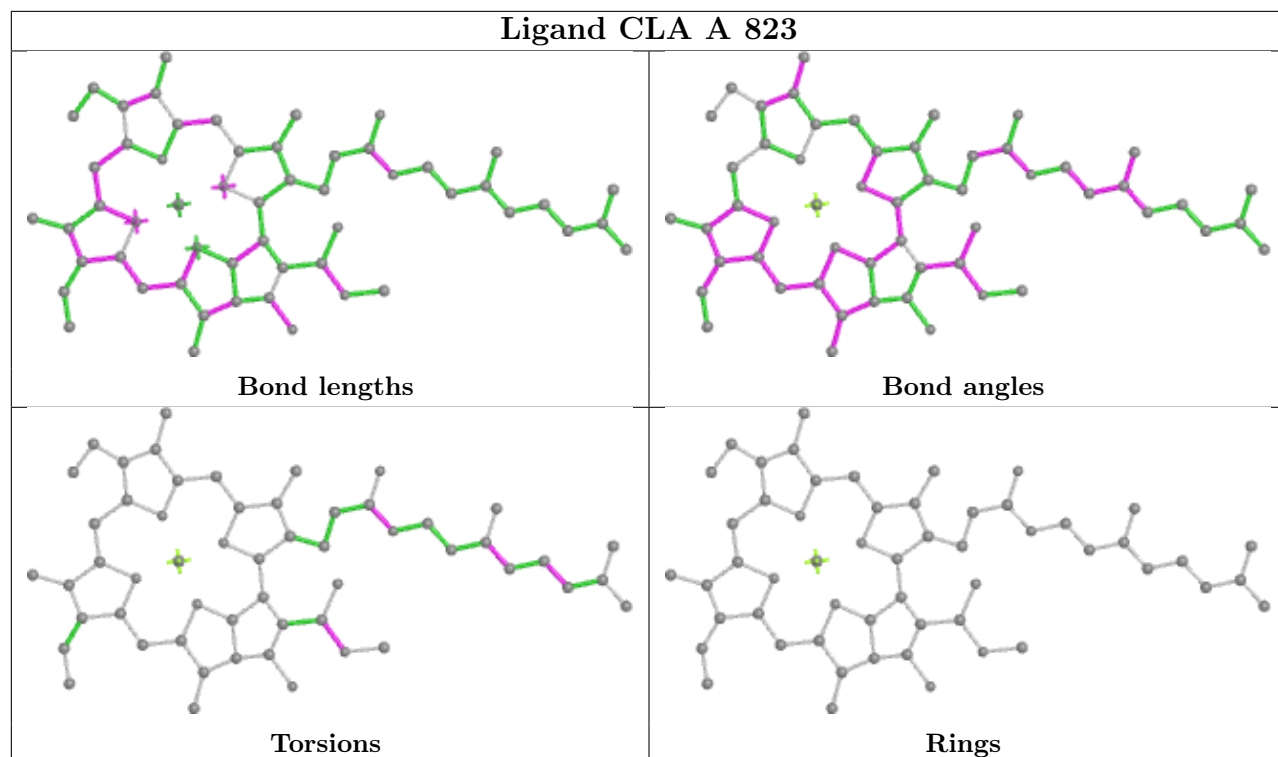
## Ligand CLA B 815



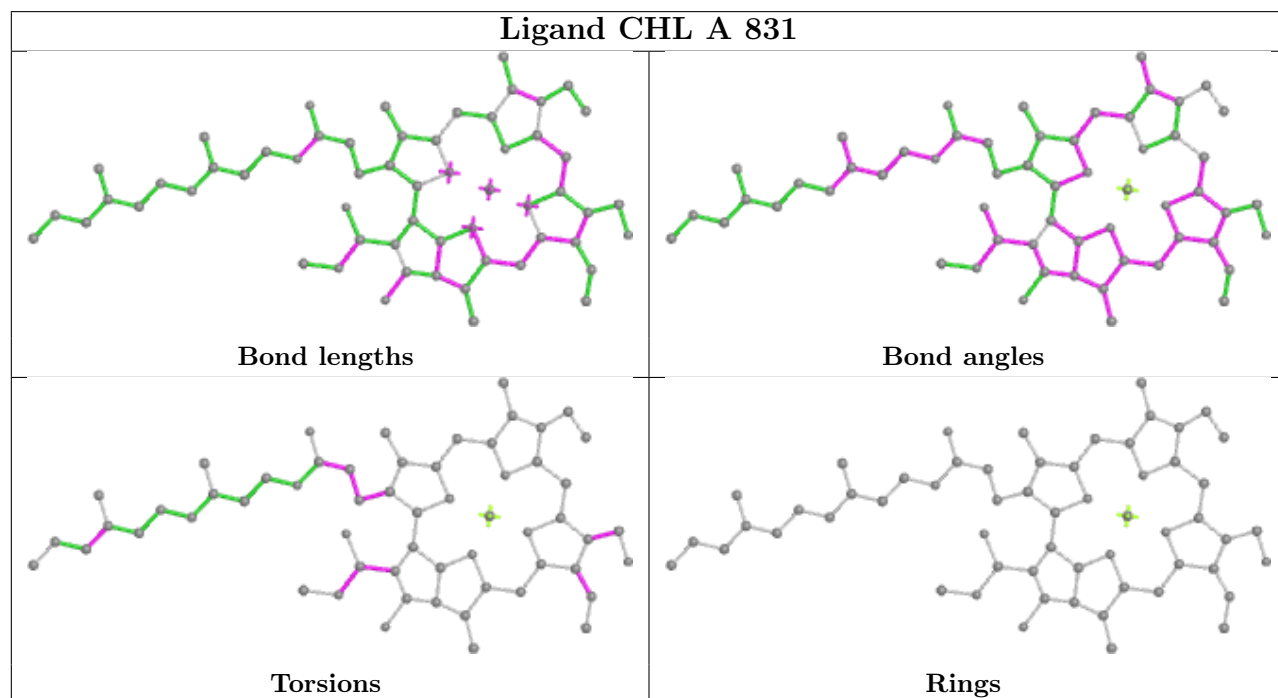
## Ligand AXT a 304

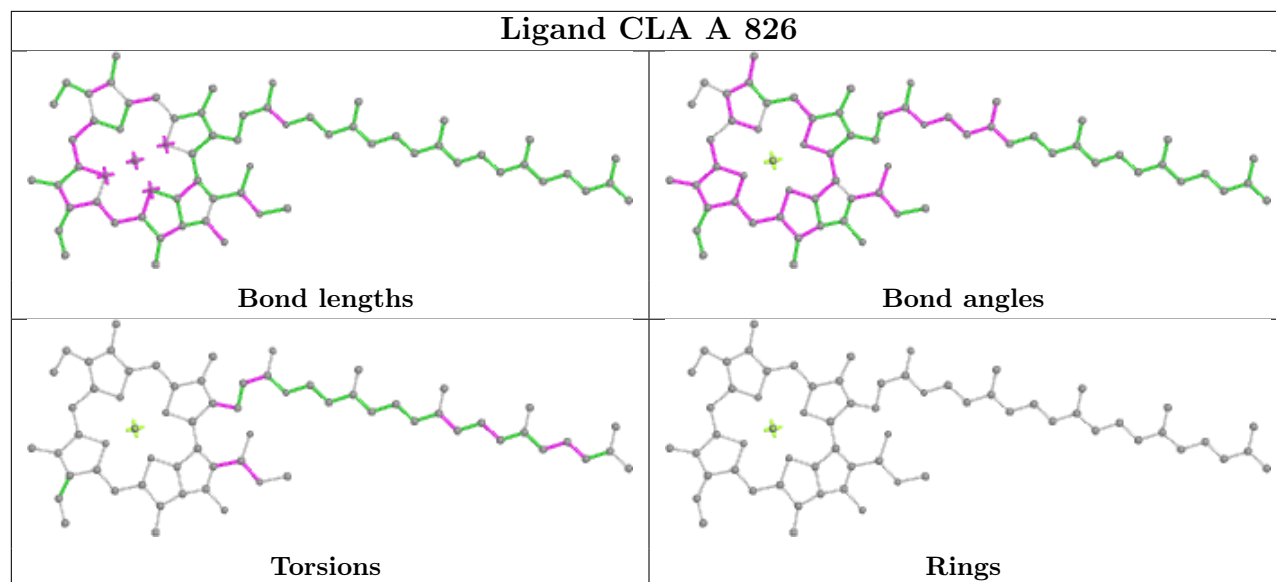
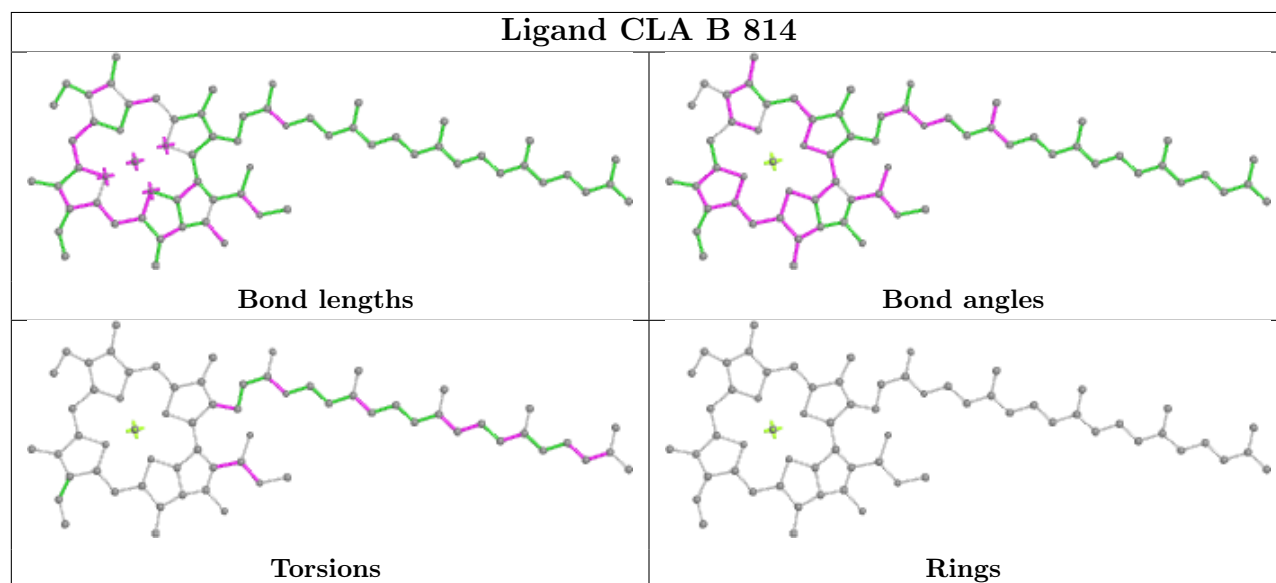


## Ligand CLA A 823



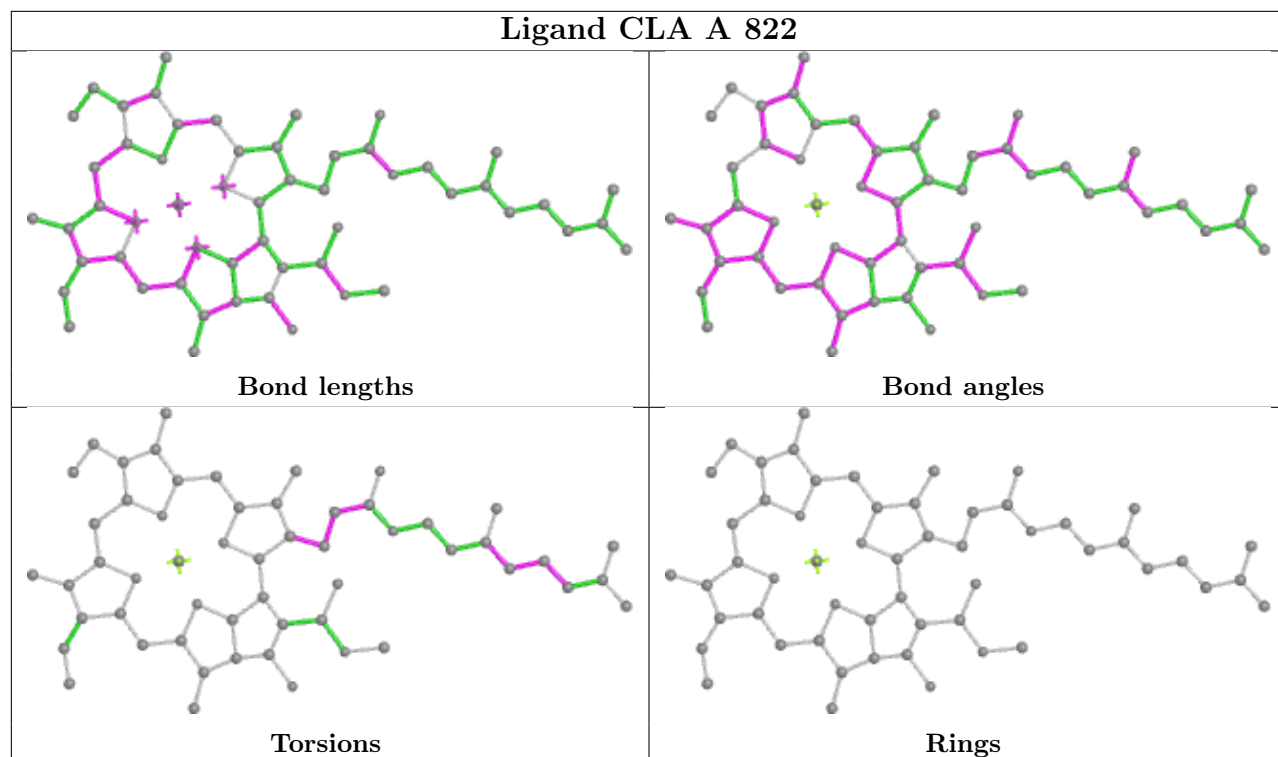
## Ligand CHL A 831



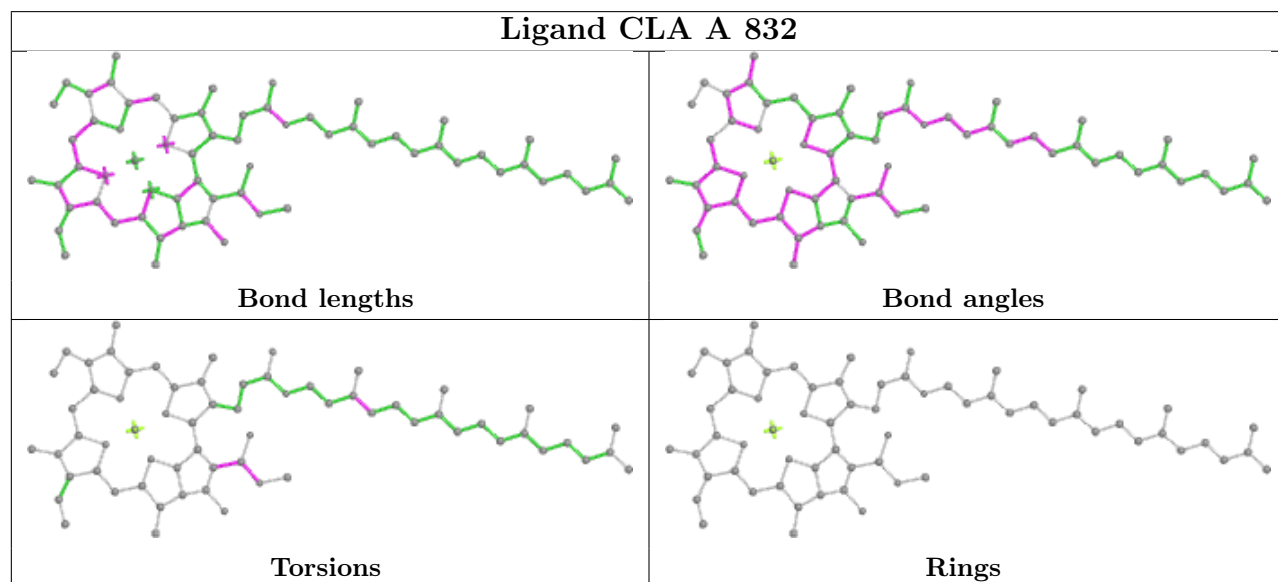
**Ligand CLA A 826****Ligand CLA B 814**



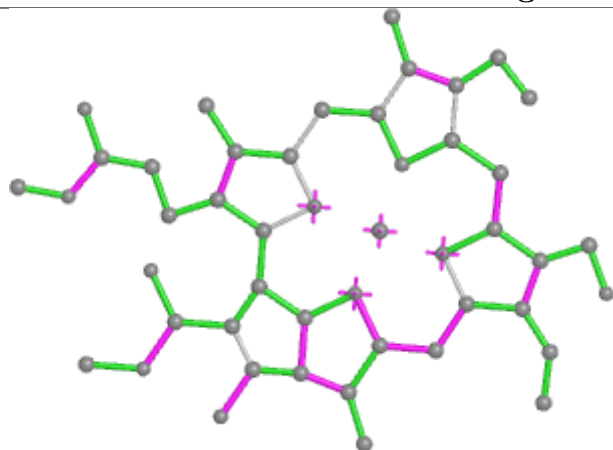
## Ligand CLA A 822



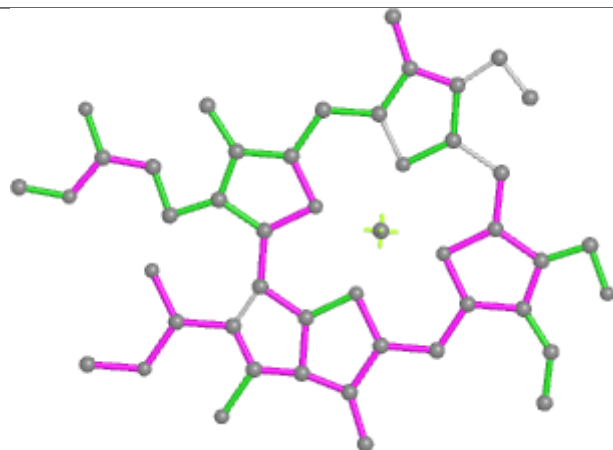
## Ligand CLA A 832



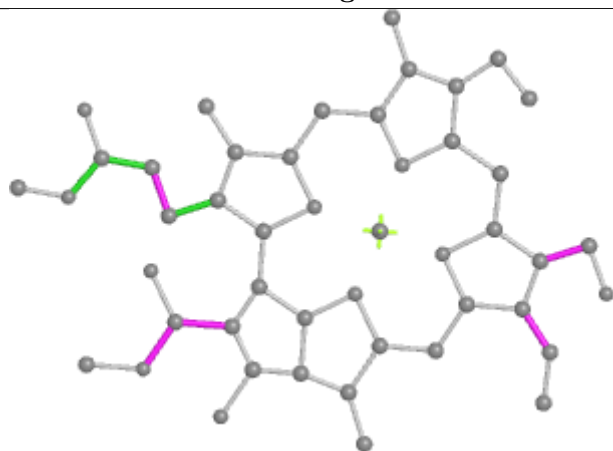
## Ligand CHL 6 320



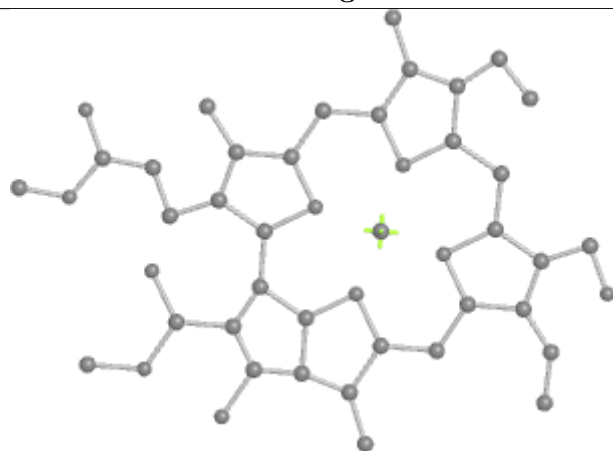
Bond lengths



Bond angles

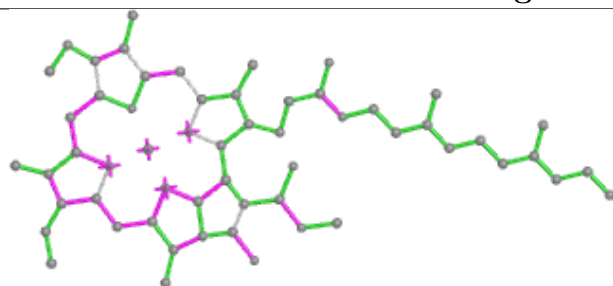


Torsions

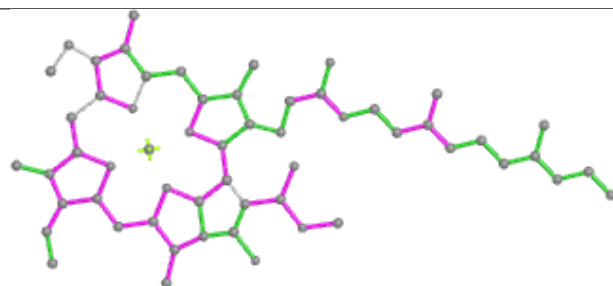


Rings

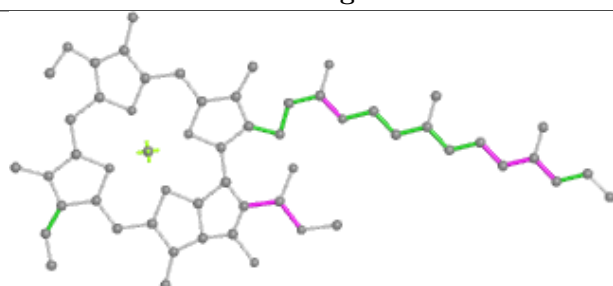
## Ligand CLA B 824



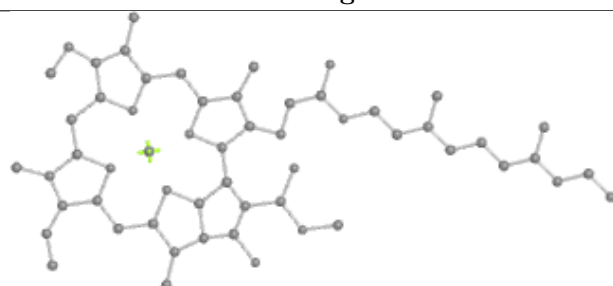
Bond lengths



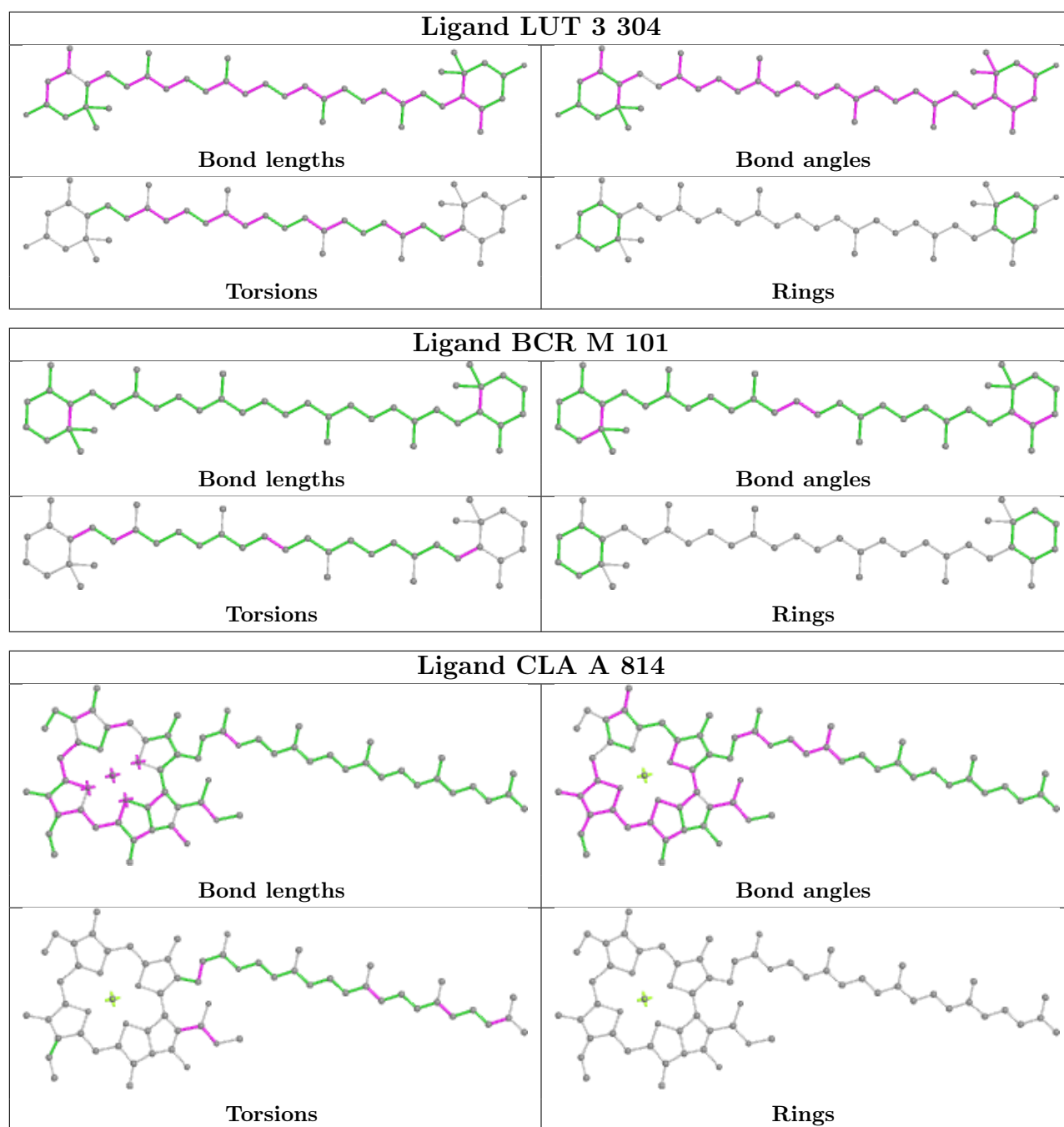
Bond angles



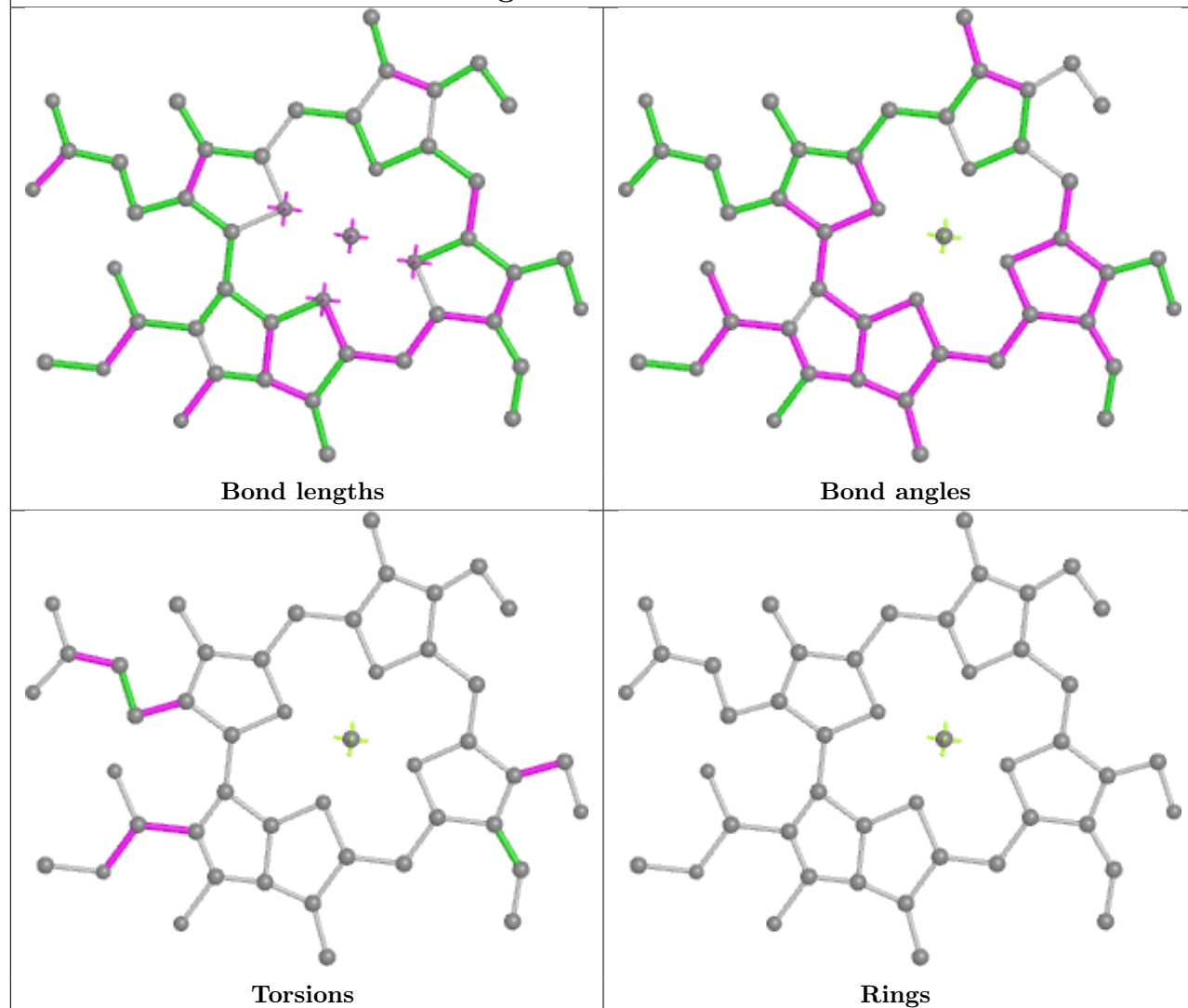
Torsions



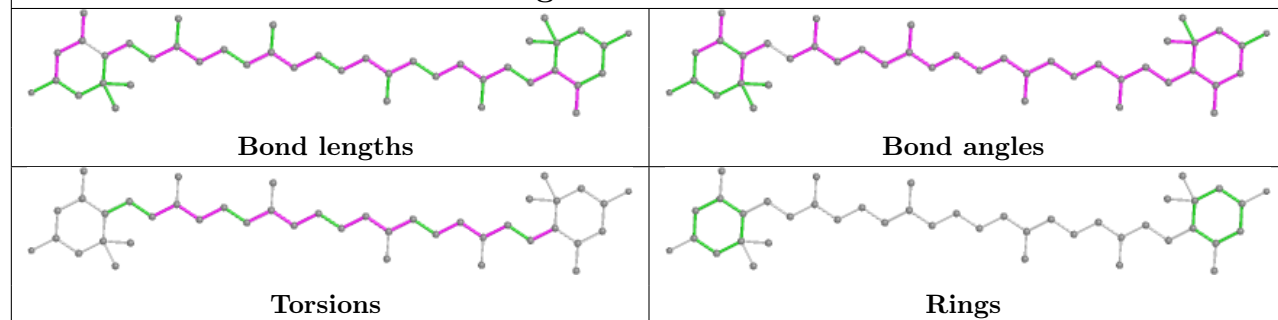
Rings



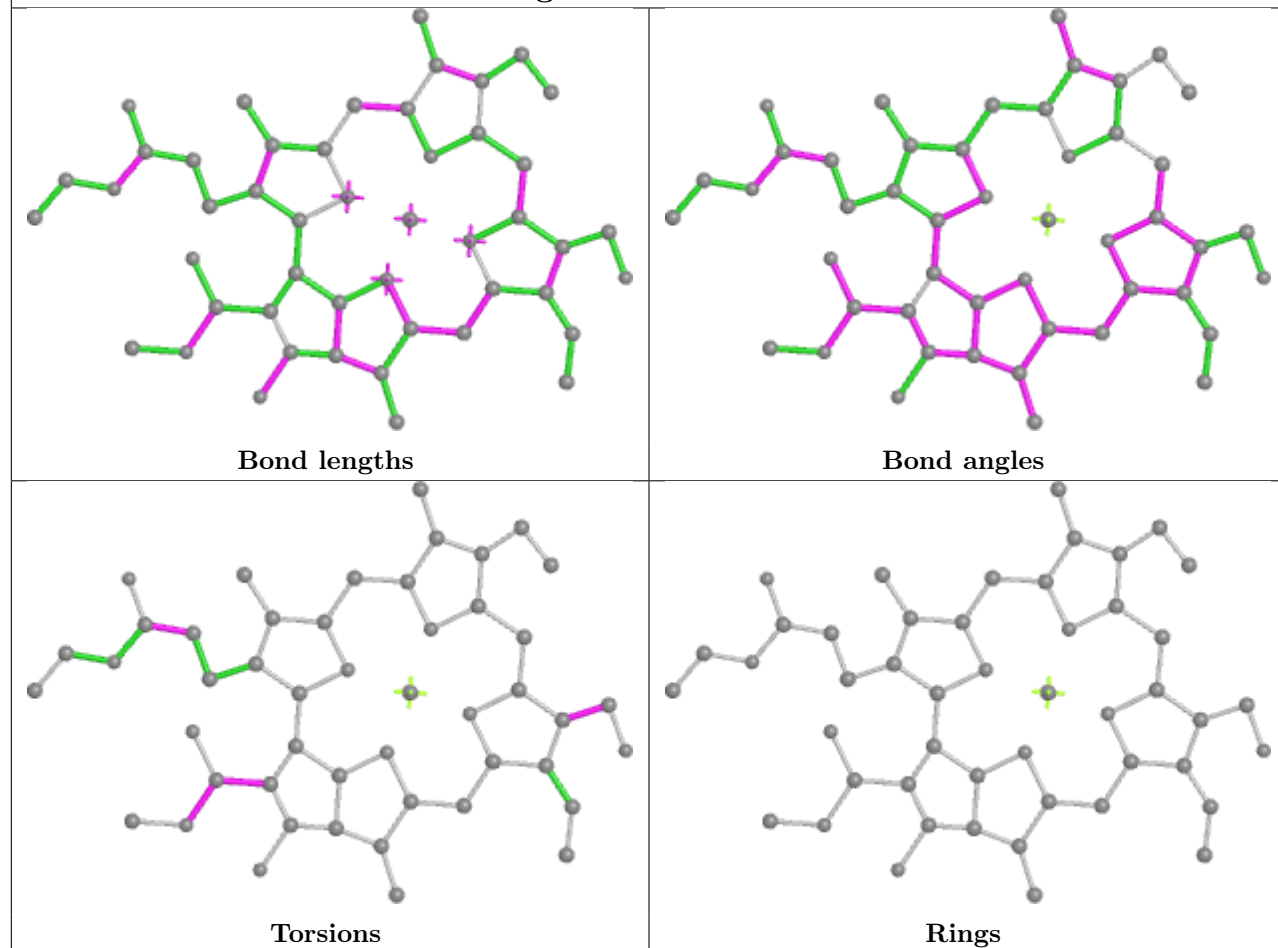
## Ligand CHL 6 318



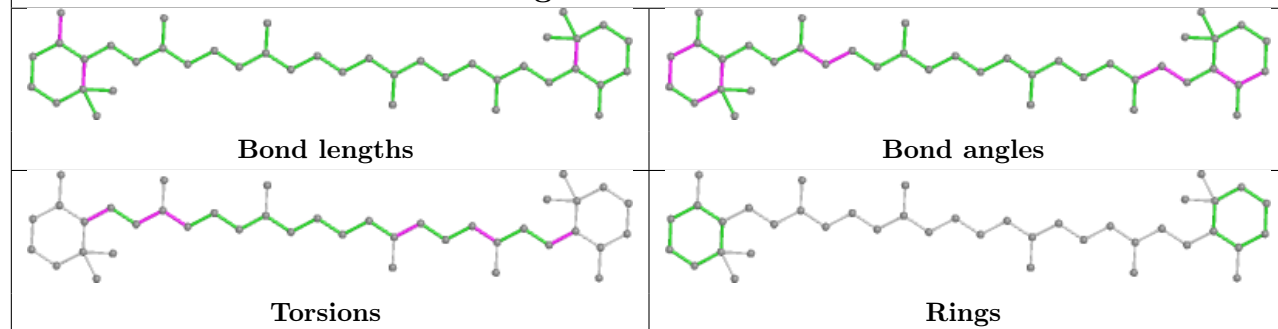
## Ligand LUT 8 302



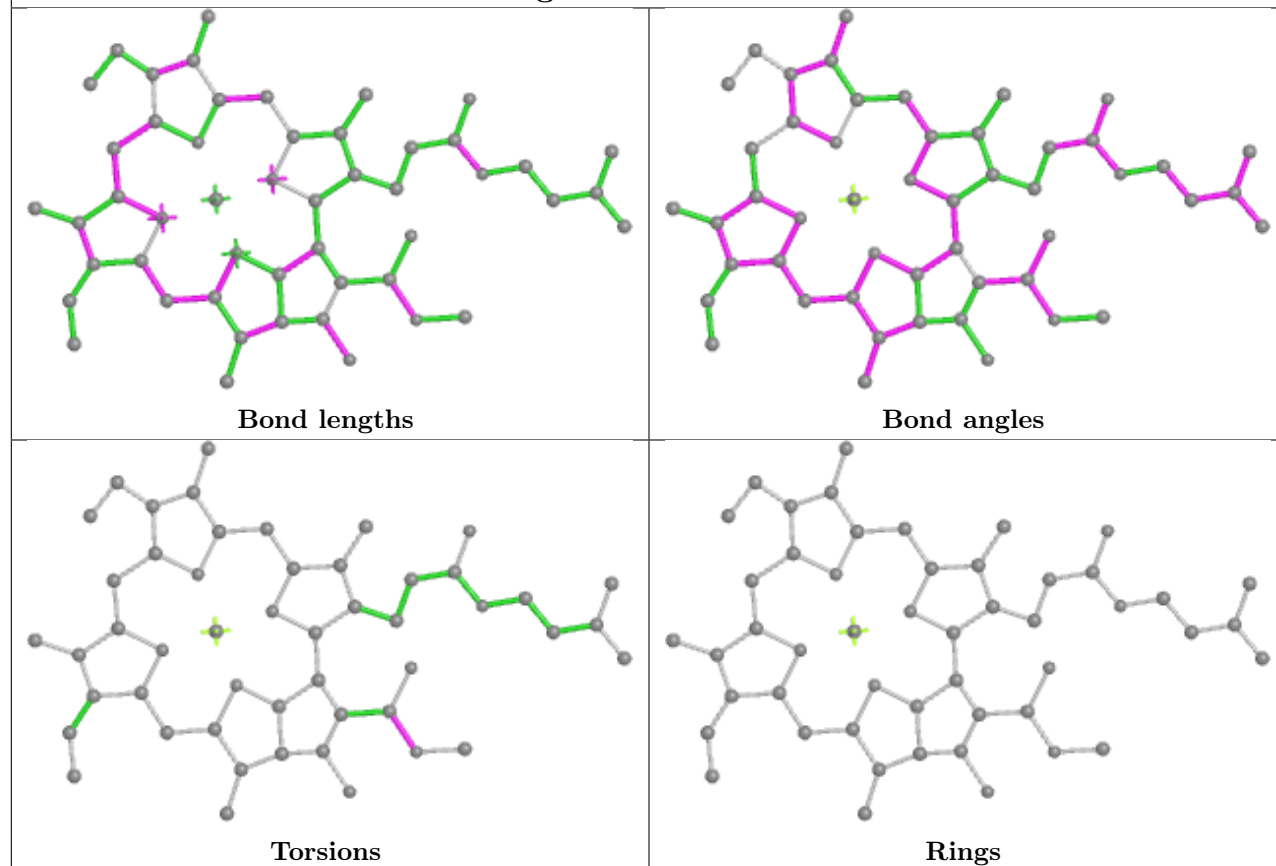
## Ligand CHL a 320



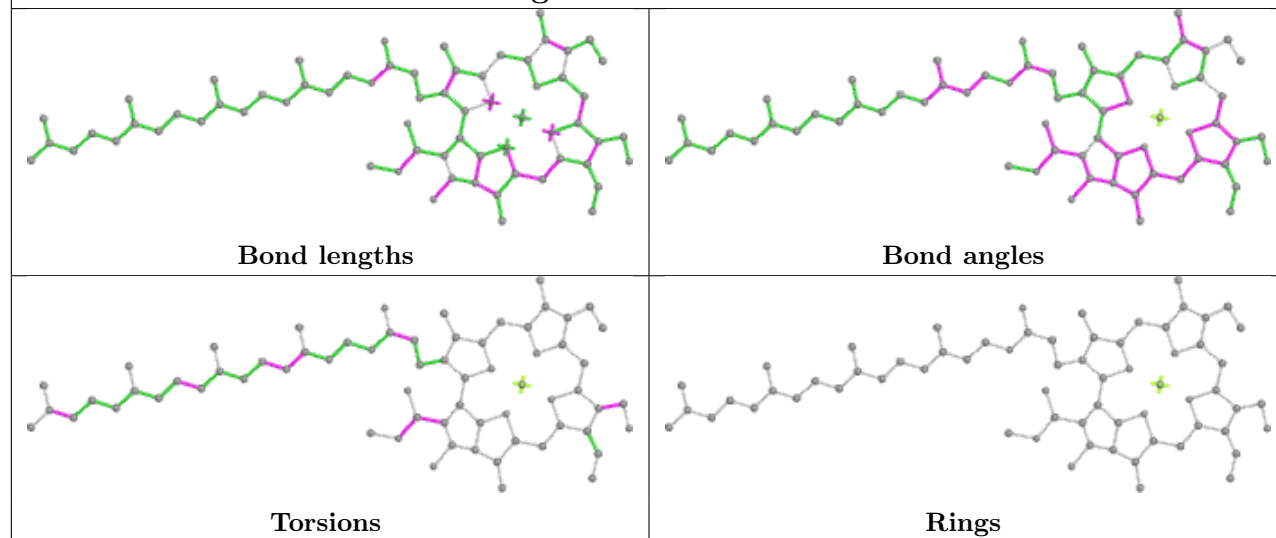
## Ligand BCR 3 303



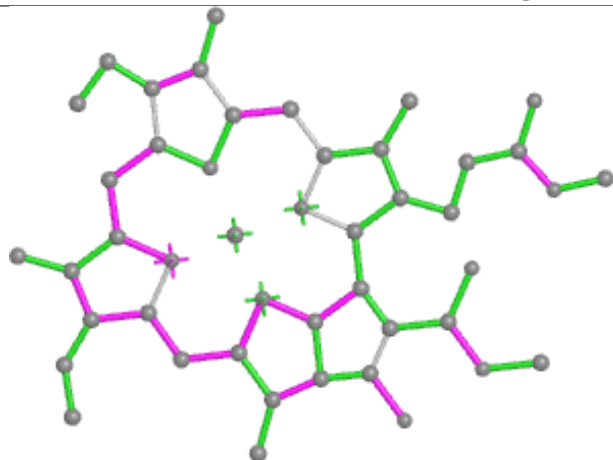
## Ligand CLA 8 317



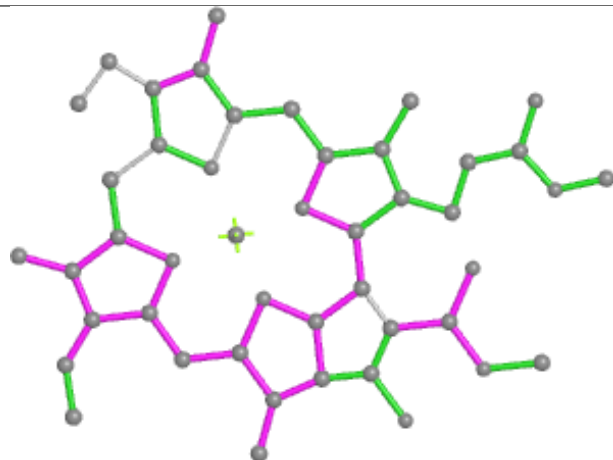
## Ligand CHL A 840



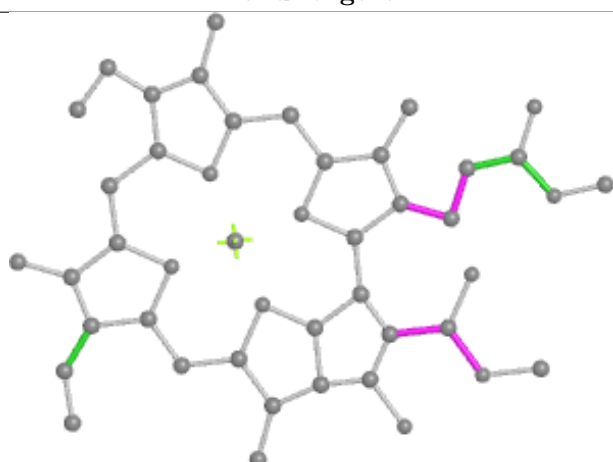
## Ligand CLA b 310



Bond lengths



Bond angles

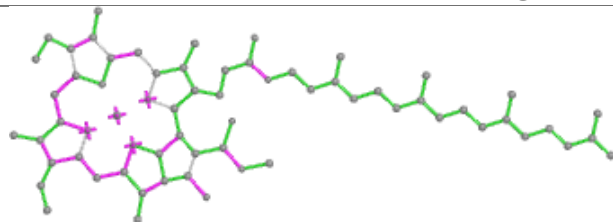


Torsions

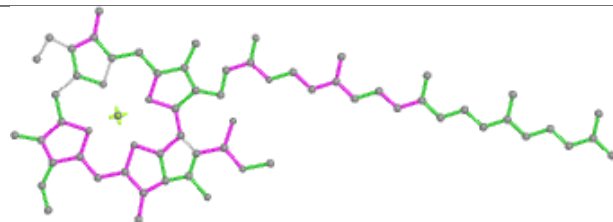


Rings

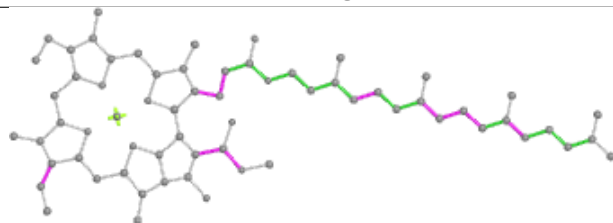
## Ligand CLA B 822



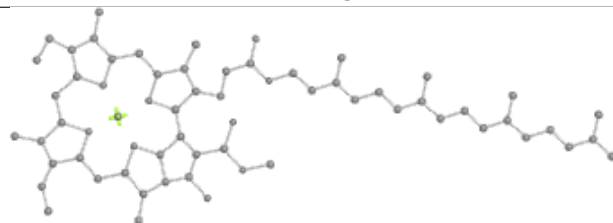
Bond lengths



Bond angles

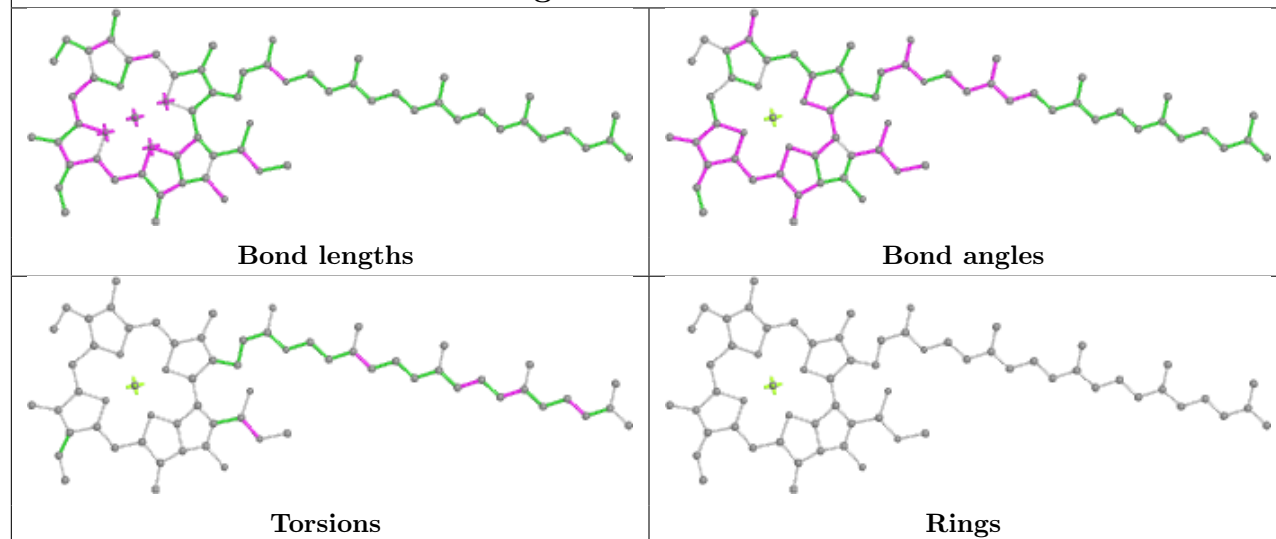


Torsions

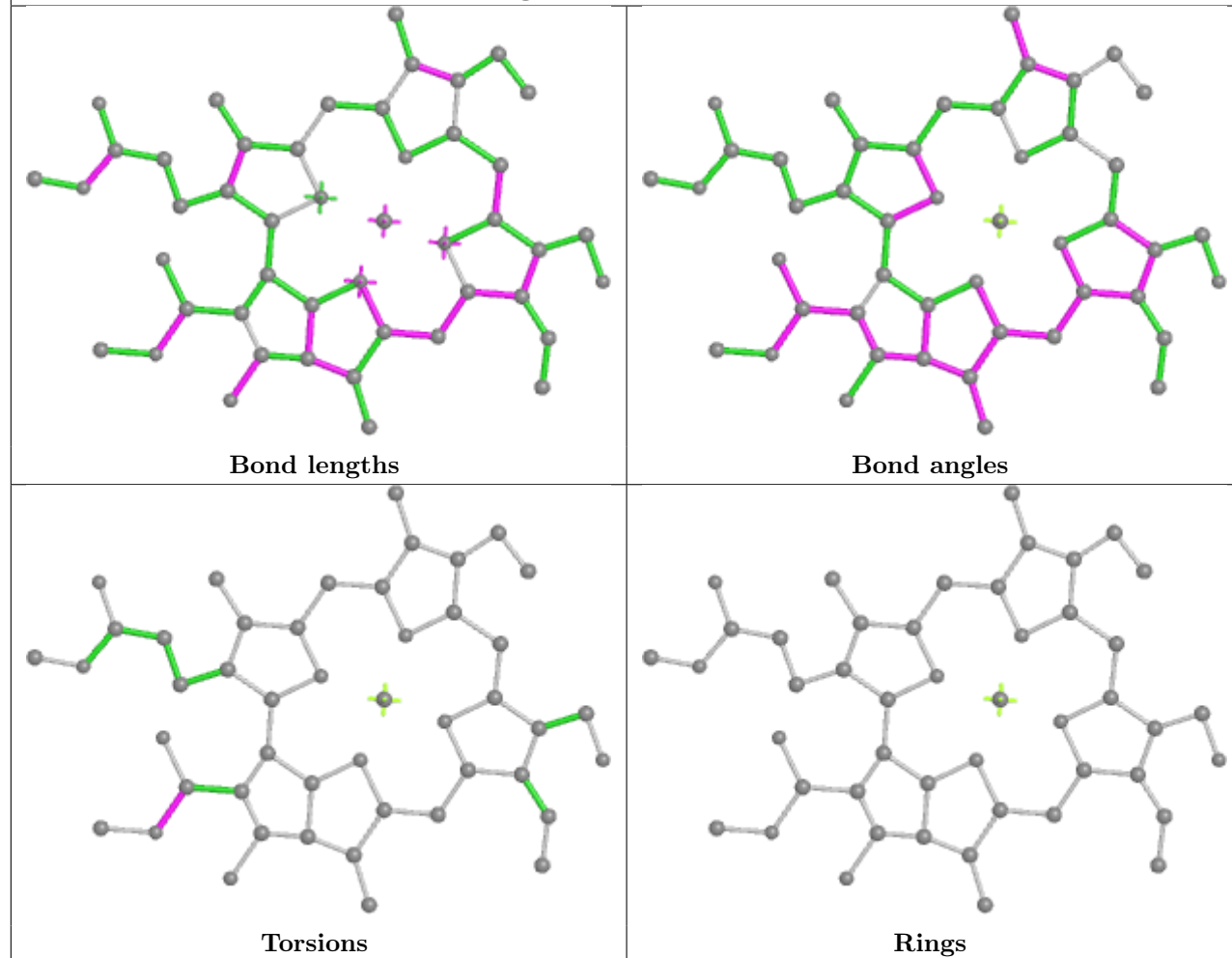


Rings

## Ligand CLA F 301

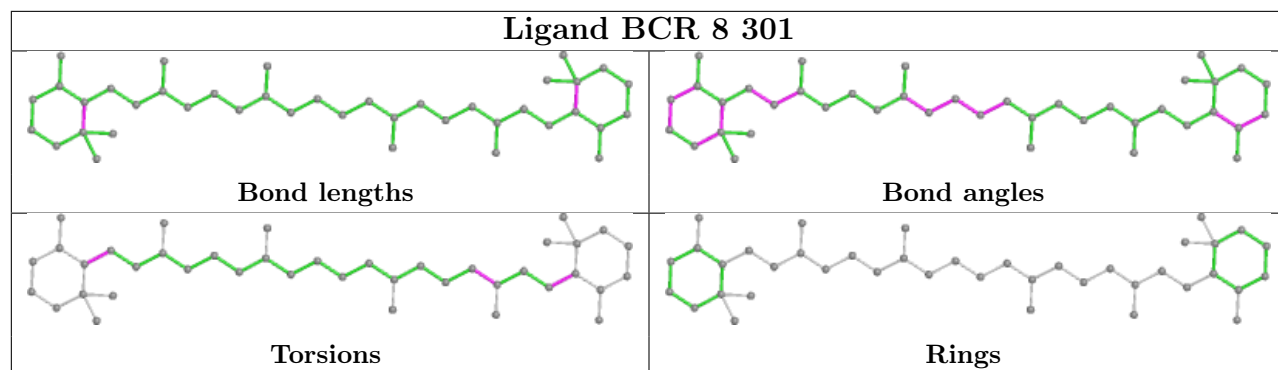


## Ligand CHL 7 319

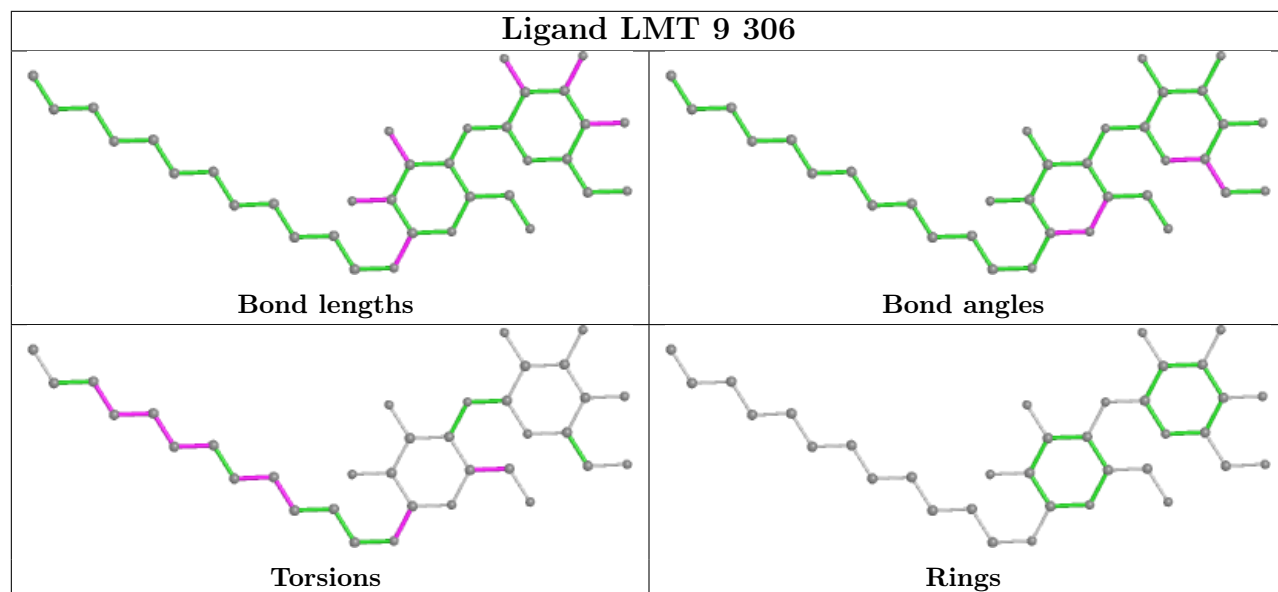




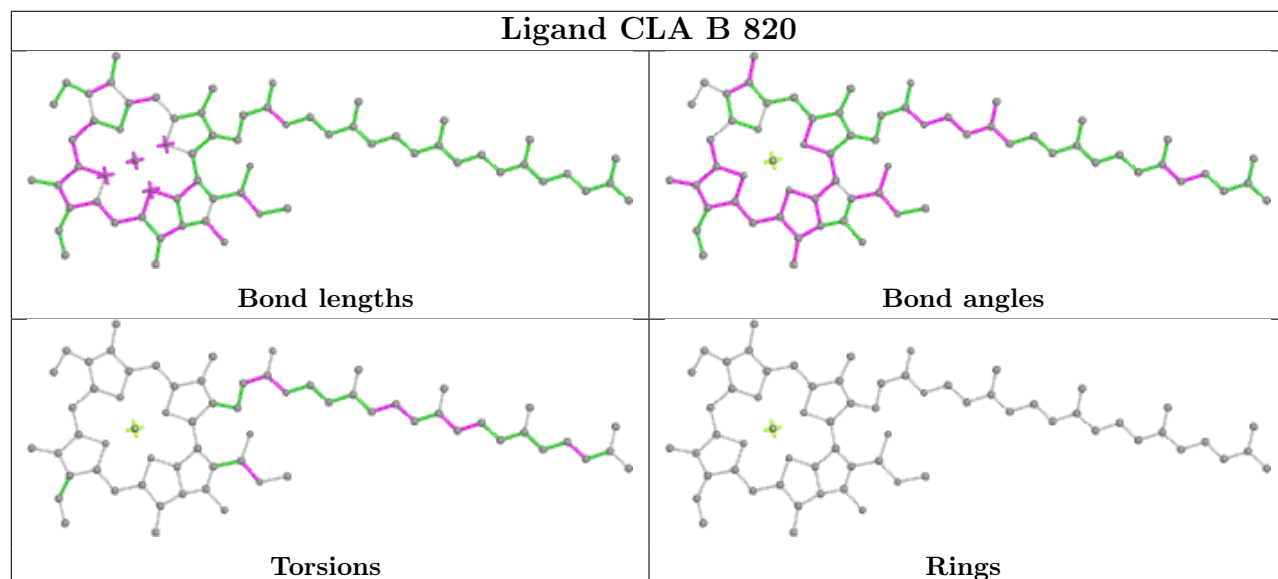
## Ligand BCR 8 301



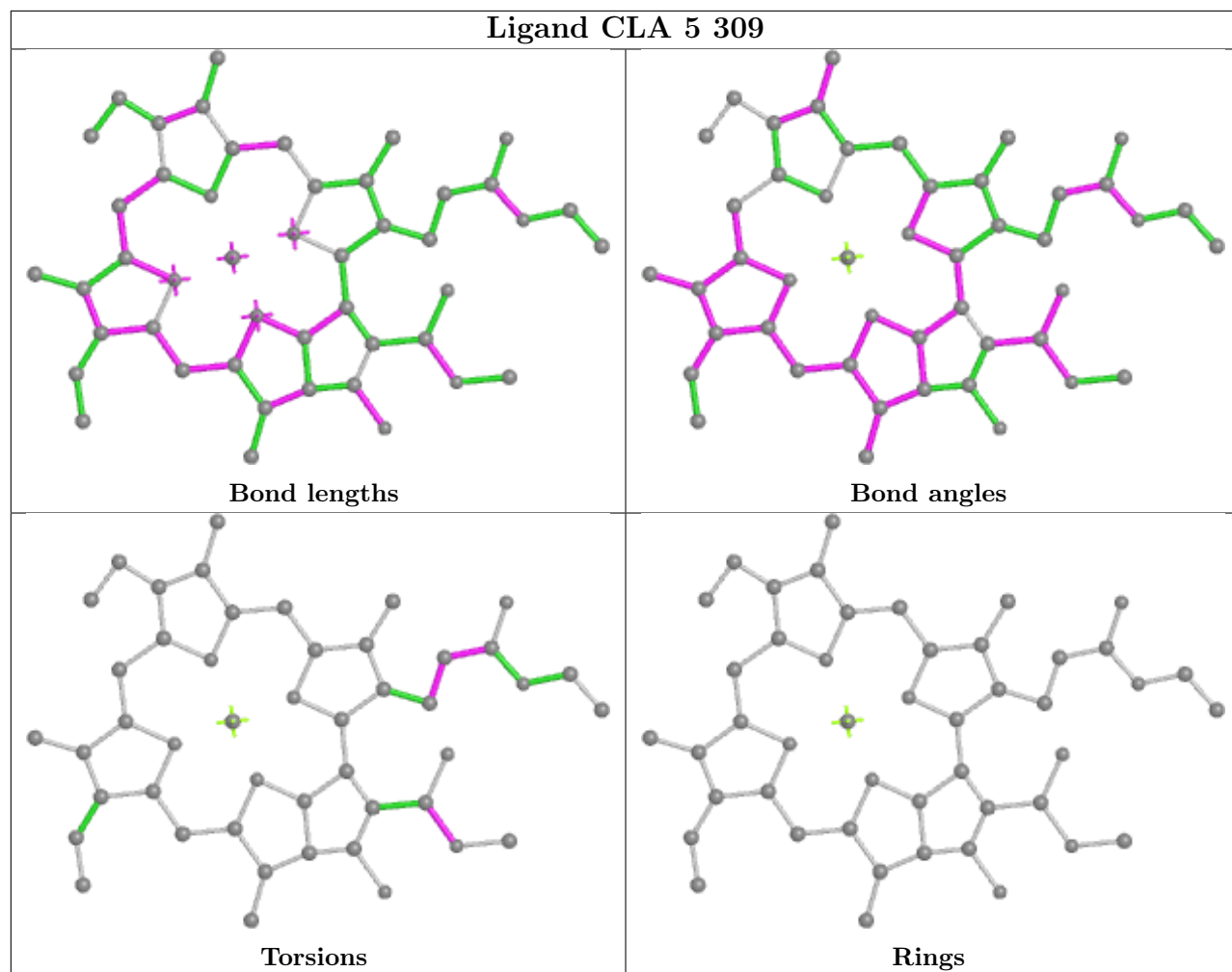
## Ligand LMT 9 306

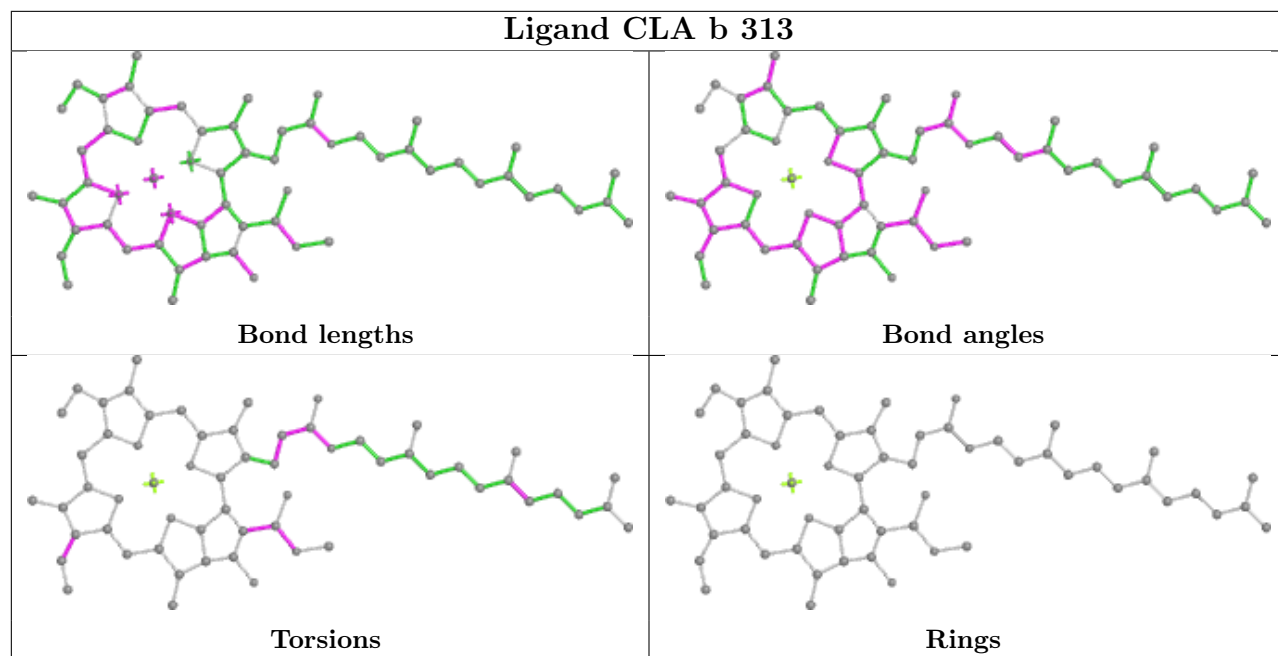
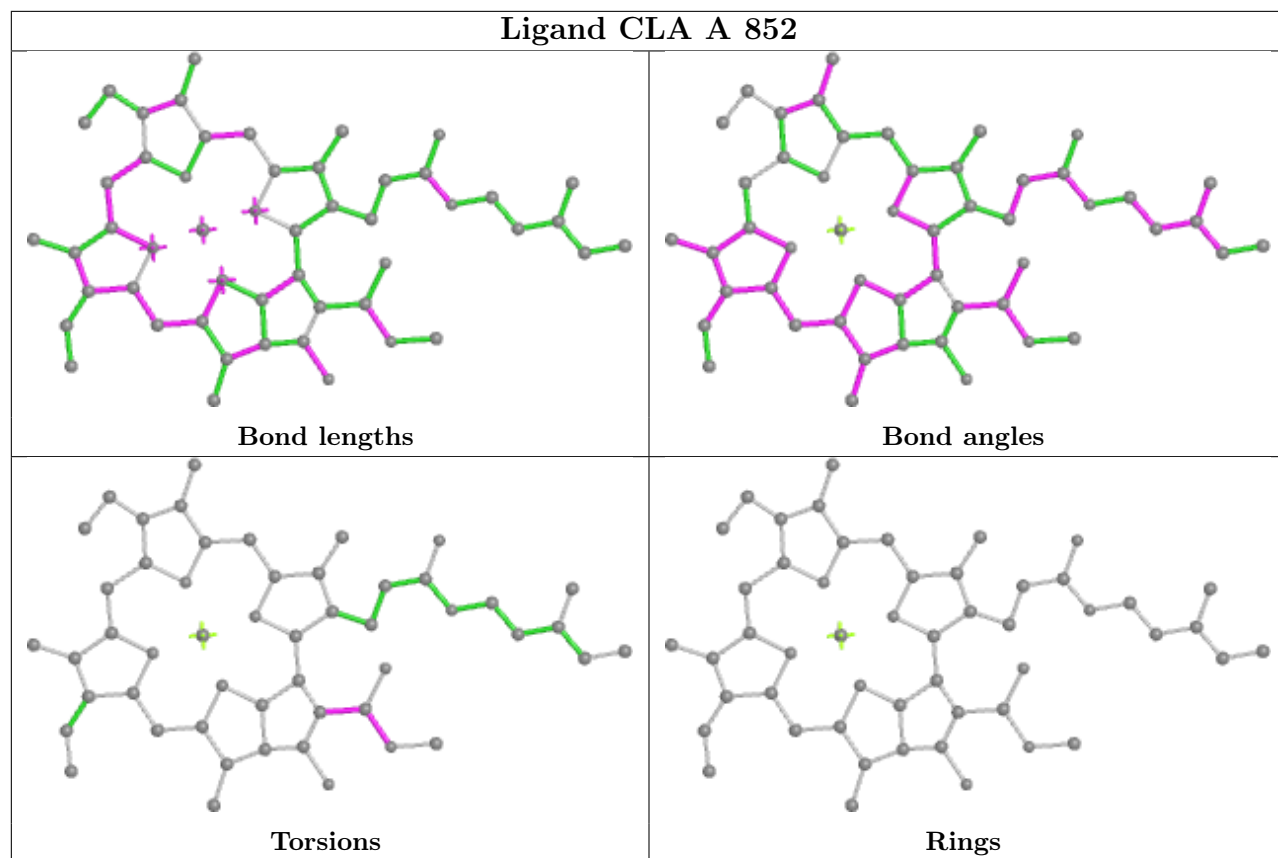


## Ligand CLA B 820

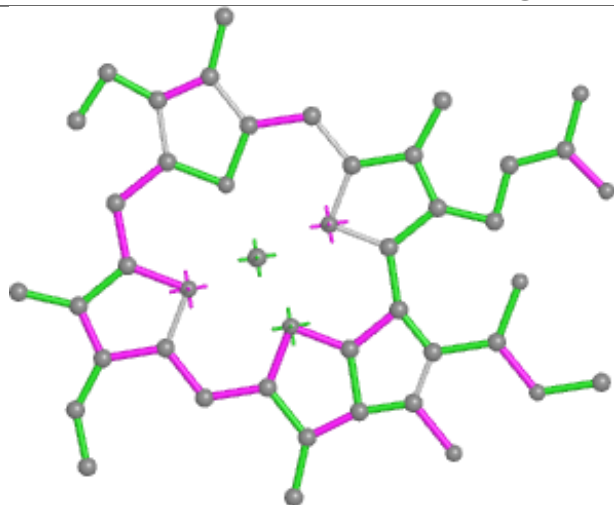


## Ligand CLA 5 309

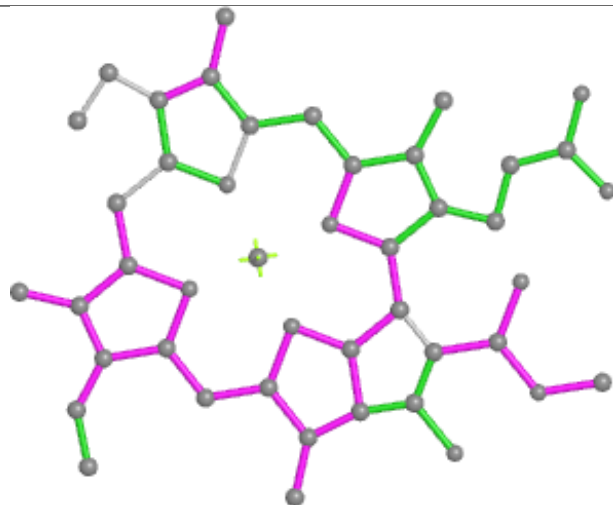




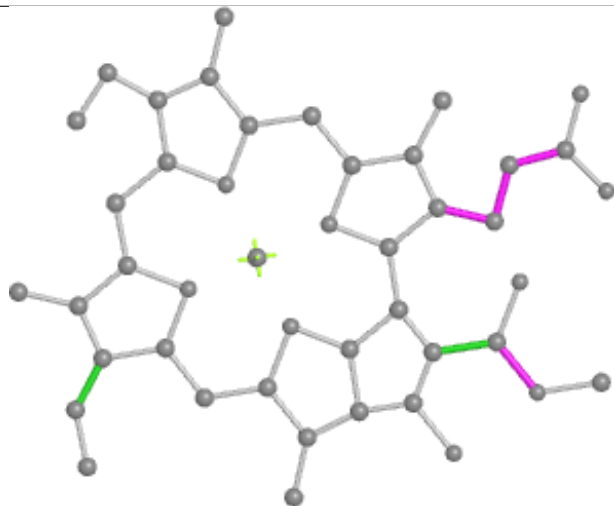
## Ligand CLA L 307



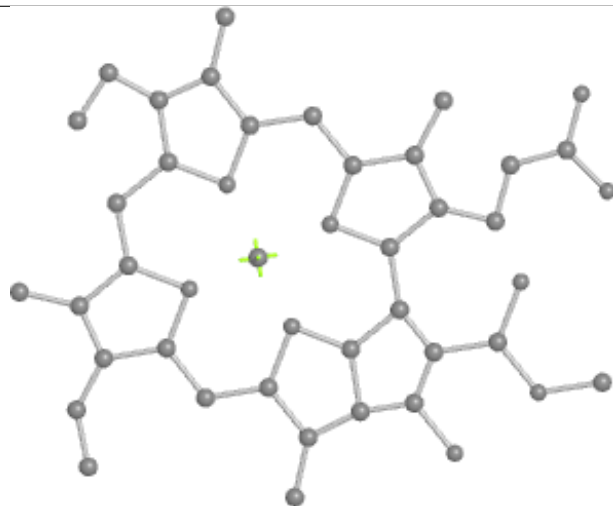
Bond lengths



Bond angles

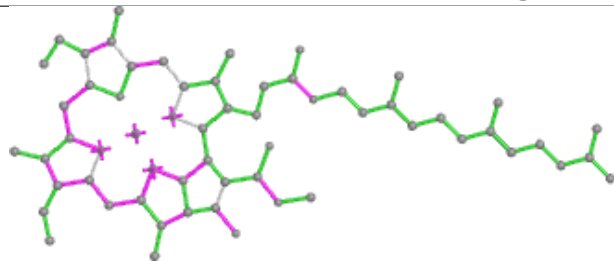


Torsions

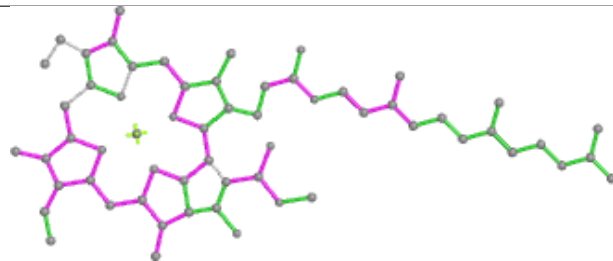


Rings

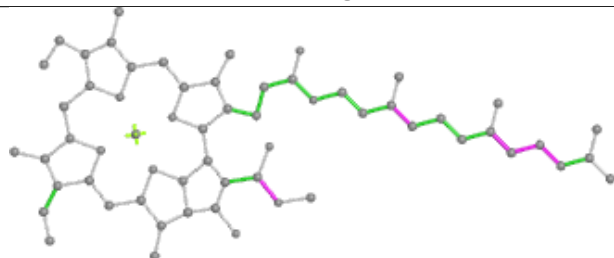
## Ligand CLA B 825



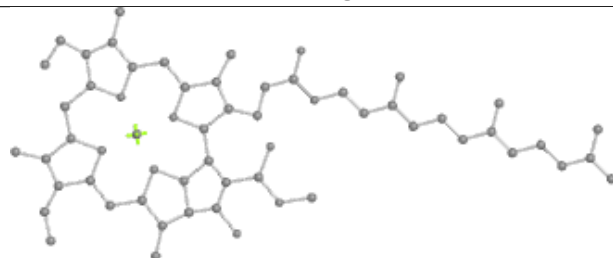
Bond lengths



Bond angles

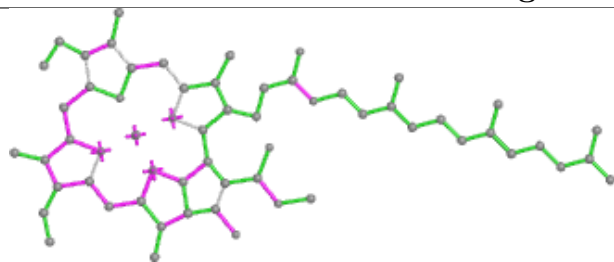


Torsions

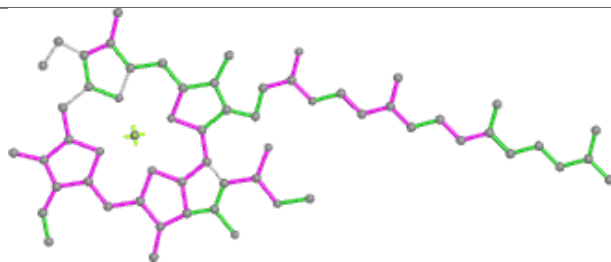


Rings

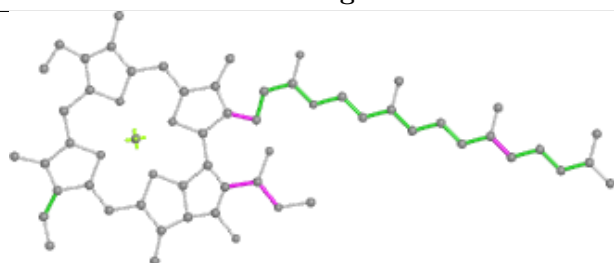
## Ligand CLA a 309



Bond lengths



Bond angles

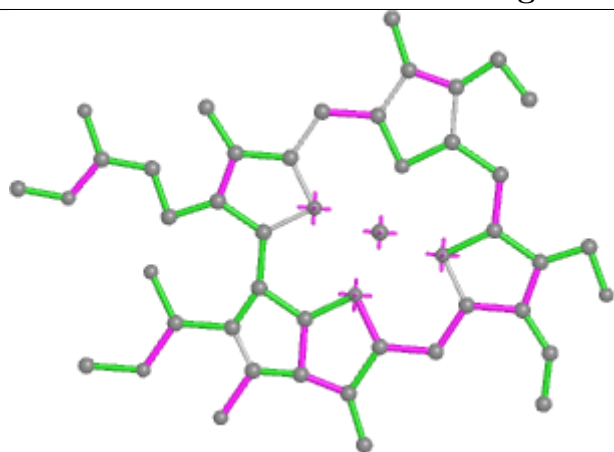


Torsions

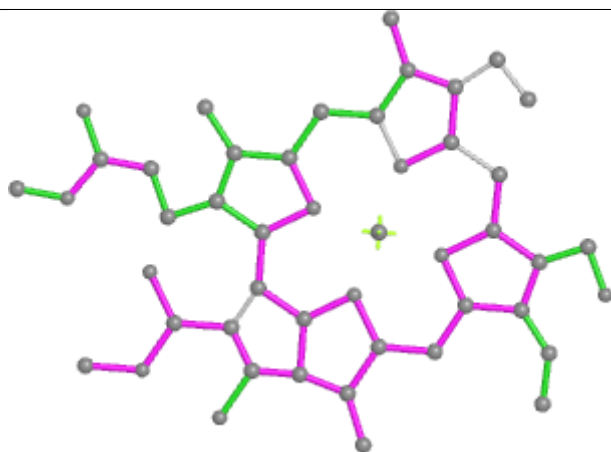


Rings

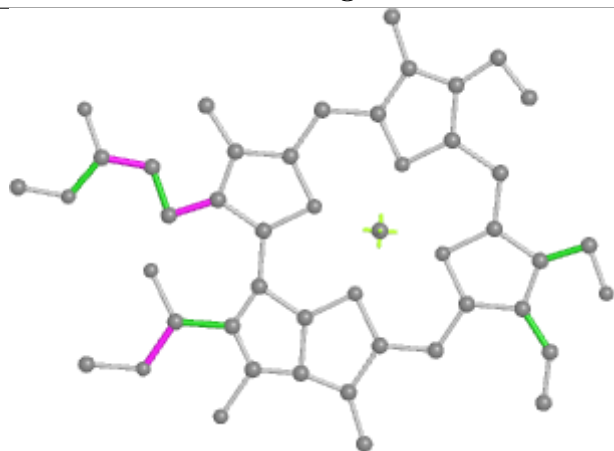
## Ligand CHL 5 322



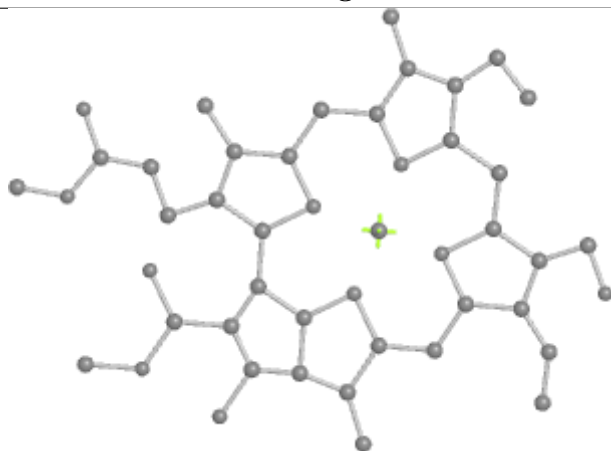
Bond lengths



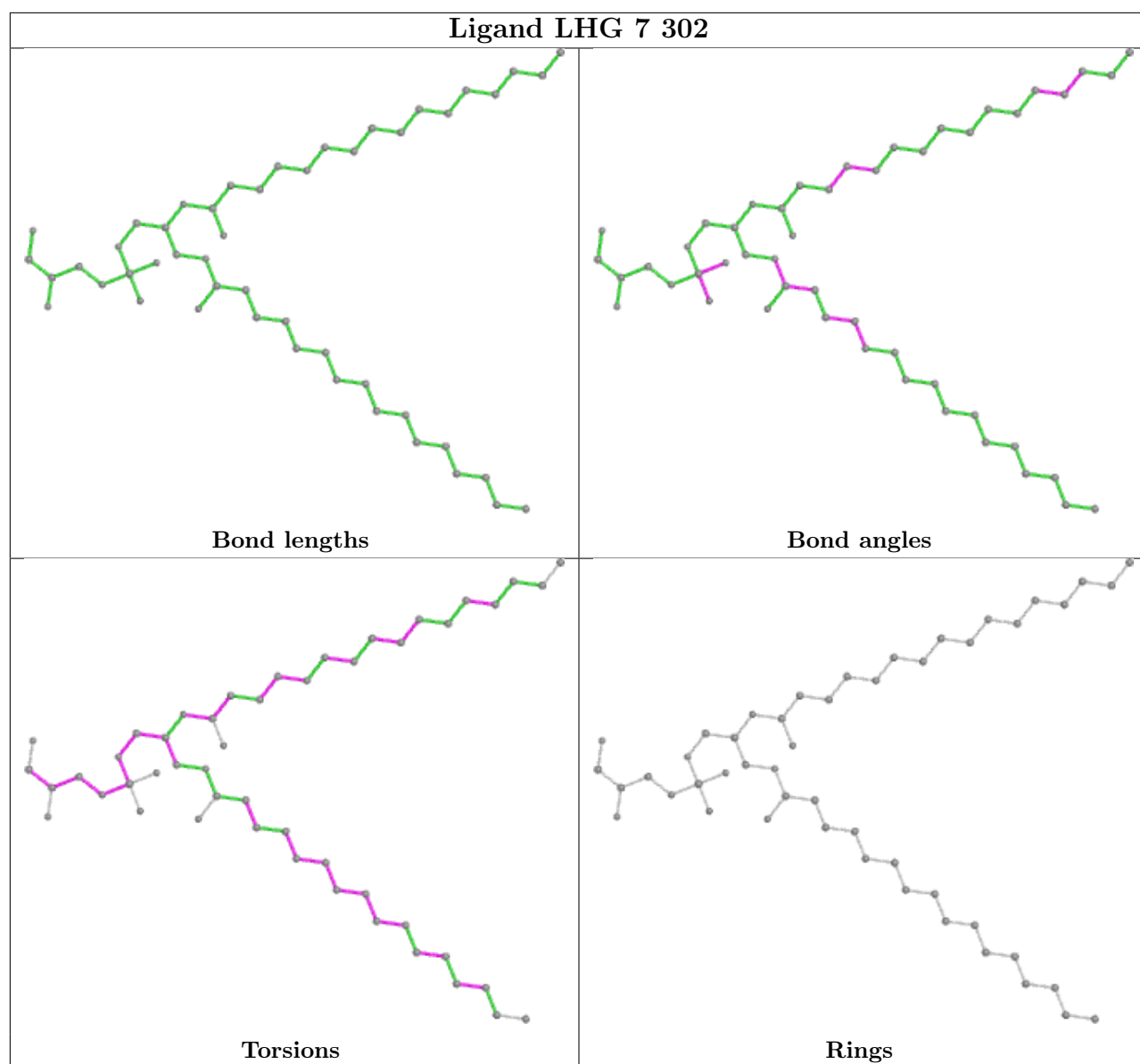
Bond angles



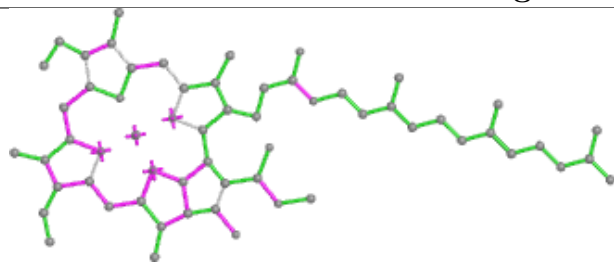
Torsions



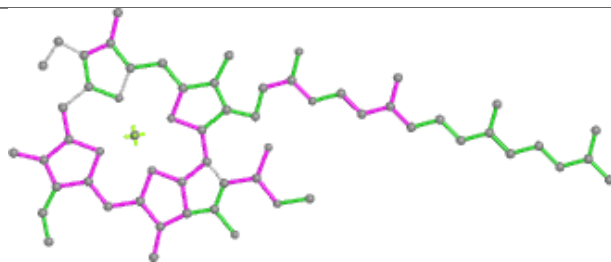
Rings



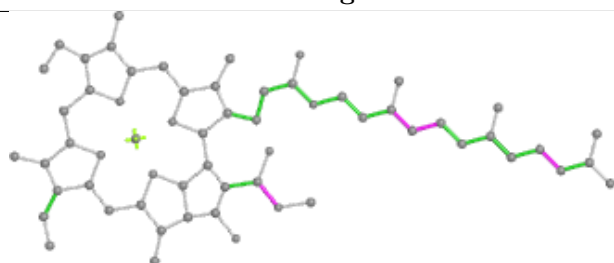
## Ligand CLA A 836



Bond lengths



Bond angles

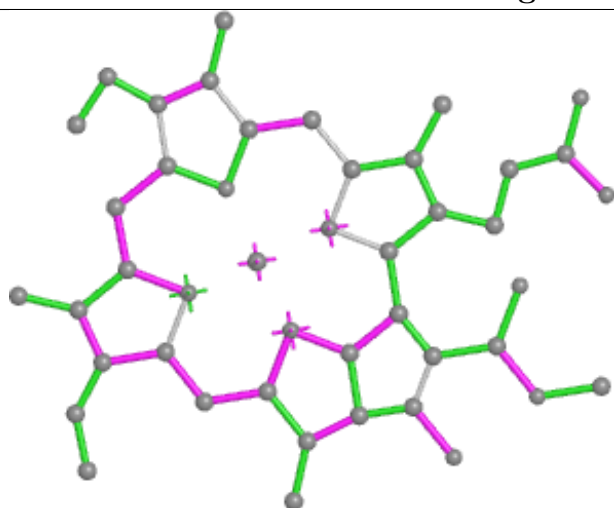


Torsions

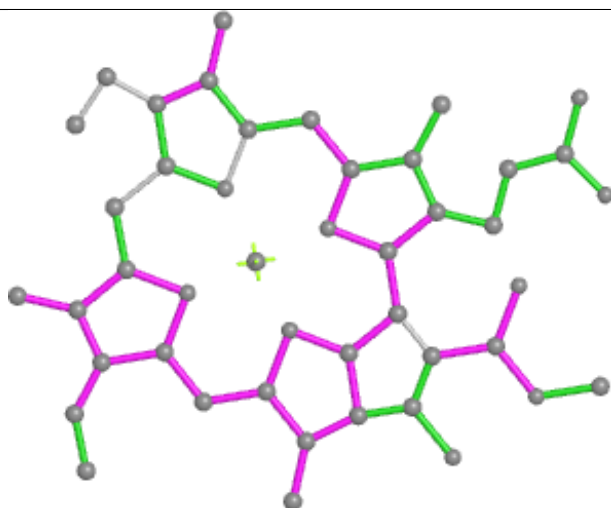


Rings

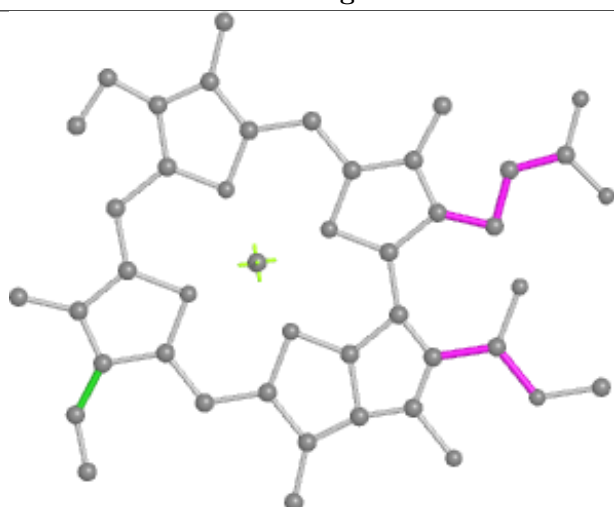
## Ligand CLA a 316



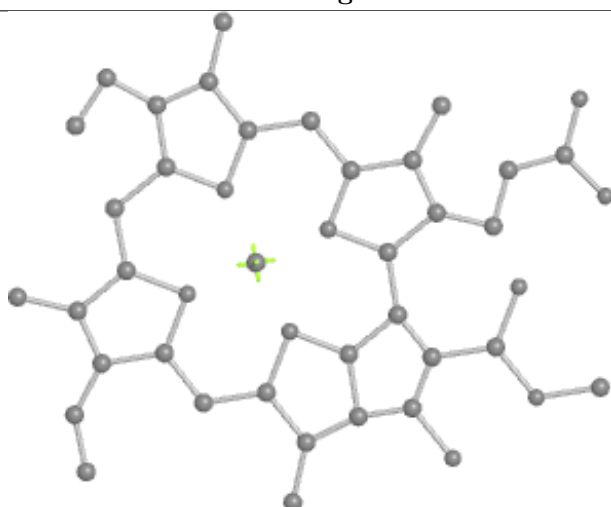
Bond lengths



Bond angles

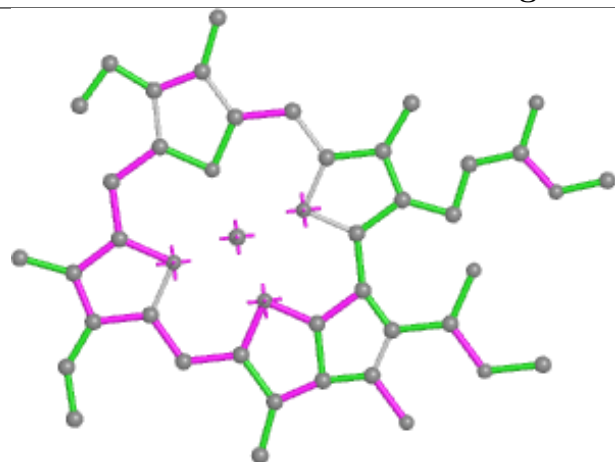


Torsions

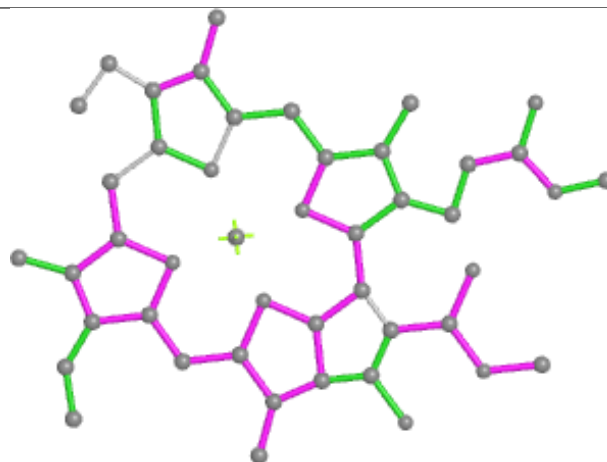


Rings

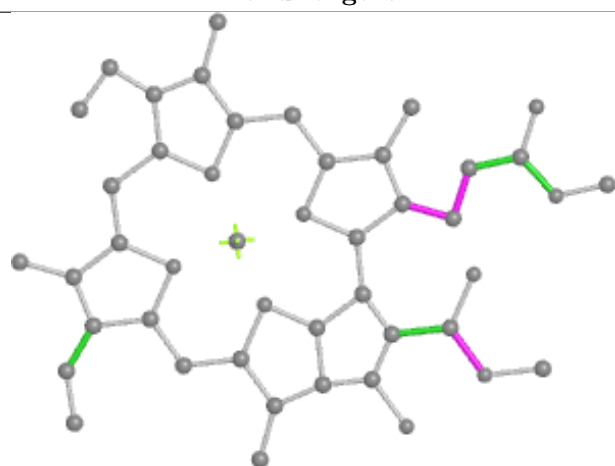
## Ligand CLA b 311



Bond lengths



Bond angles



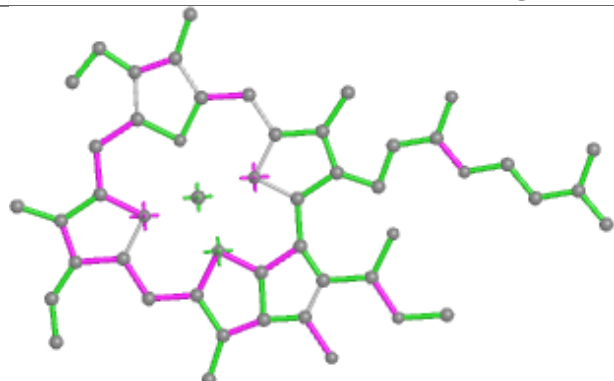
Torsions



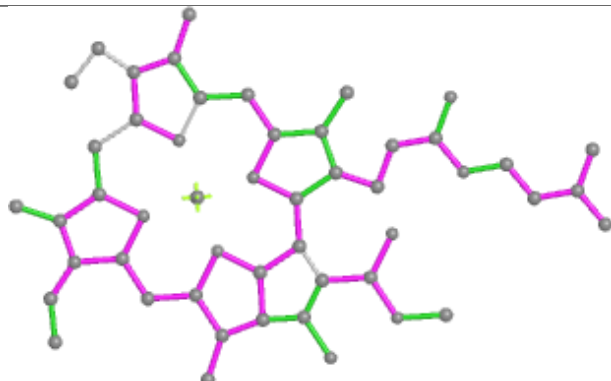
Rings



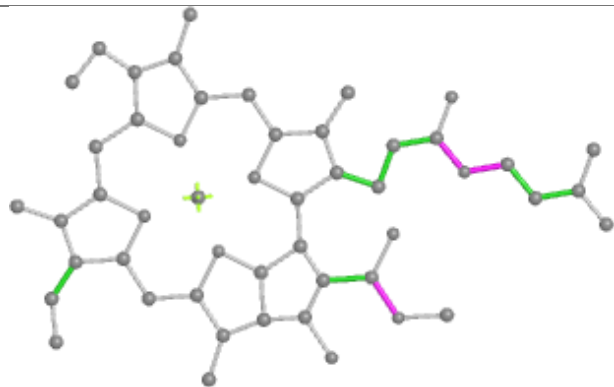
## Ligand CLA G 204



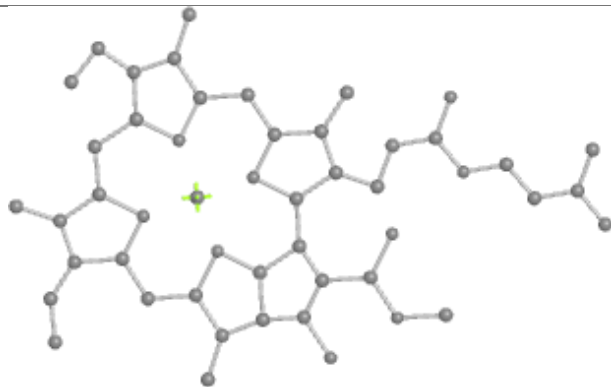
Bond lengths



Bond angles

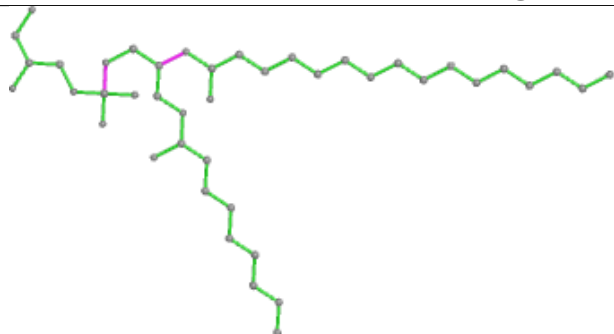


Torsions

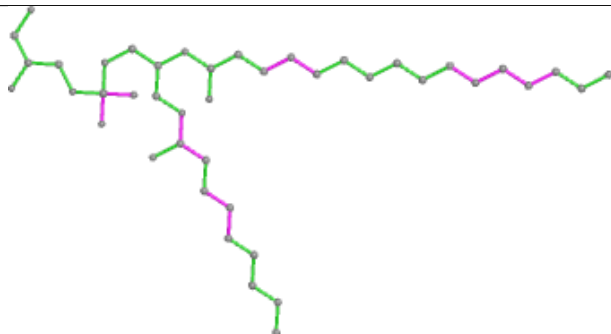


Rings

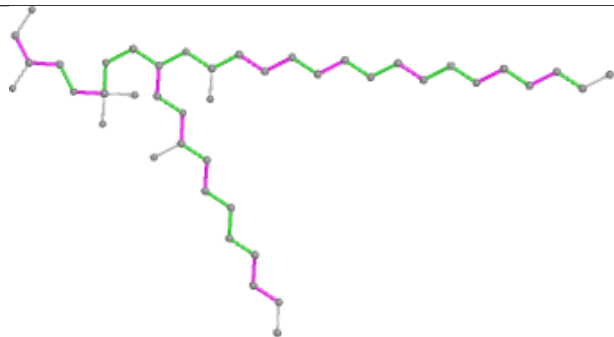
## Ligand LHG A 809



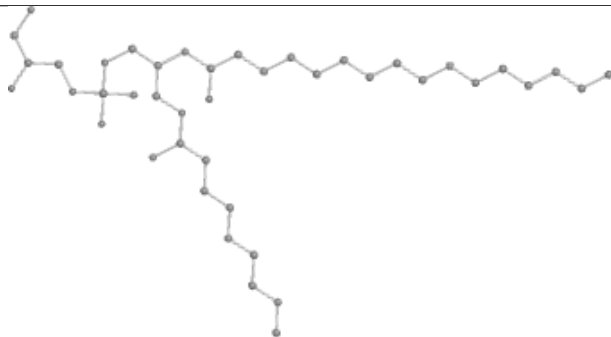
Bond lengths



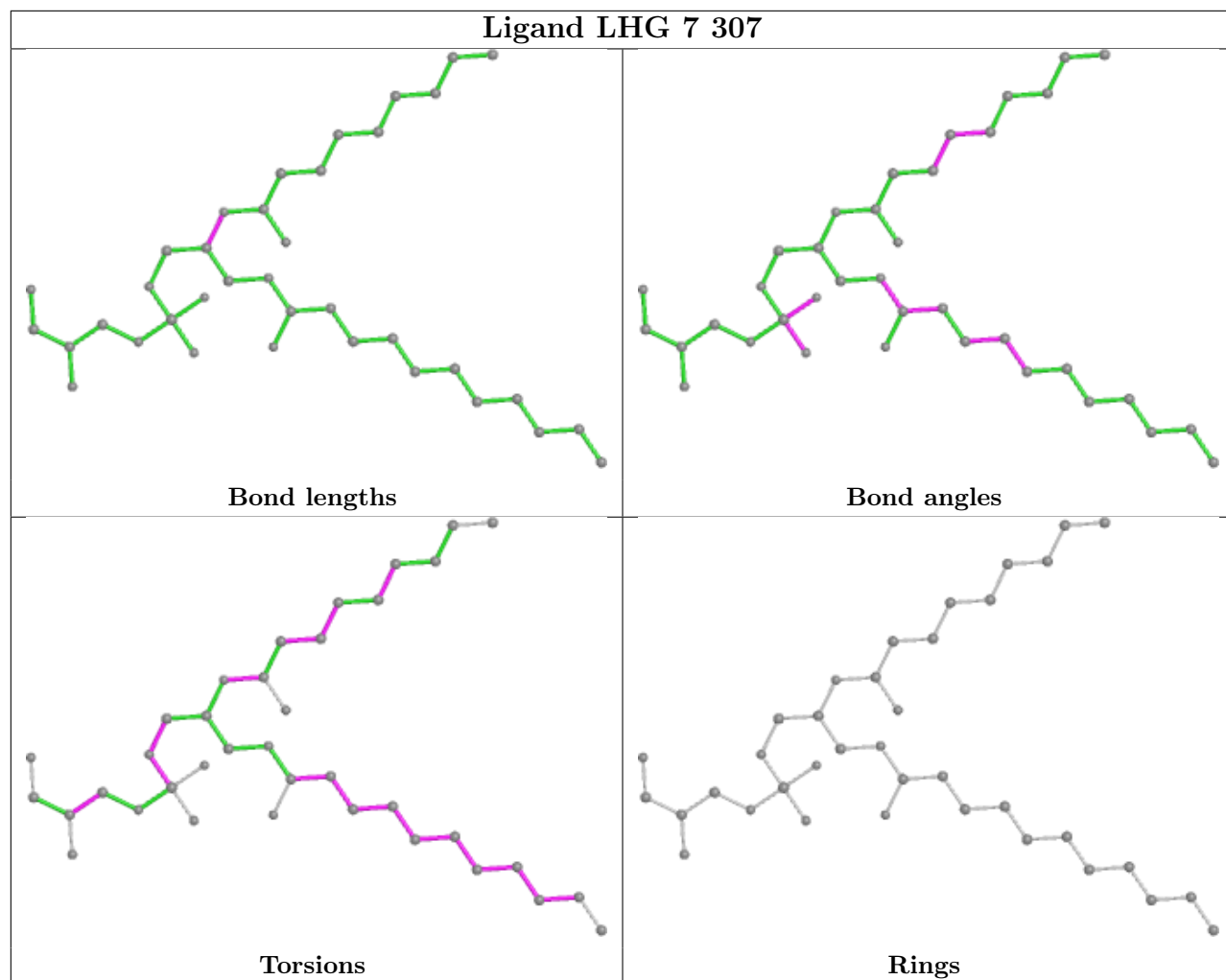
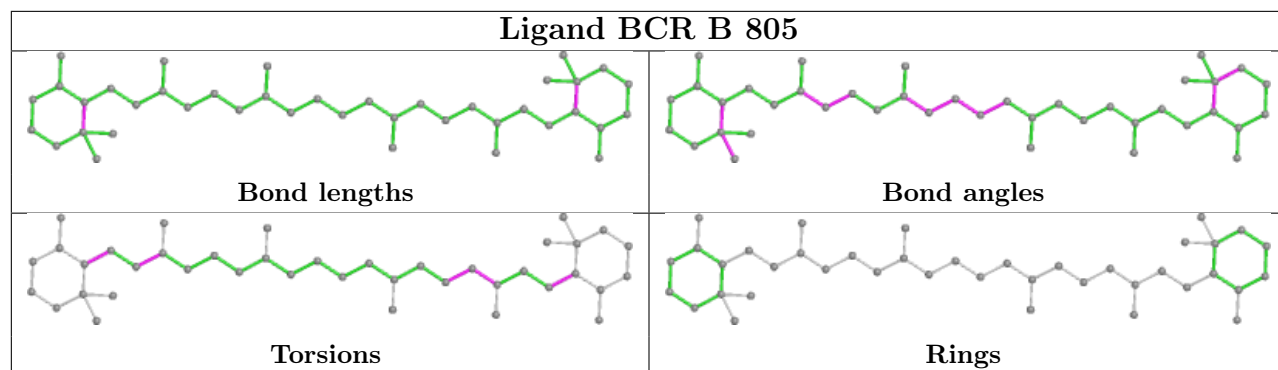
Bond angles



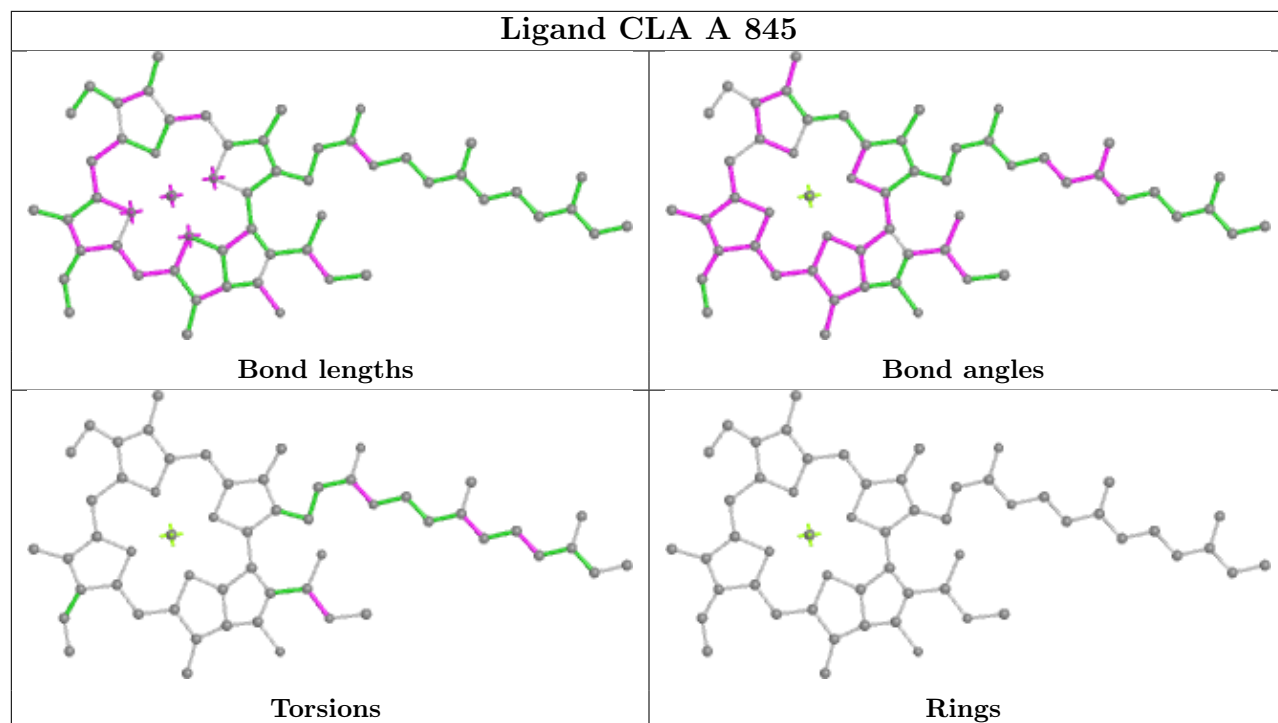
Torsions



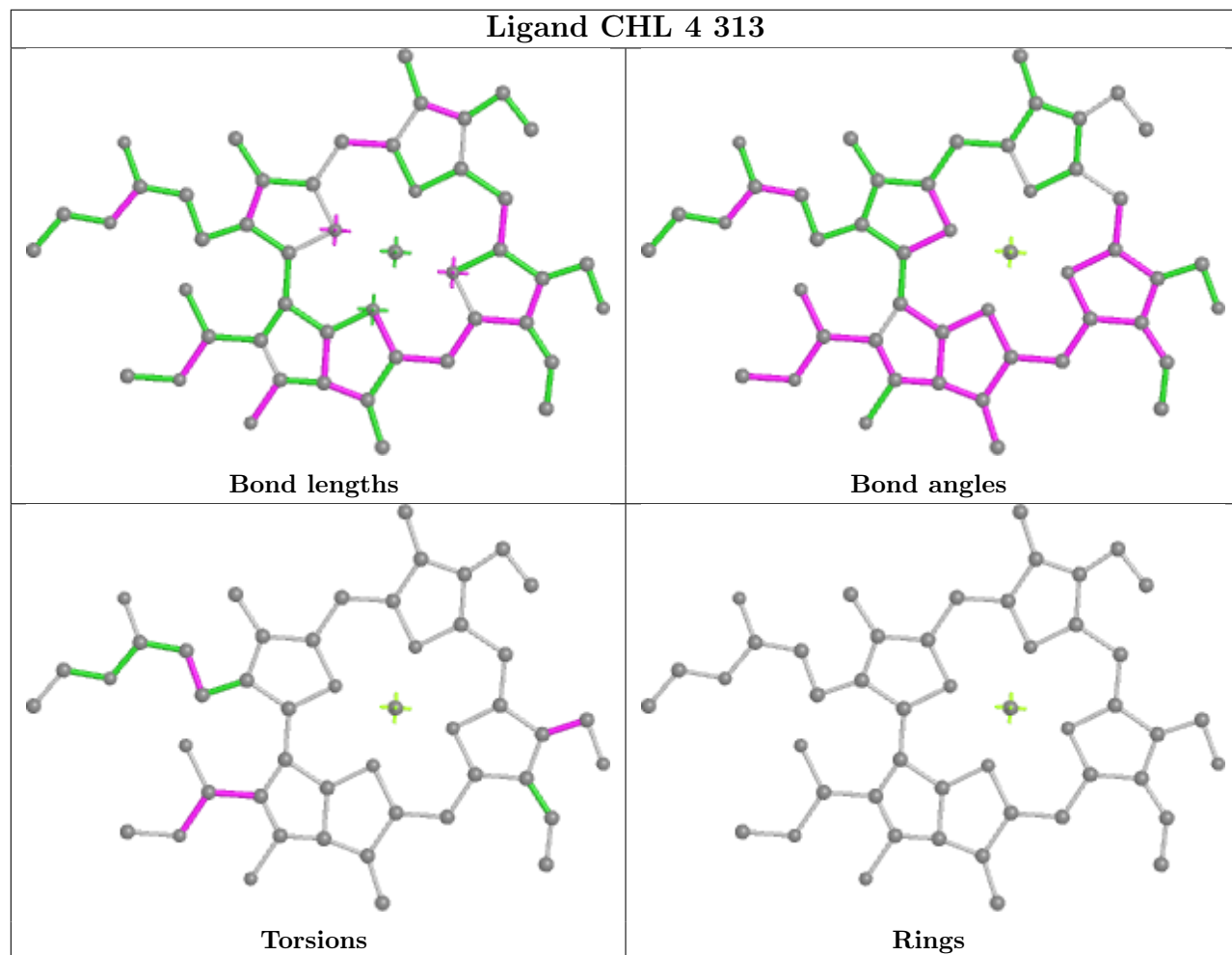
Rings



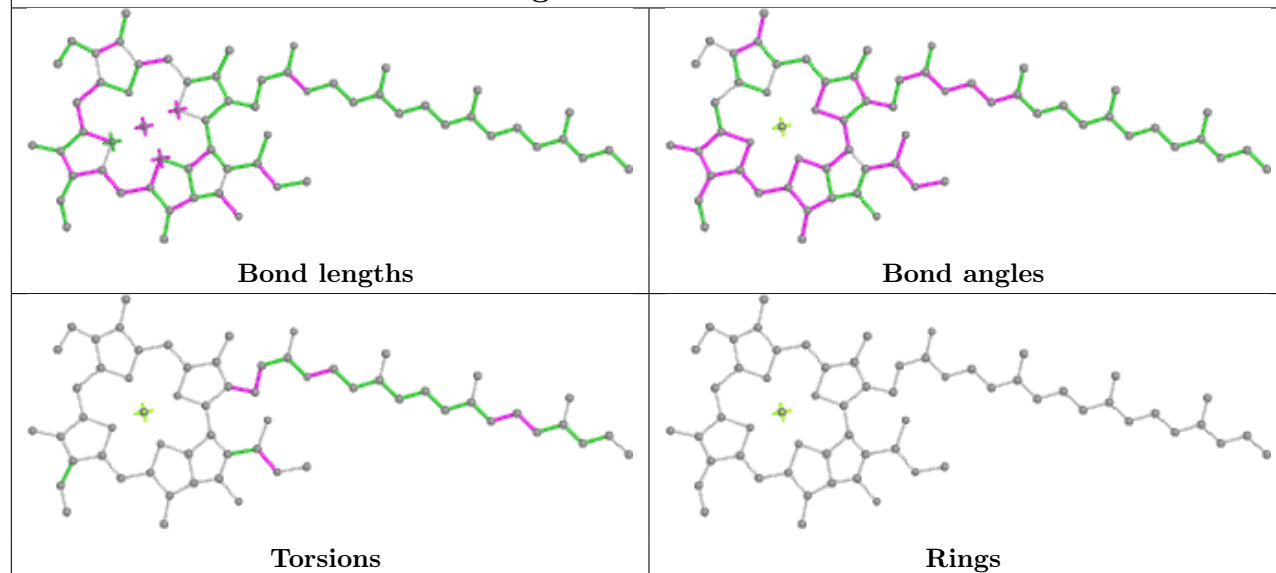
## Ligand CLA A 845



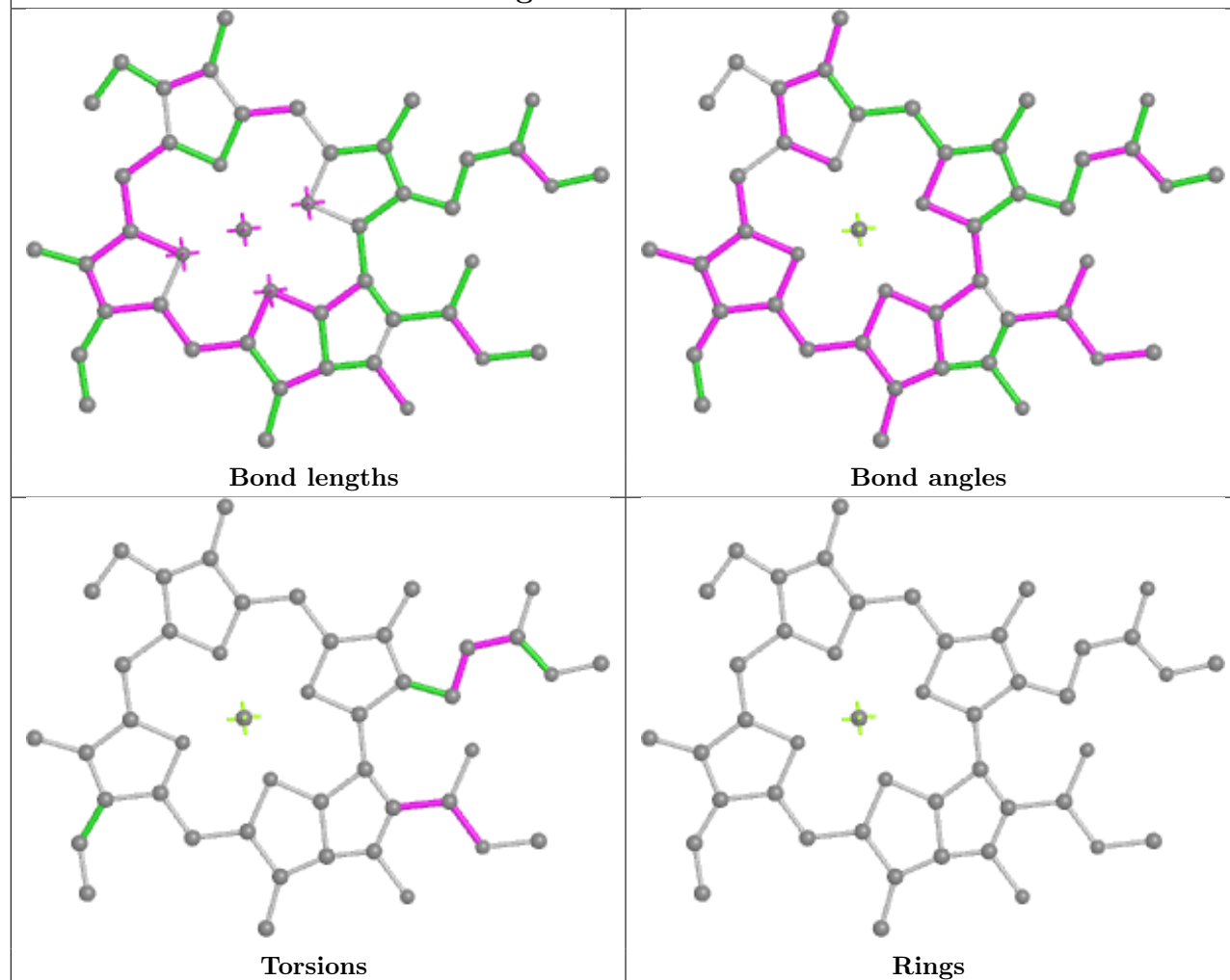
## Ligand CHL 4 313

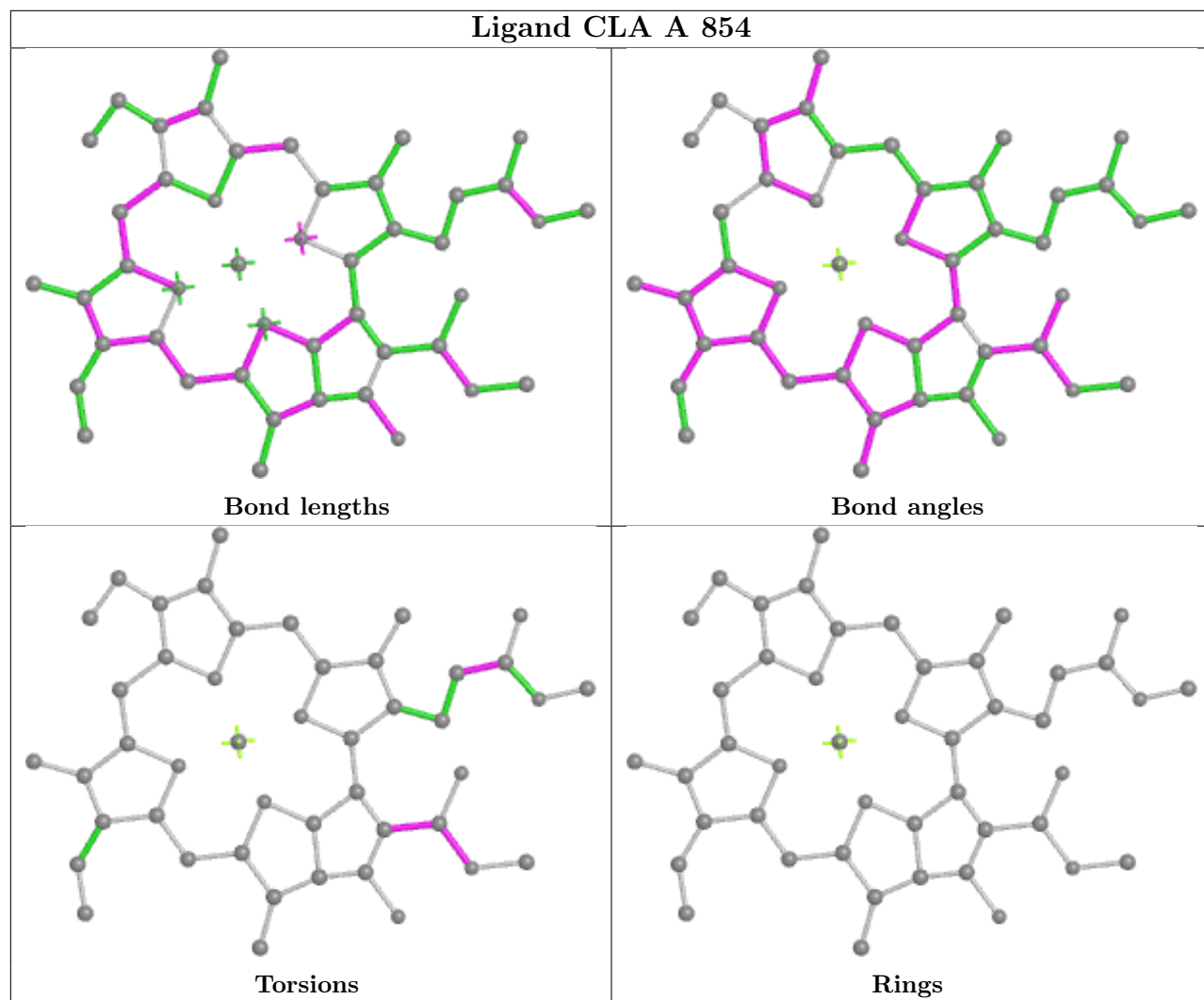
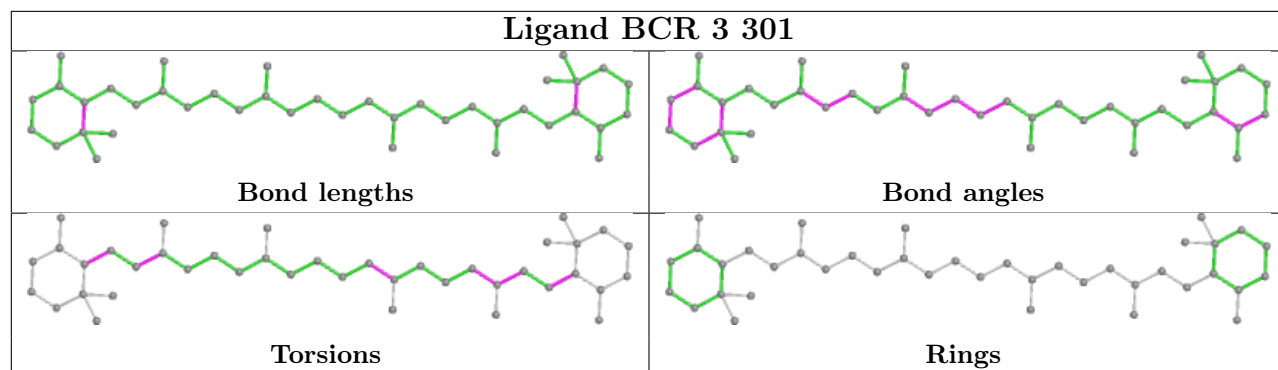


## Ligand CLA A 824

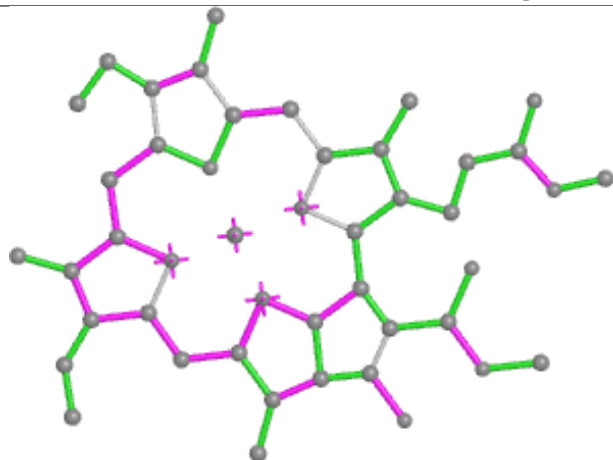


## Ligand CLA b 305

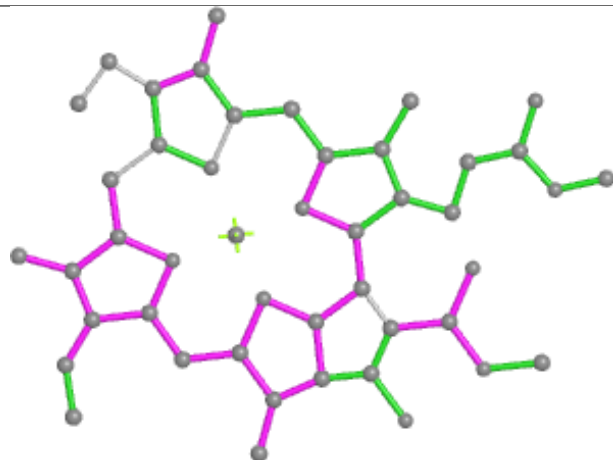




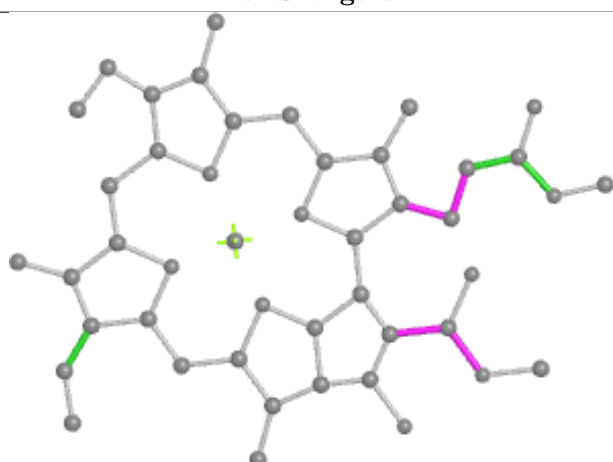
## Ligand CLA b 308



Bond lengths



Bond angles

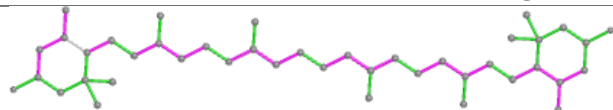


Torsions

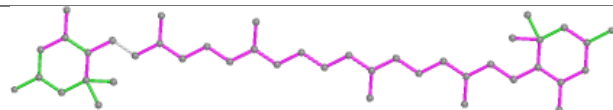


Rings

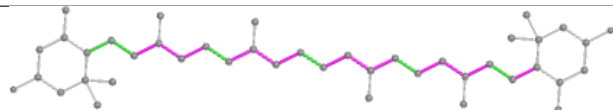
## Ligand LUT J 103



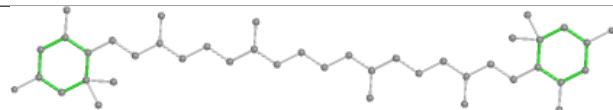
Bond lengths



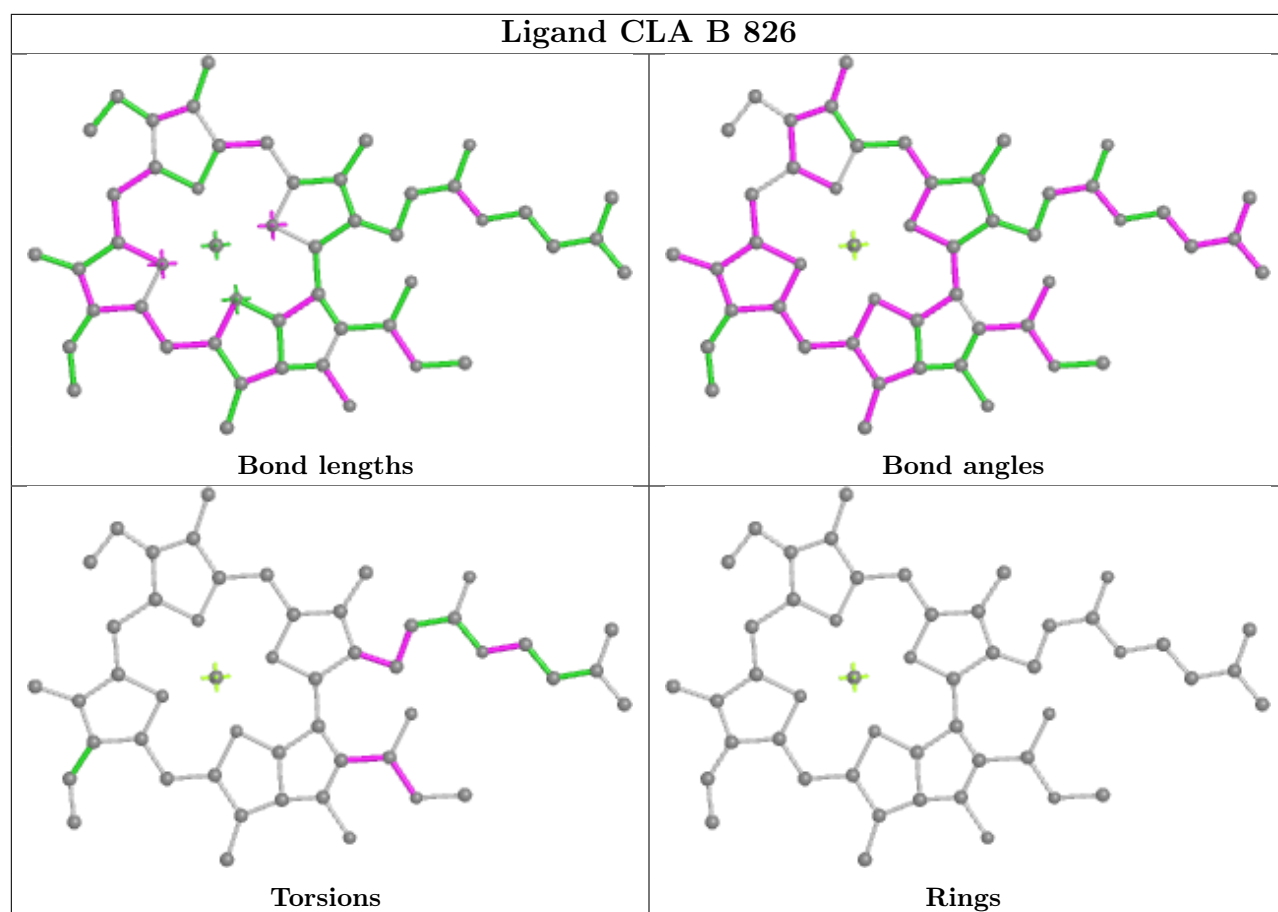
Bond angles



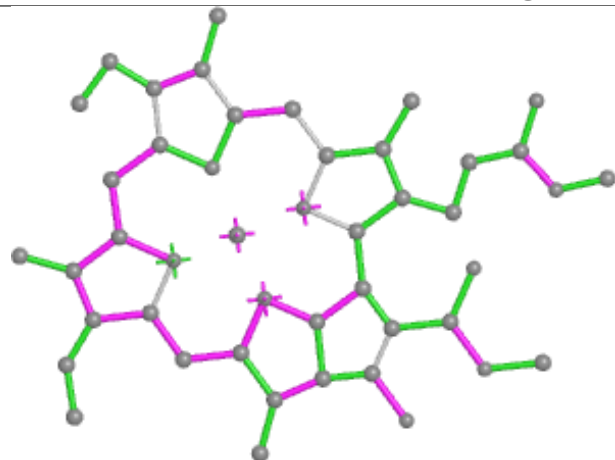
Torsions



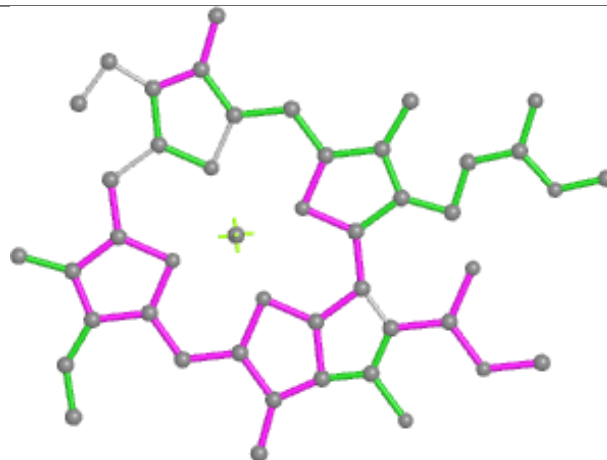
Rings



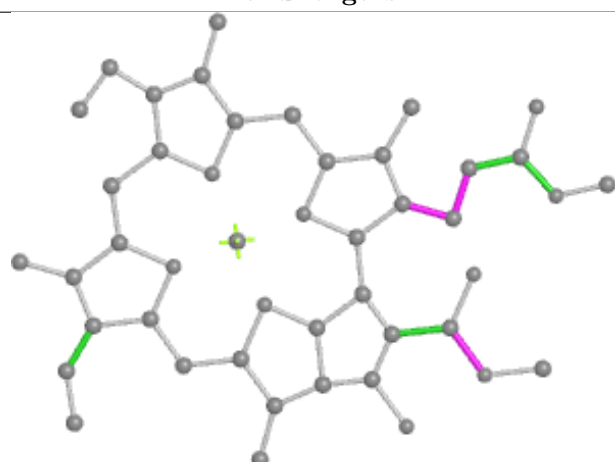
## Ligand CLA b 306



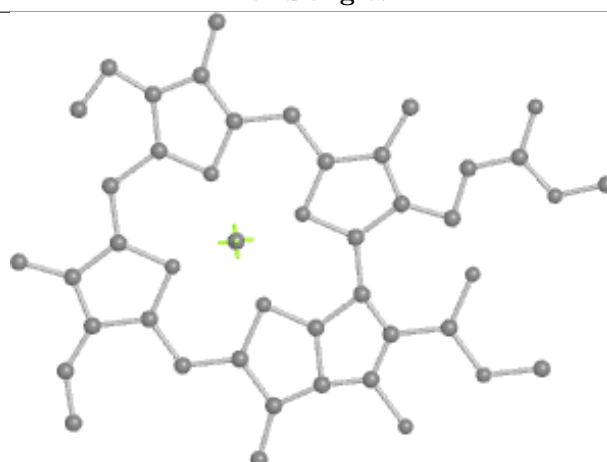
Bond lengths



Bond angles

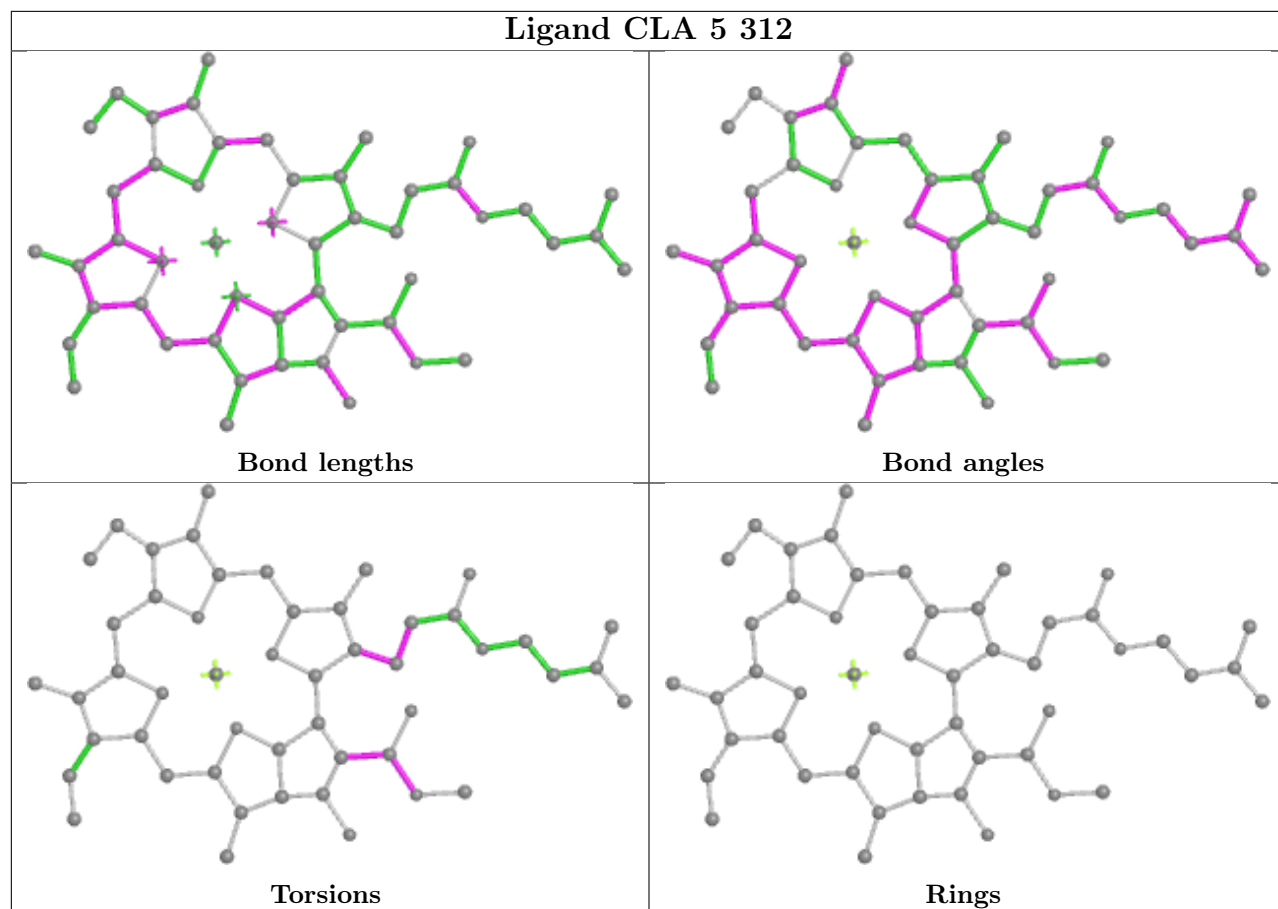


Torsions

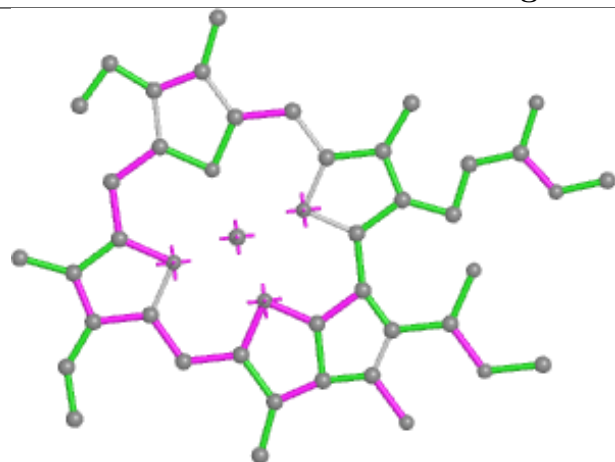


Rings

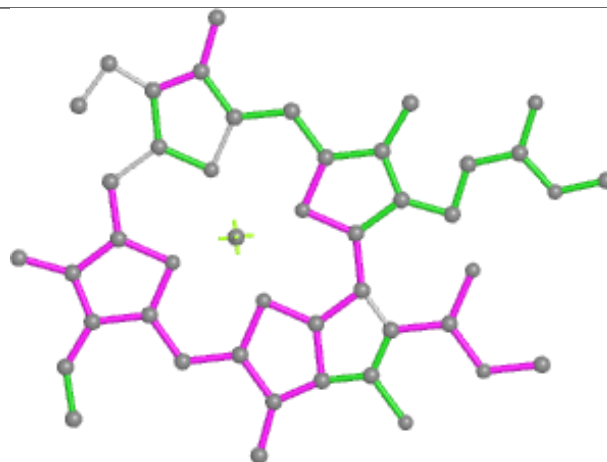




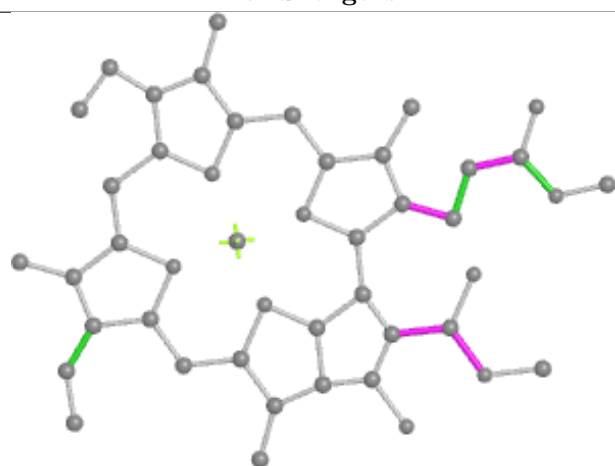
## Ligand CLA 6 322



Bond lengths



Bond angles

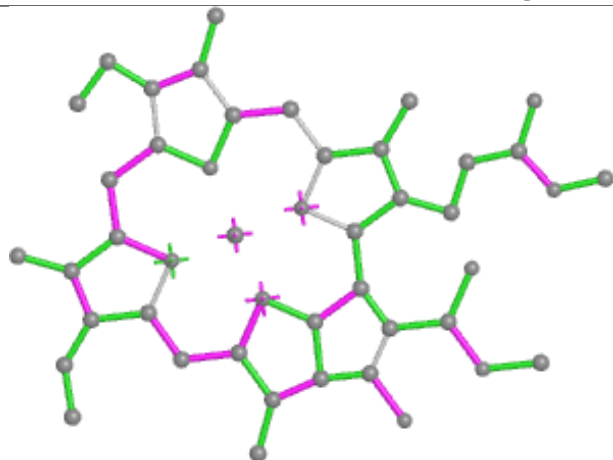


Torsions

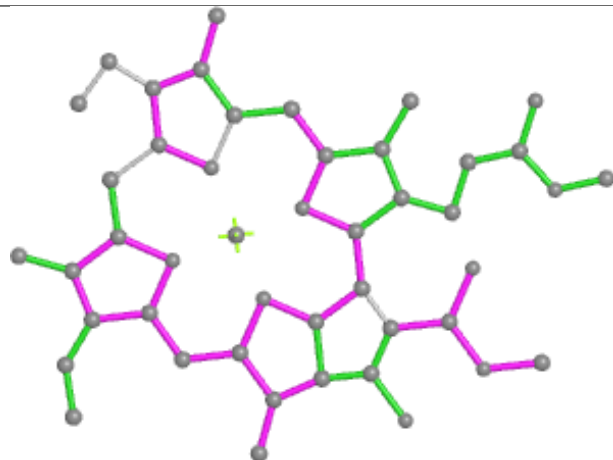


Rings

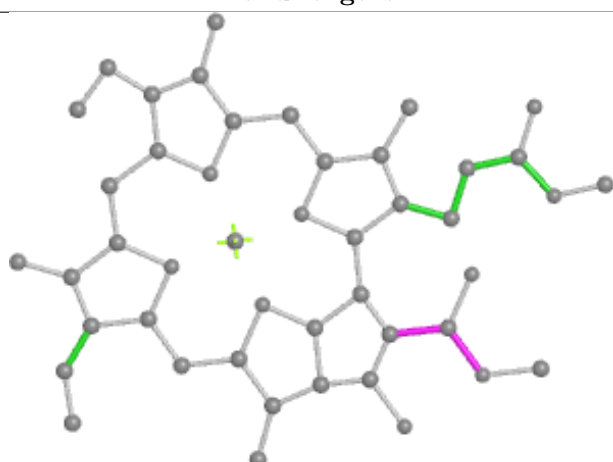
## Ligand CLA 8 321



Bond lengths



Bond angles

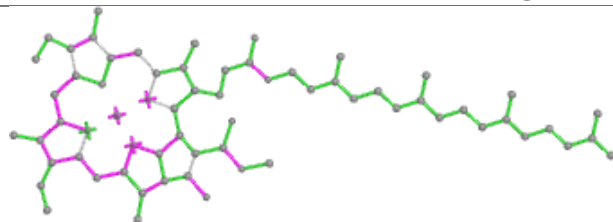


Torsions

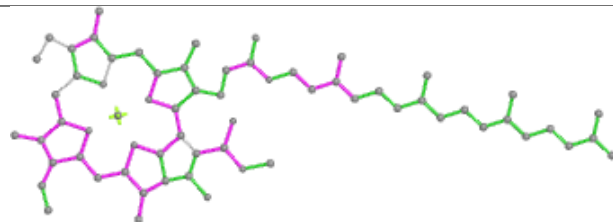


Rings

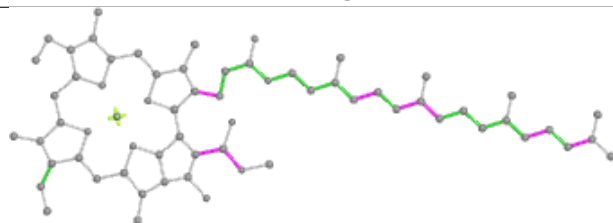
## Ligand CLA a 312



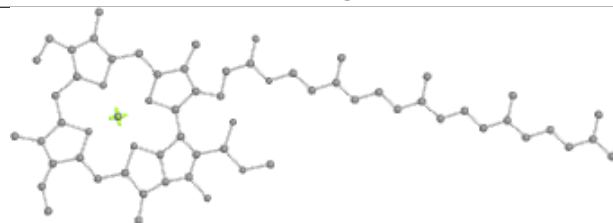
Bond lengths



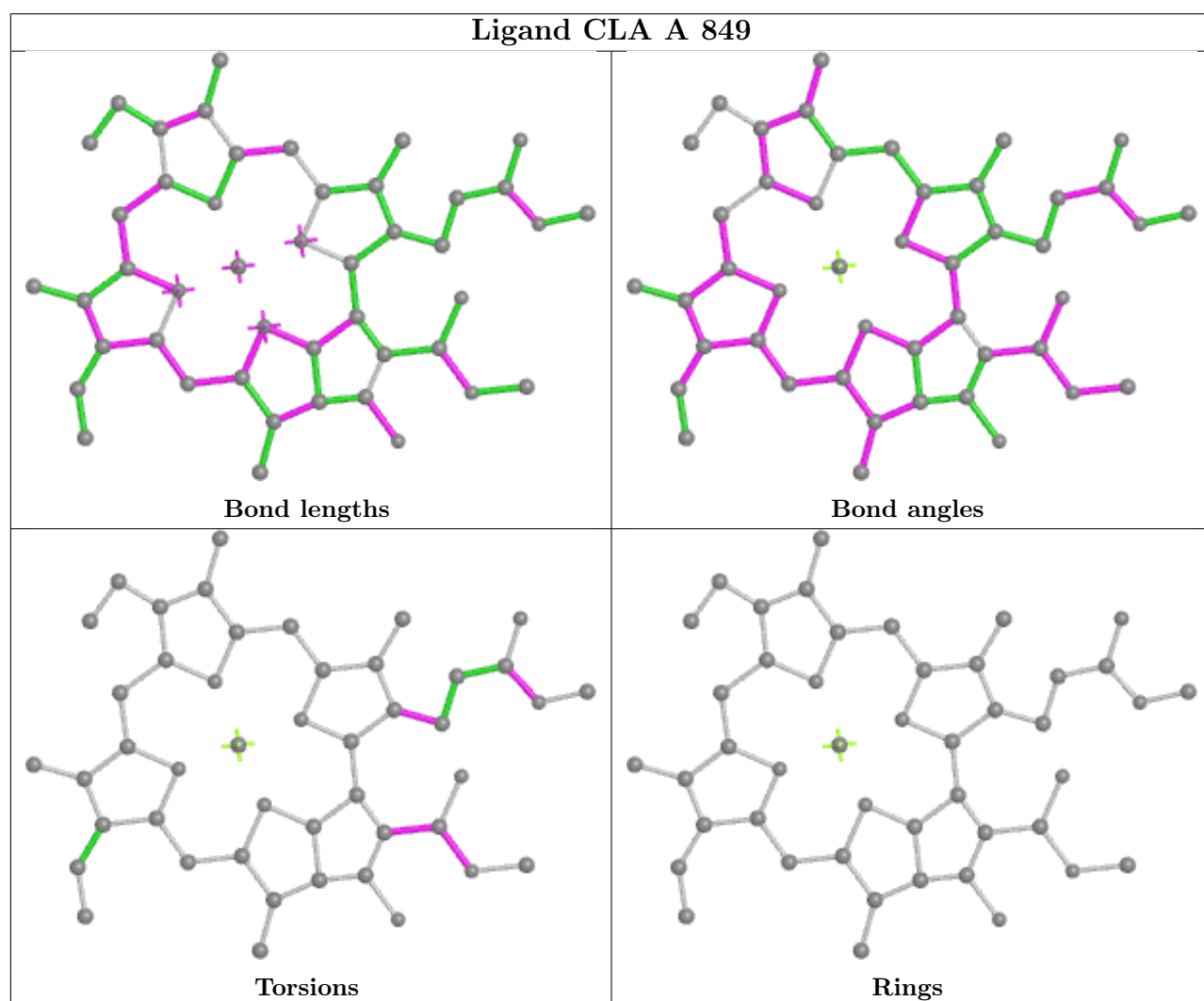
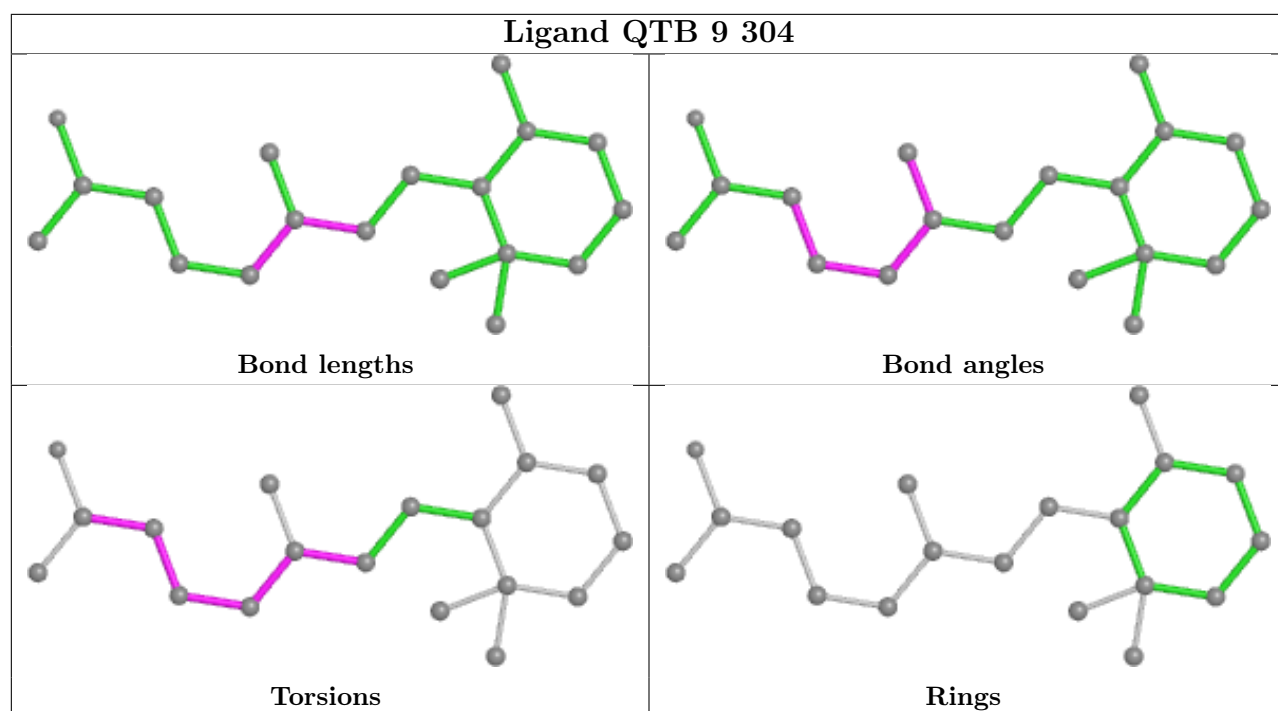
Bond angles



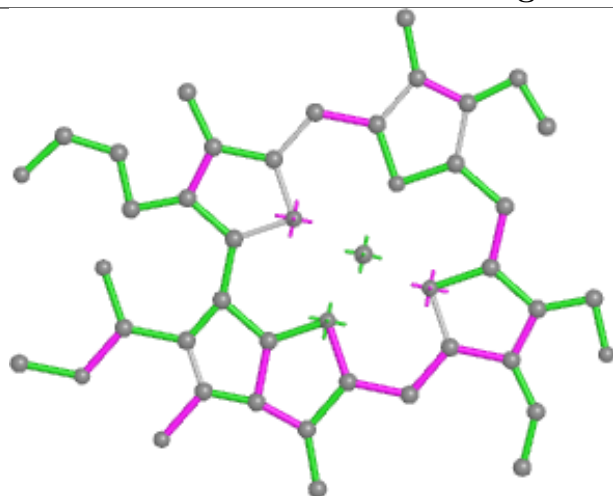
Torsions



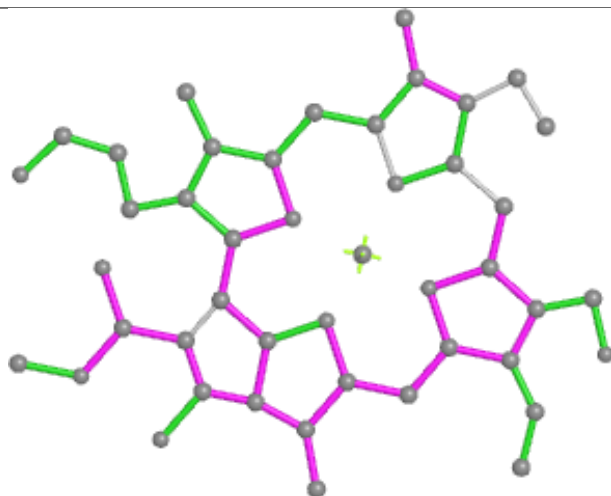
Rings



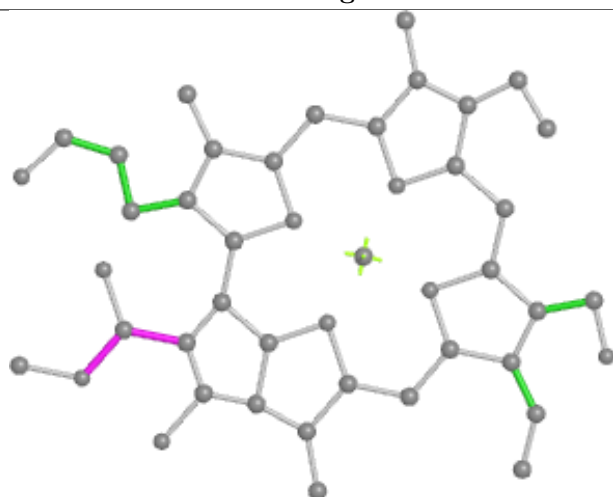
## Ligand CHL 8 319



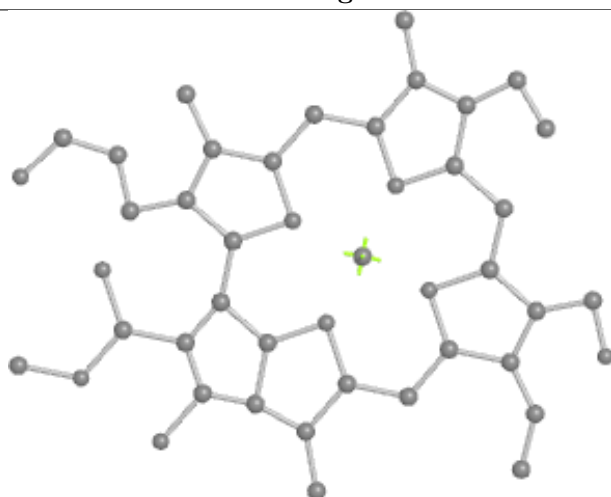
Bond lengths



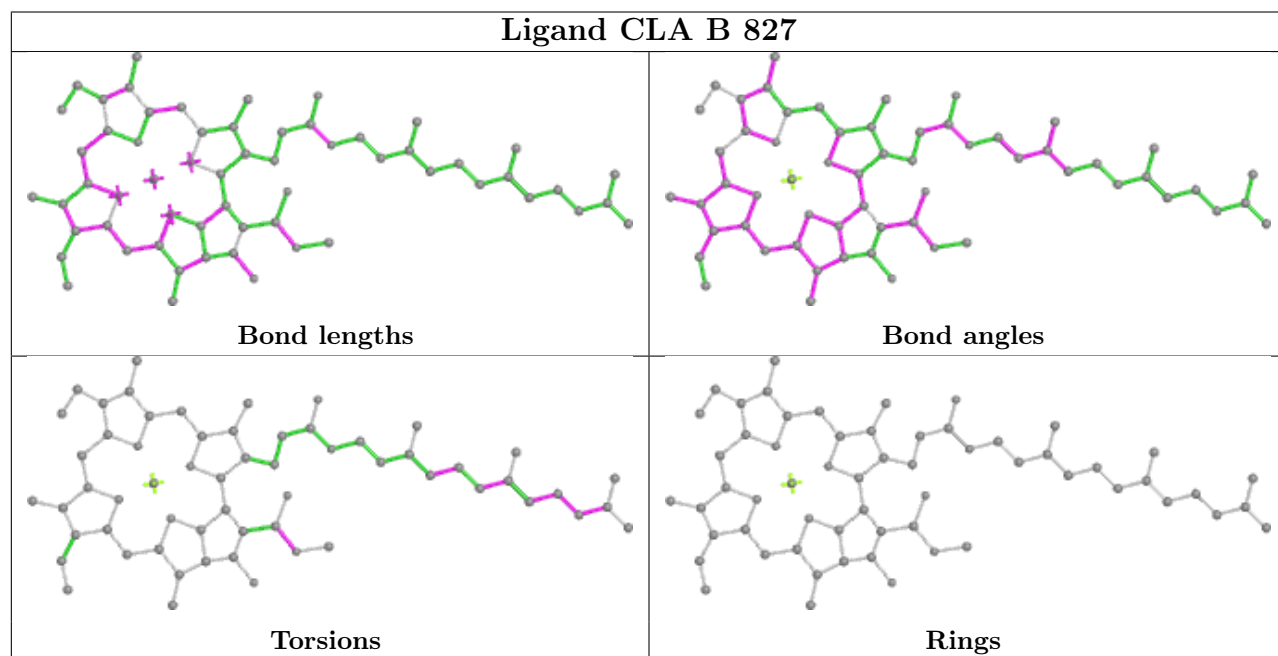
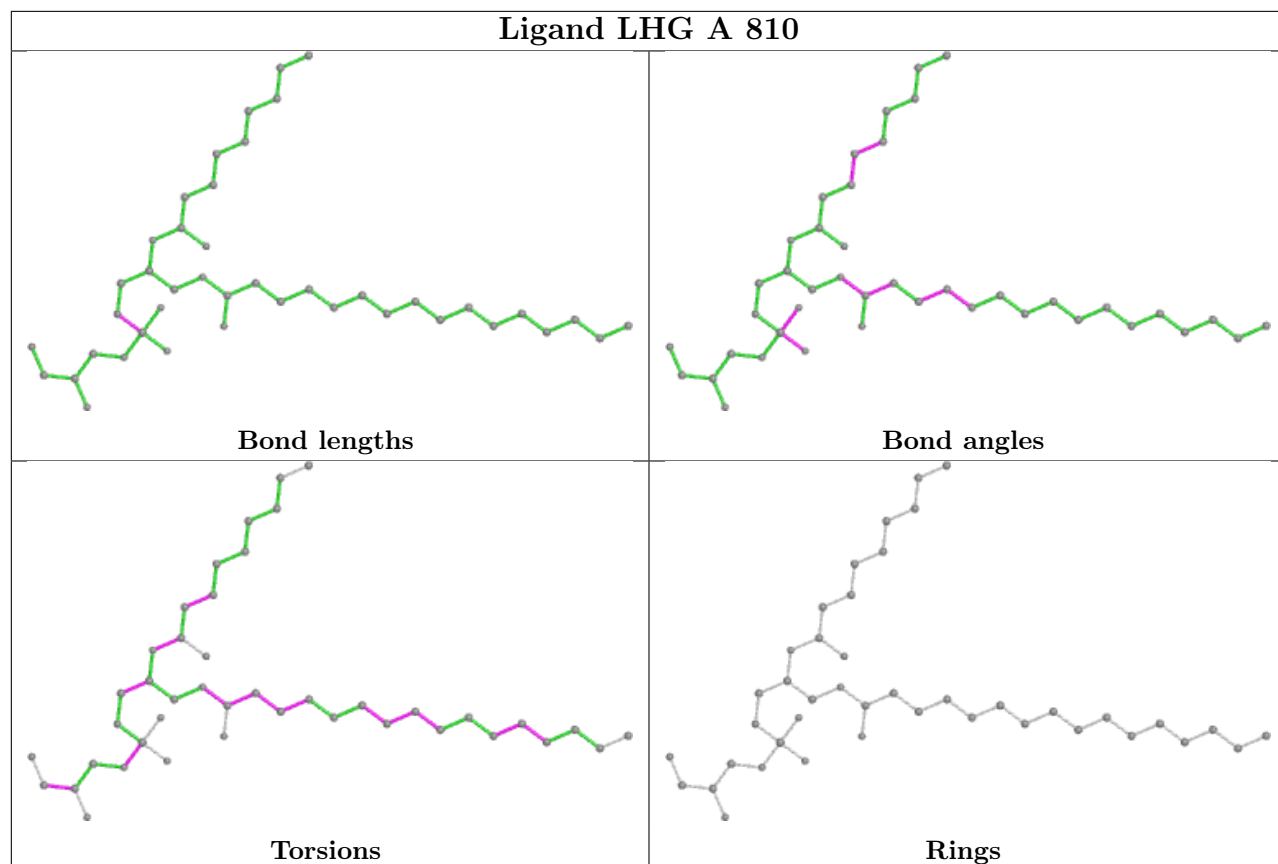
Bond angles



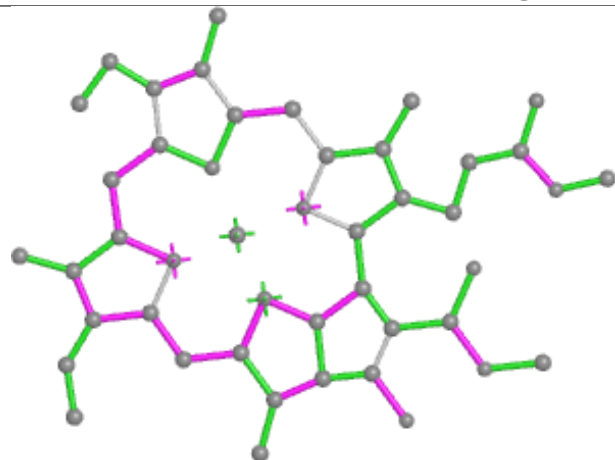
Torsions



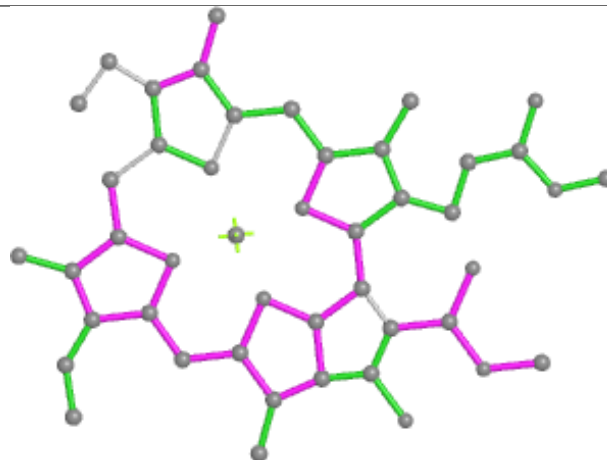
Rings



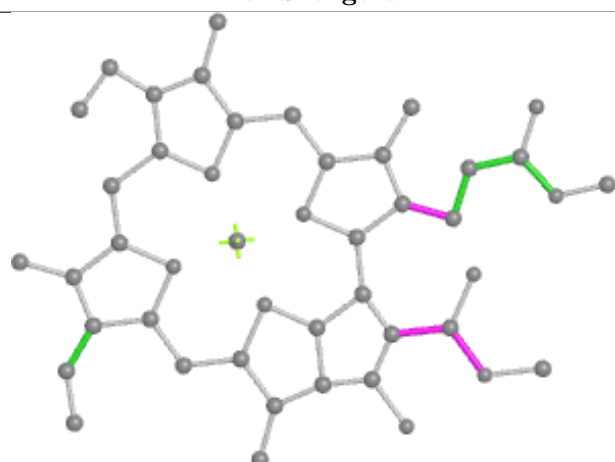
## Ligand CLA H 903



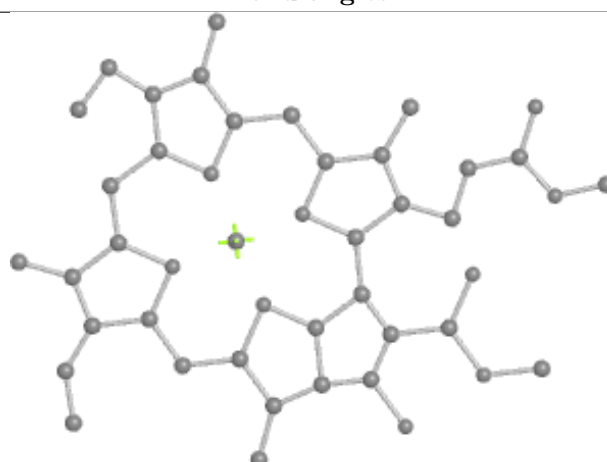
Bond lengths



Bond angles

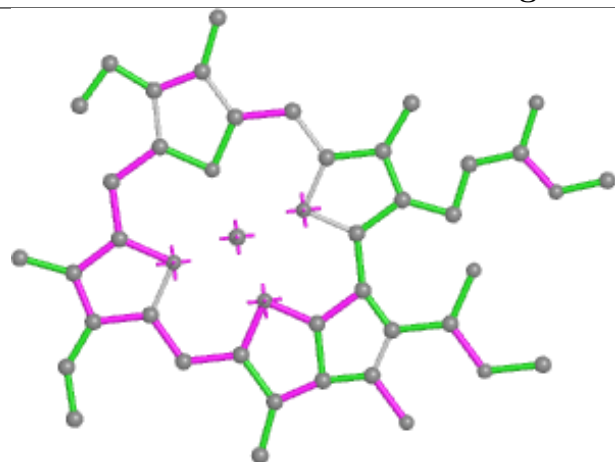


Torsions

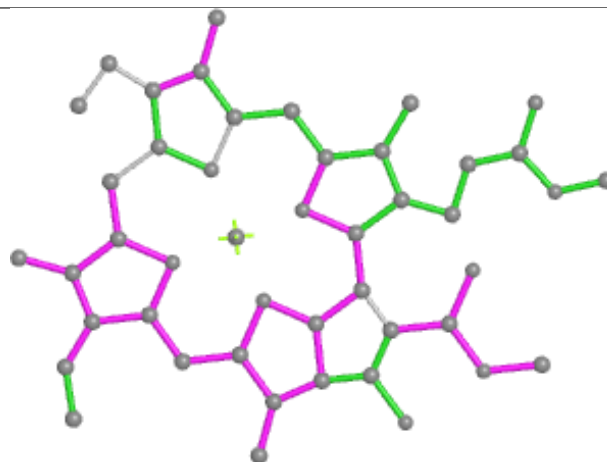


Rings

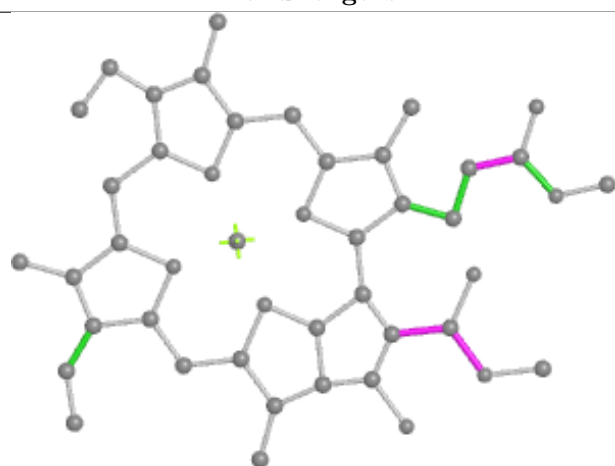
## Ligand CLA b 307



Bond lengths



Bond angles



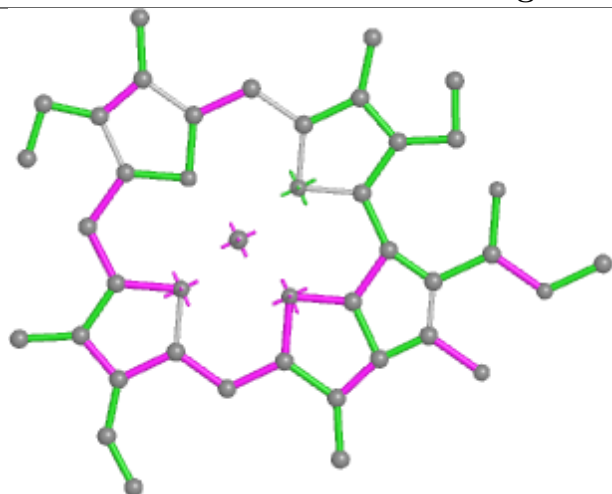
Torsions



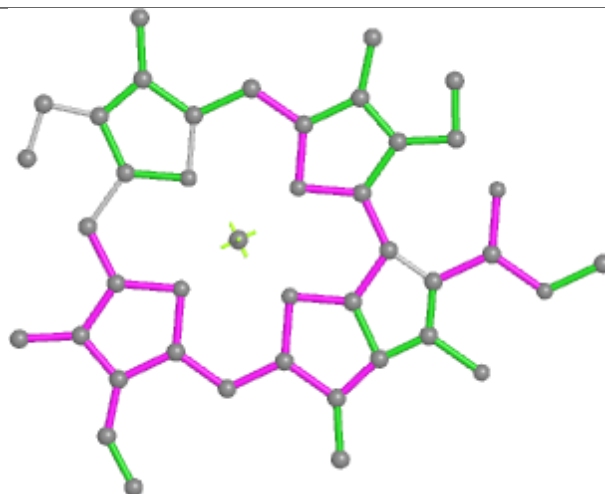
Rings



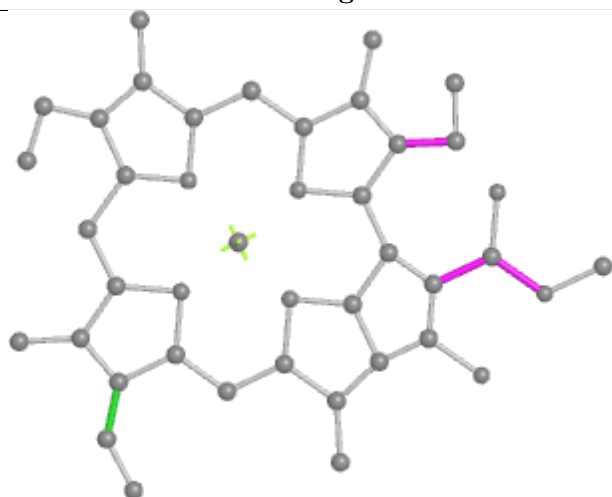
## Ligand CLA J 105



Bond lengths



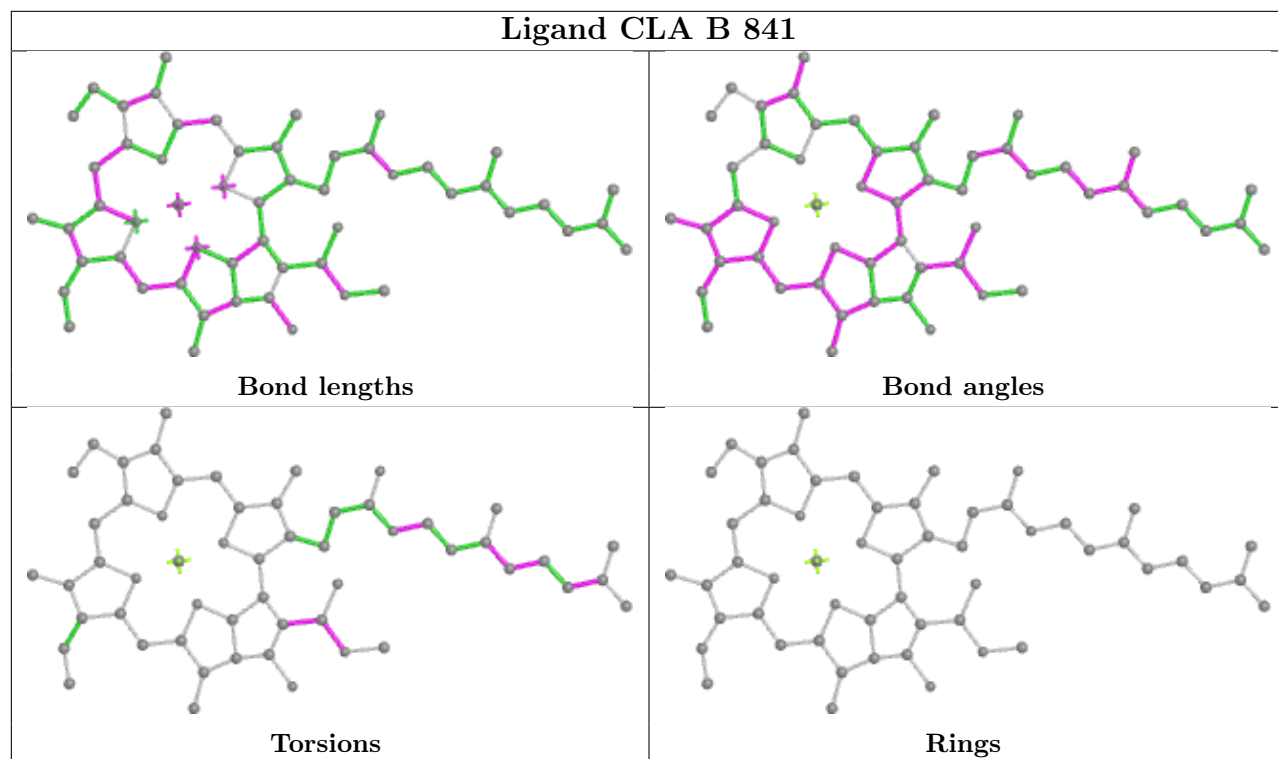
Bond angles

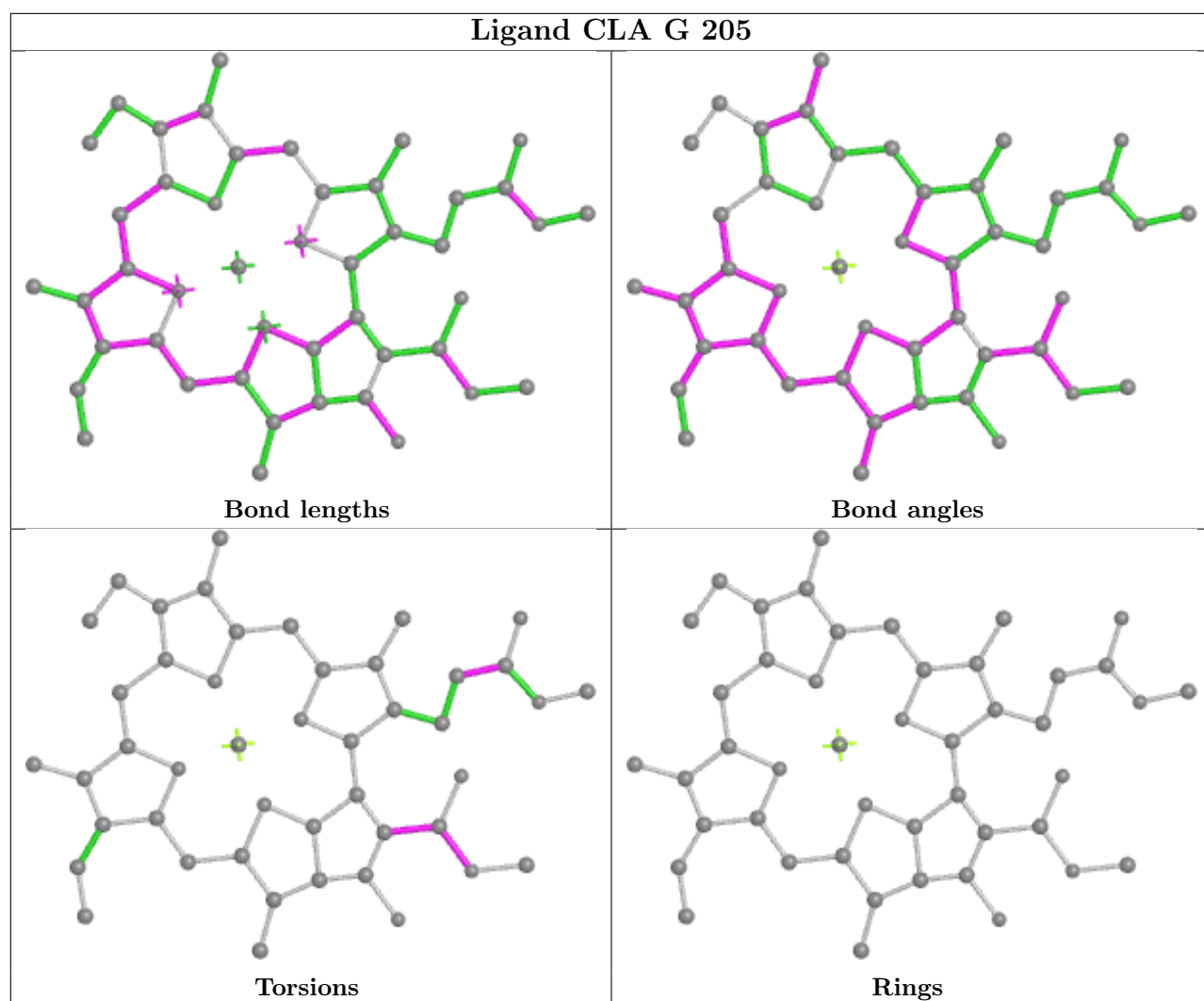


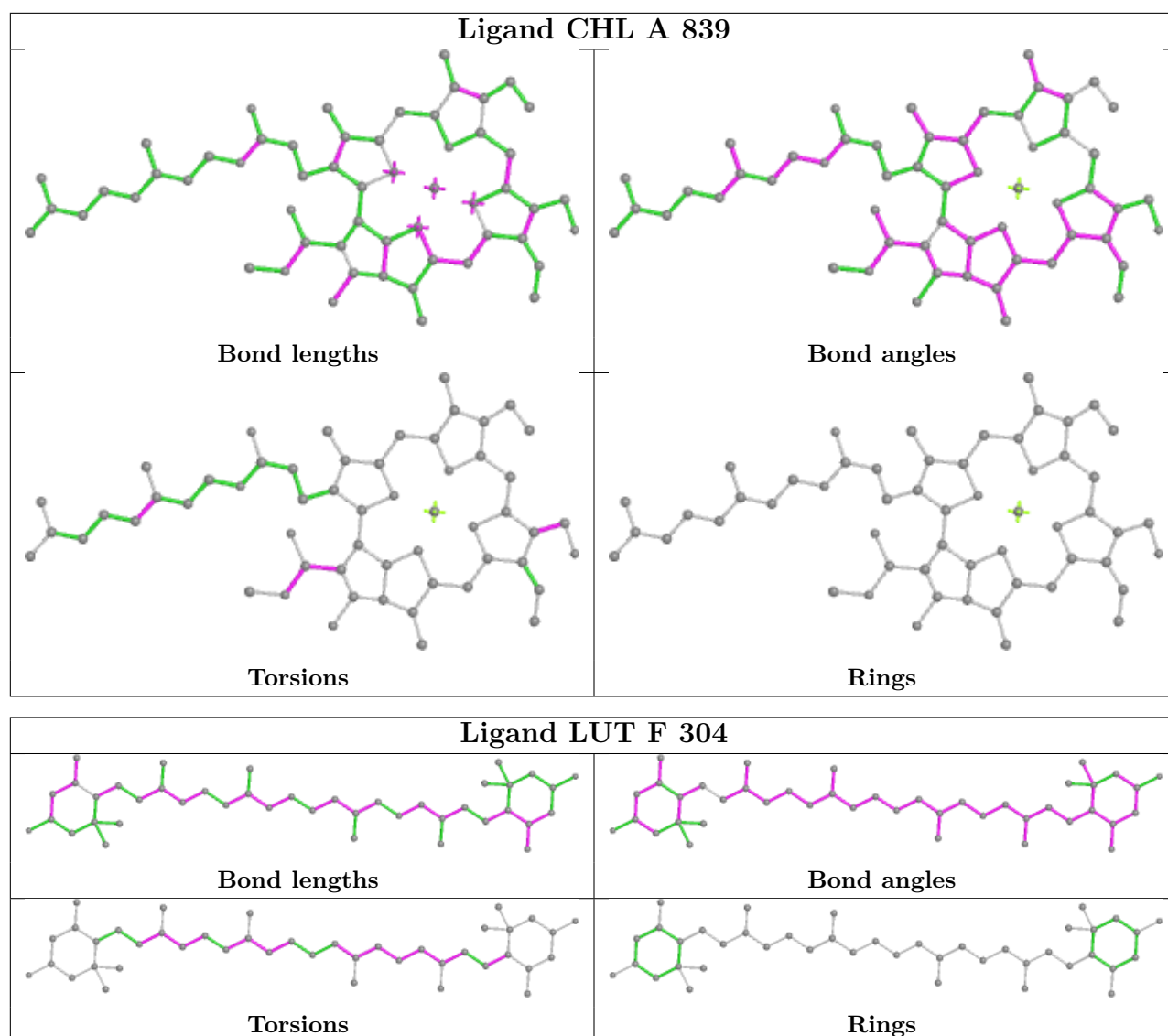
Torsions



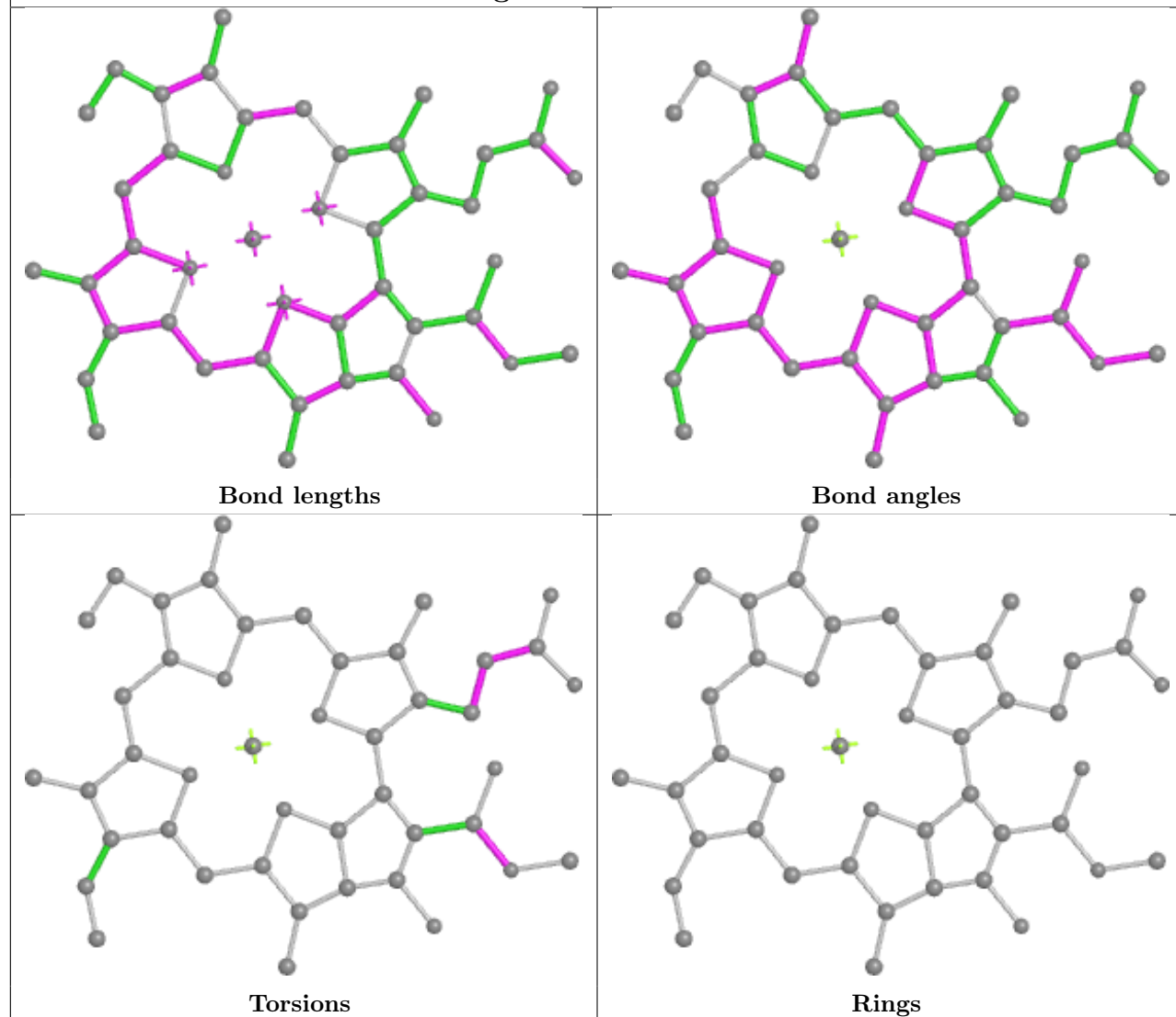
Rings



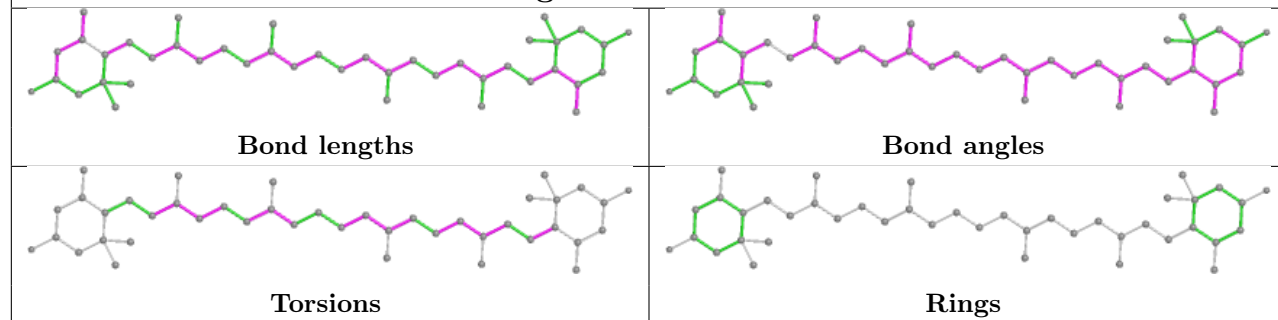




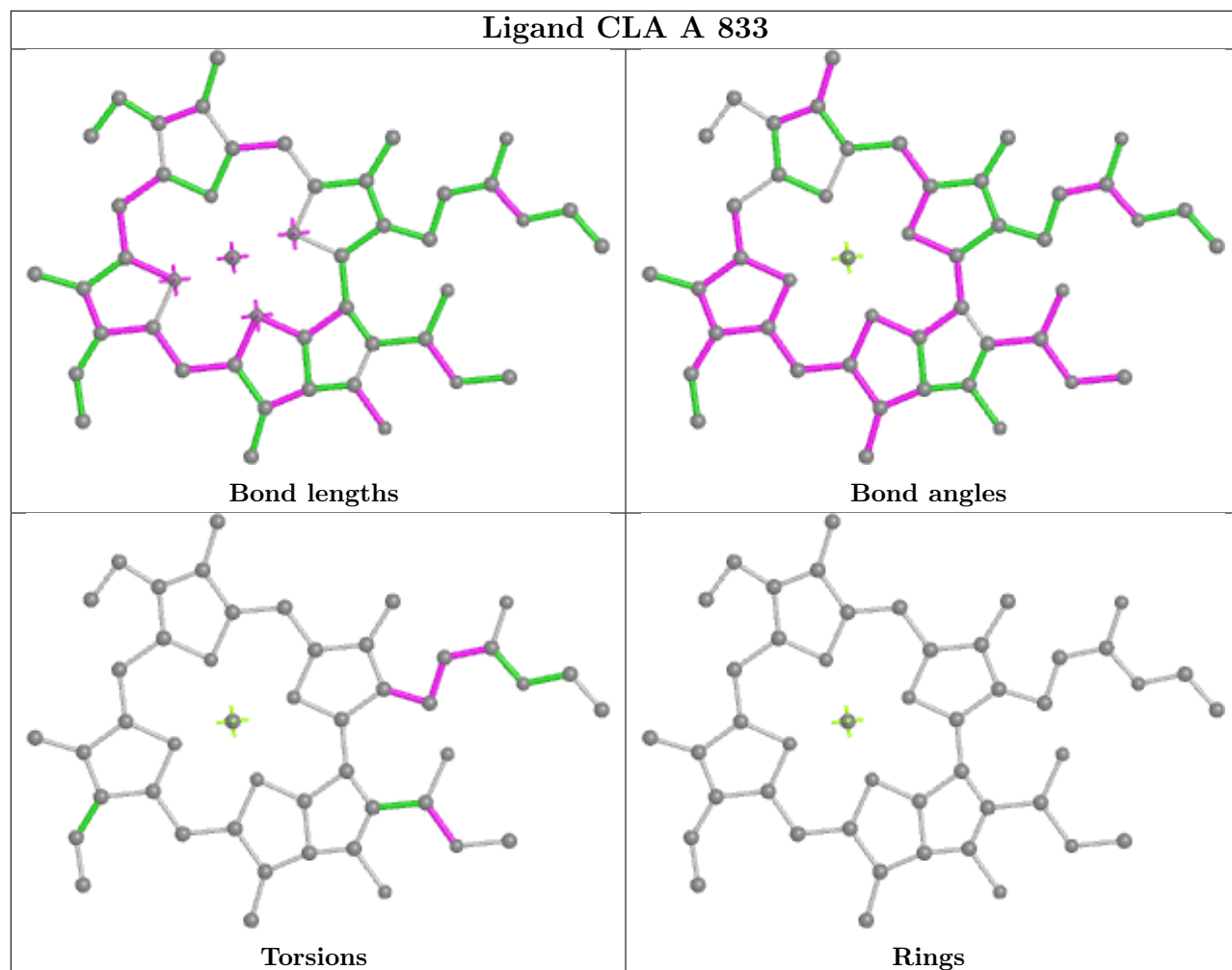
## Ligand CLA 5 314



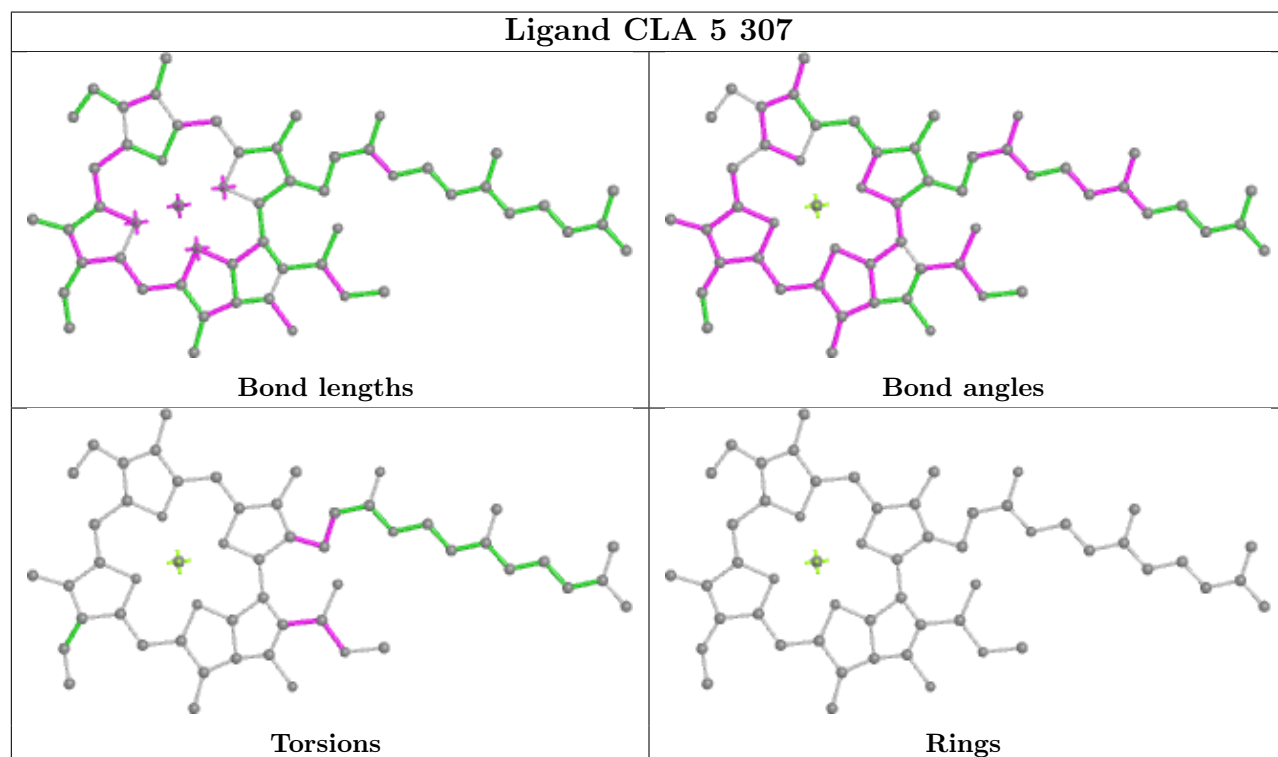
## Ligand LUT 4 303



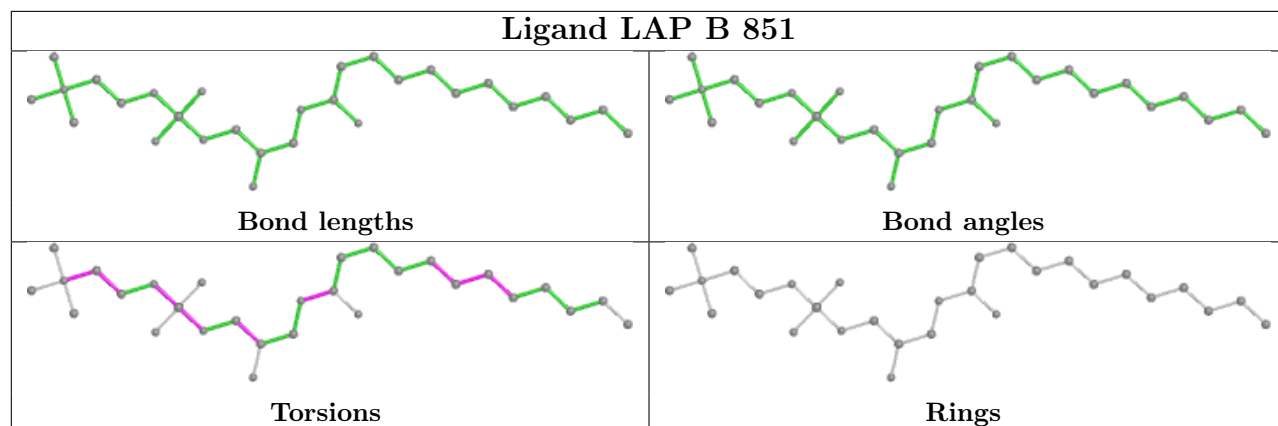
## Ligand CLA A 833



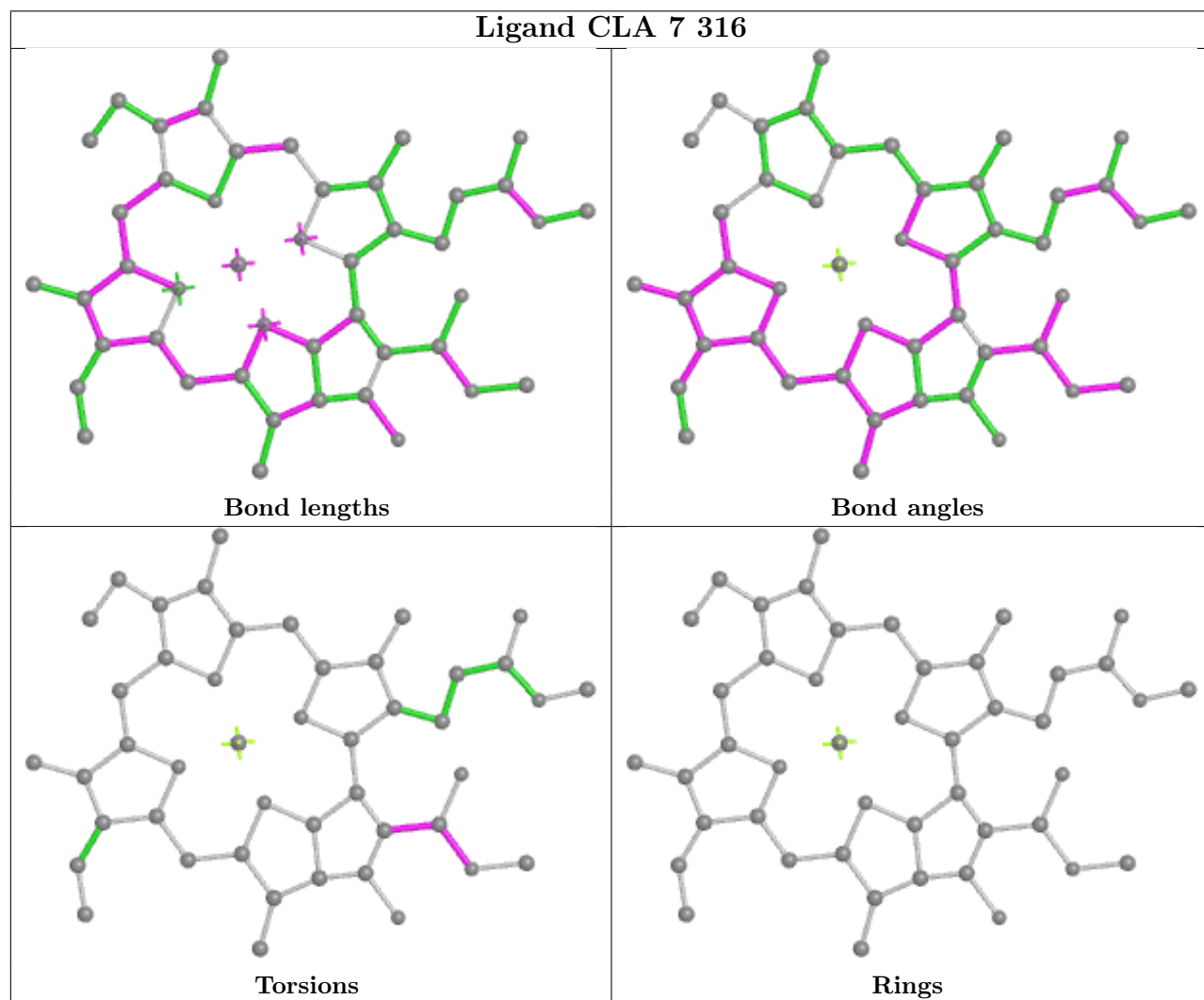
## Ligand CLA 5 307

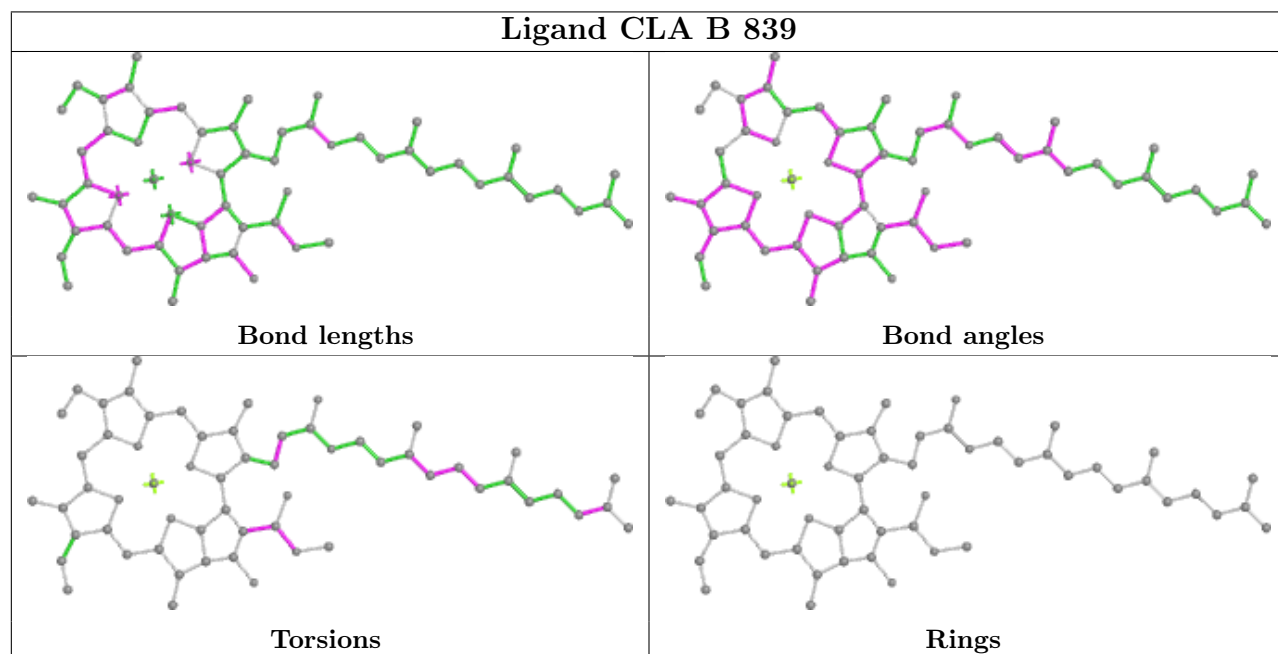
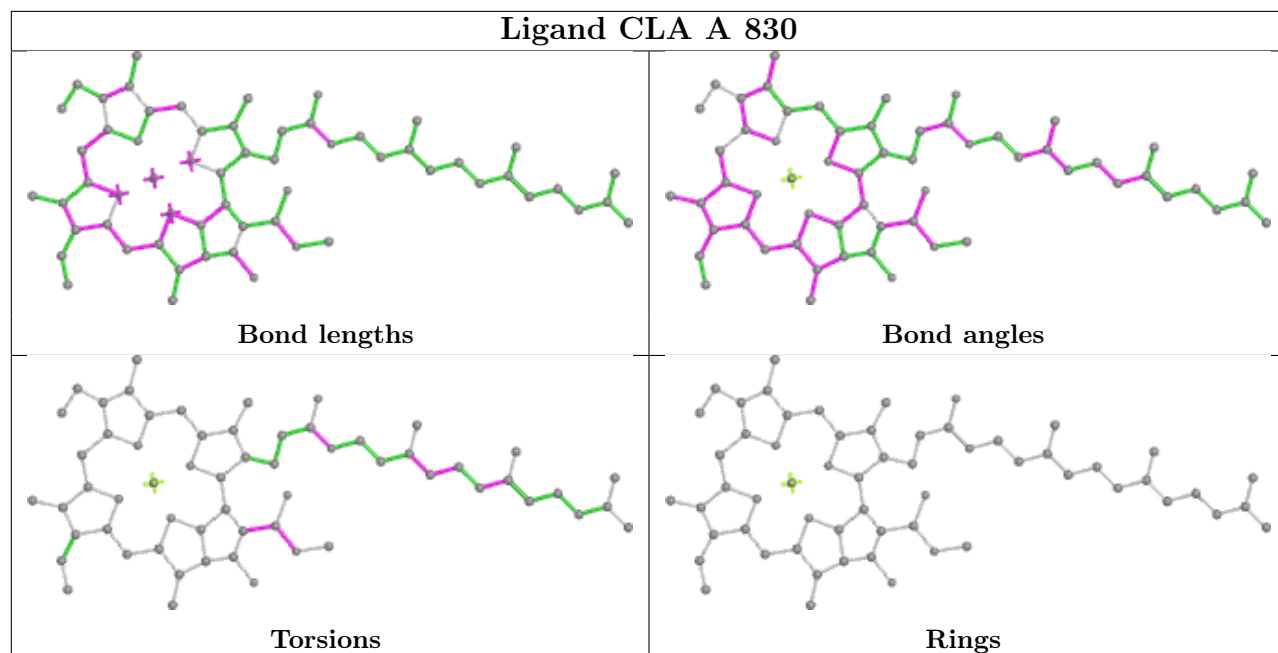


## Ligand LAP B 851

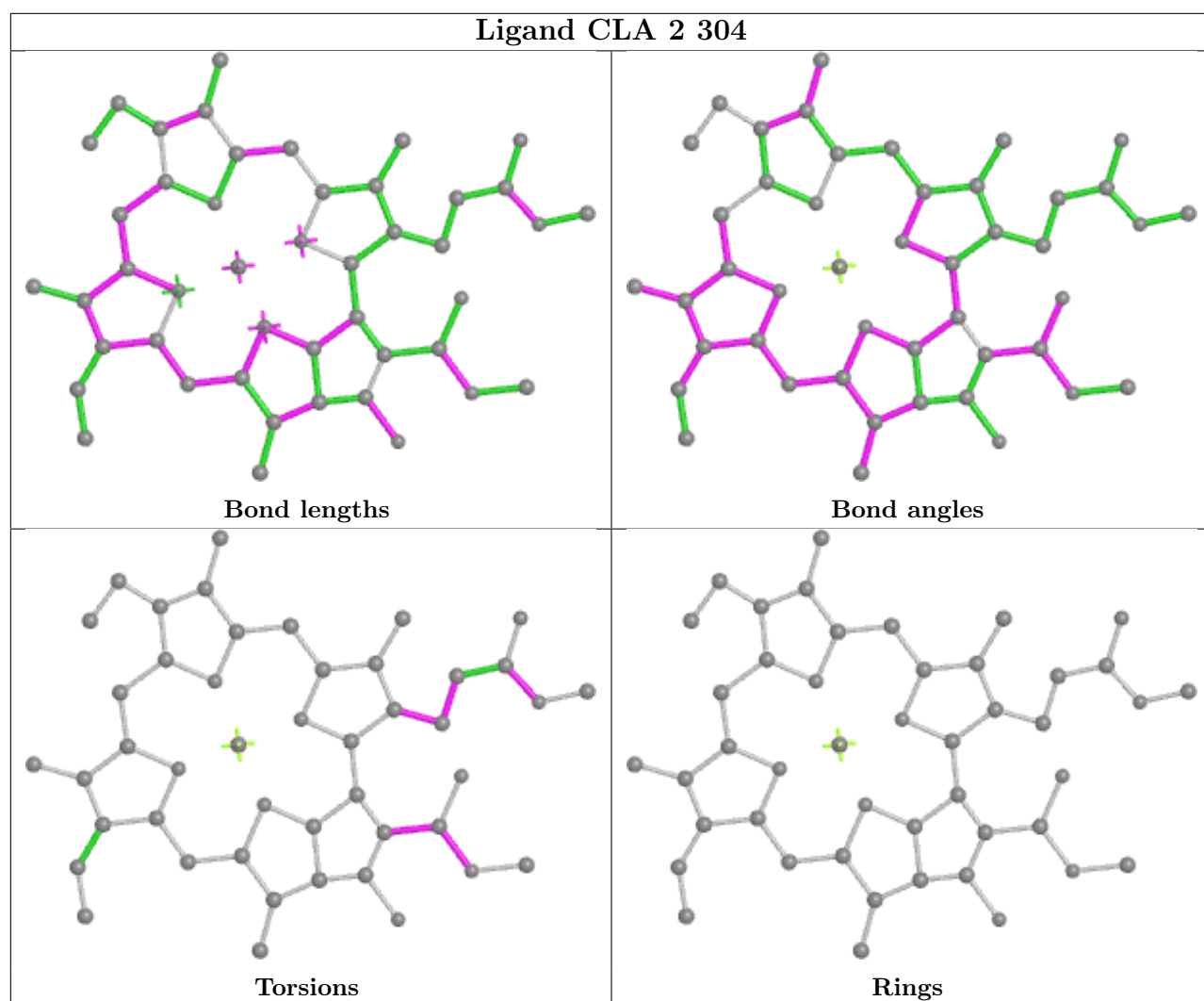
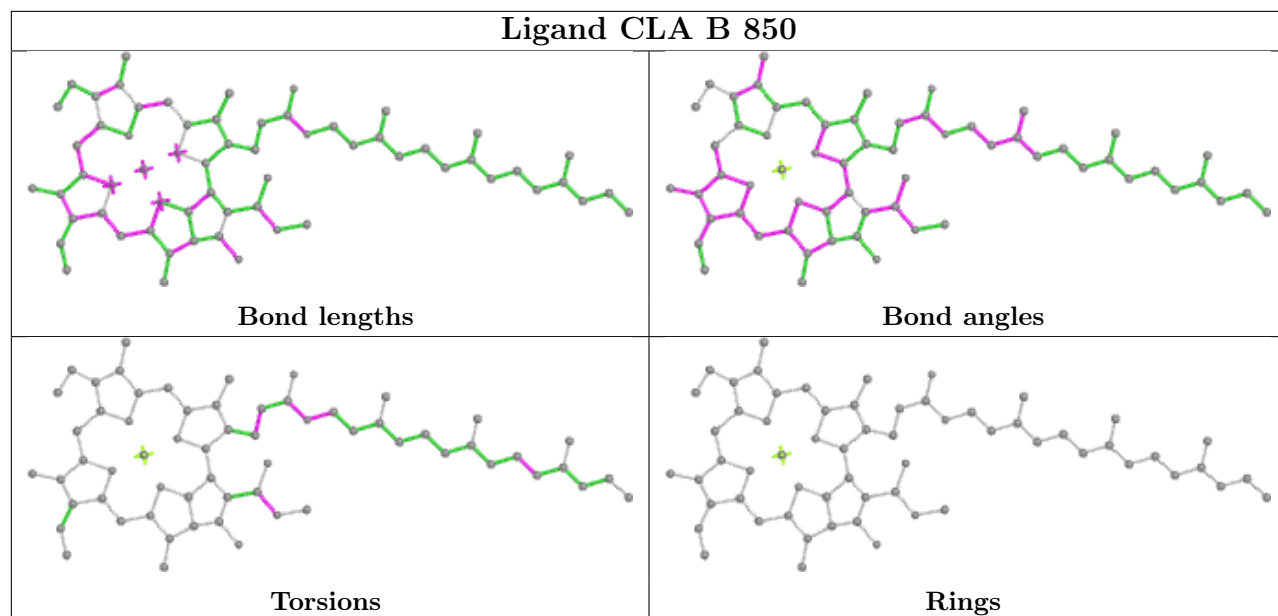


## Ligand CLA 7 316

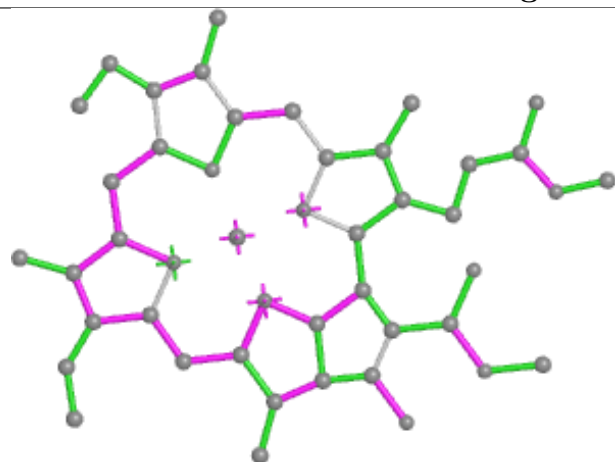




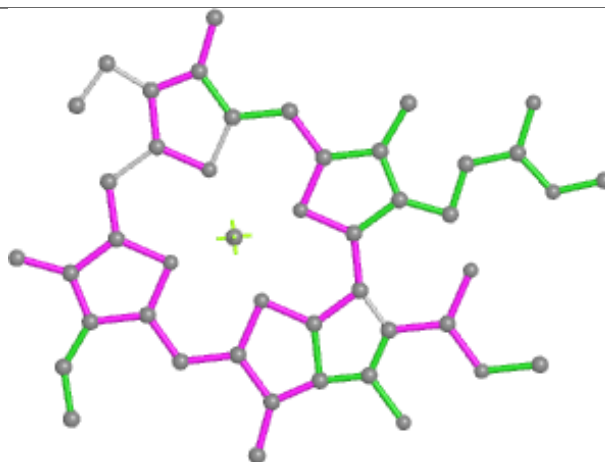




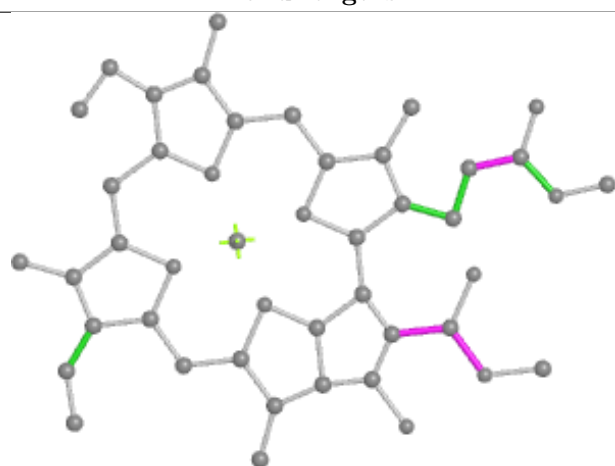
## Ligand CLA 3 308



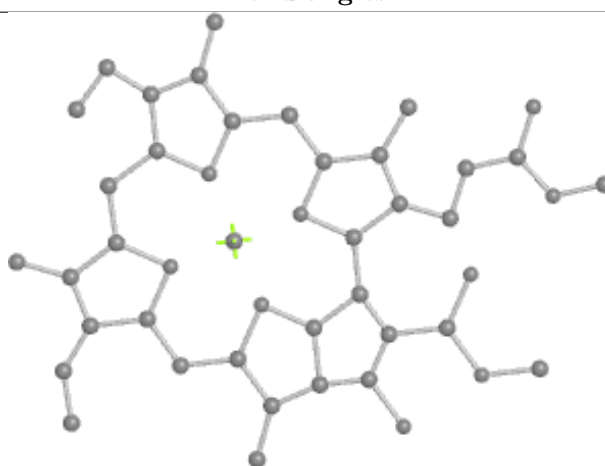
Bond lengths



Bond angles

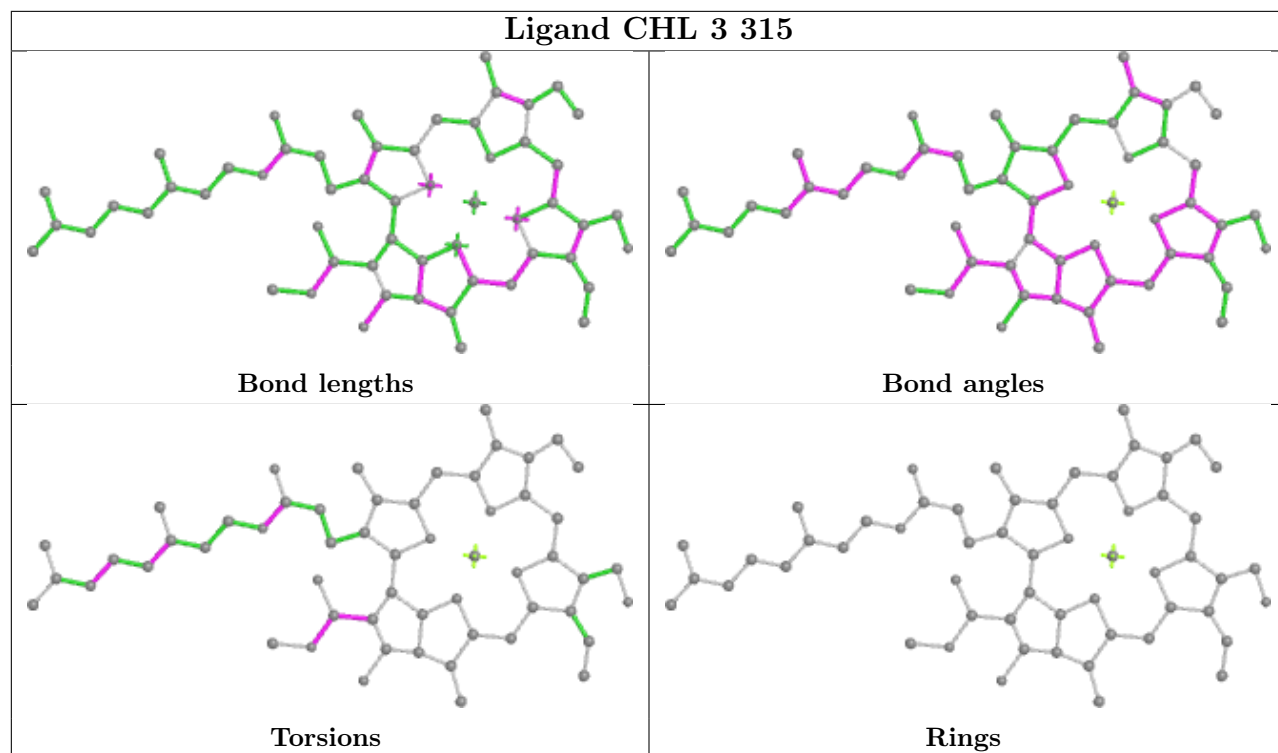


Torsions

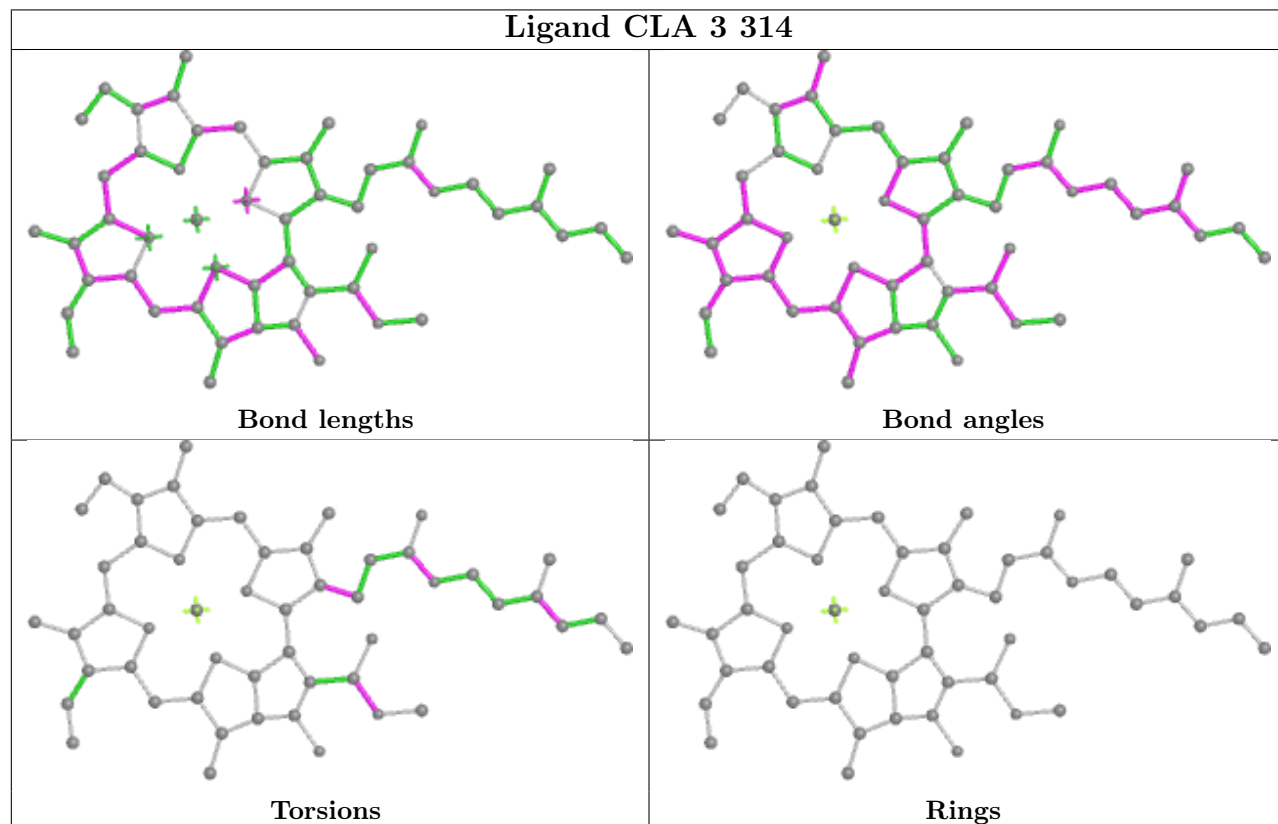


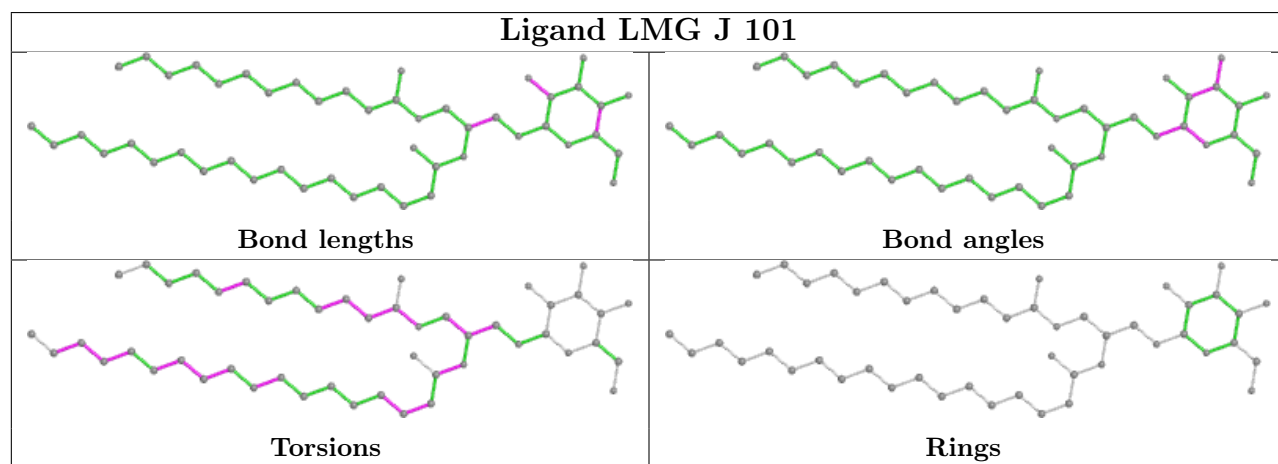
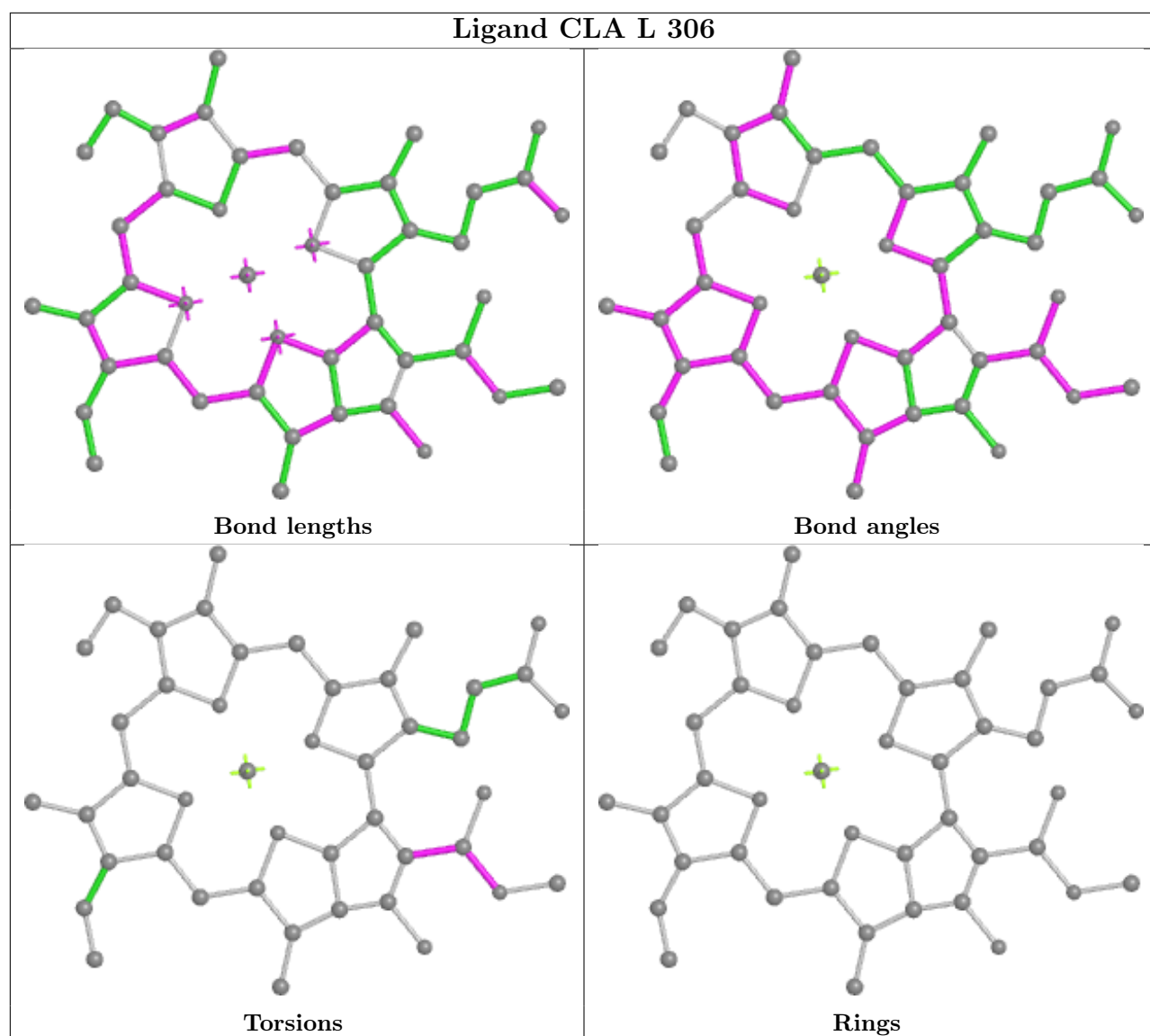
Rings

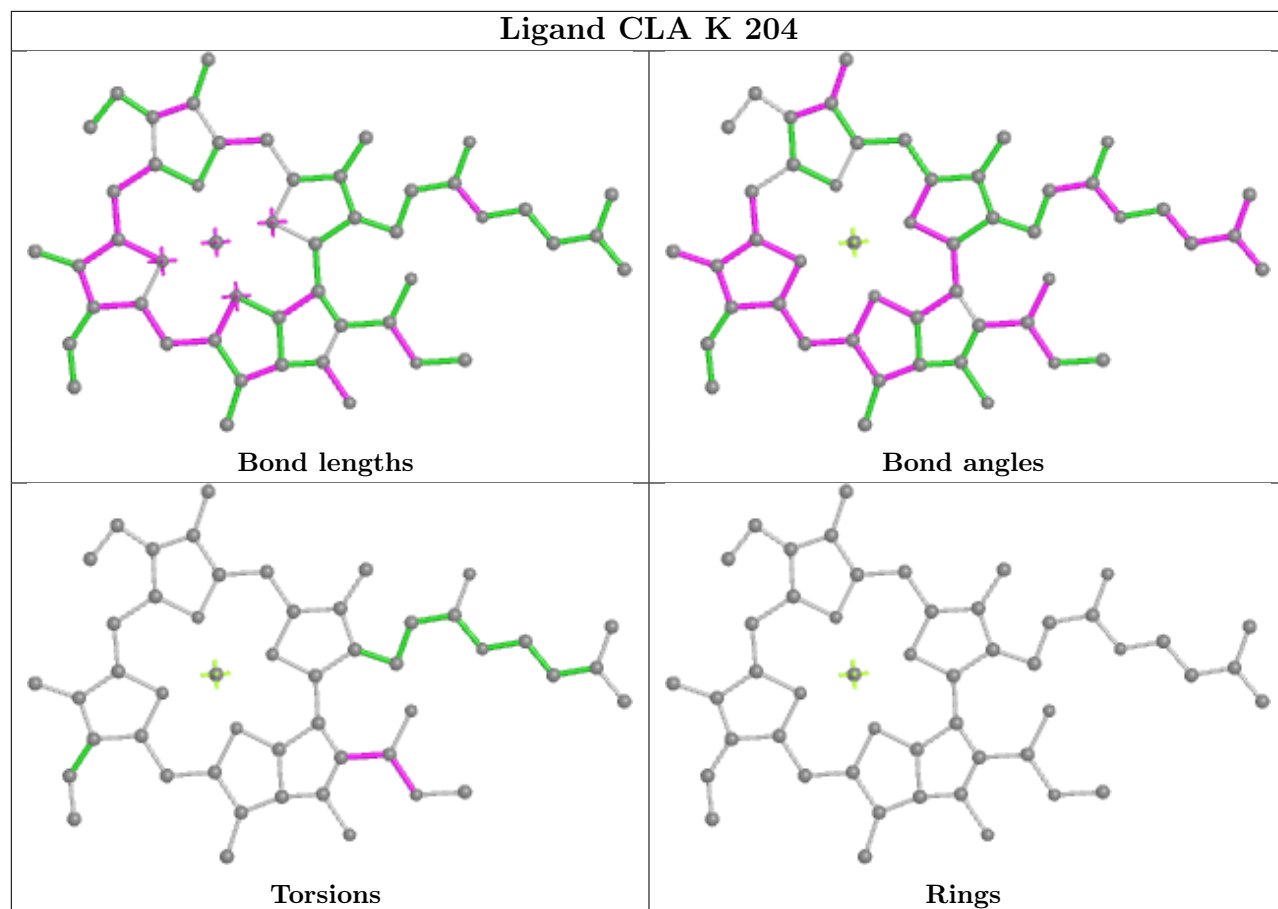
## Ligand CHL 3 315



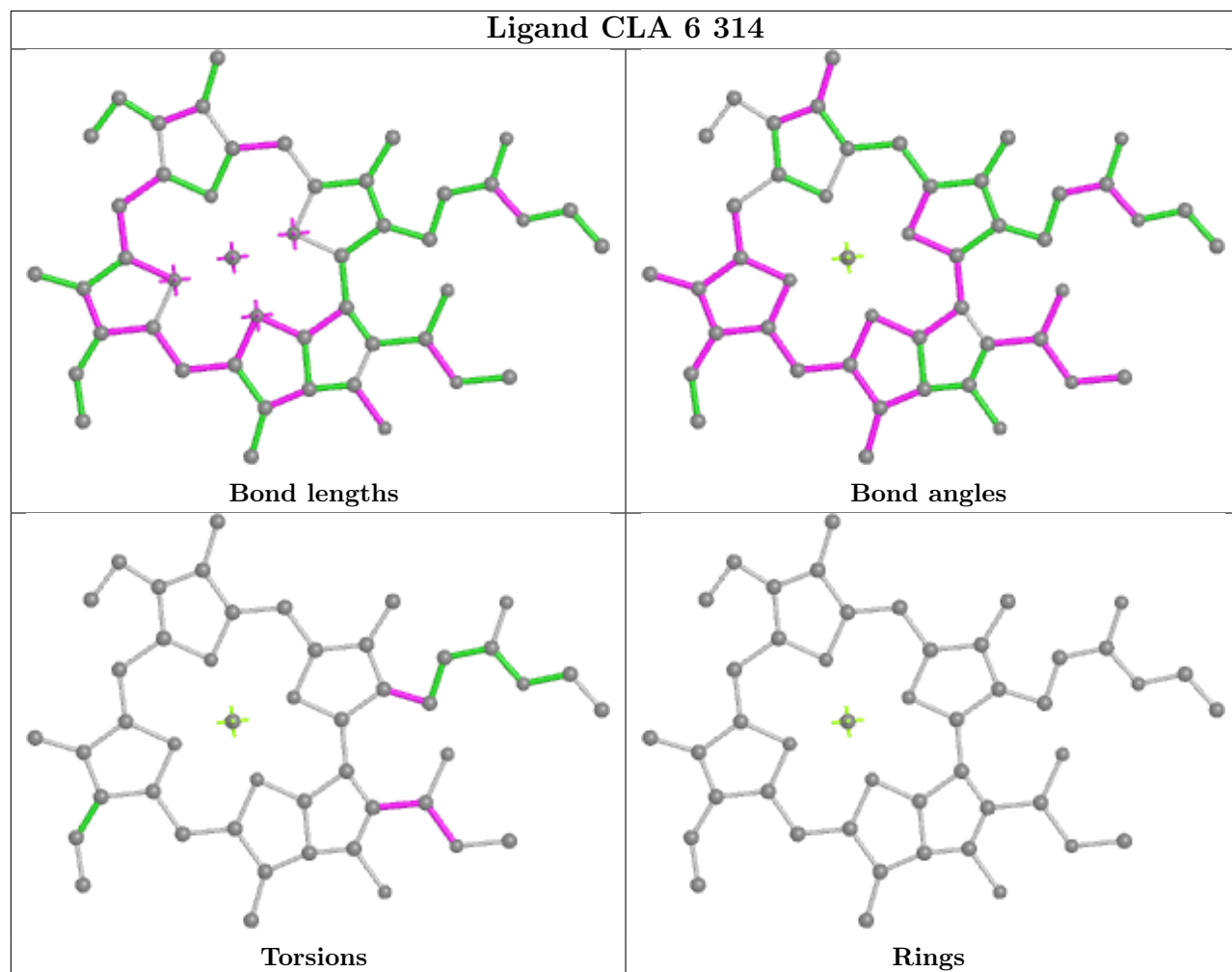
## Ligand CLA 3 314



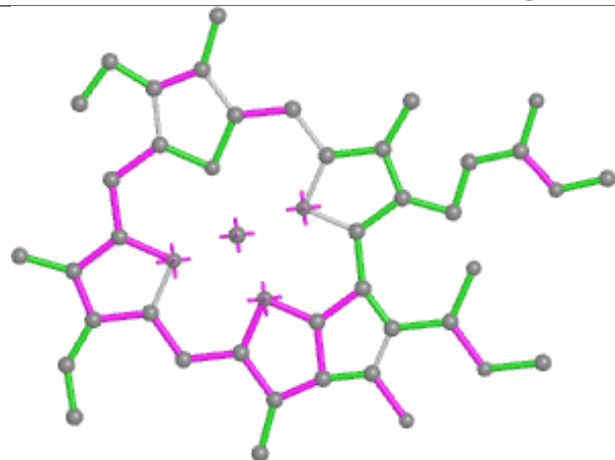




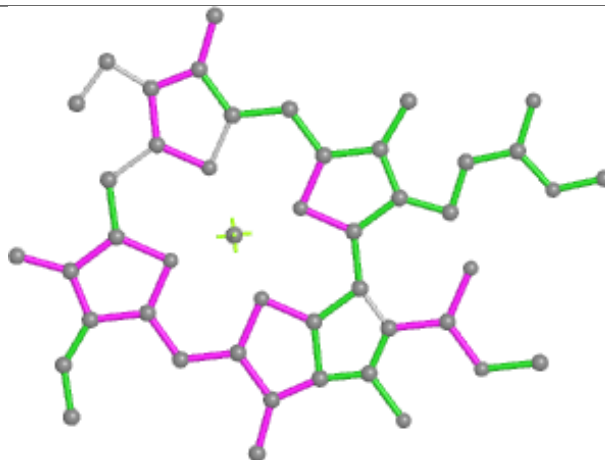
## Ligand CLA 6 314



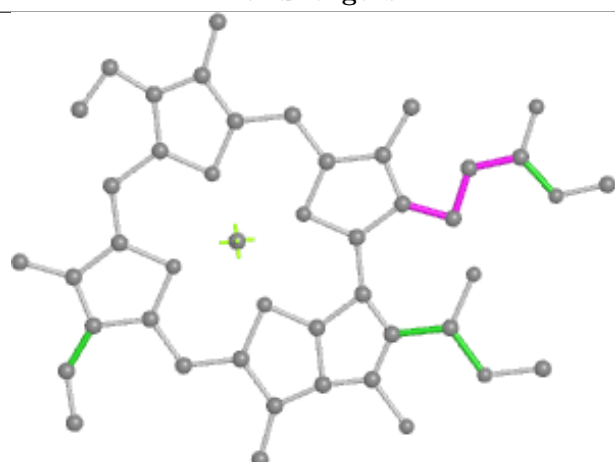
## Ligand CLA 6 306



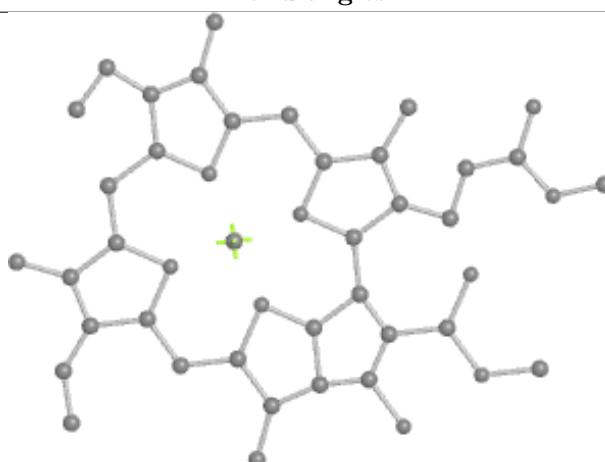
Bond lengths



Bond angles

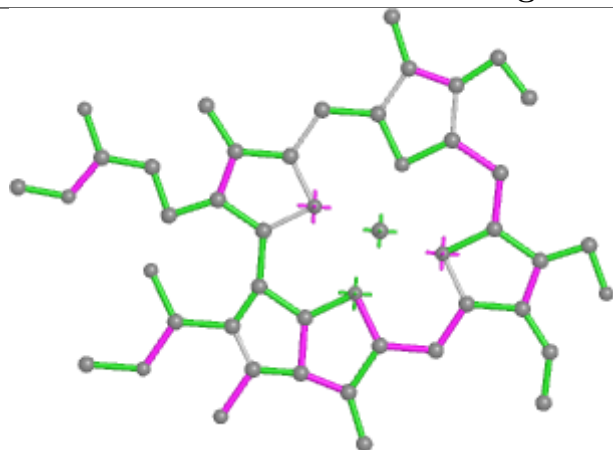


Torsions

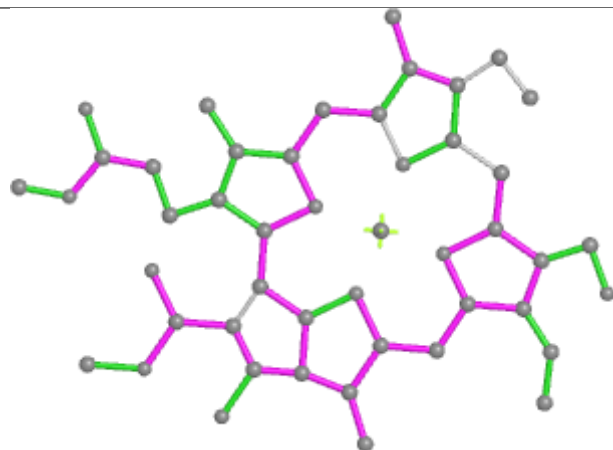


Rings

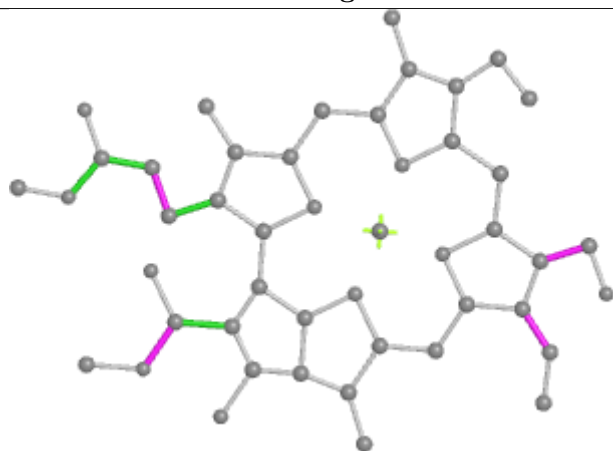
## Ligand CHL 5 317



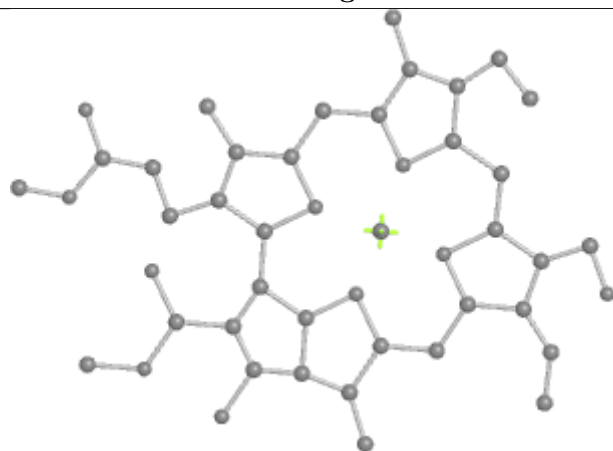
Bond lengths



Bond angles



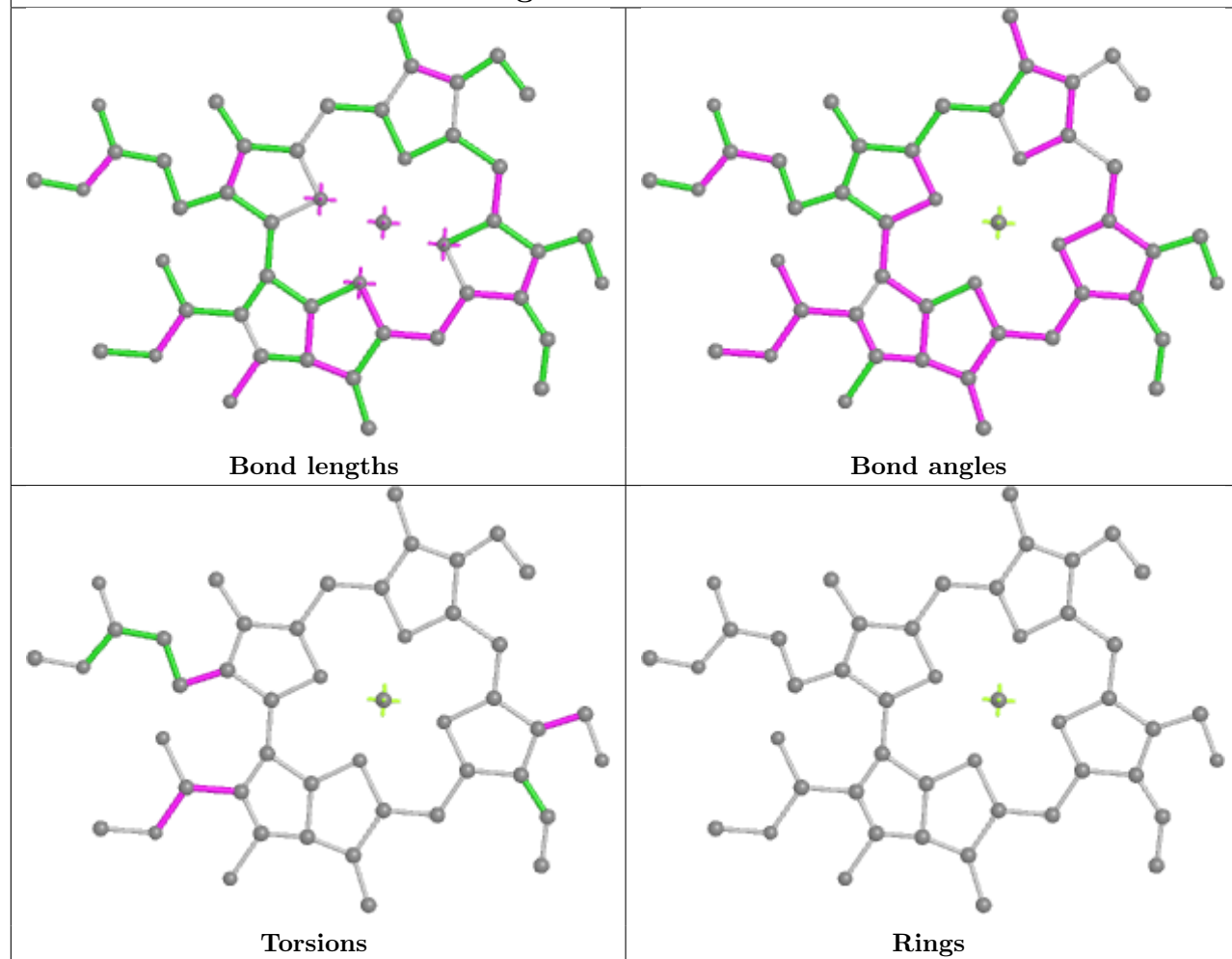
Torsions



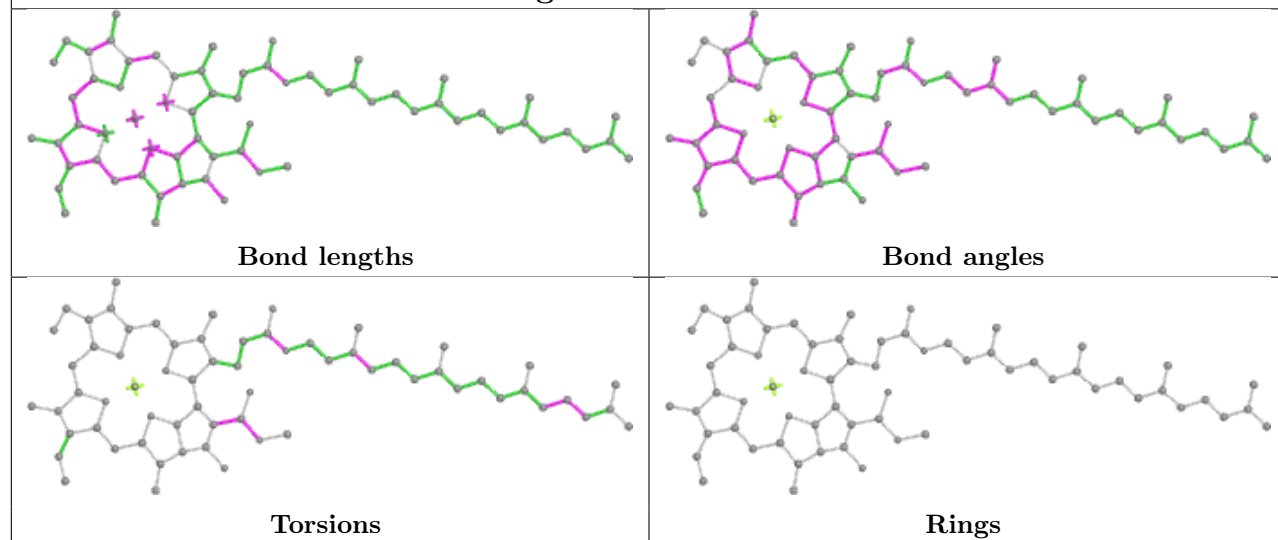
Rings



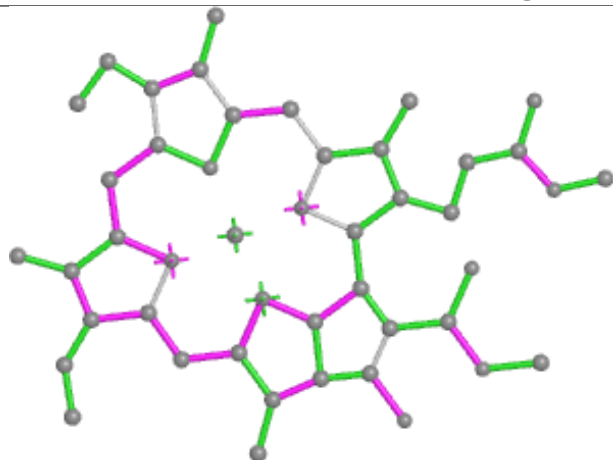
## Ligand CHL 6 317



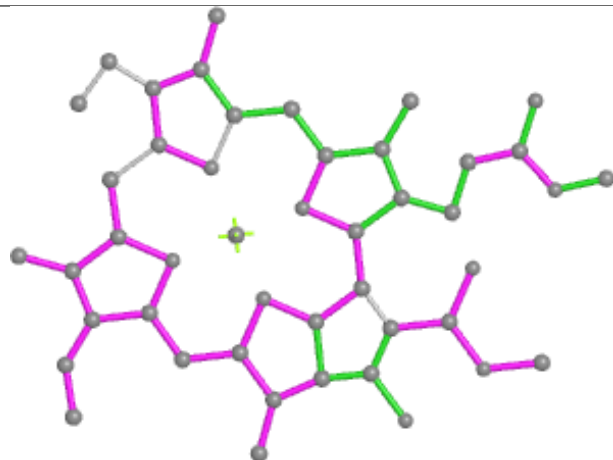
## Ligand CLA 3 312



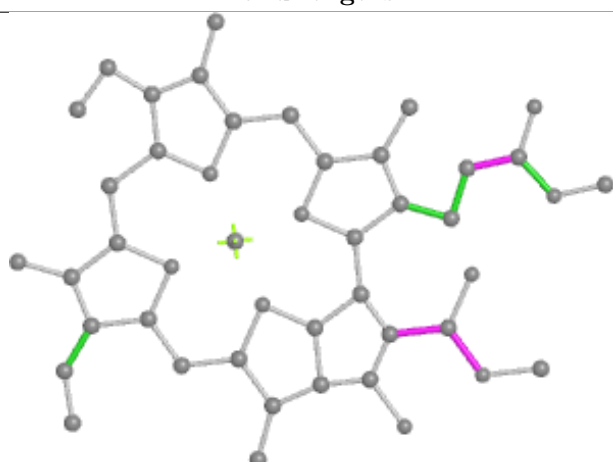
## Ligand CLA 5 311



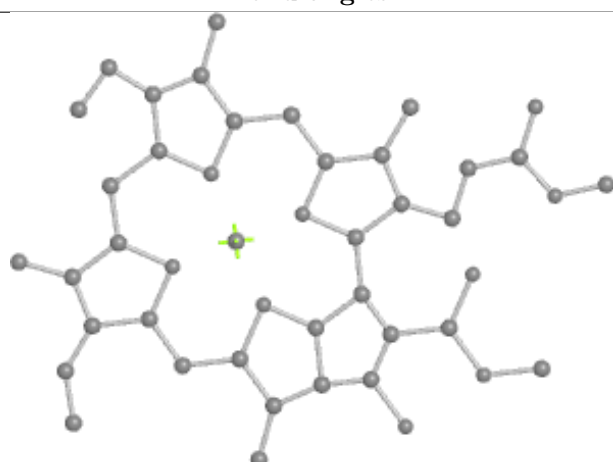
Bond lengths



Bond angles

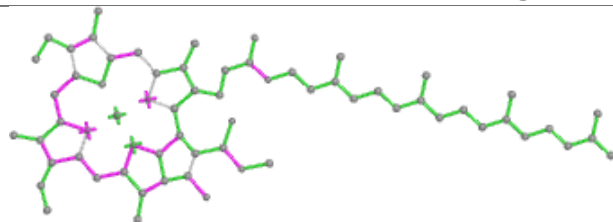


Torsions

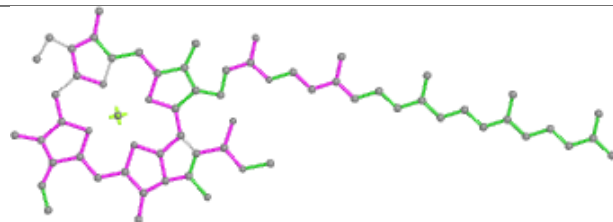


Rings

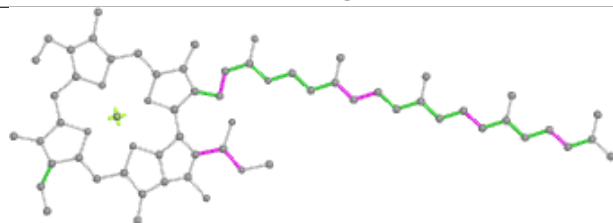
## Ligand CLA B 832



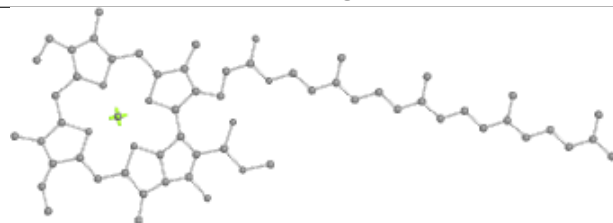
Bond lengths



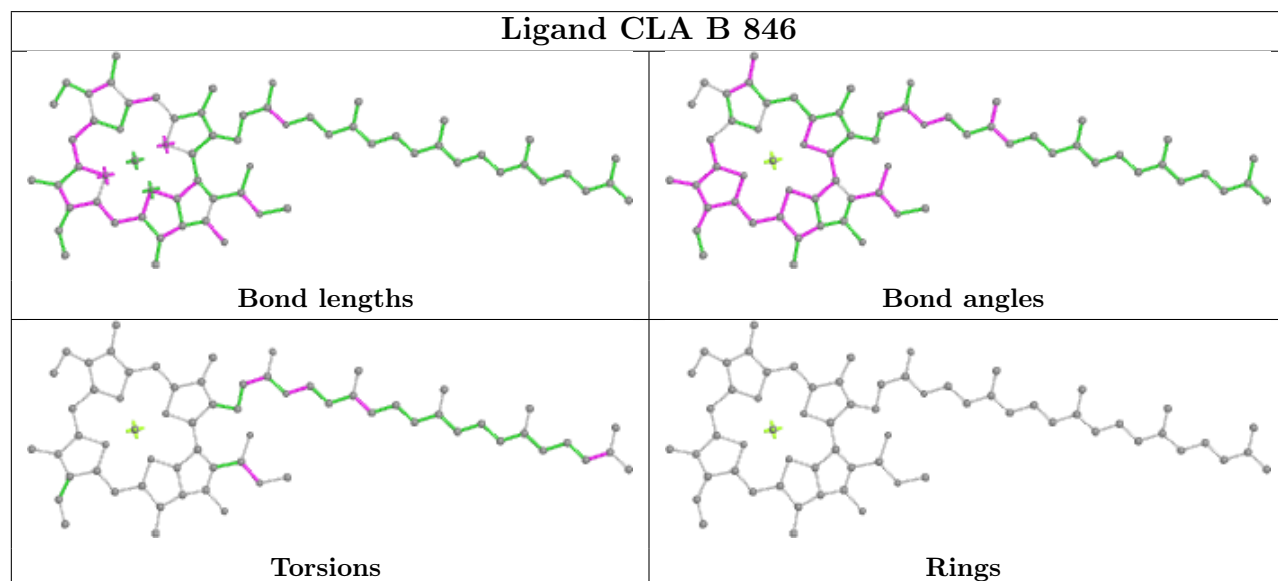
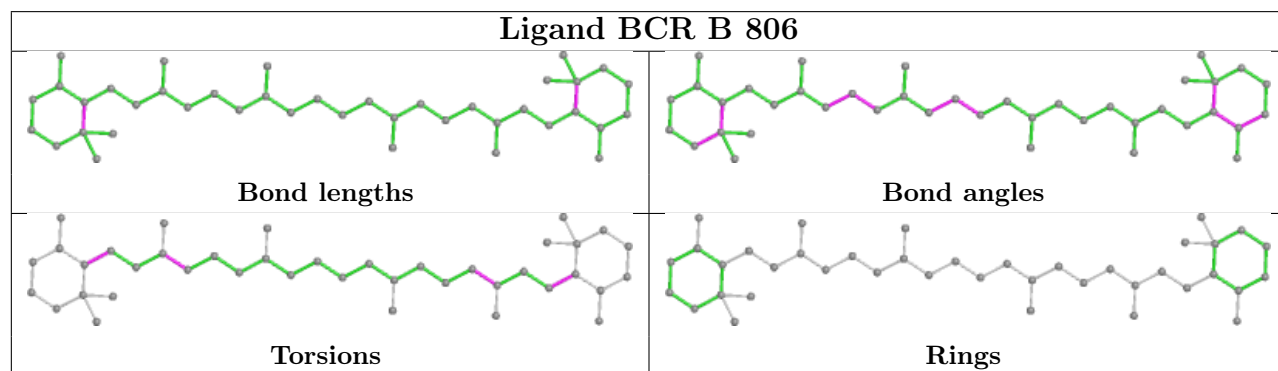
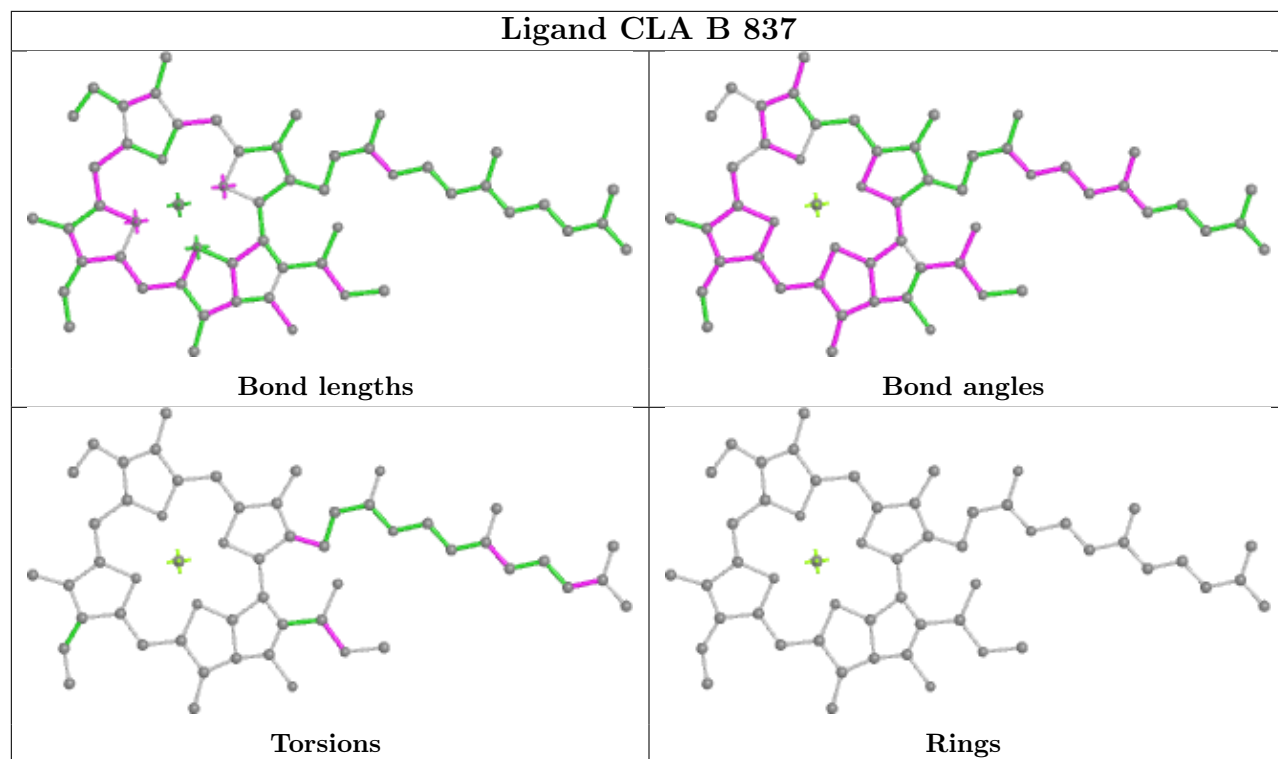
Bond angles

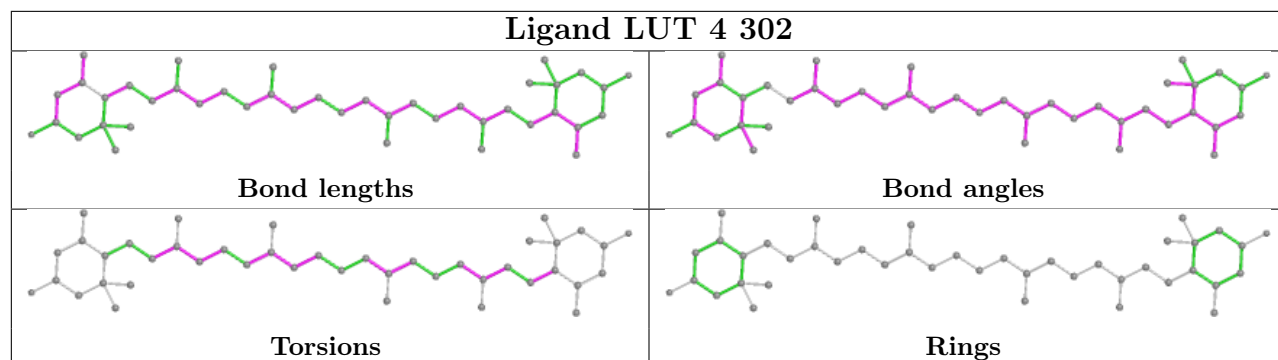
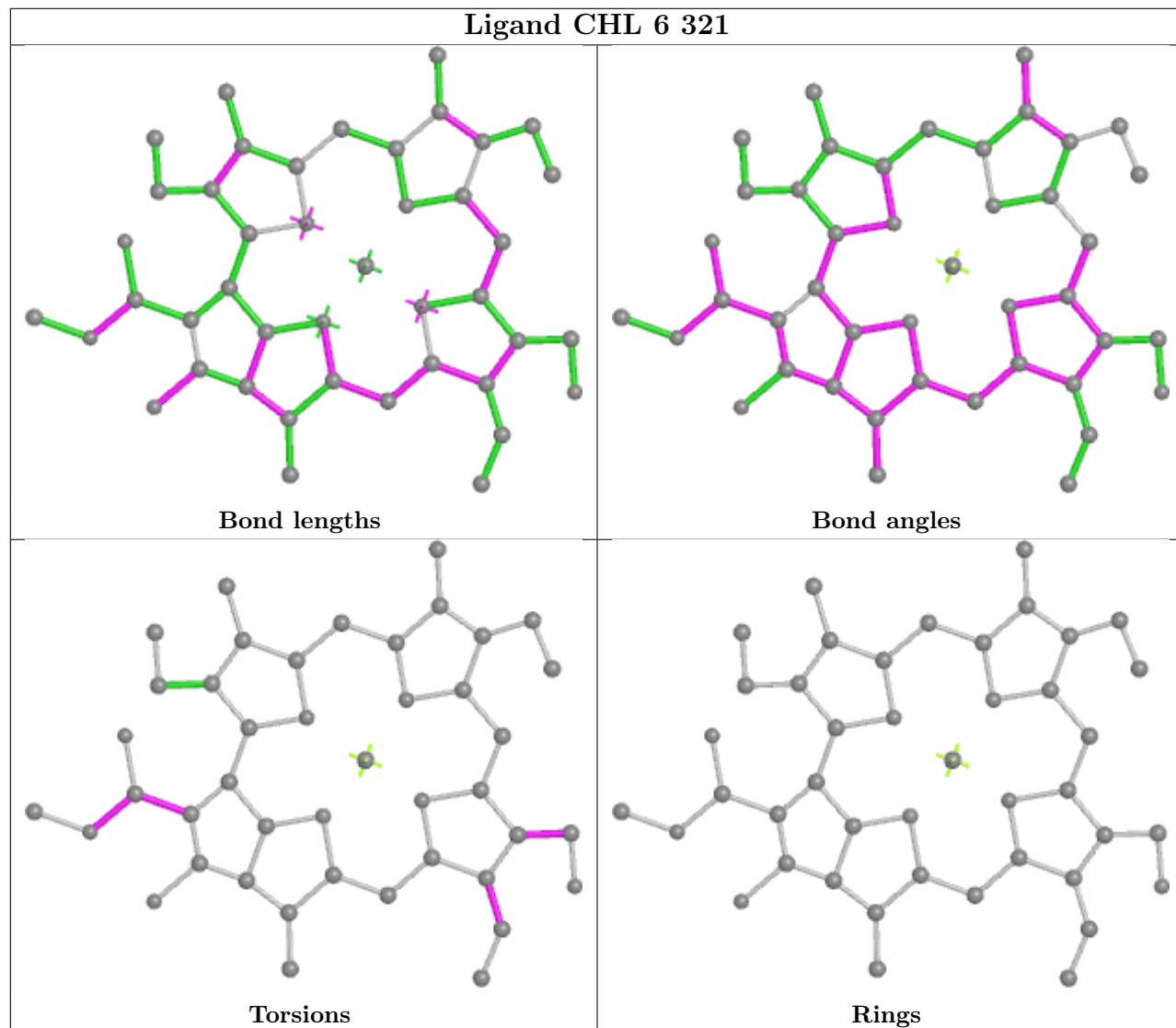


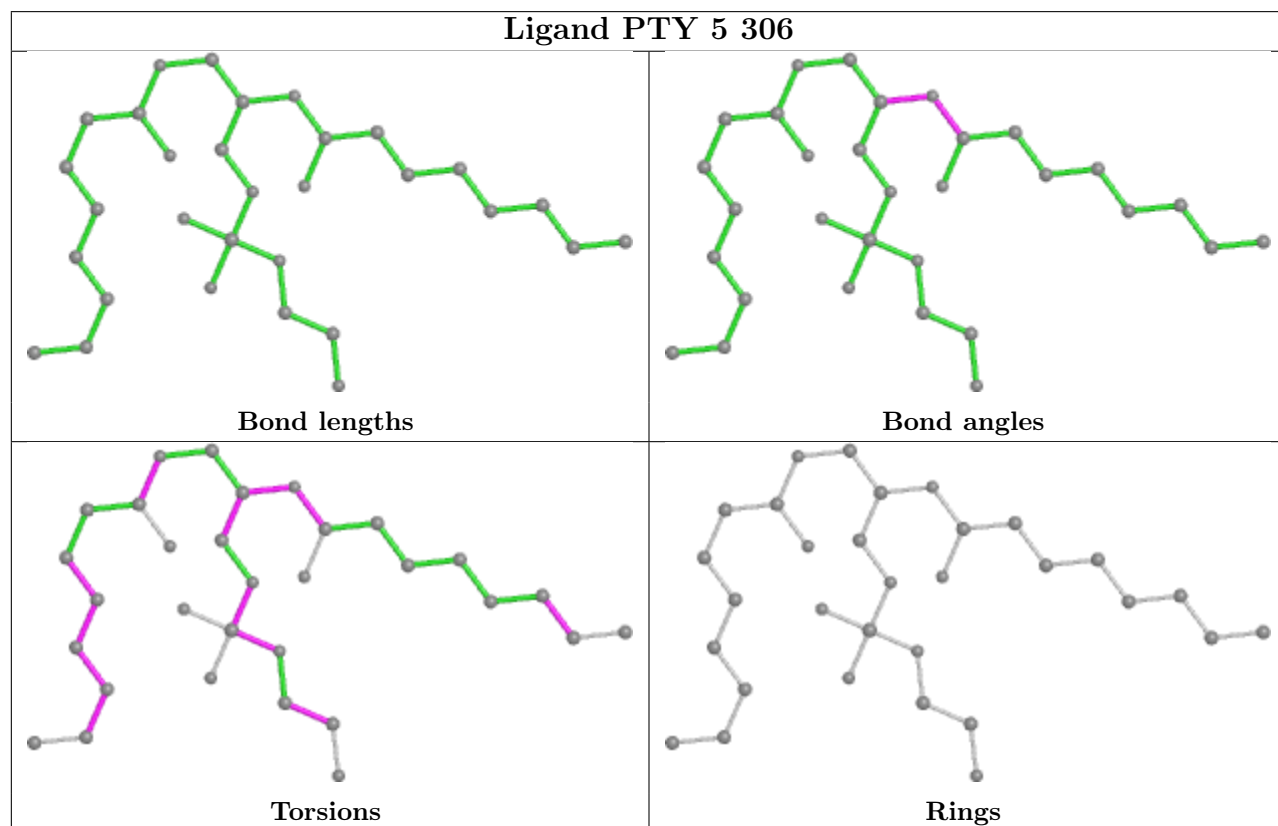
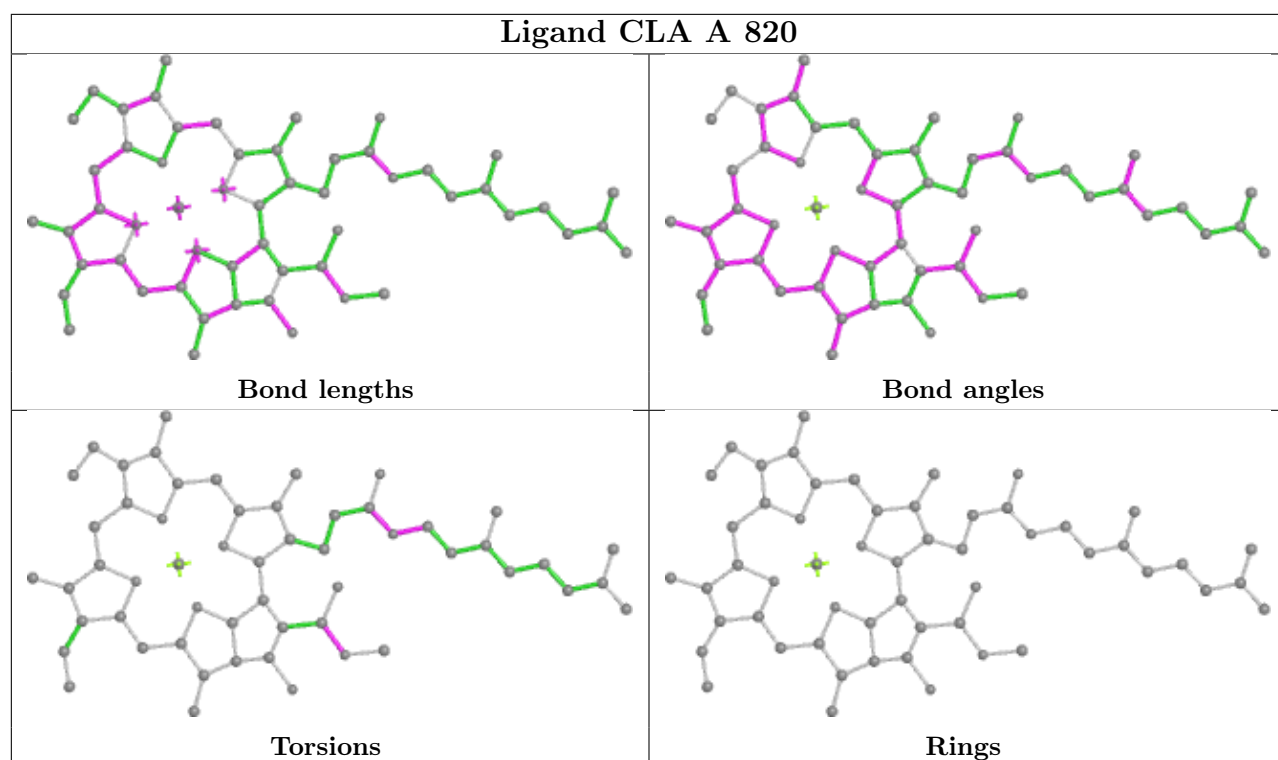
Torsions



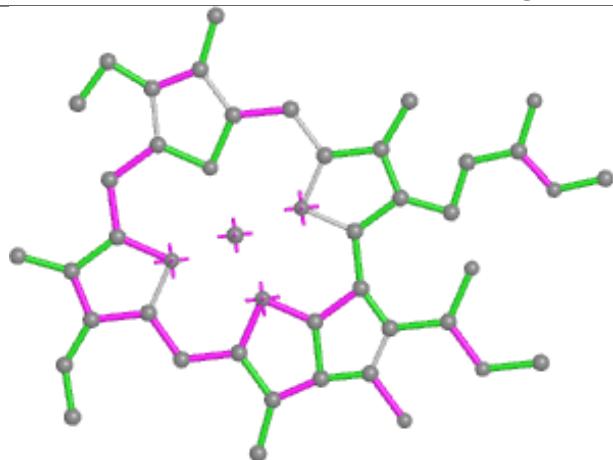
Rings



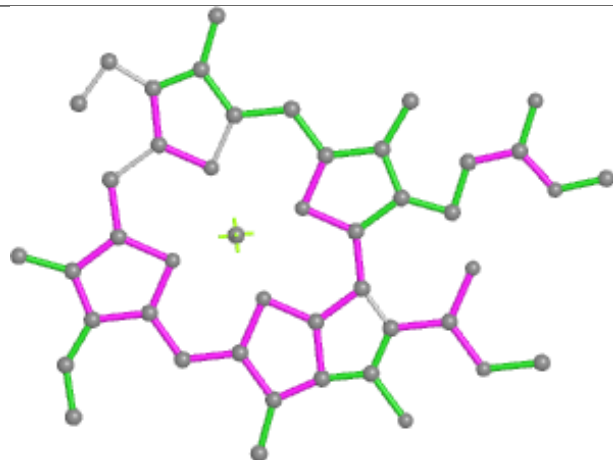
**Ligand LUT 4 302****Ligand CHL 6 321**



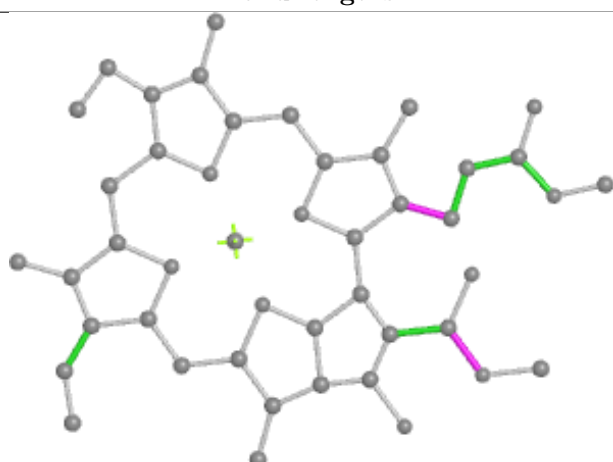
## Ligand CLA 7 322



Bond lengths



Bond angles

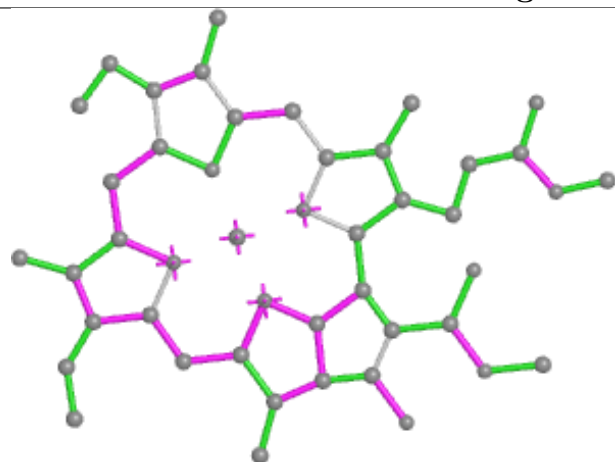


Torsions

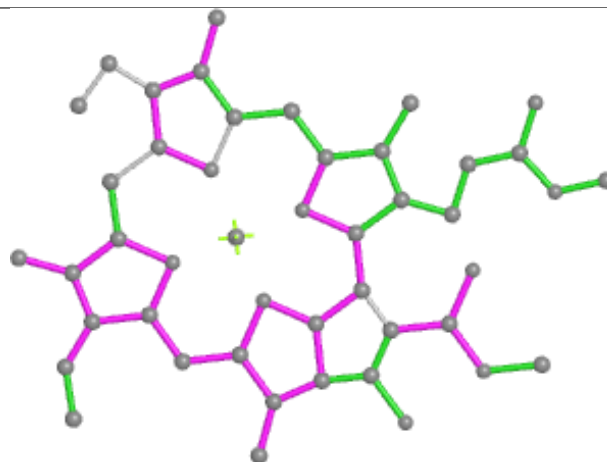


Rings

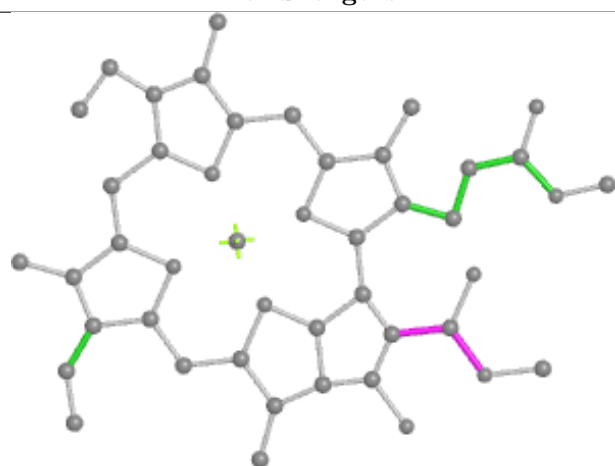
## Ligand CLA B 838



Bond lengths



Bond angles

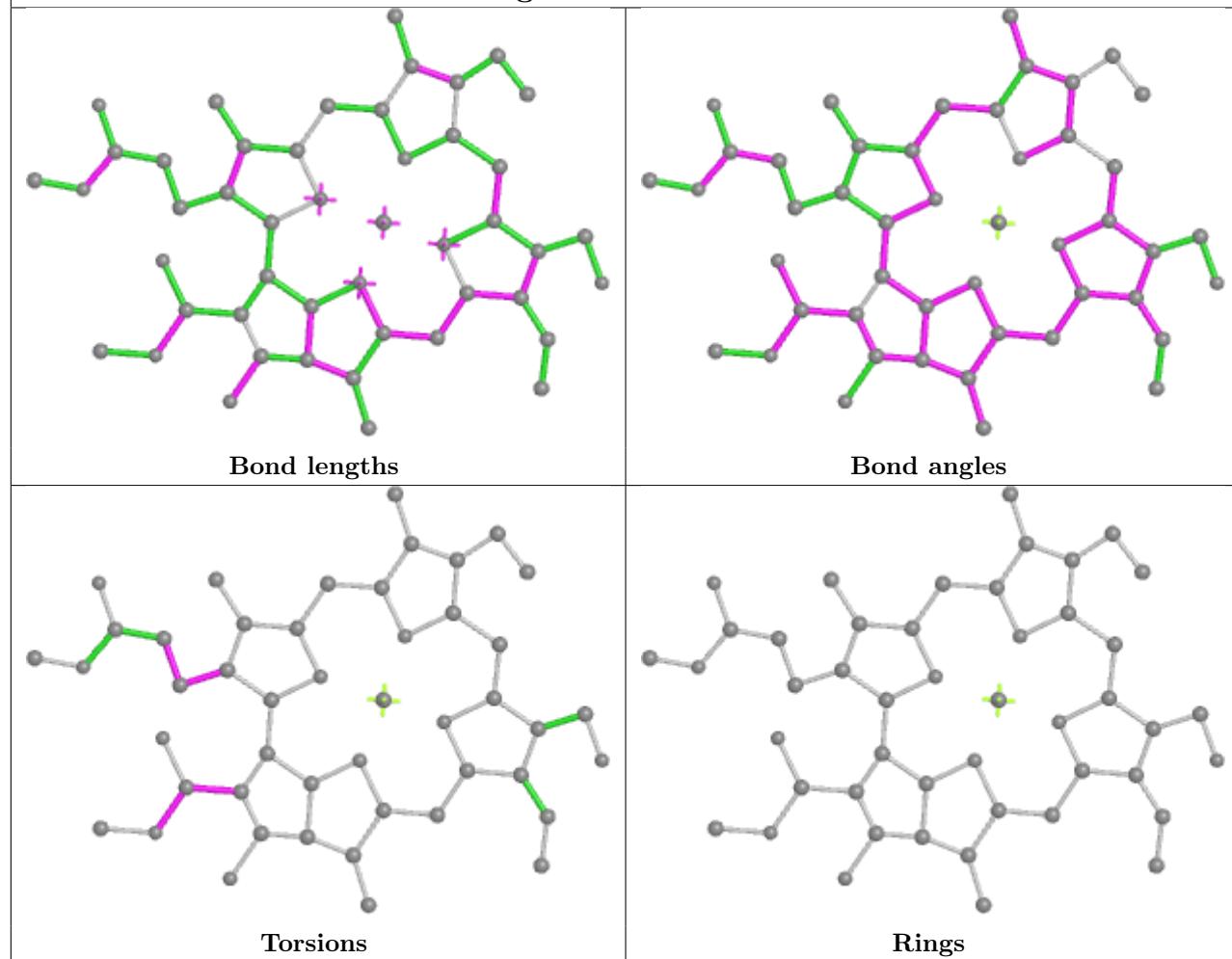


Torsions

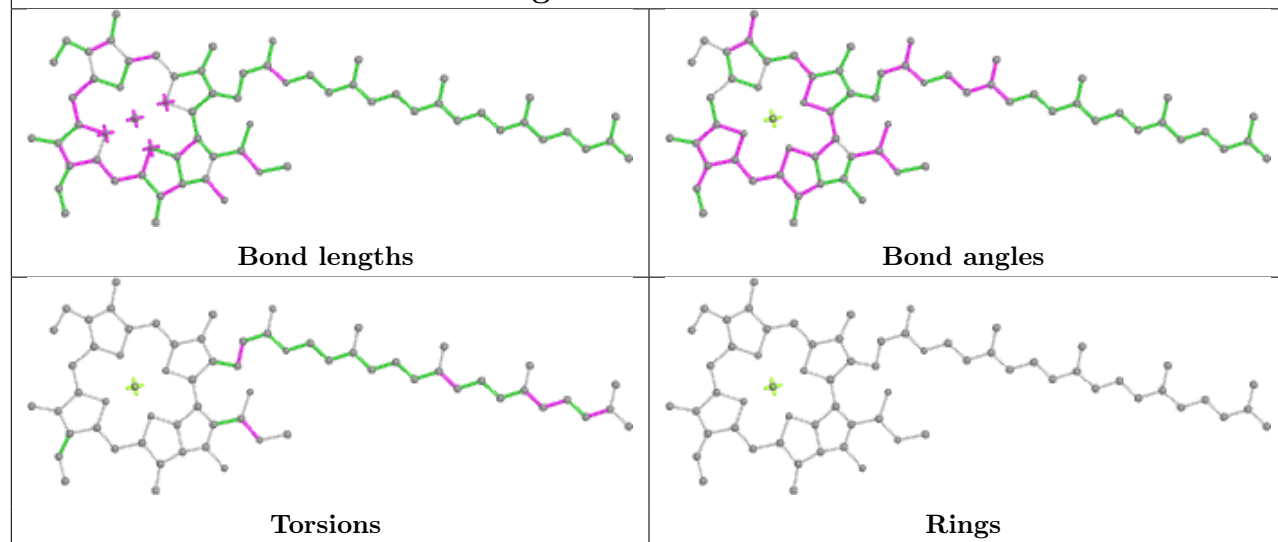


Rings

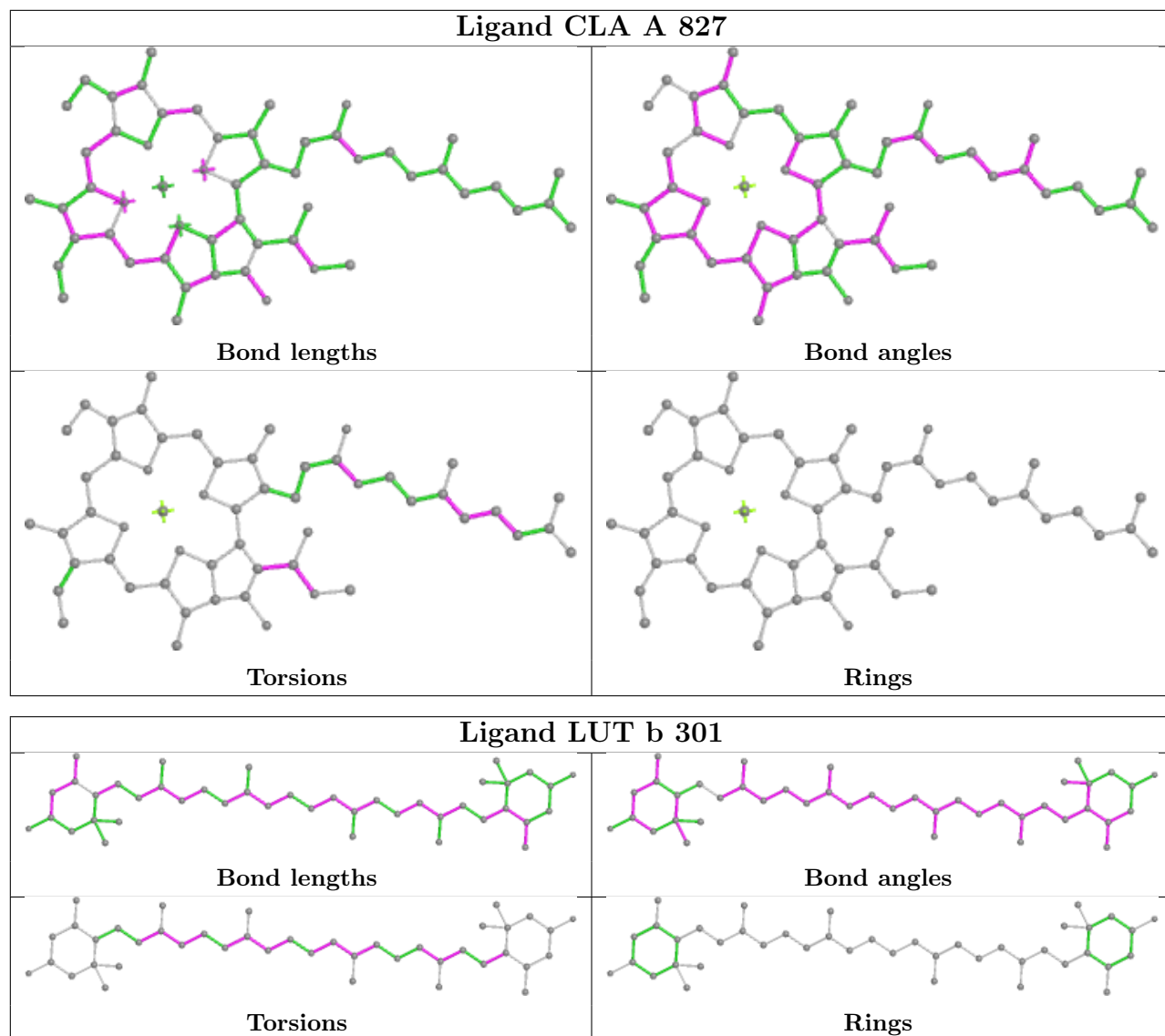
## Ligand CHL 6 319



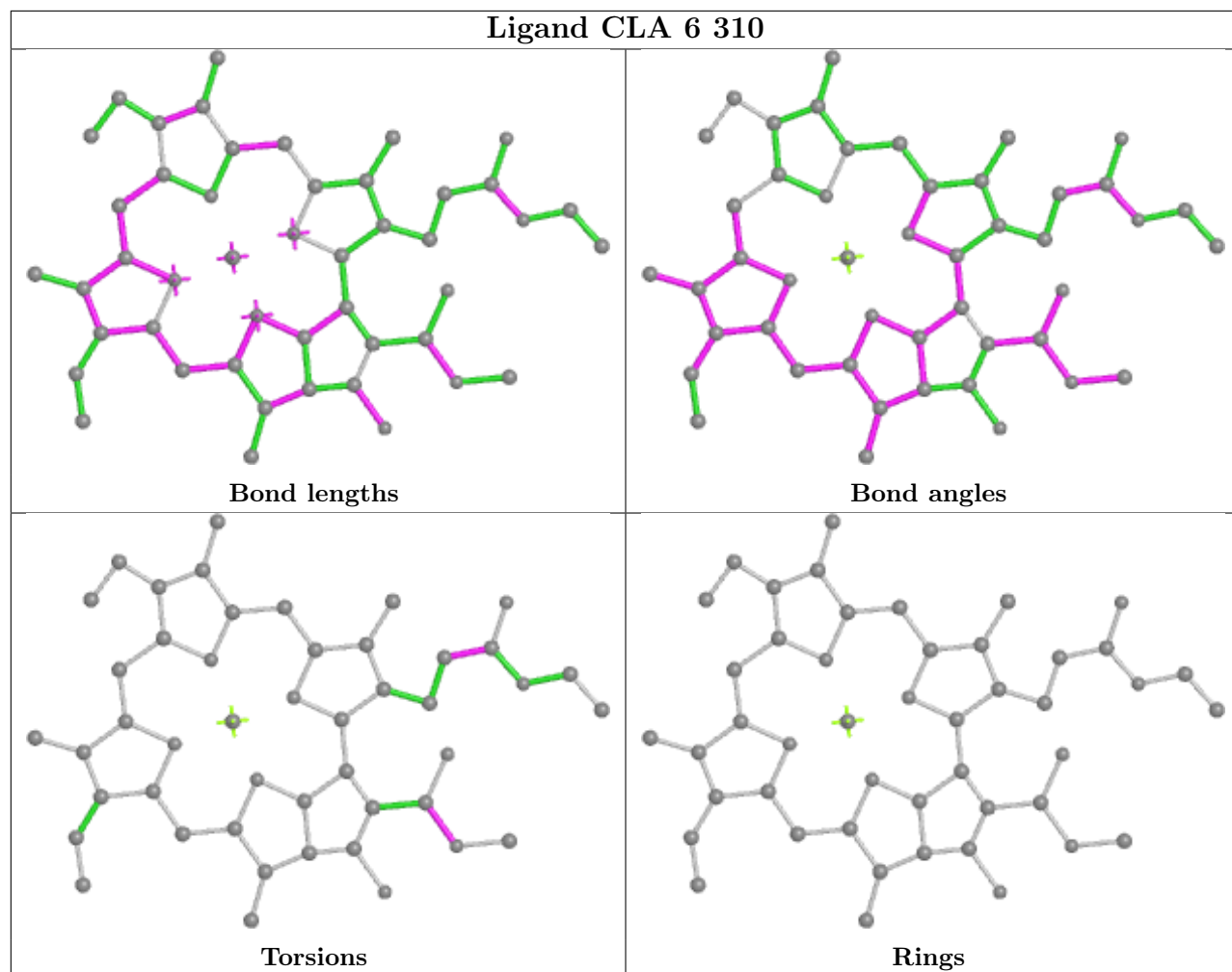
## Ligand CLA B 812



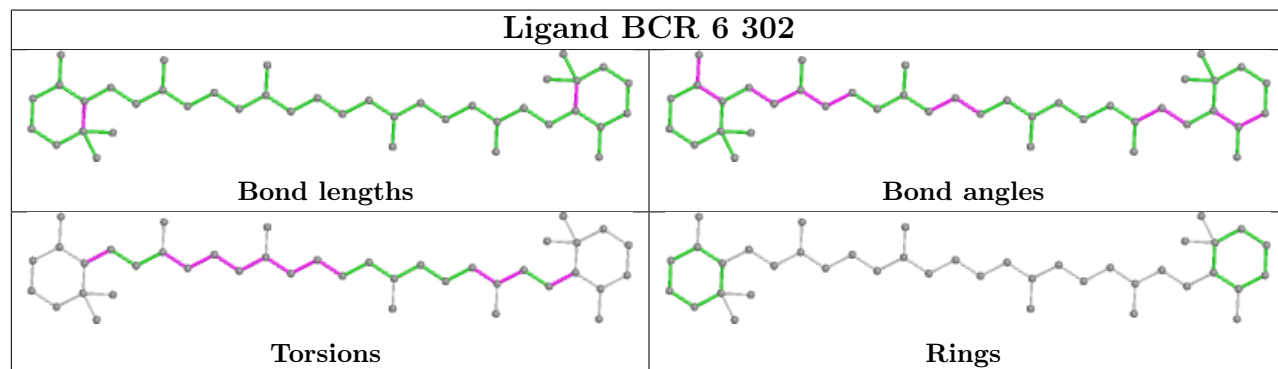


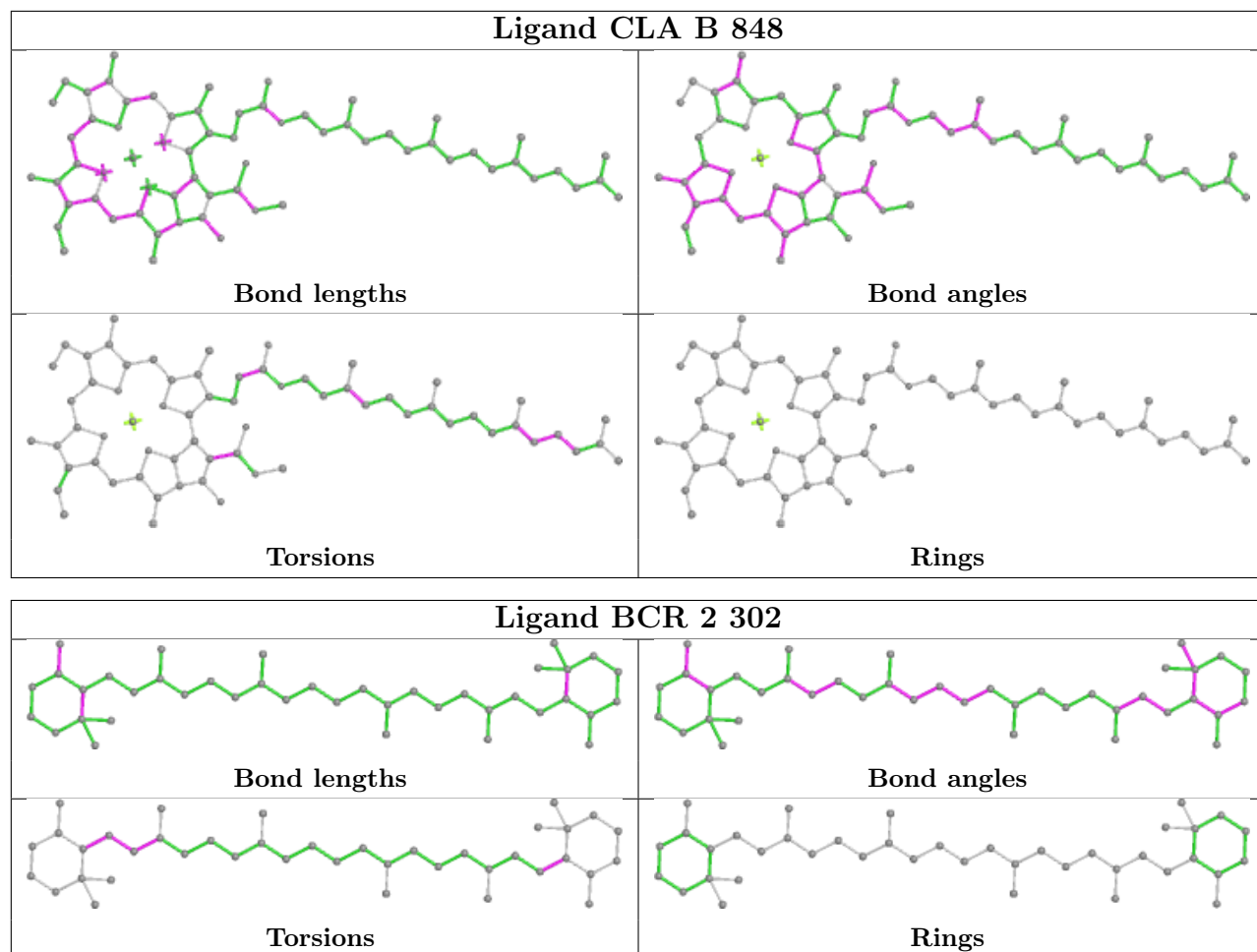


## Ligand CLA 6 310

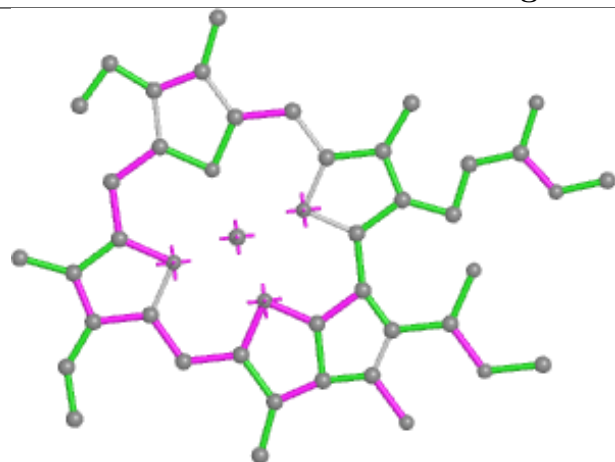


## Ligand BCR 6 302

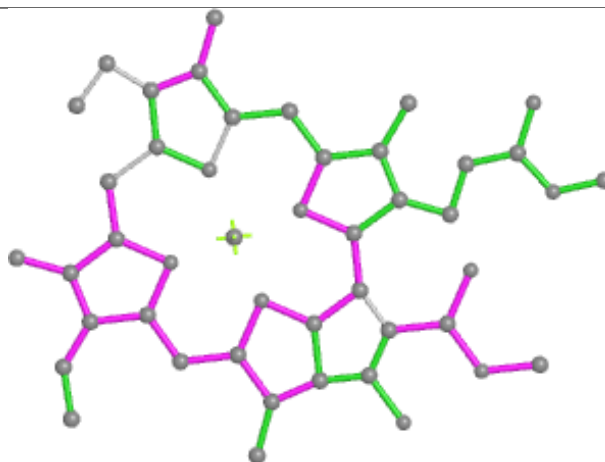




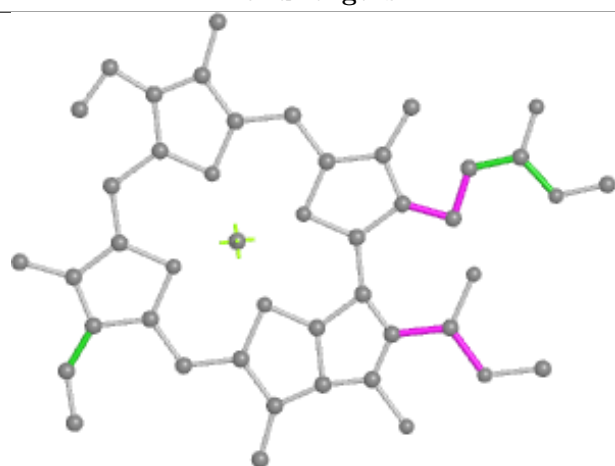
## Ligand CLA 2 315



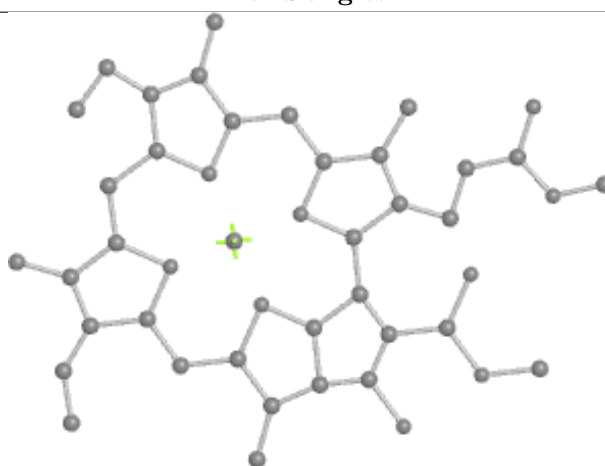
Bond lengths



Bond angles

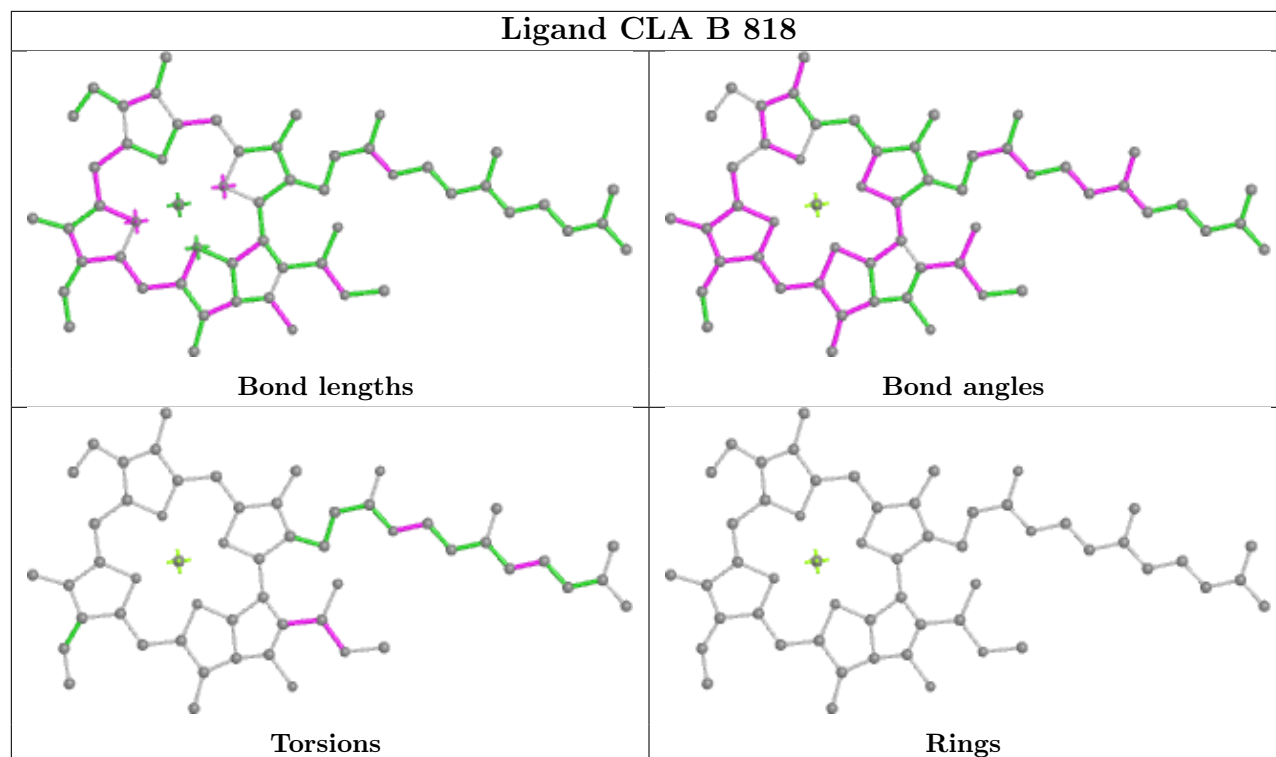


Torsions

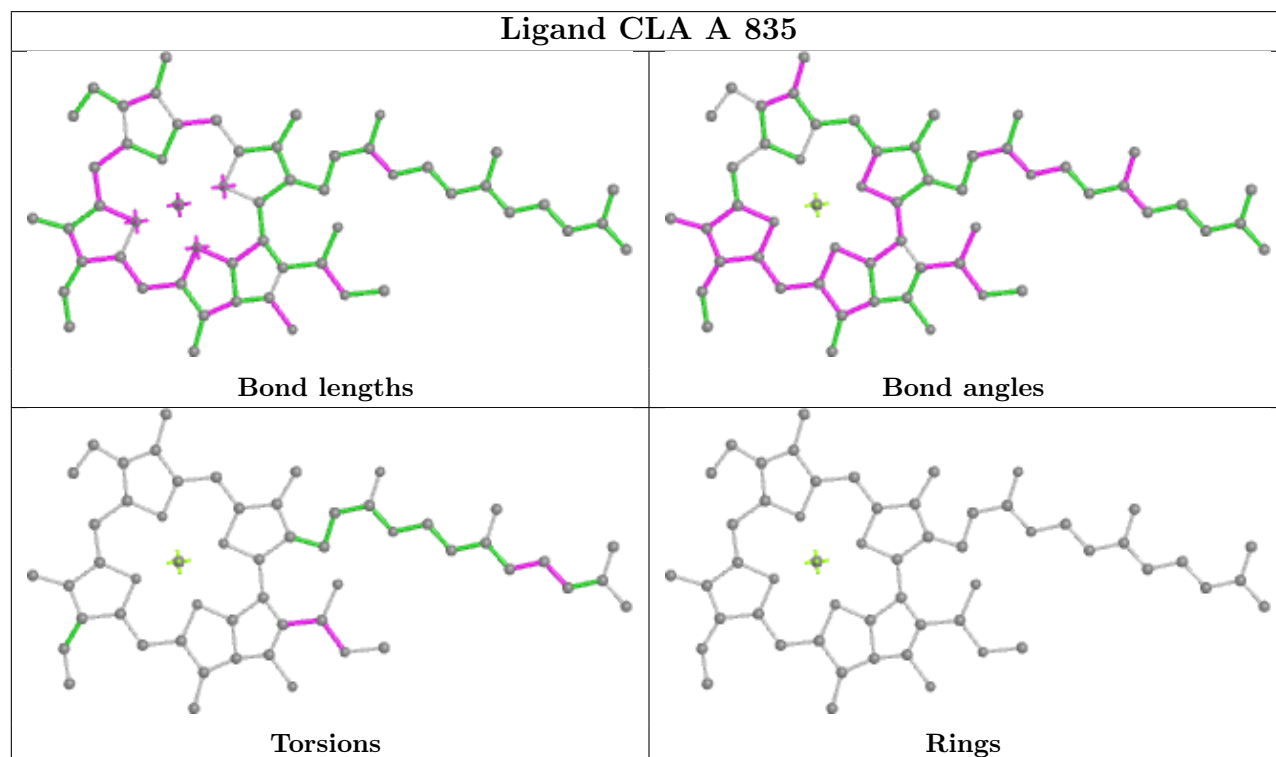


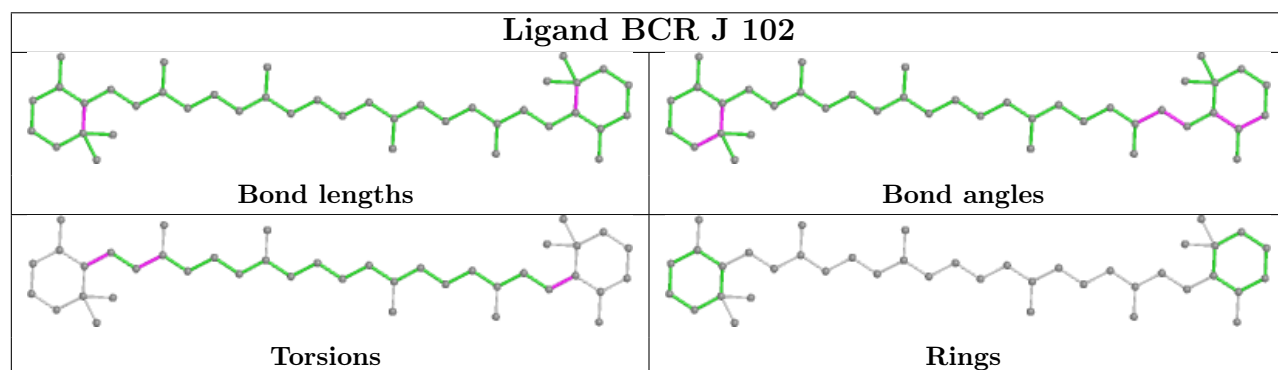
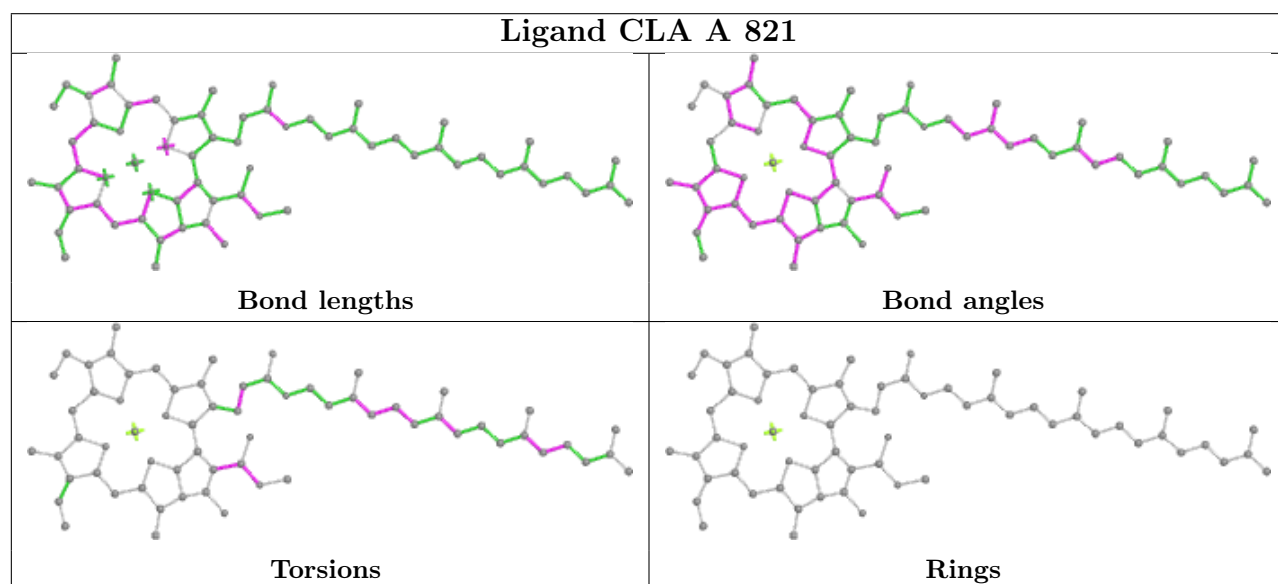
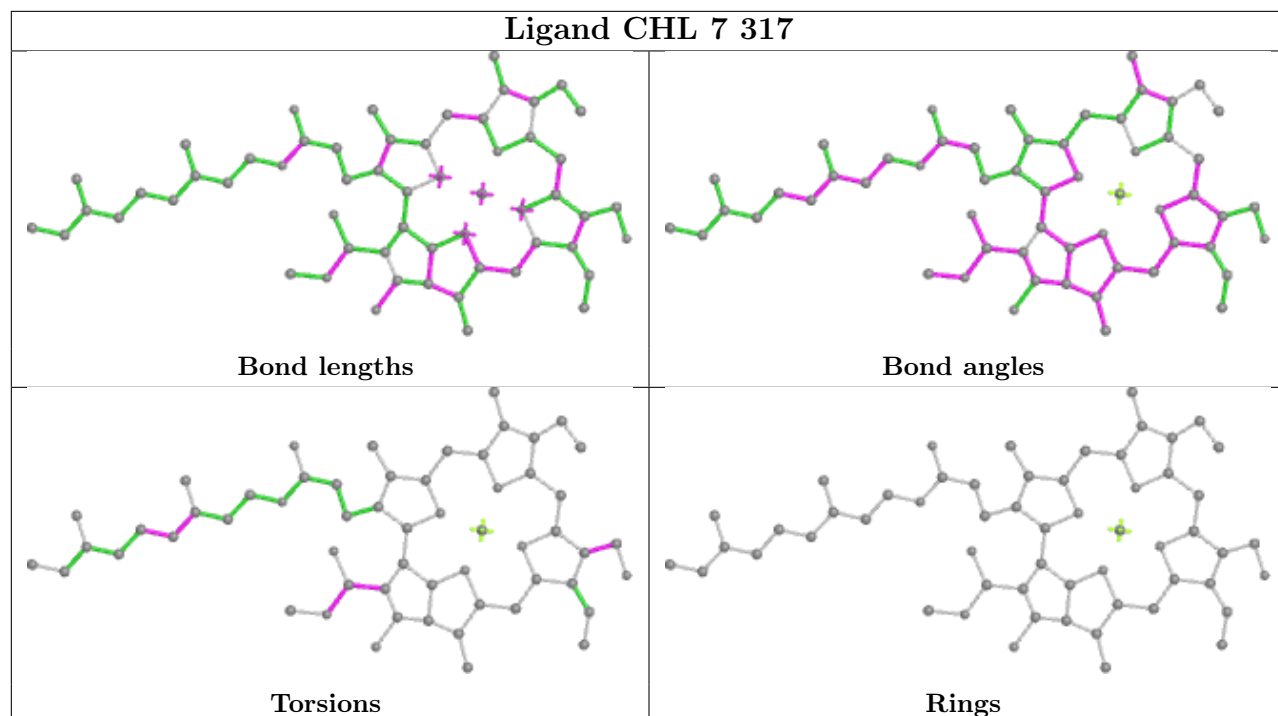
Rings

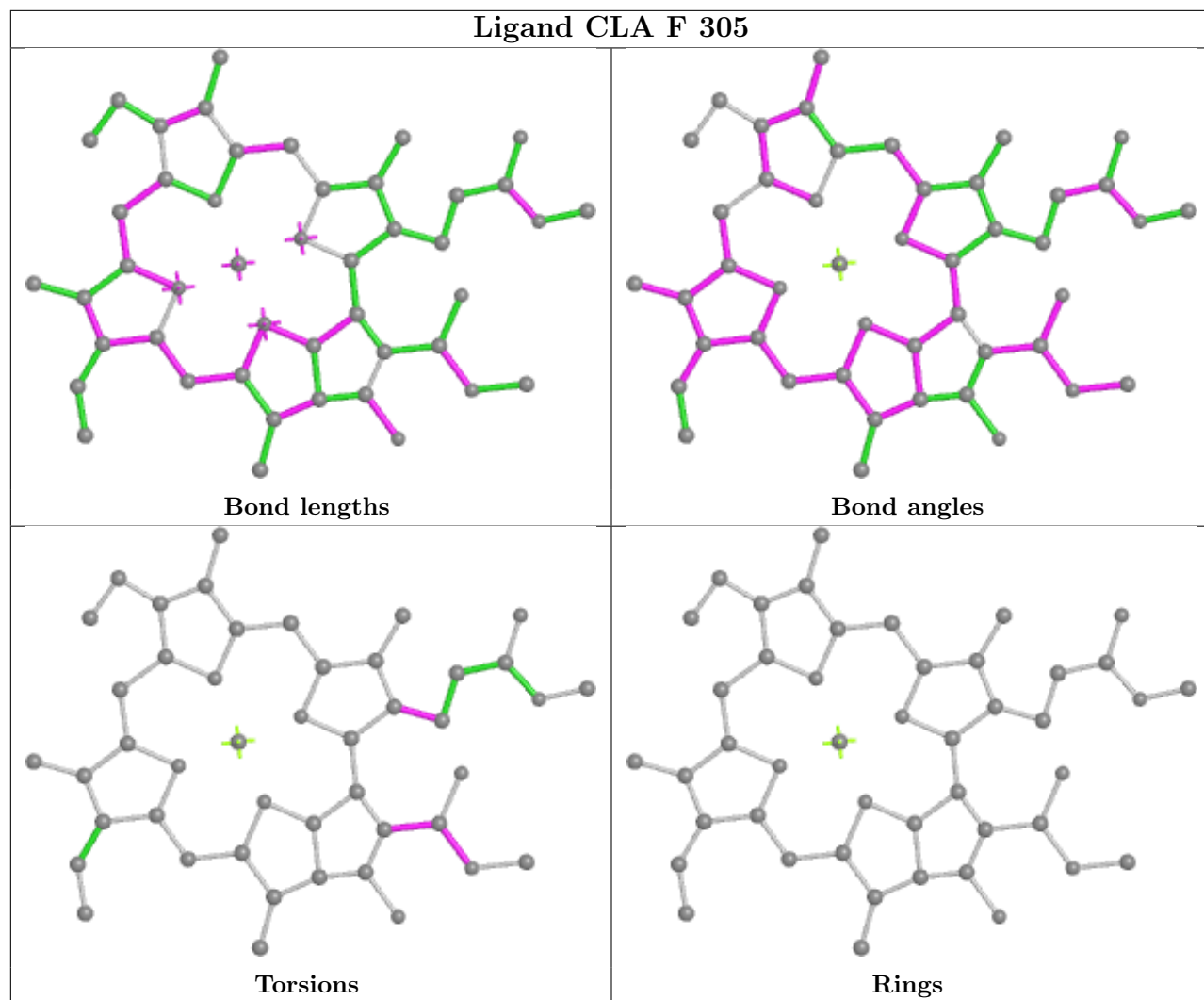
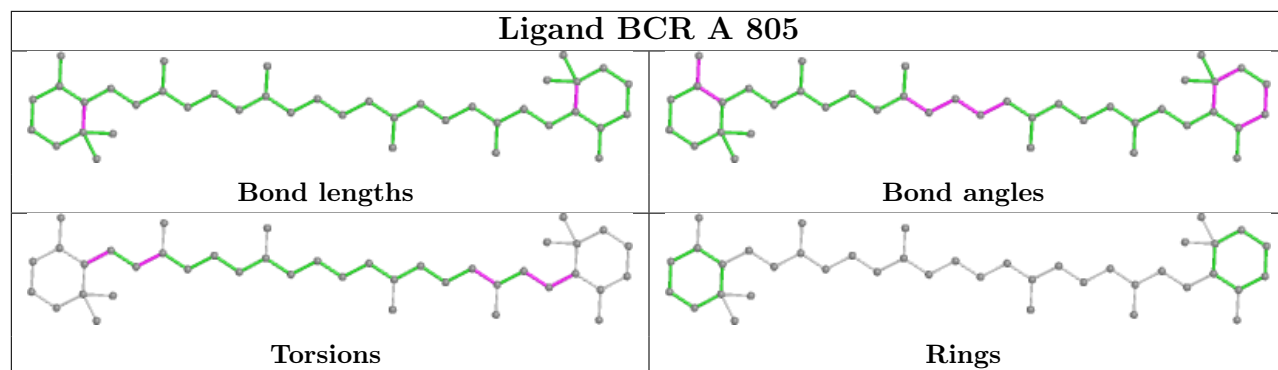
## Ligand CLA B 818



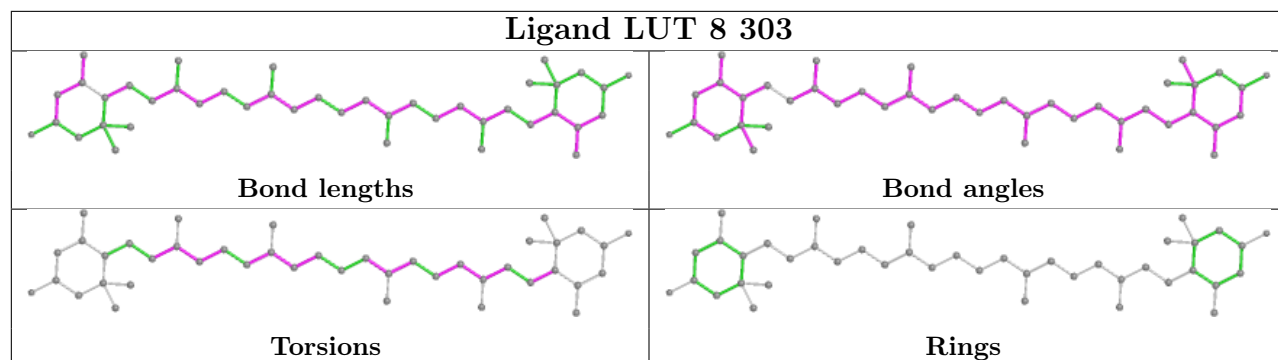
## Ligand CLA A 835



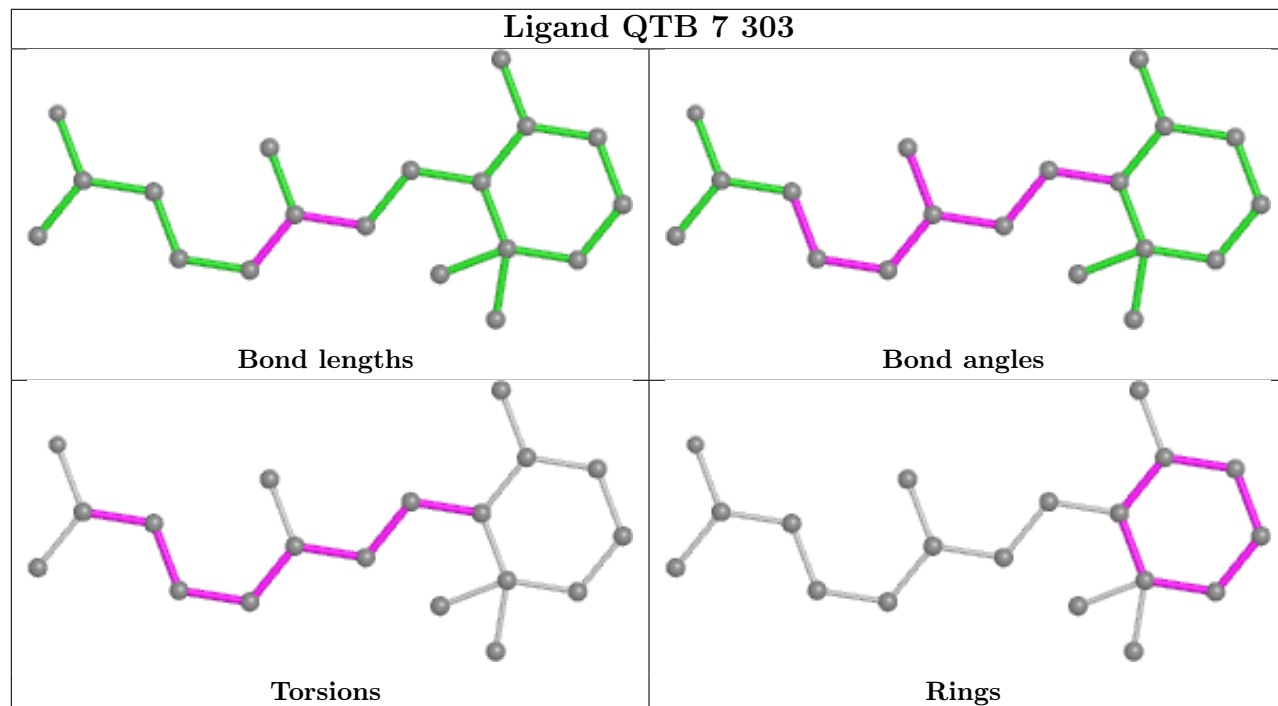




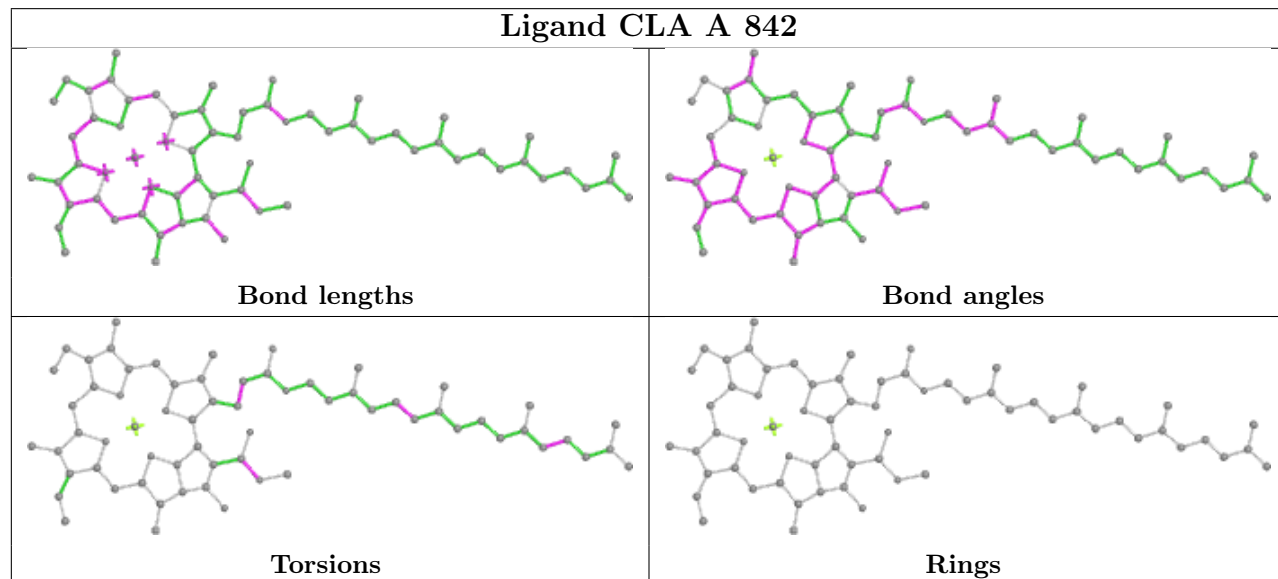
## Ligand LUT 8 303



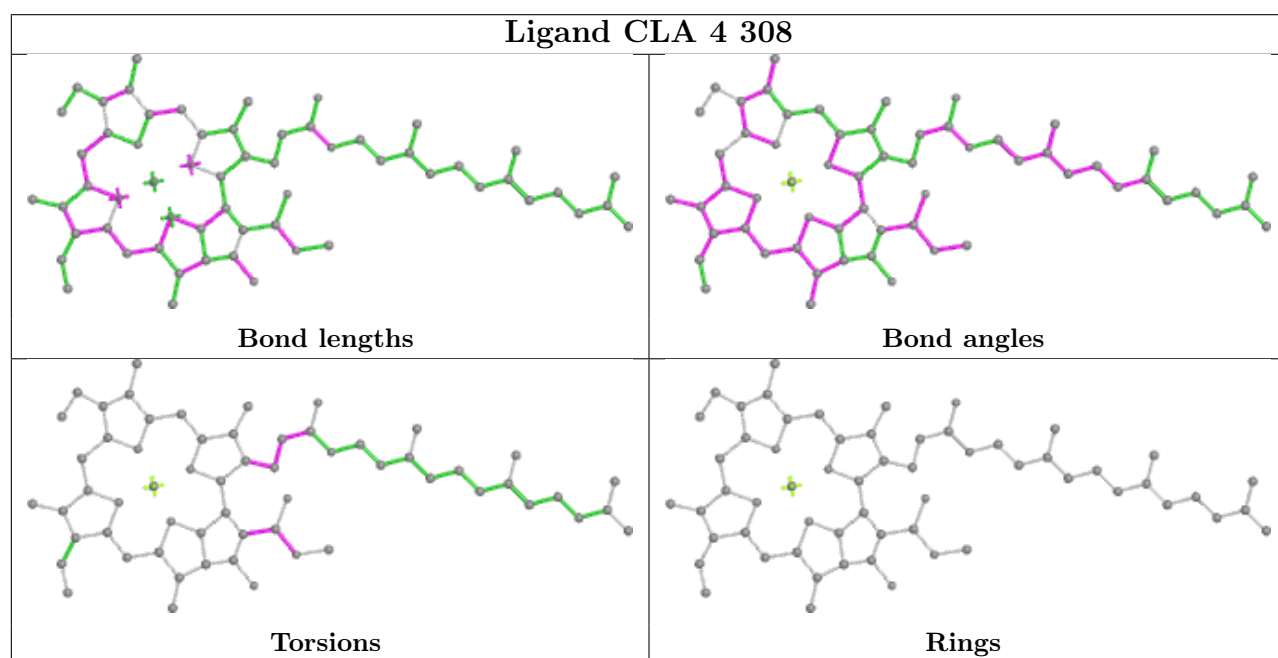
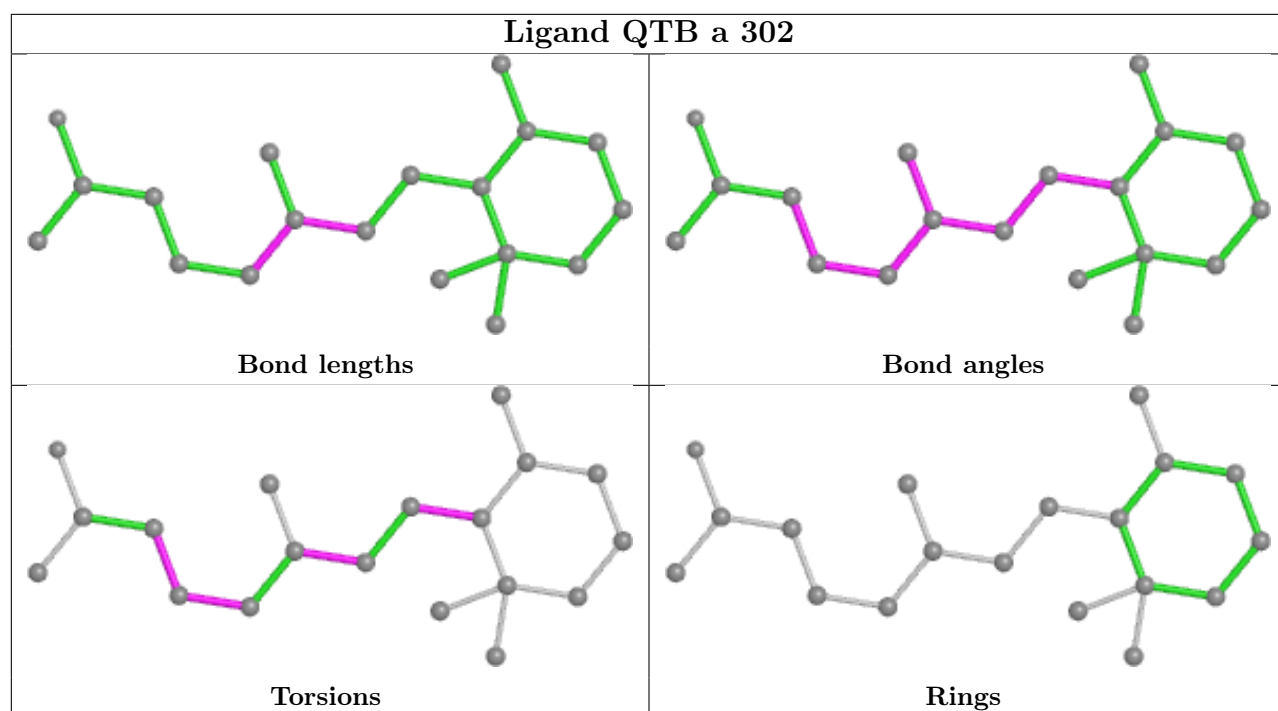
## Ligand QTB 7 303



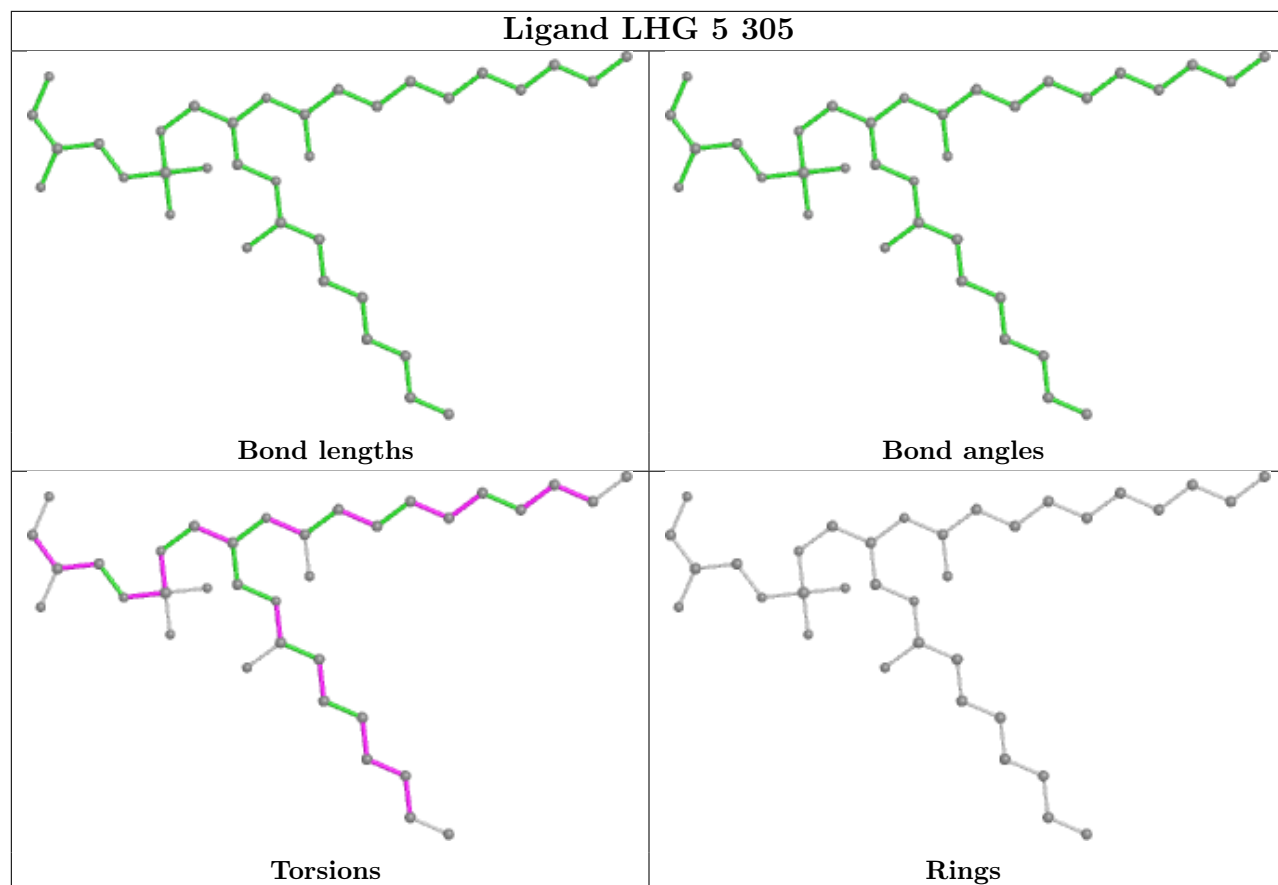
## Ligand CLA A 842



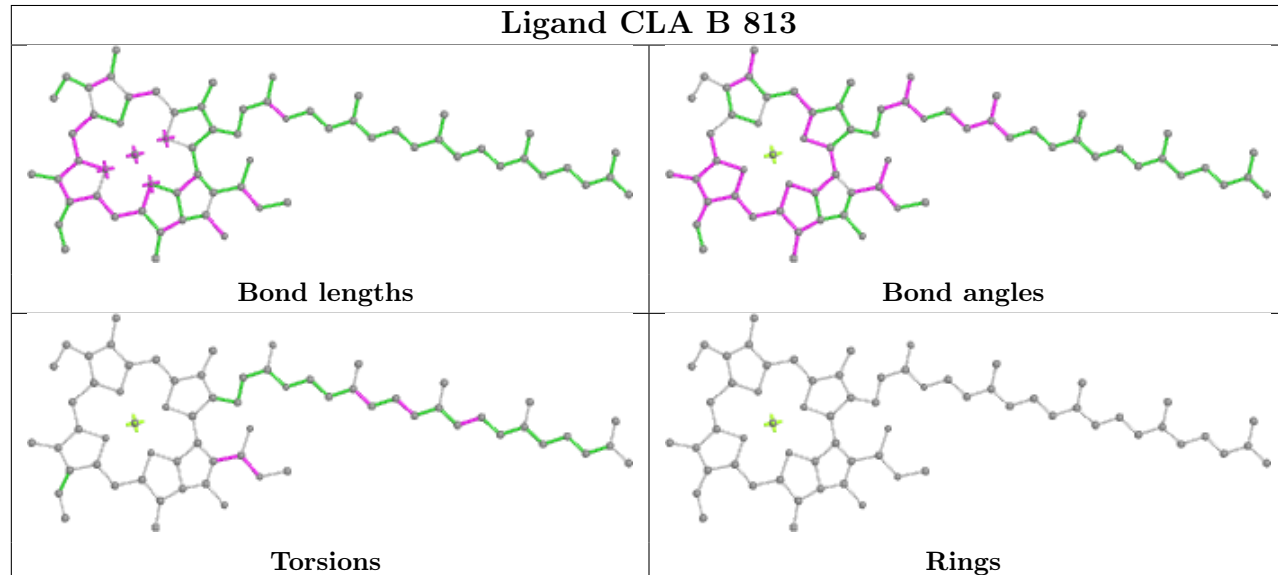


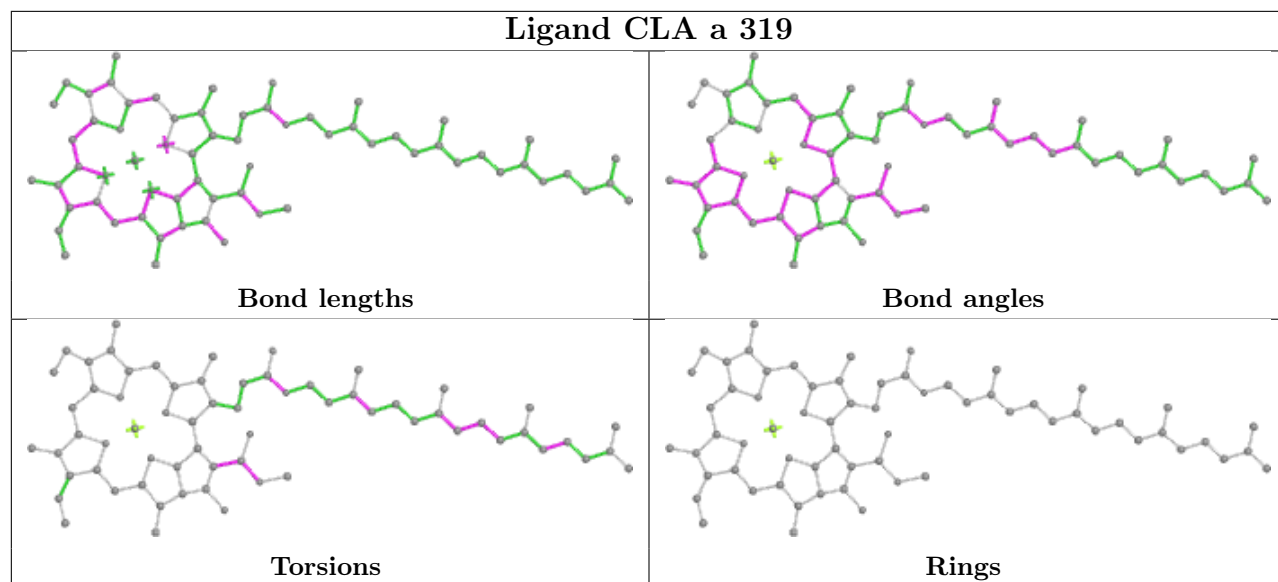
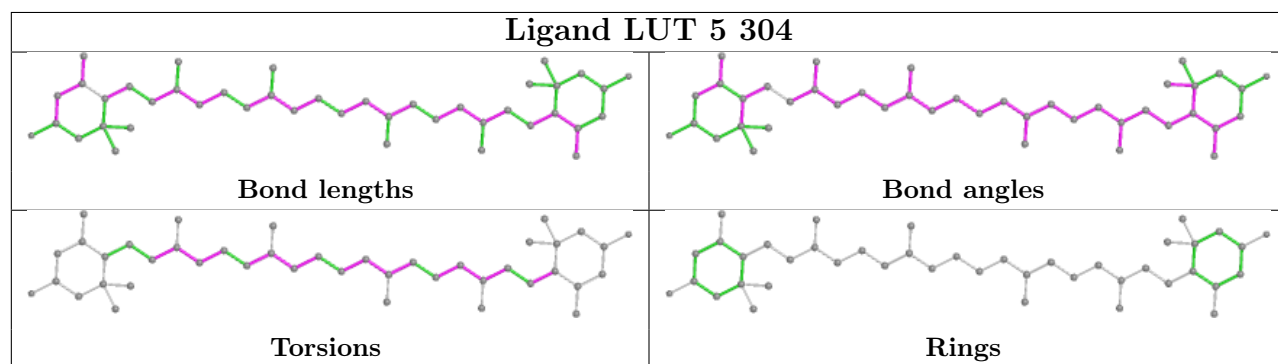


## Ligand LHG 5 305

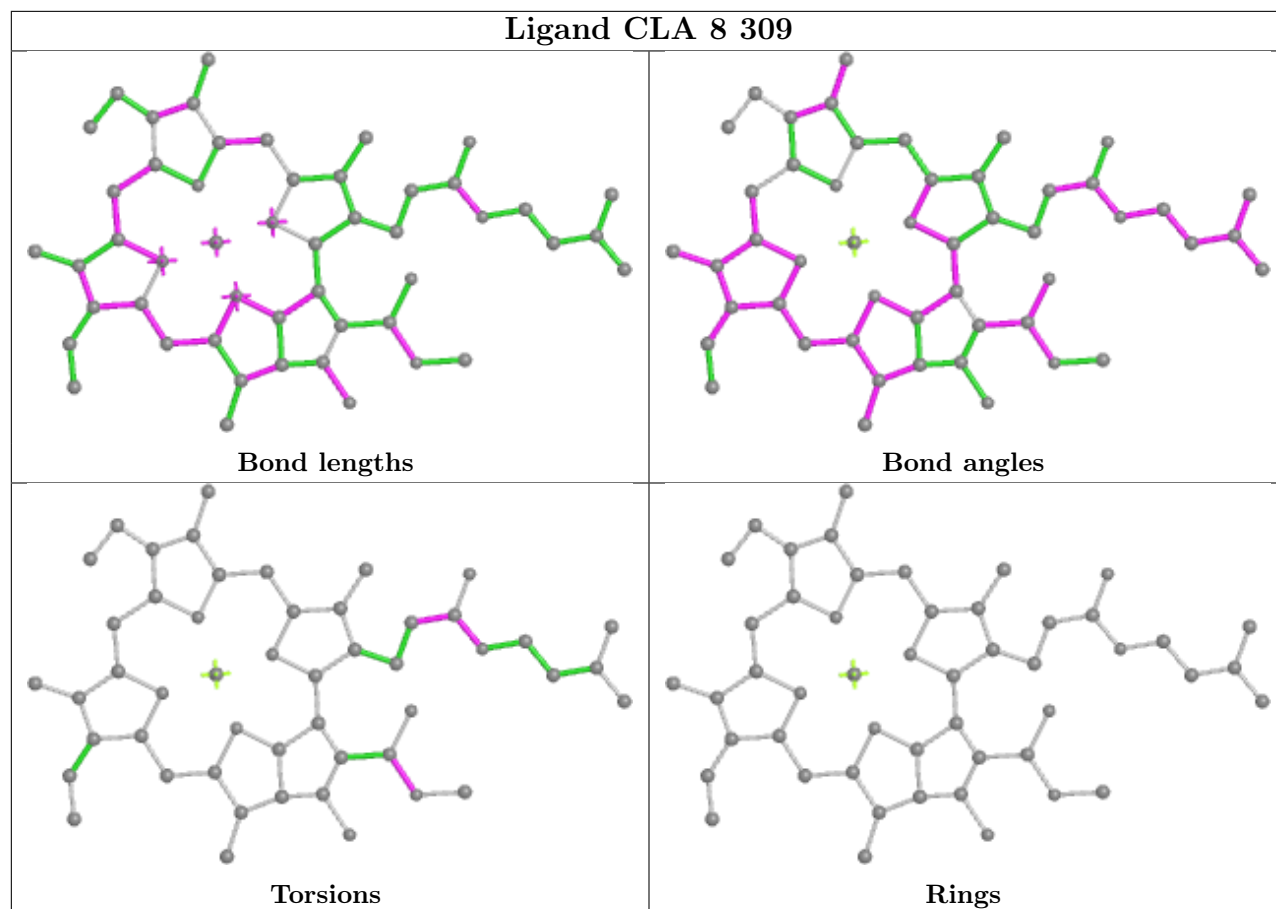


## Ligand CLA B 813

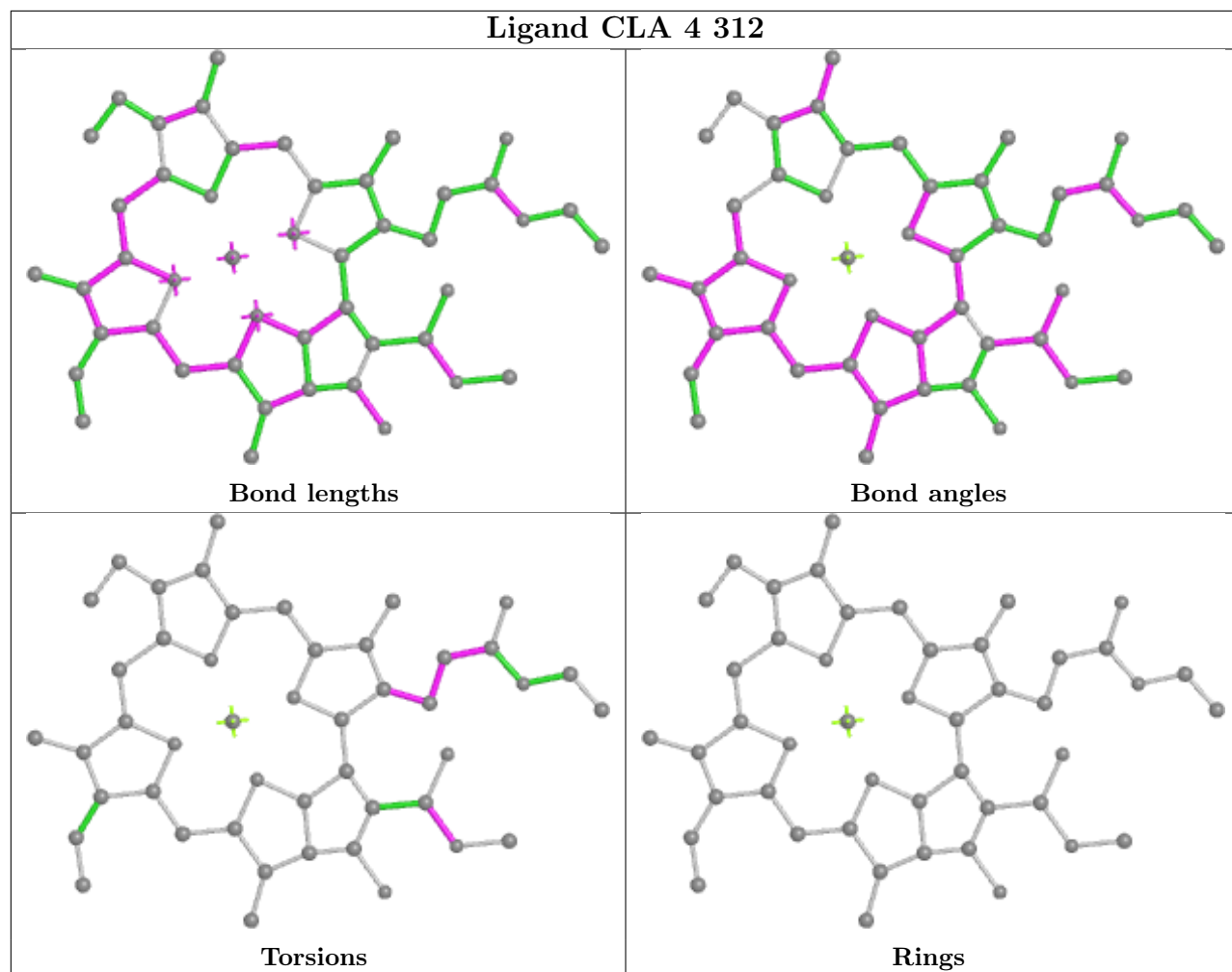


**Ligand CLA a 319****Ligand LUT 5 304**

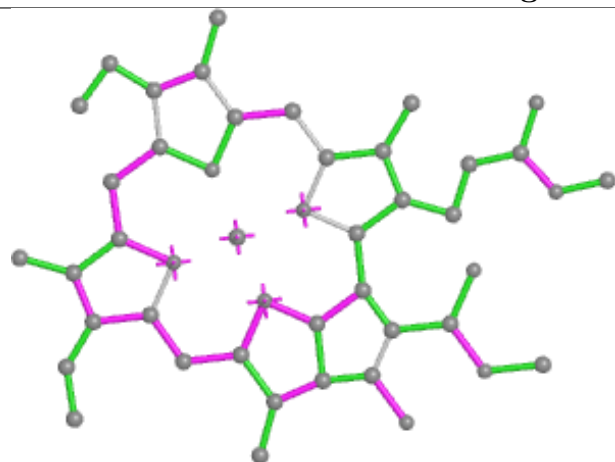
## Ligand CLA 8 309



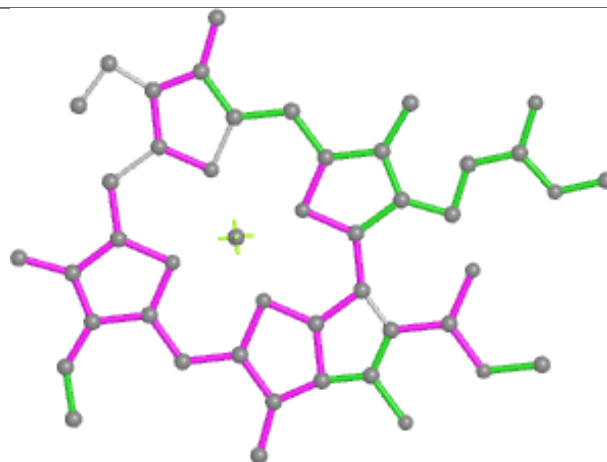
## Ligand CLA 4 312



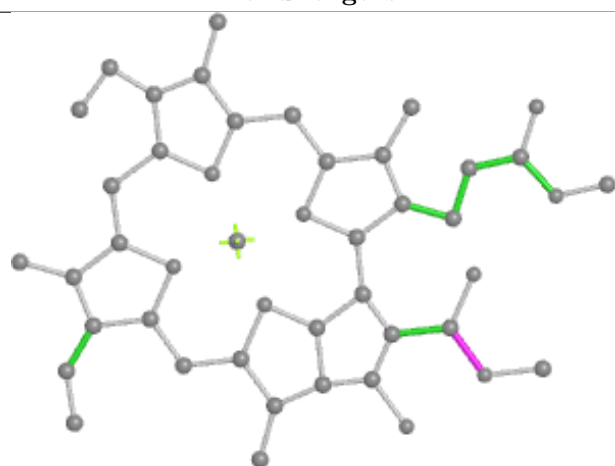
## Ligand CLA 2 314



Bond lengths



Bond angles

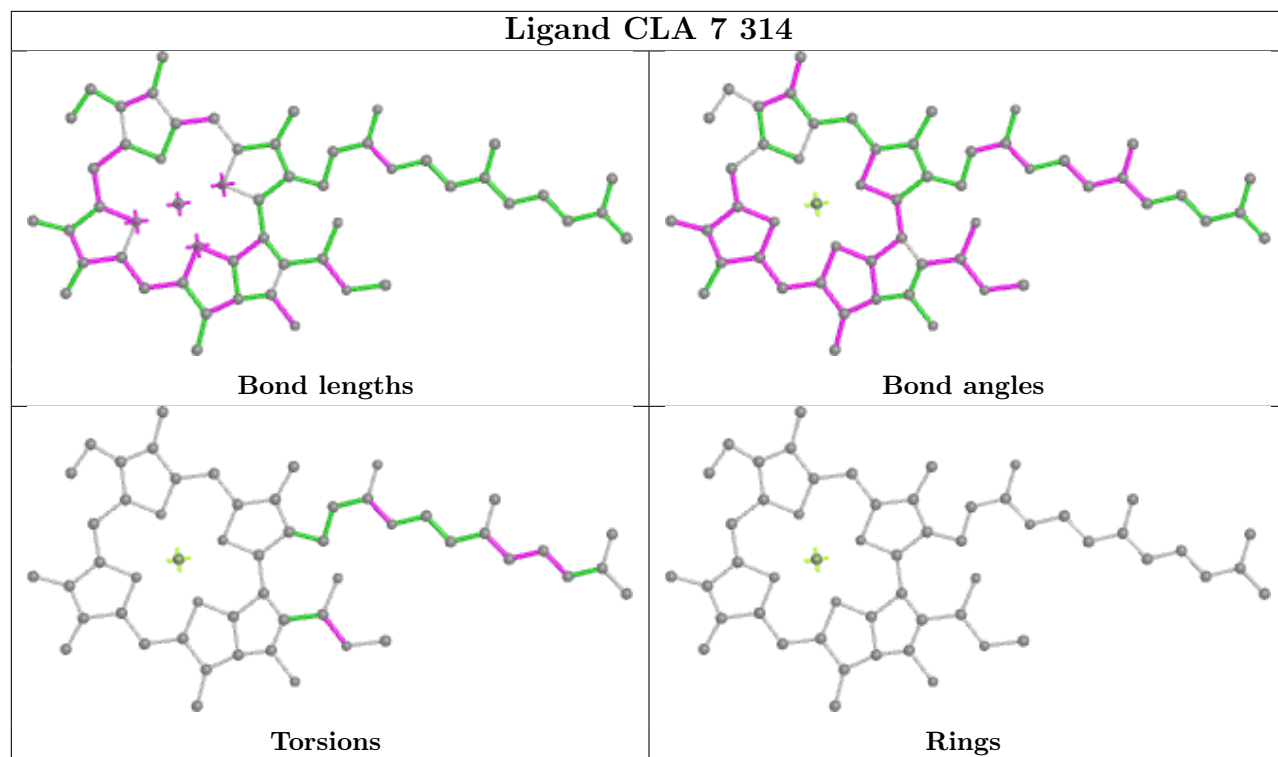


Torsions

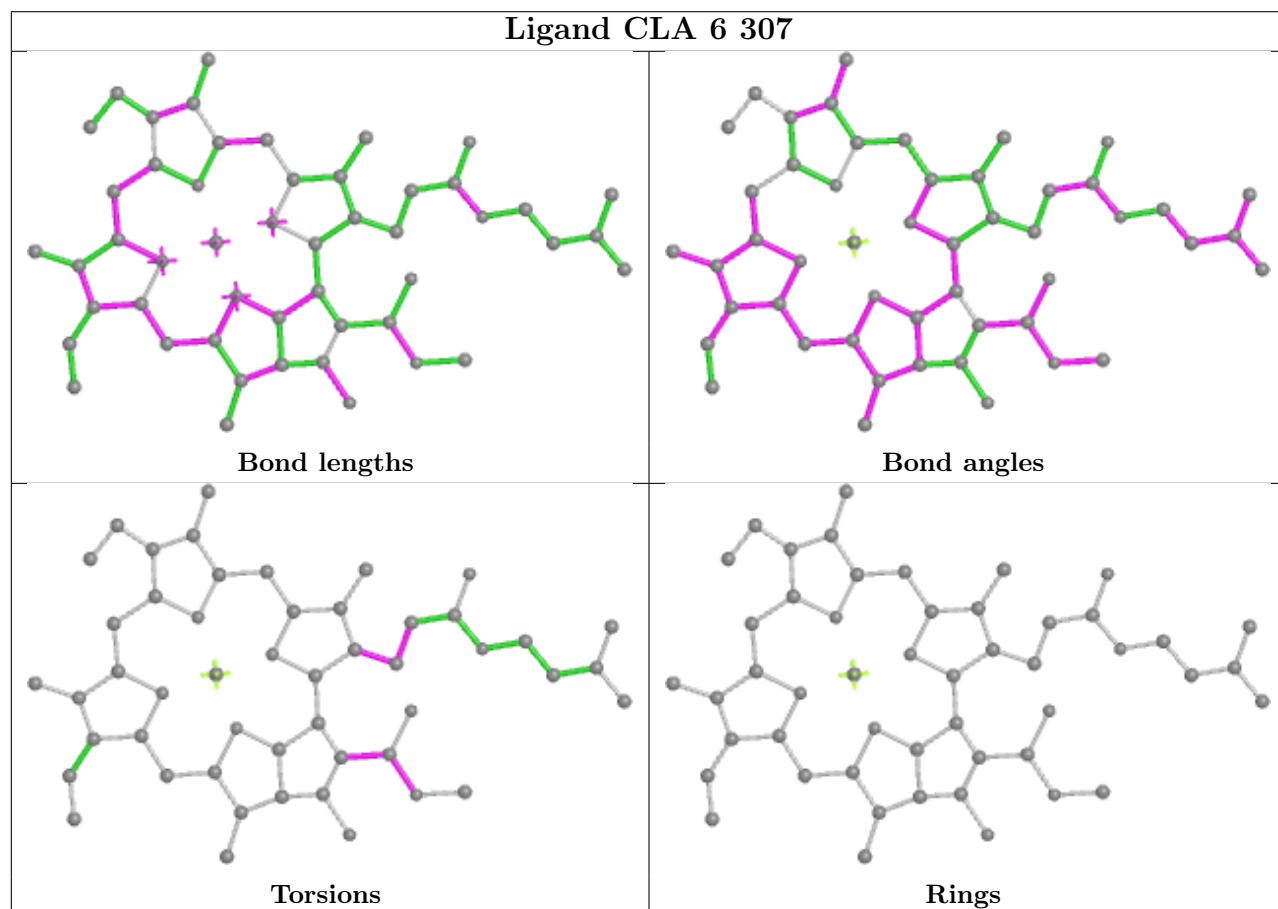


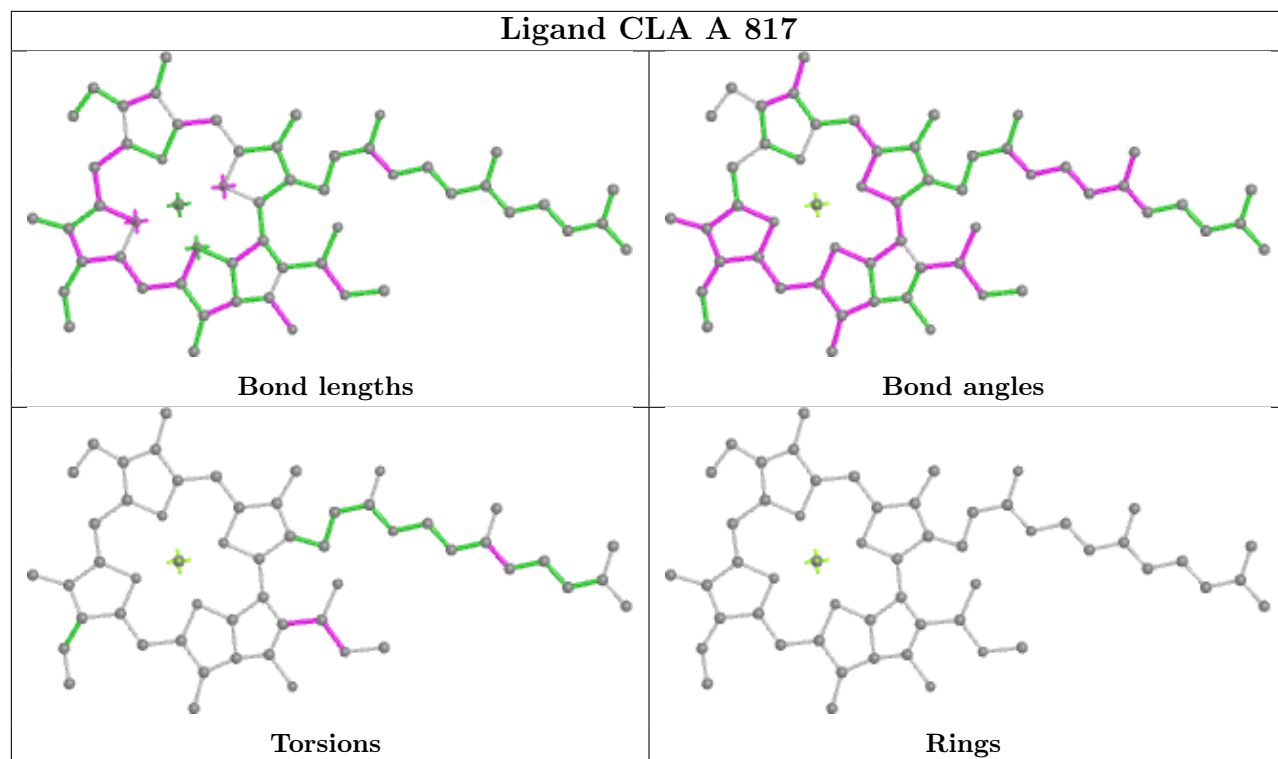
Rings

## Ligand CLA 7 314

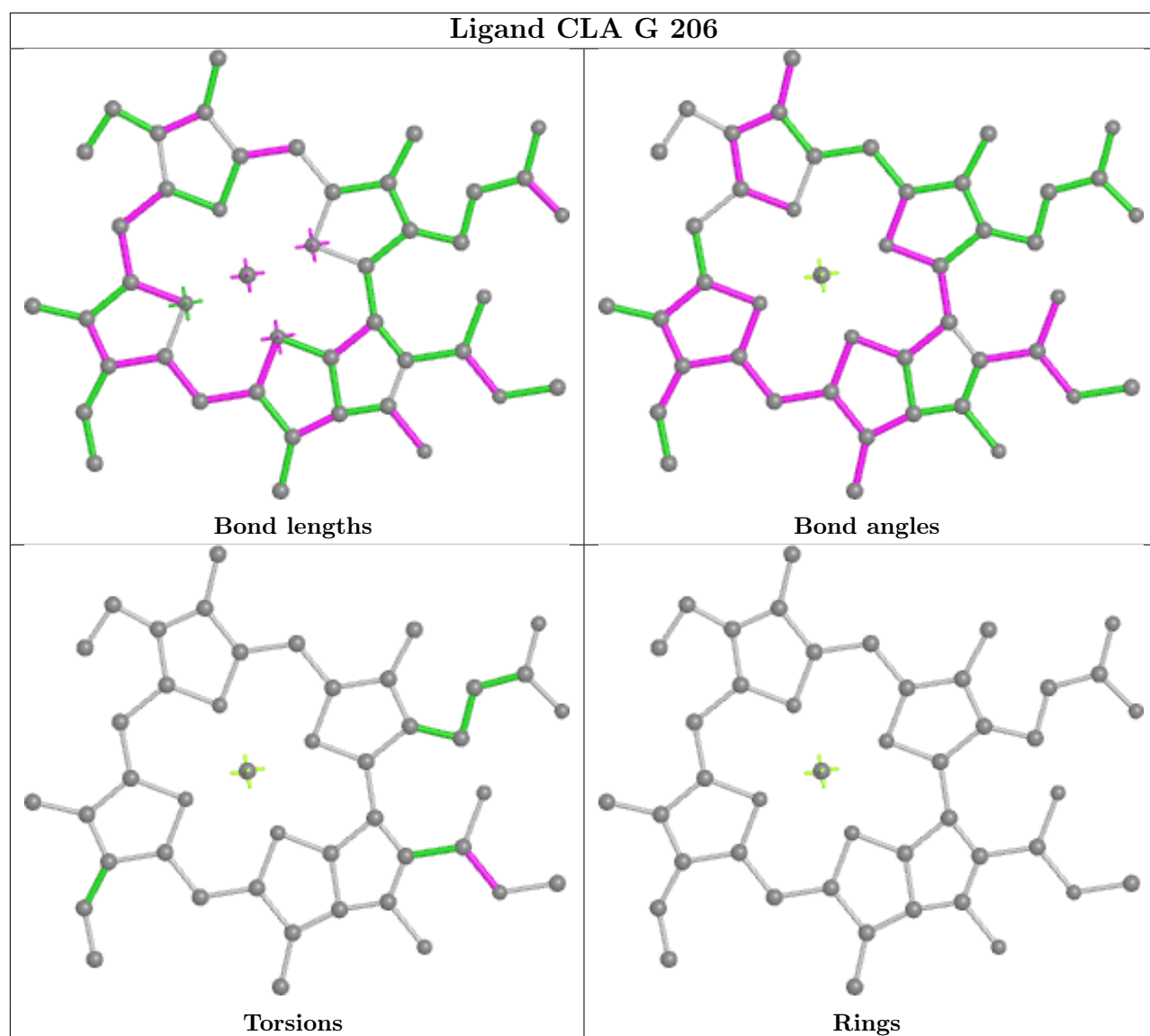


## Ligand CLA 6 307

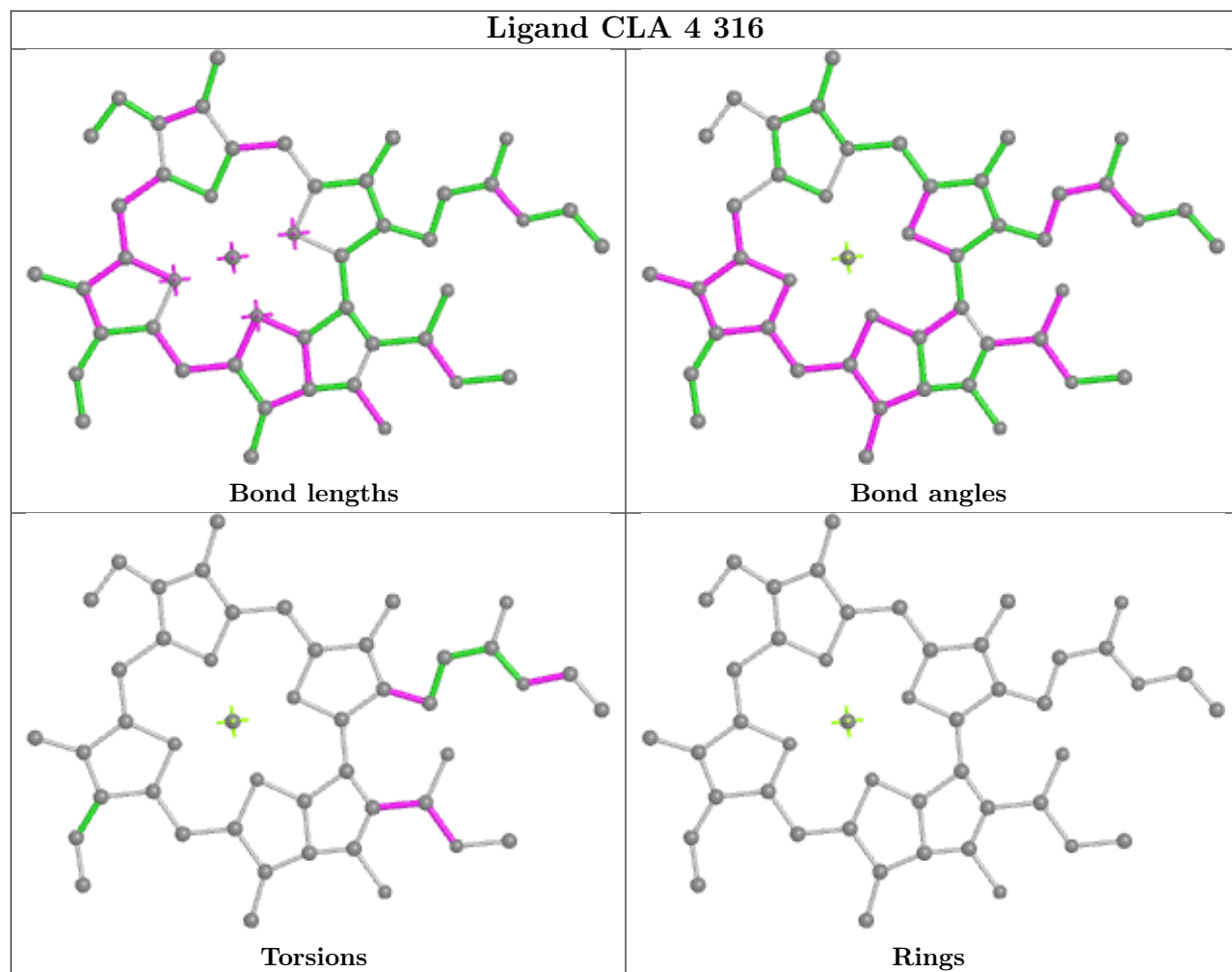




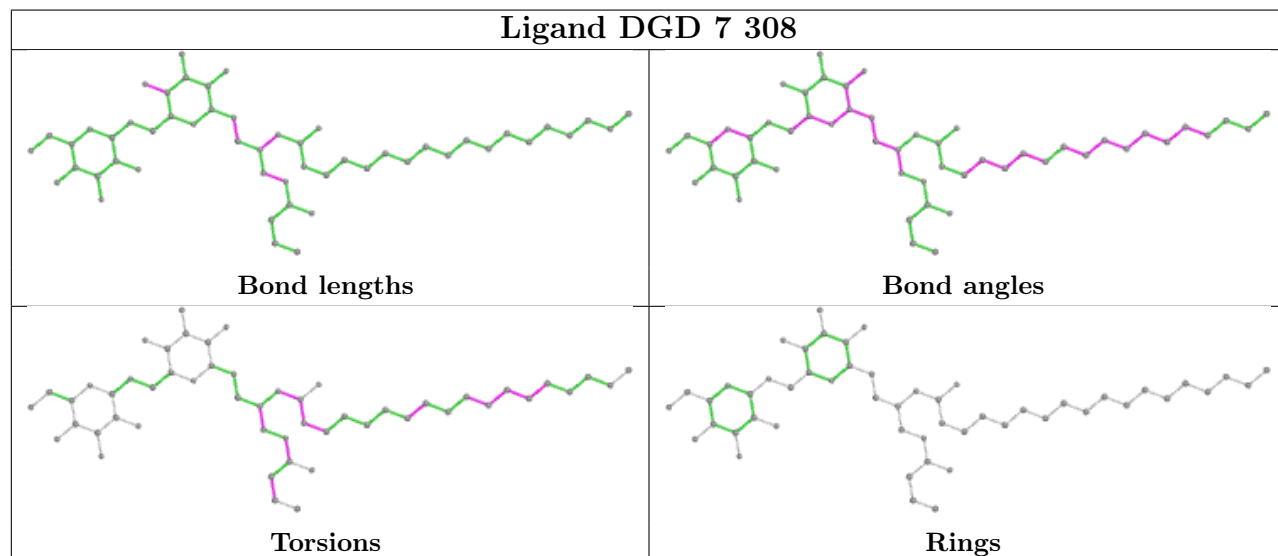


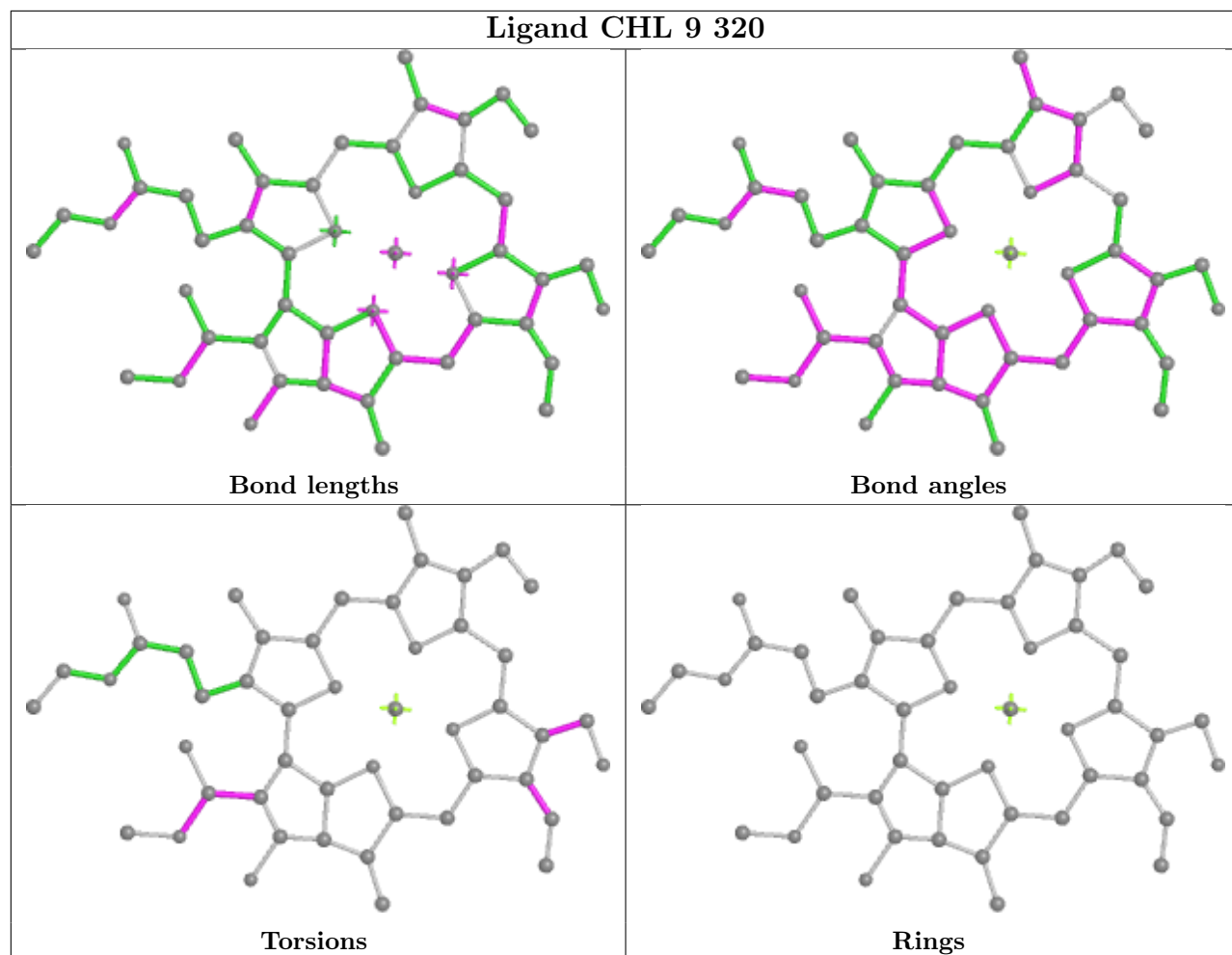


## Ligand CLA 4 316

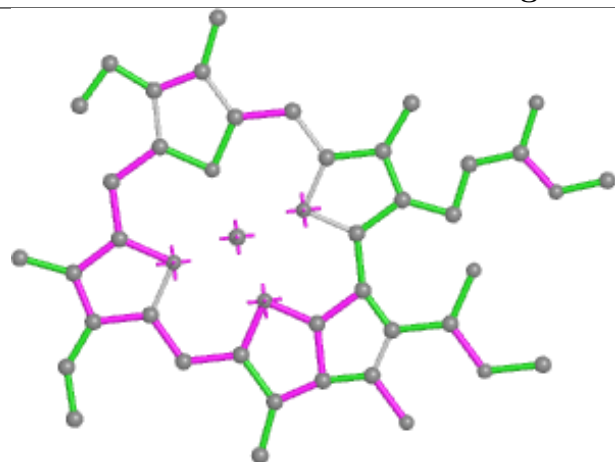


## Ligand DGD 7 308

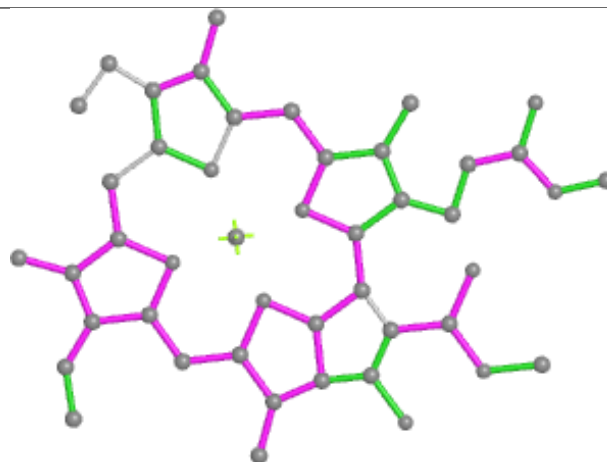




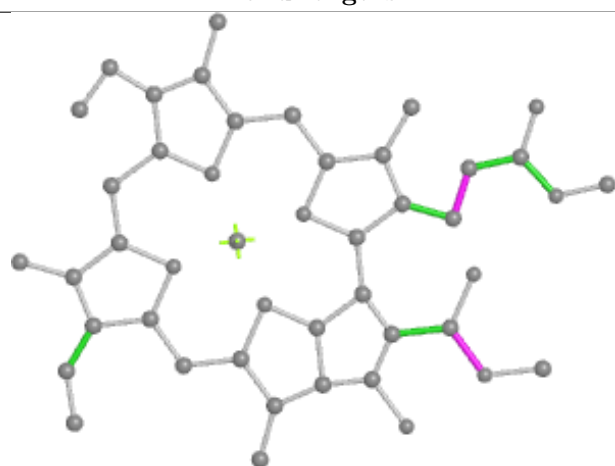
## Ligand CLA 5 320



Bond lengths



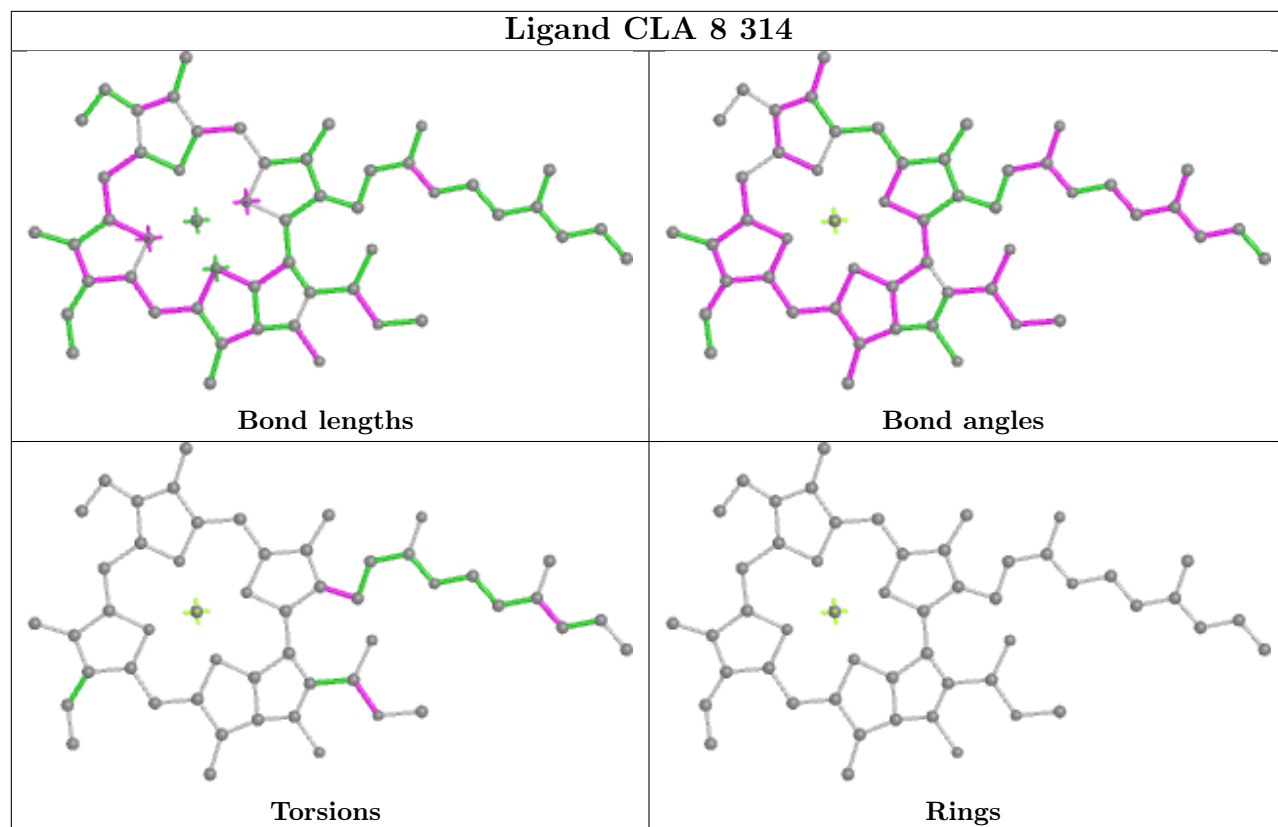
Bond angles



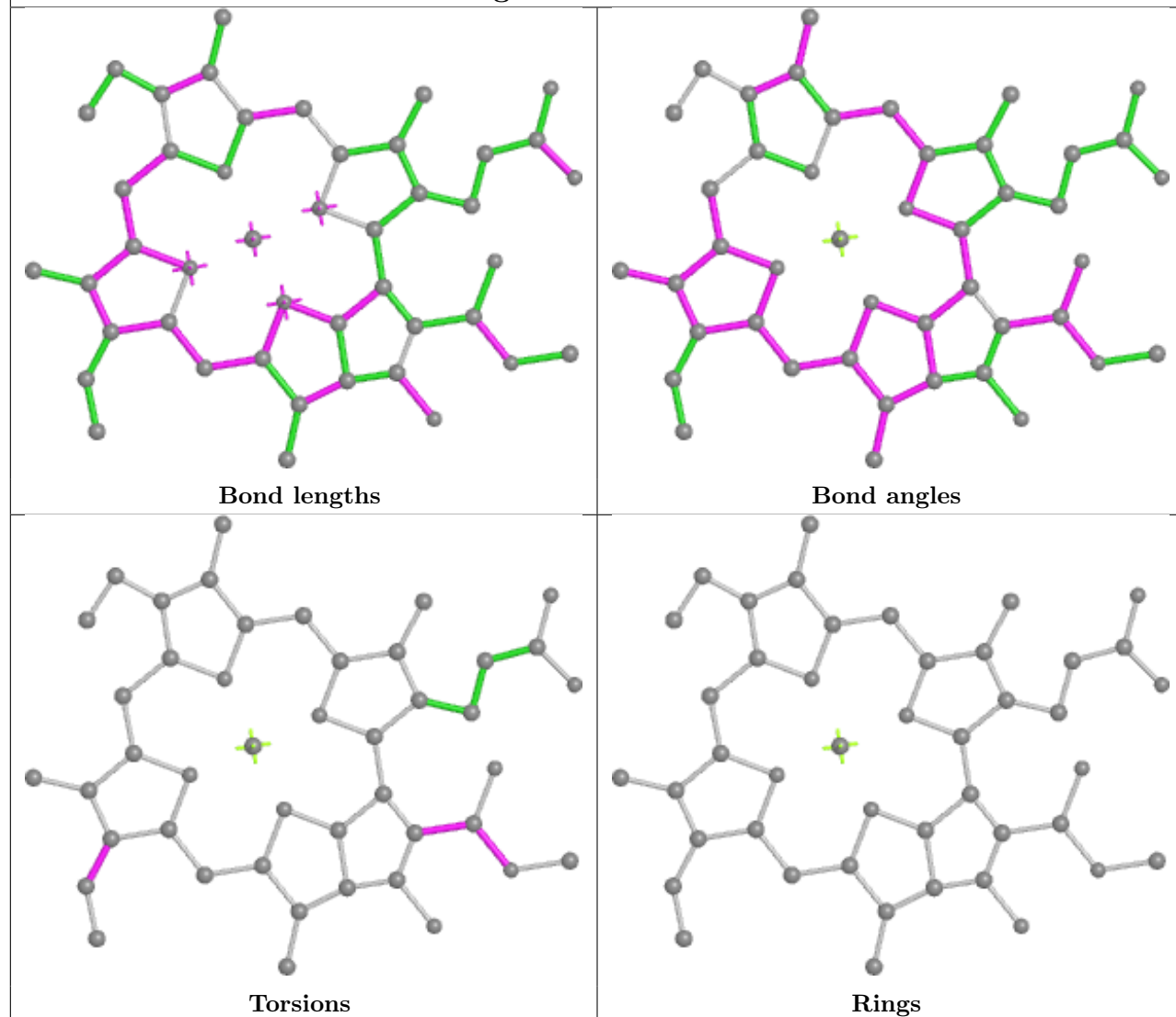
Torsions



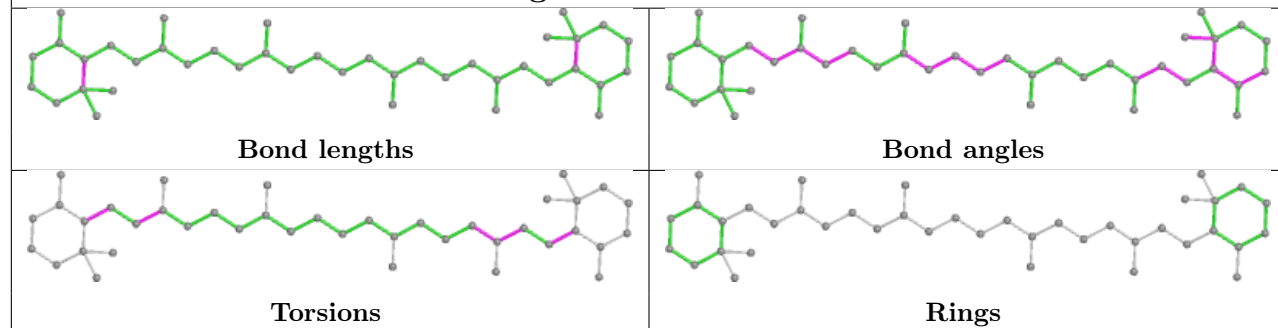
Rings

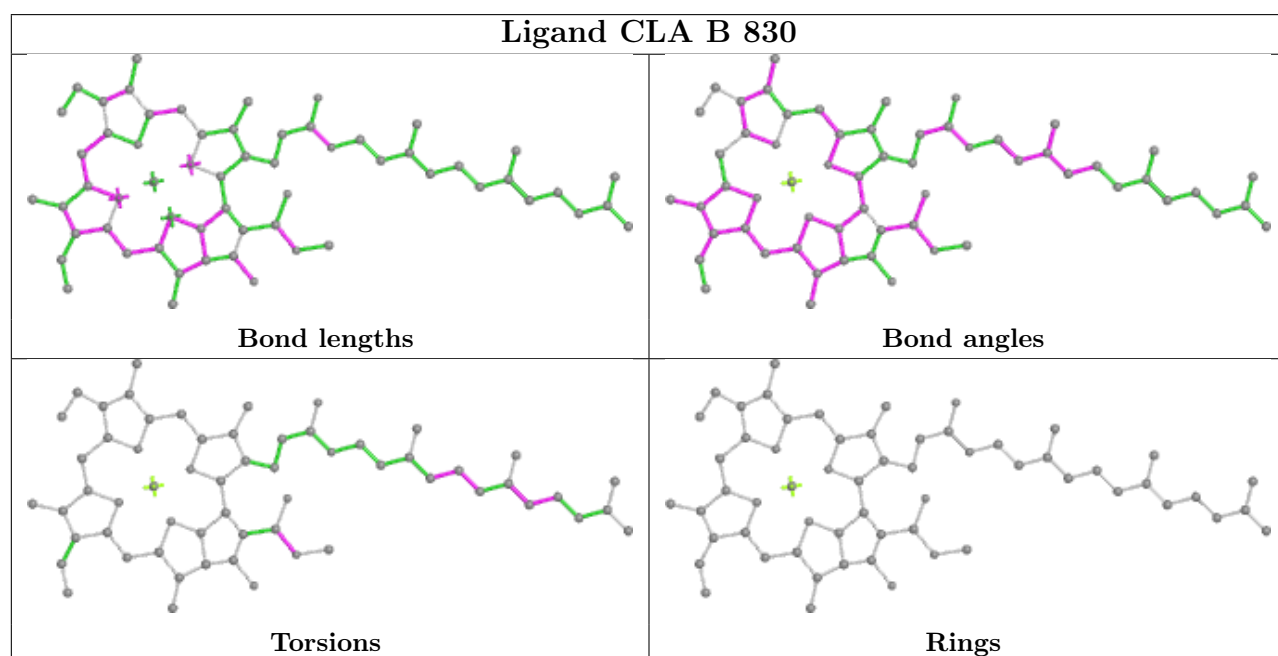
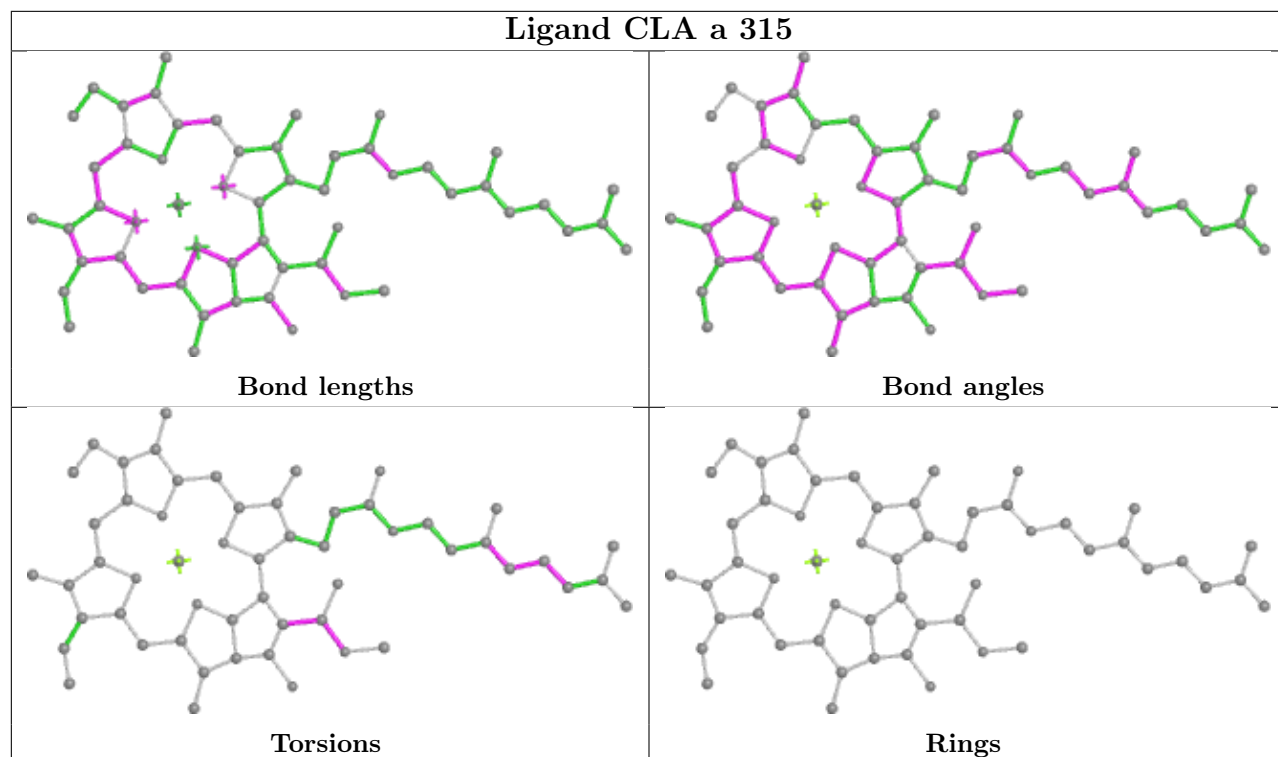
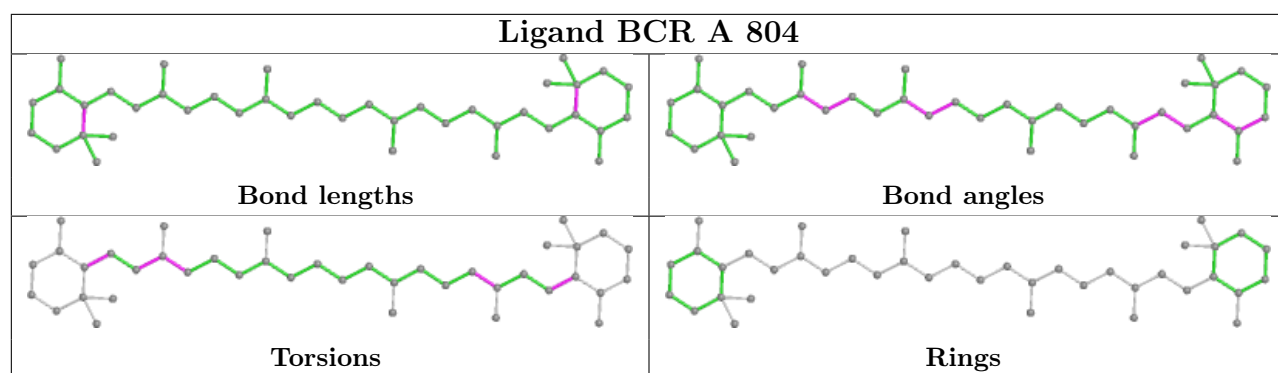


## Ligand CLA 4 320

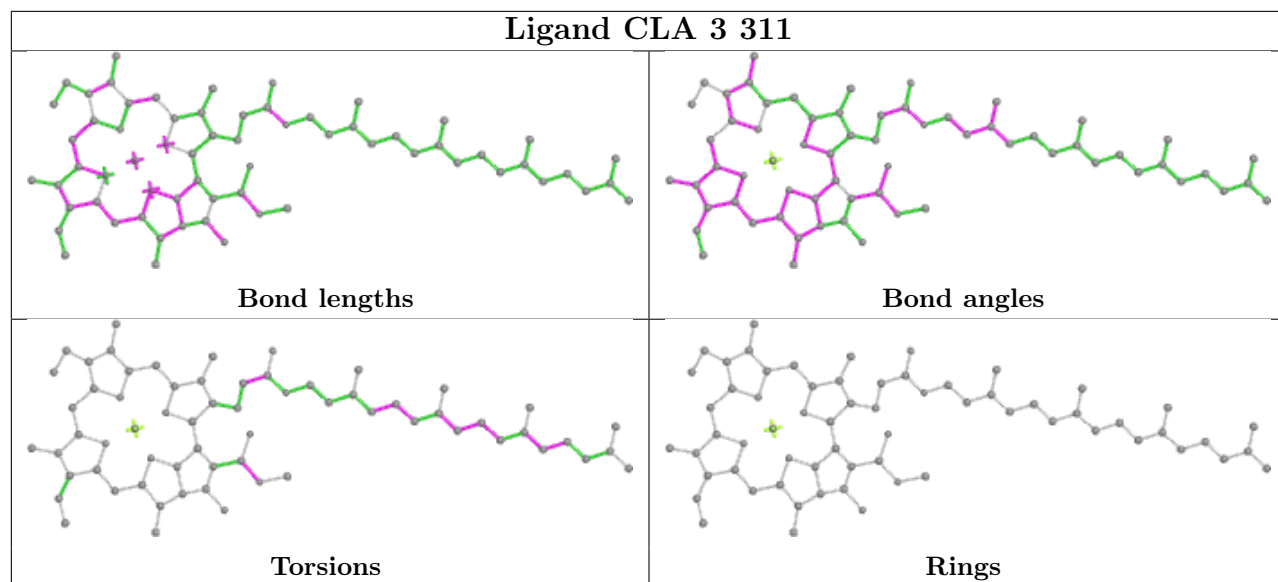


## Ligand BCR K 202

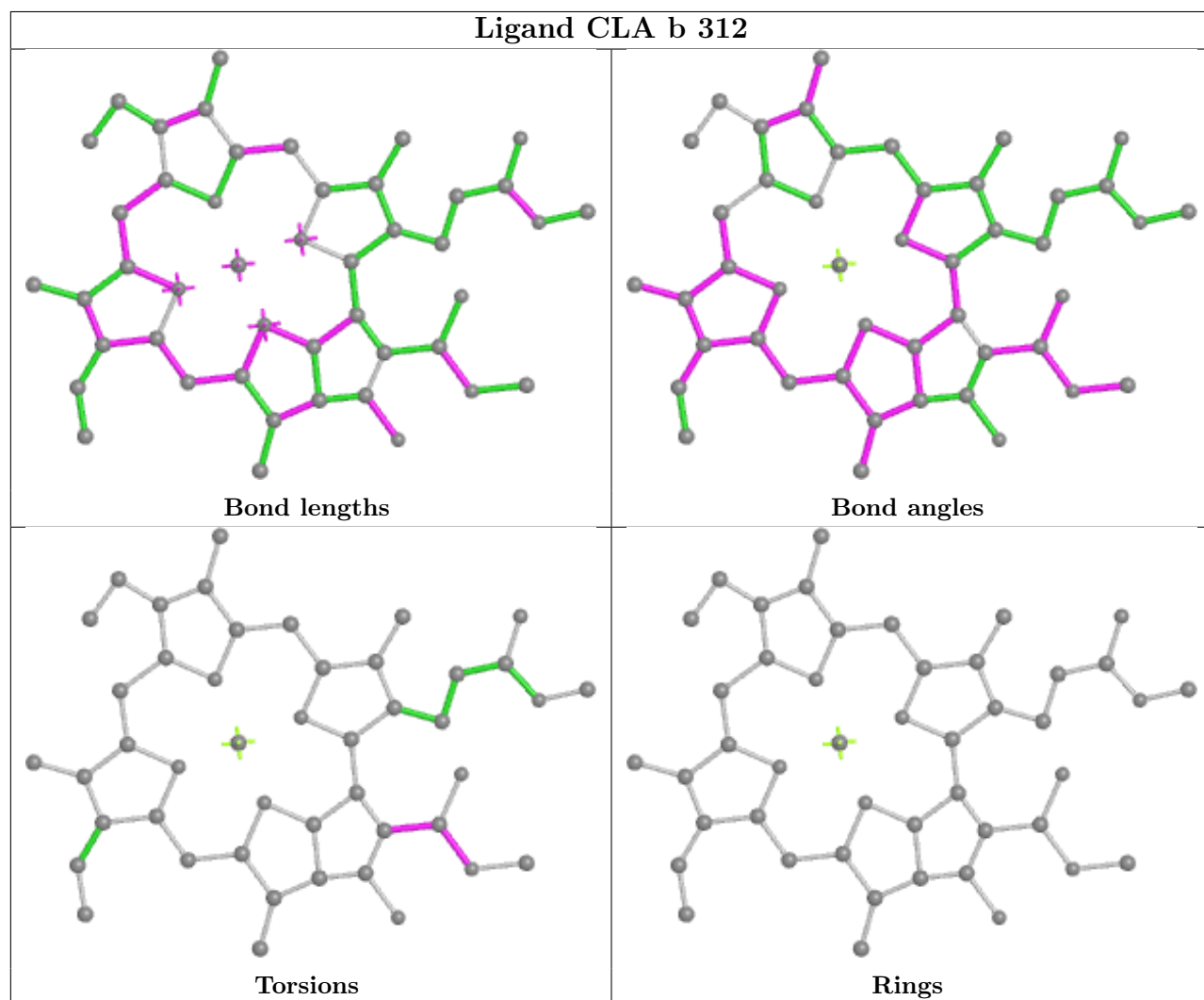




## Ligand CLA 3 311

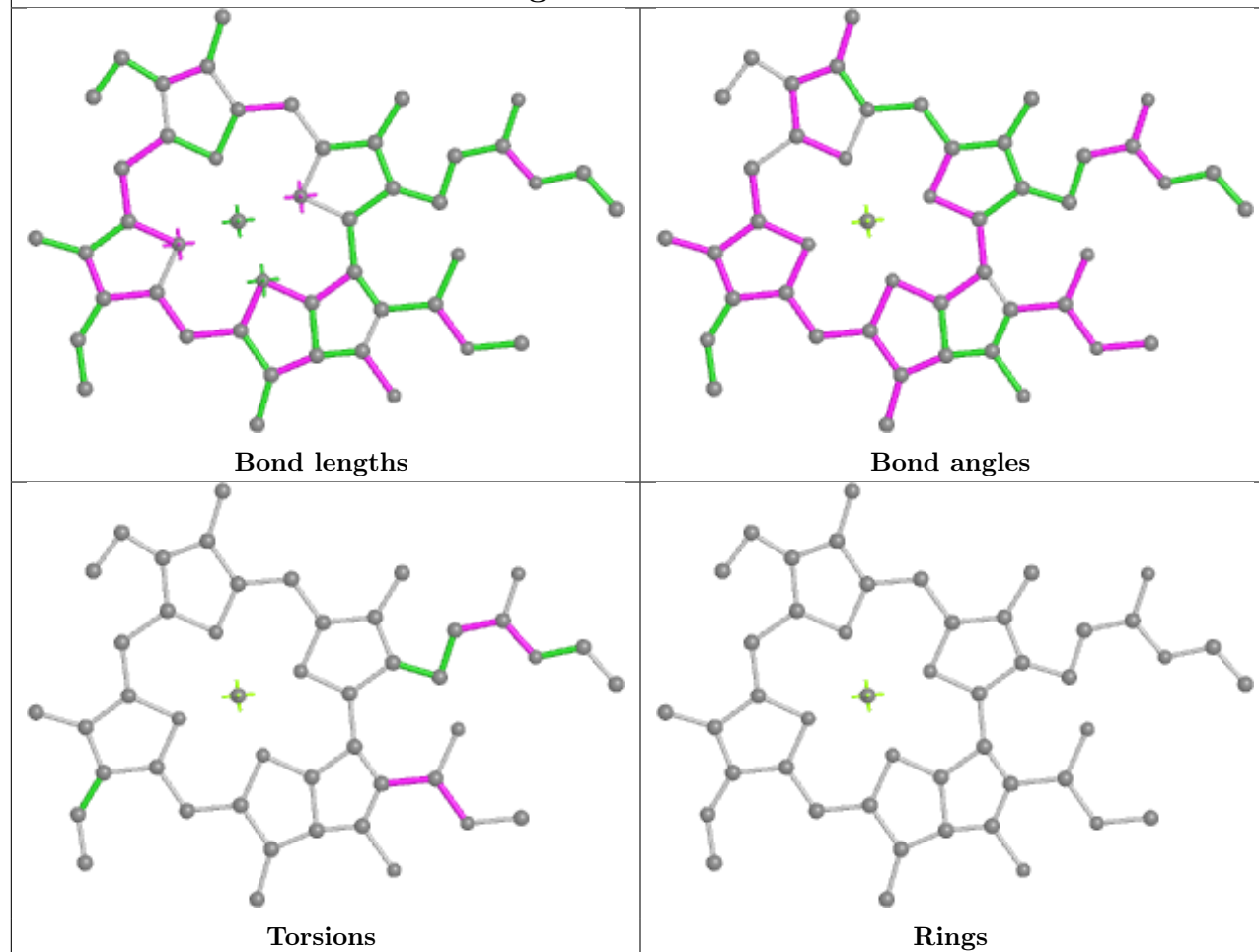


## Ligand CLA b 312

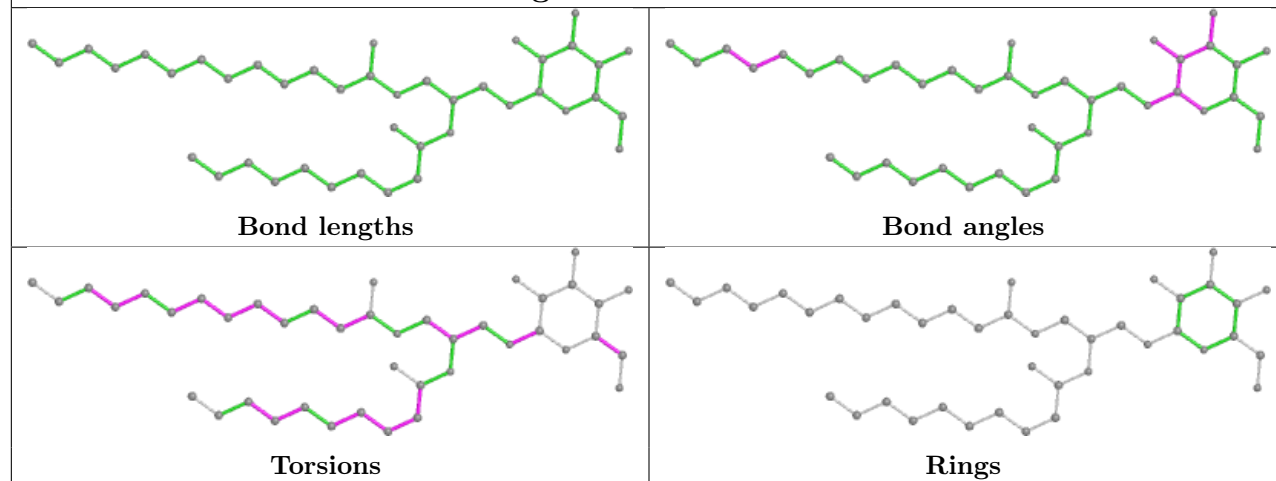




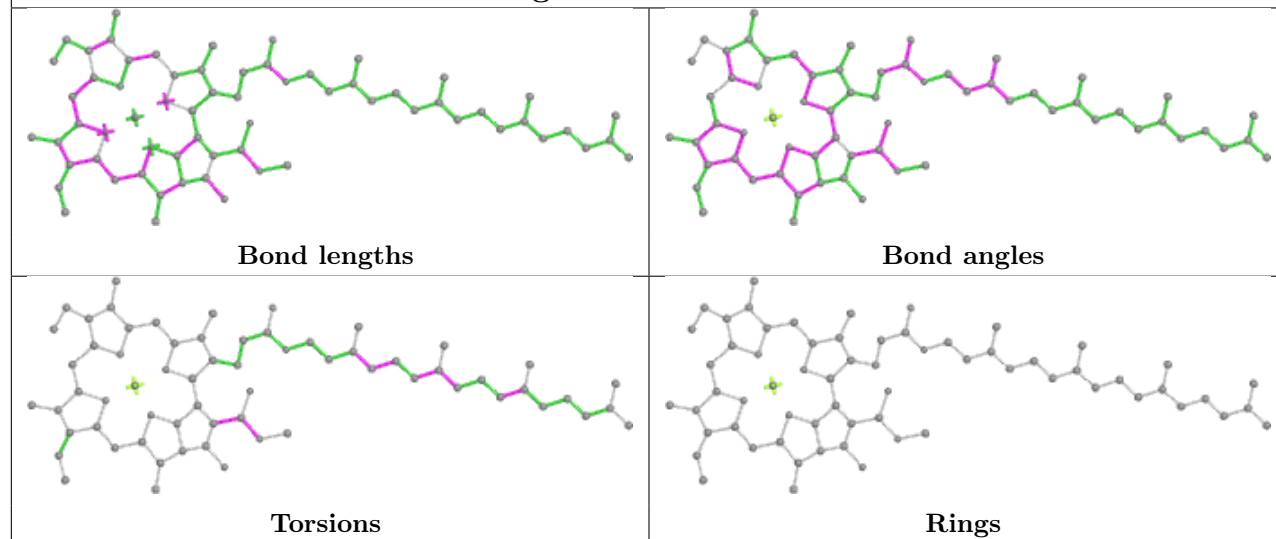
## Ligand CLA 7 321



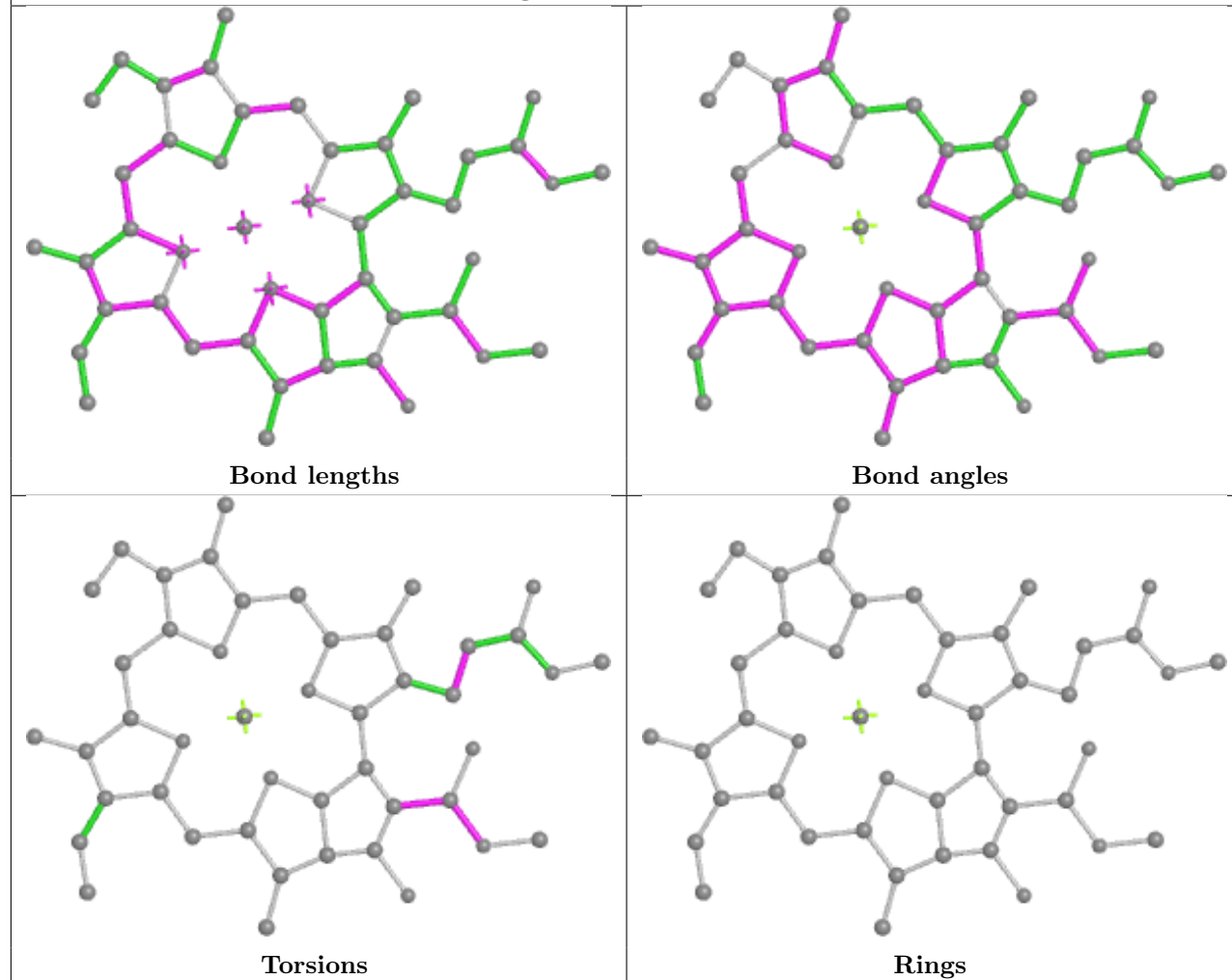
## Ligand LMG a 301

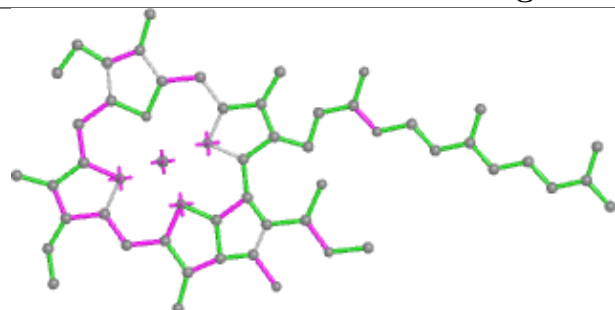


## Ligand CLA B 817

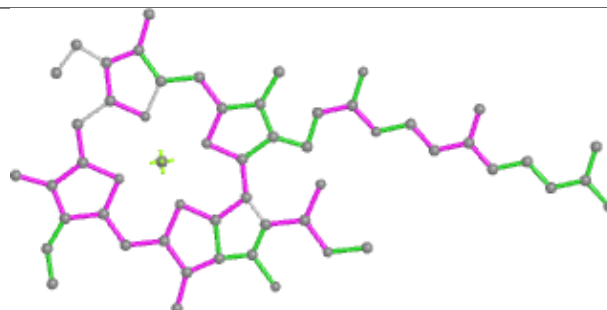


## Ligand CLA b 303

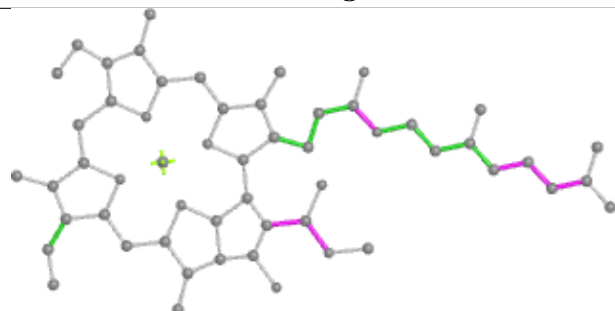


**Ligand CLA B 823**

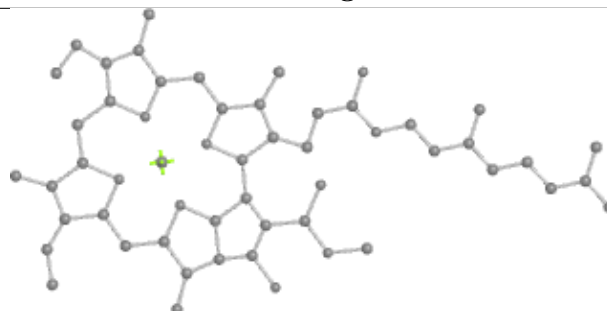
Bond lengths



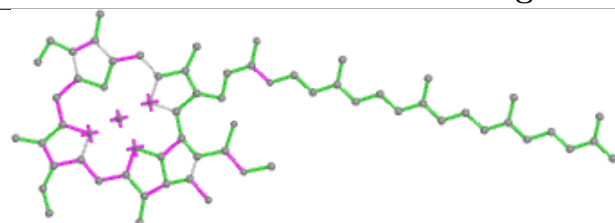
Bond angles



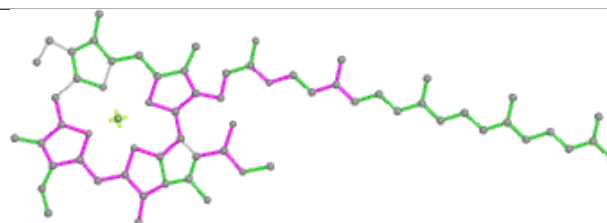
Torsions



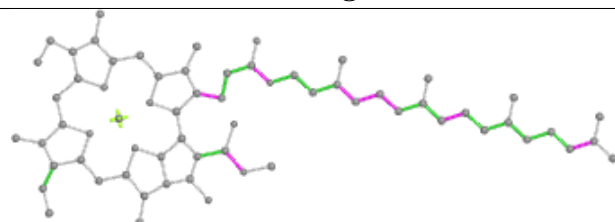
Rings

**Ligand CLA A 855**

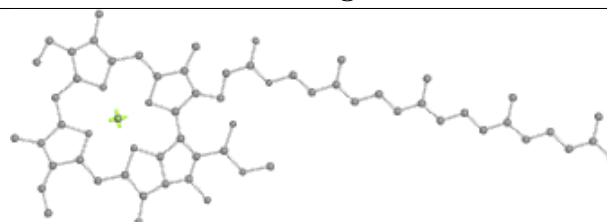
Bond lengths



Bond angles

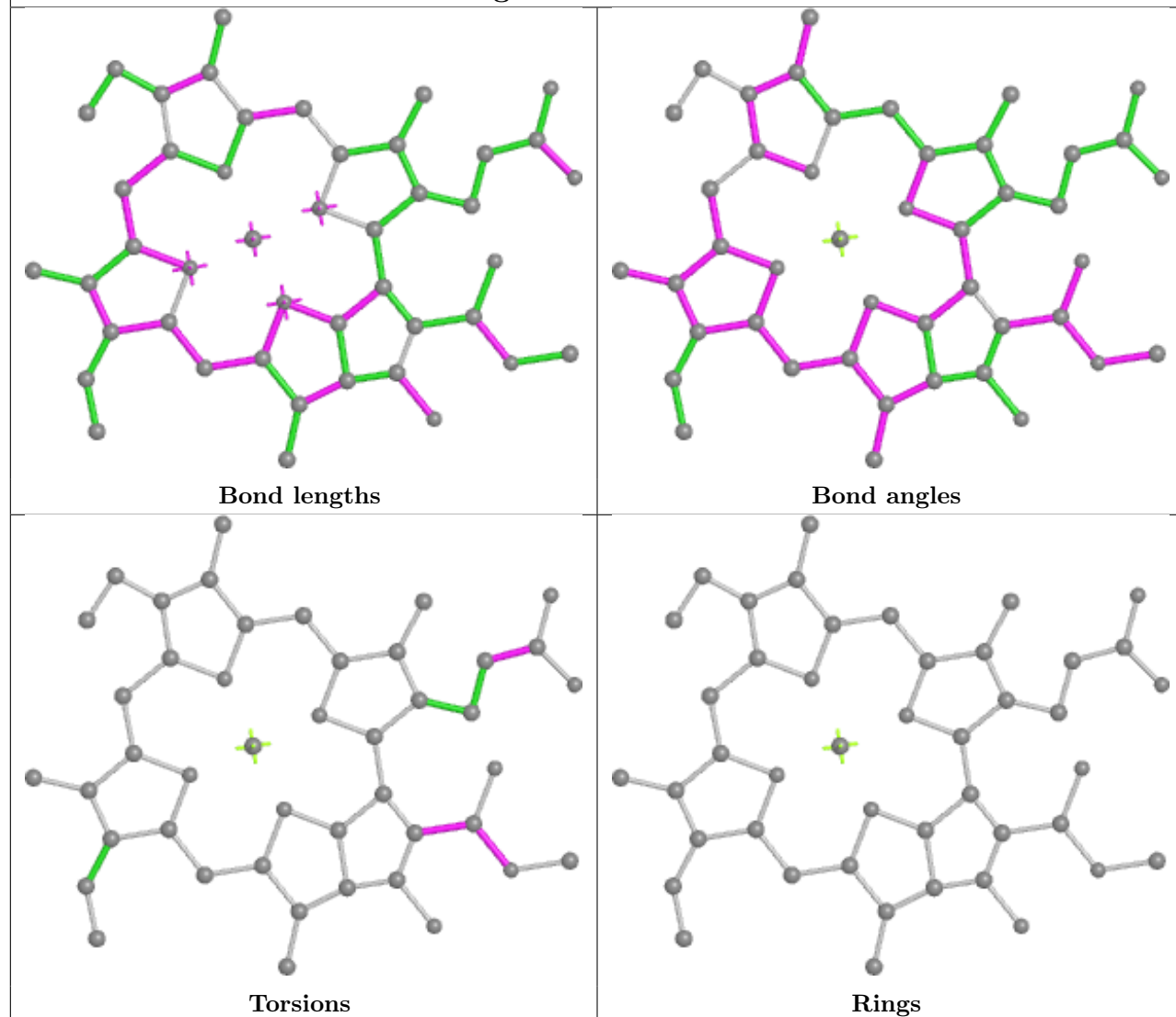


Torsions

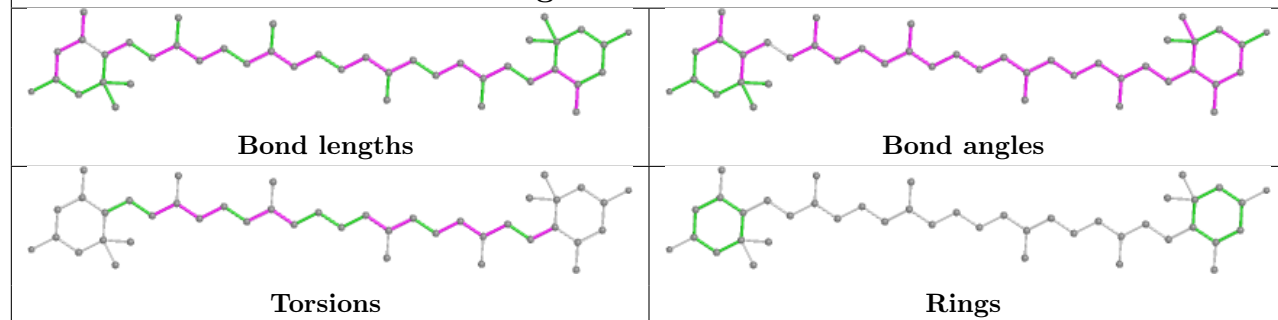


Rings

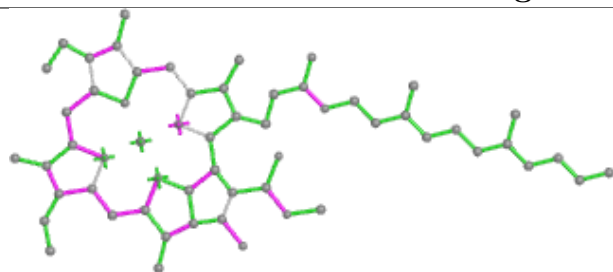
## Ligand CLA 2 305



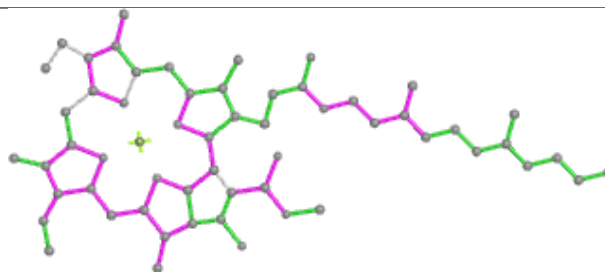
## Ligand LUT 9 303



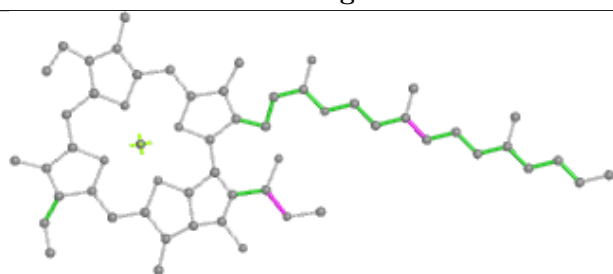
## Ligand CLA B 821



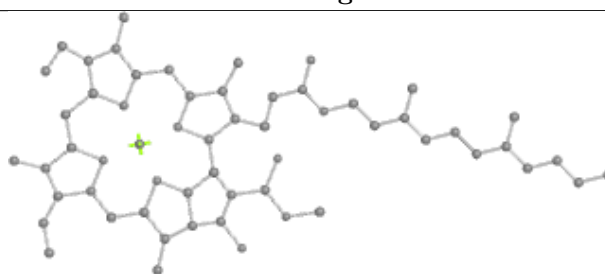
Bond lengths



Bond angles

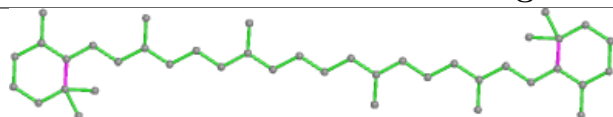


Torsions

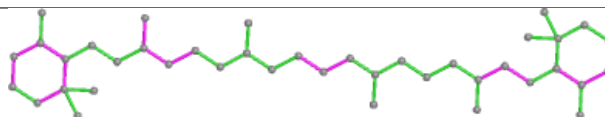


Rings

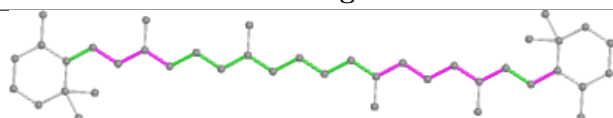
## Ligand BCR 5 302



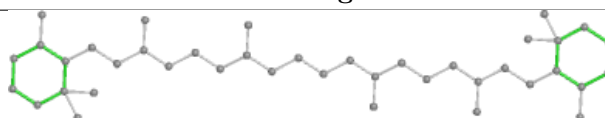
Bond lengths



Bond angles

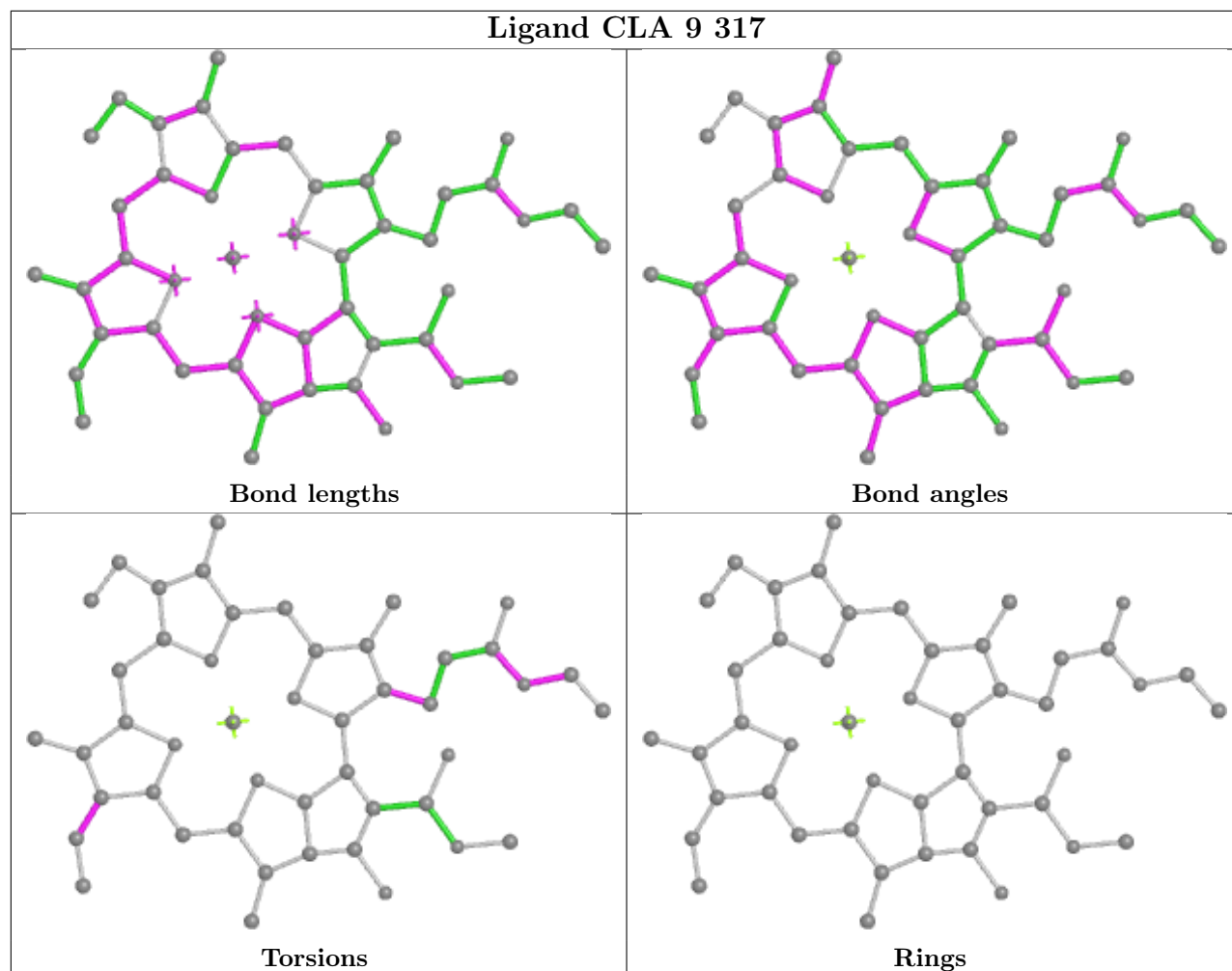


Torsions

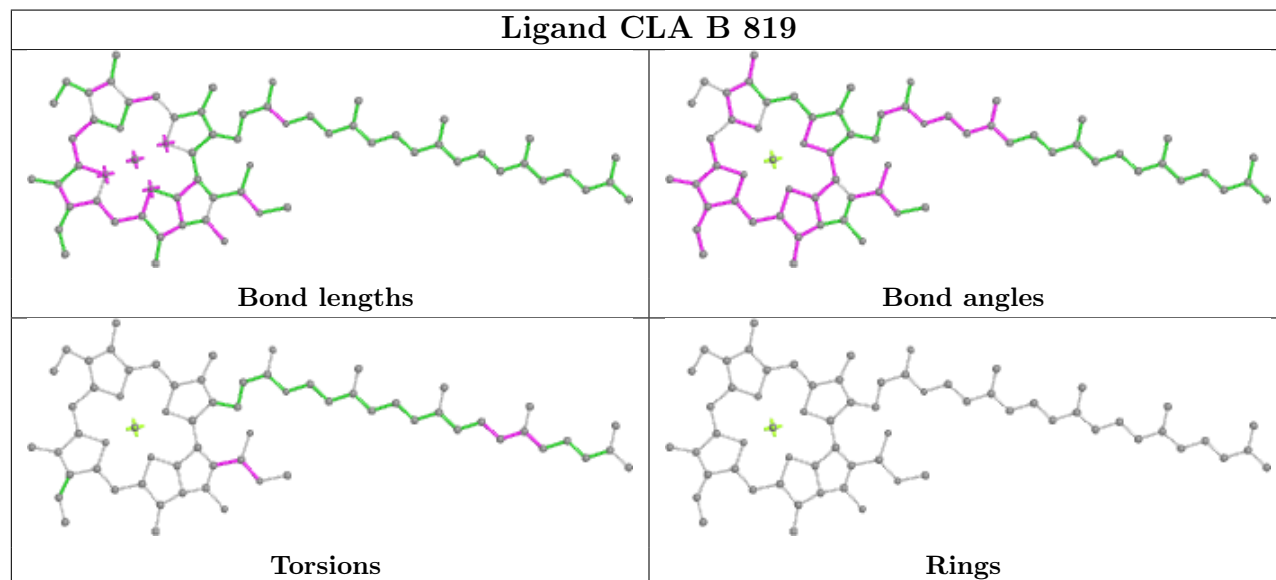


Rings

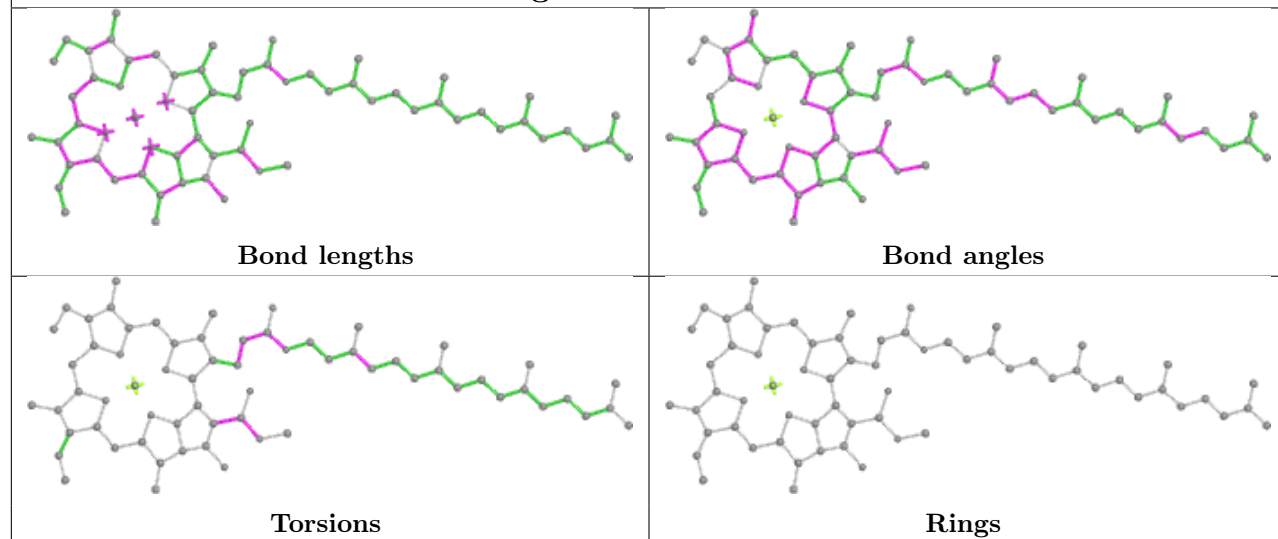
## Ligand CLA 9 317



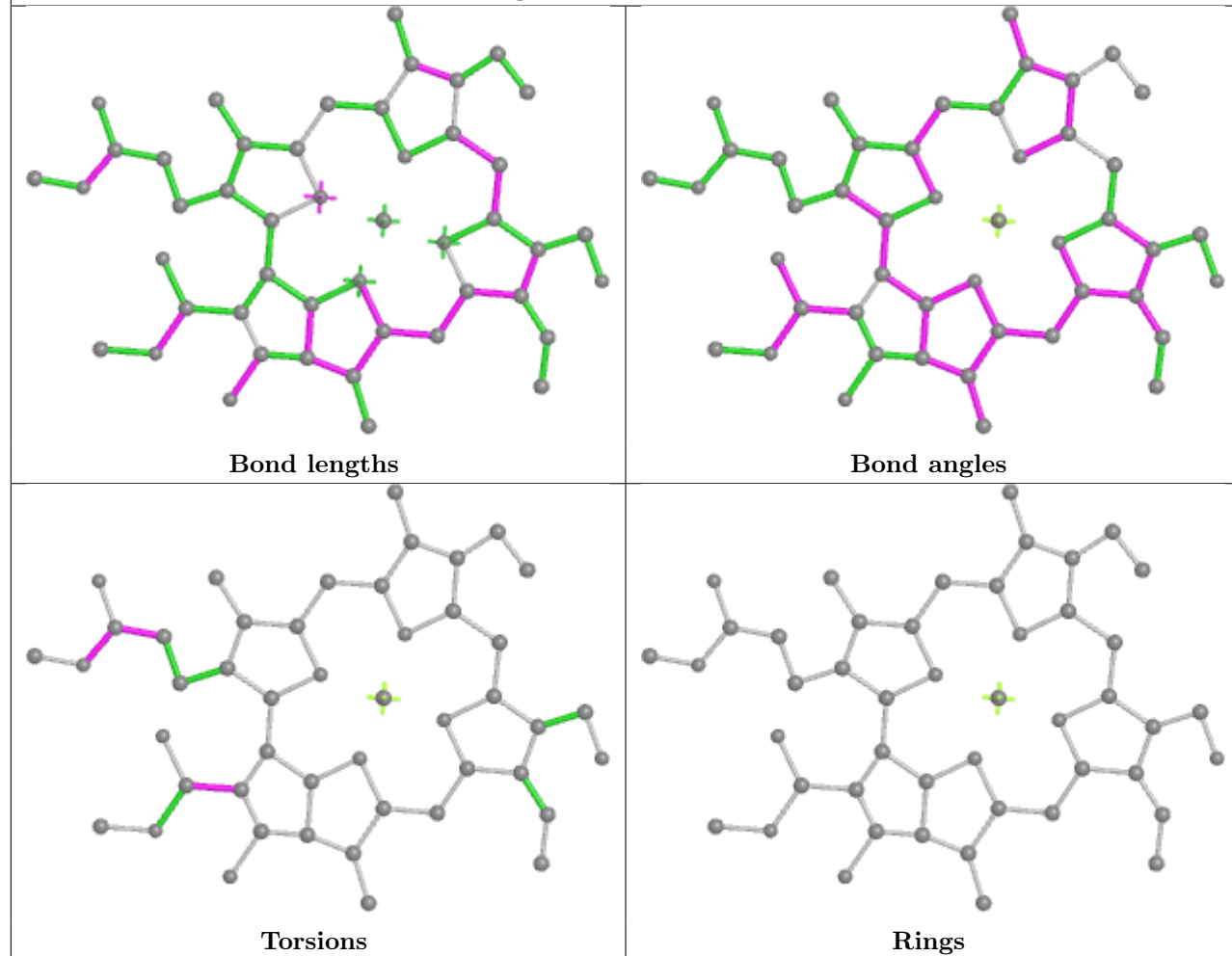
## Ligand CLA B 819

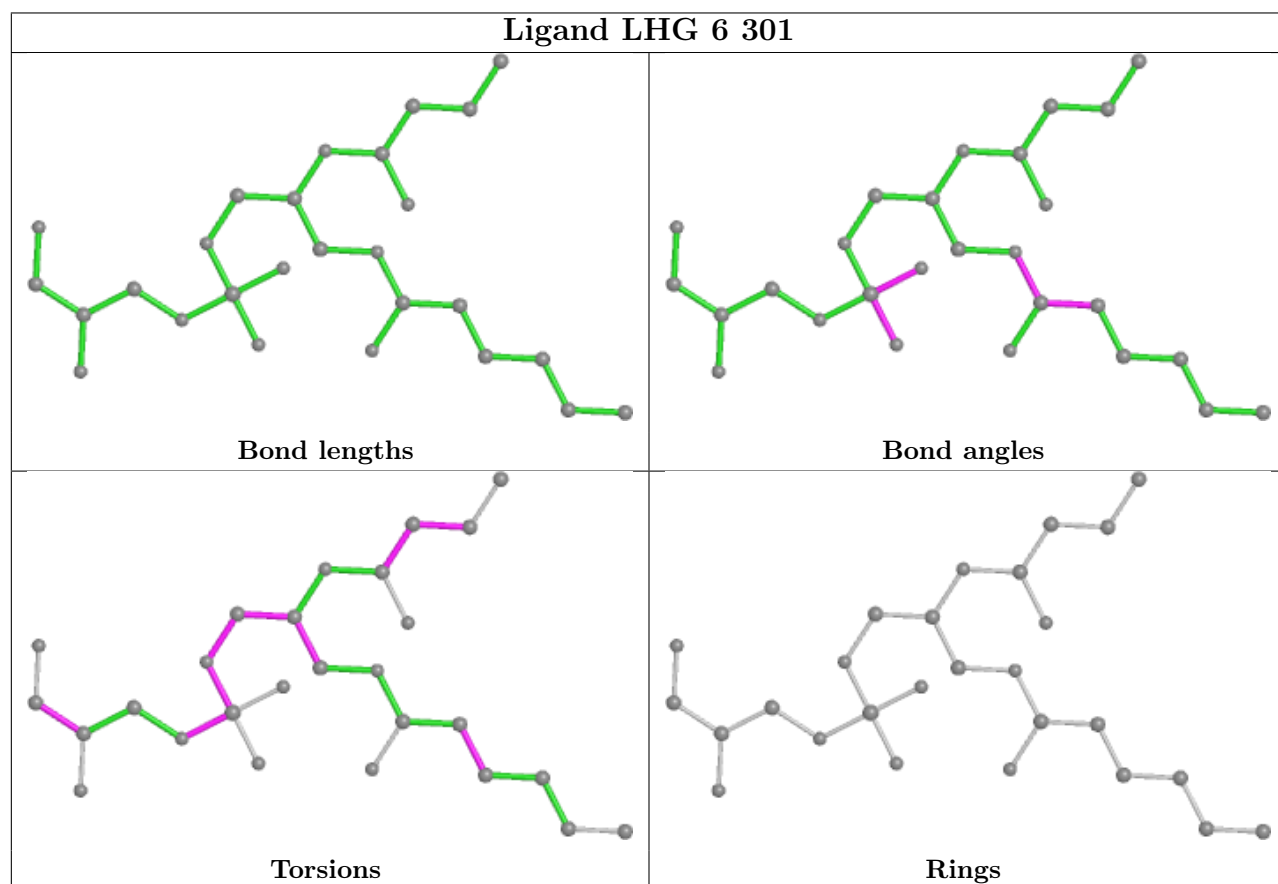
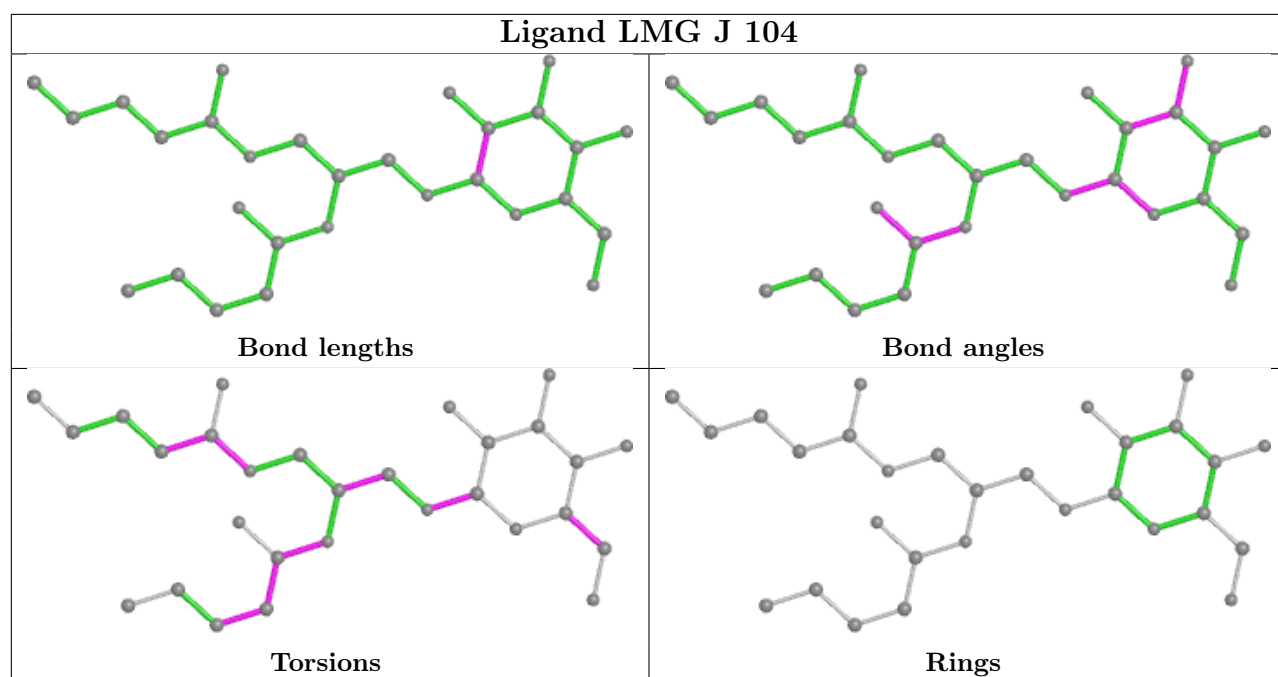


## Ligand CLA A 834

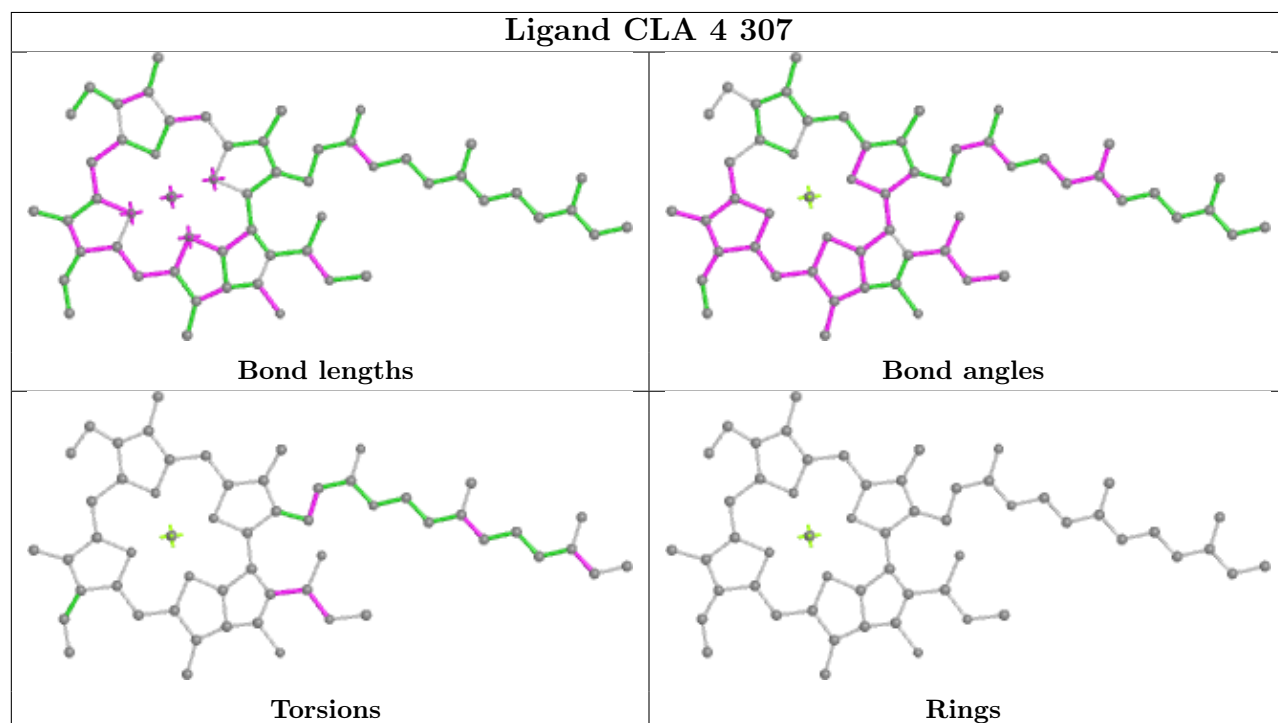
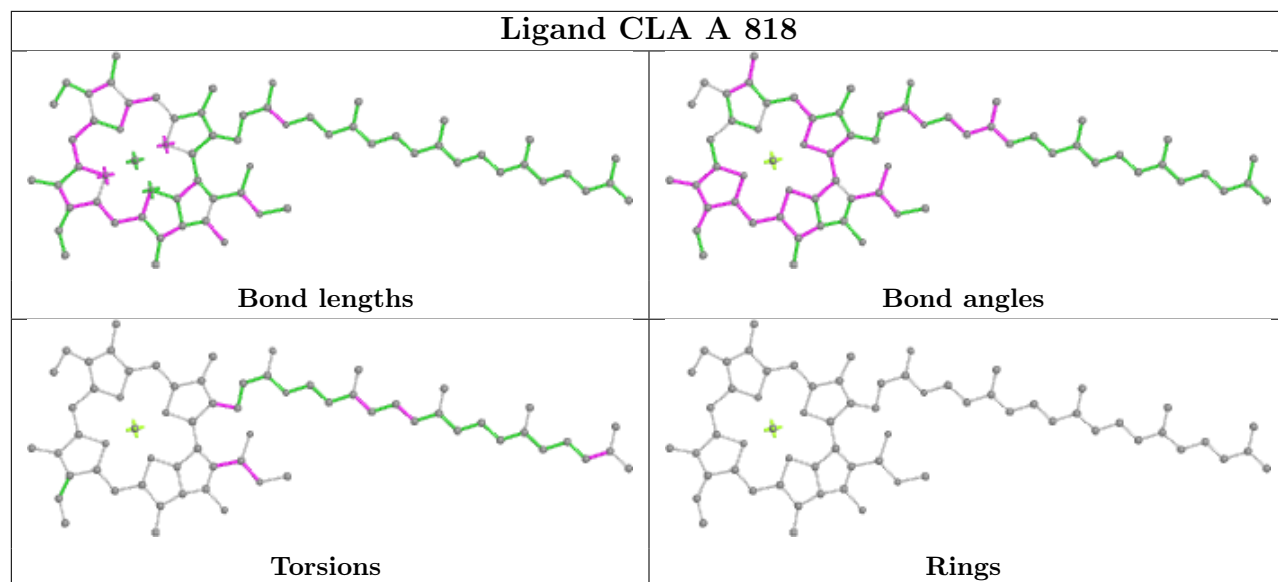


## Ligand CHL K 201

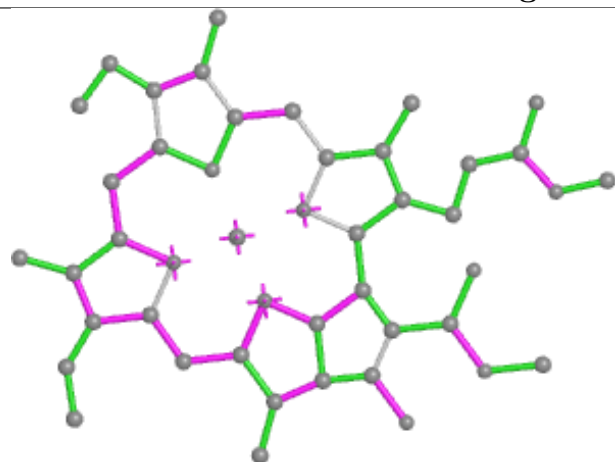




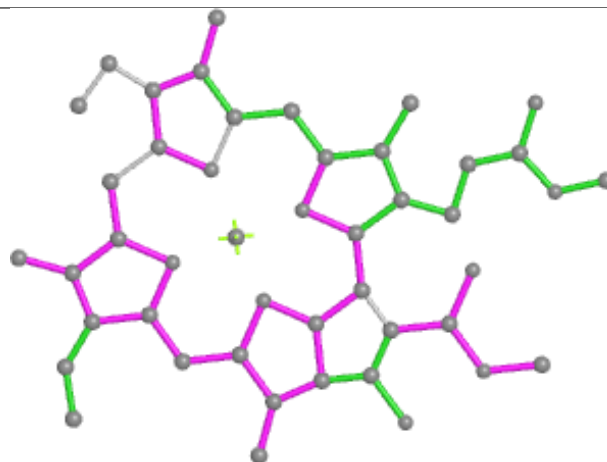




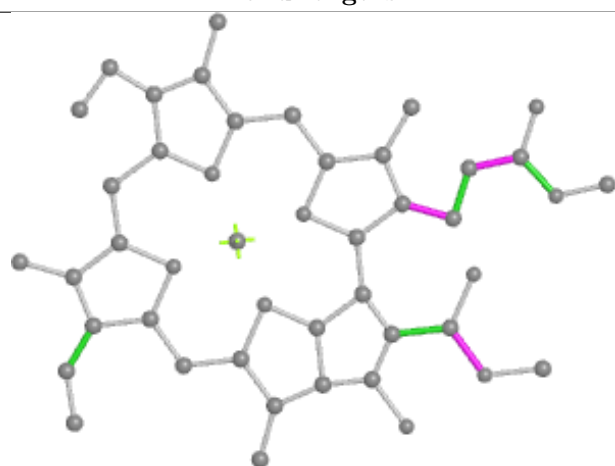
## Ligand CLA b 302



Bond lengths



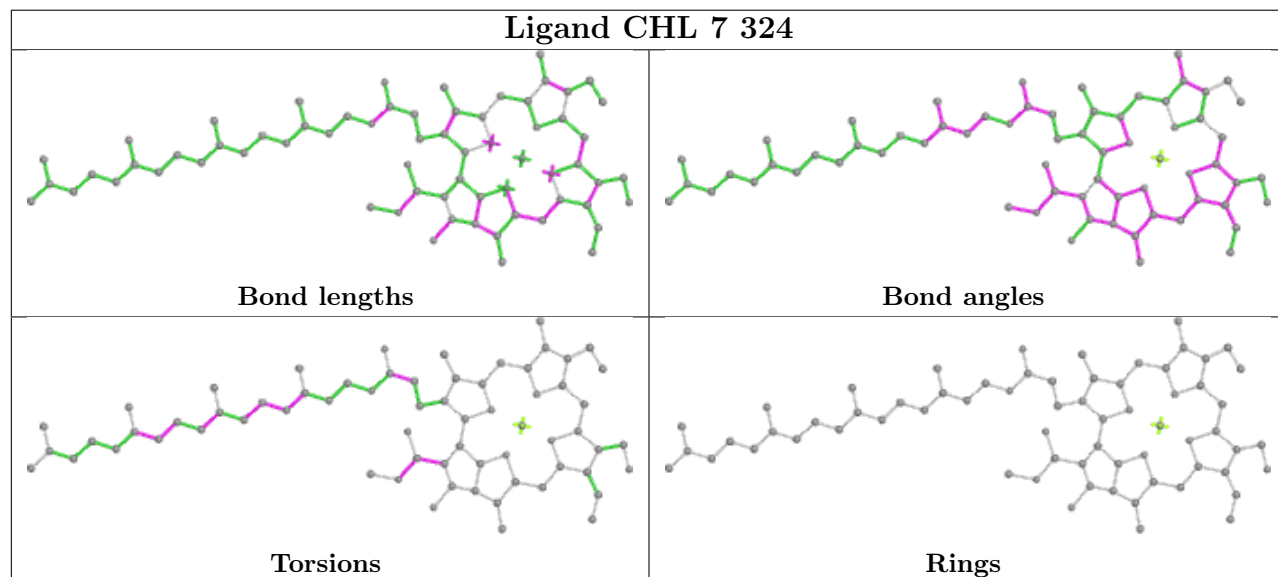
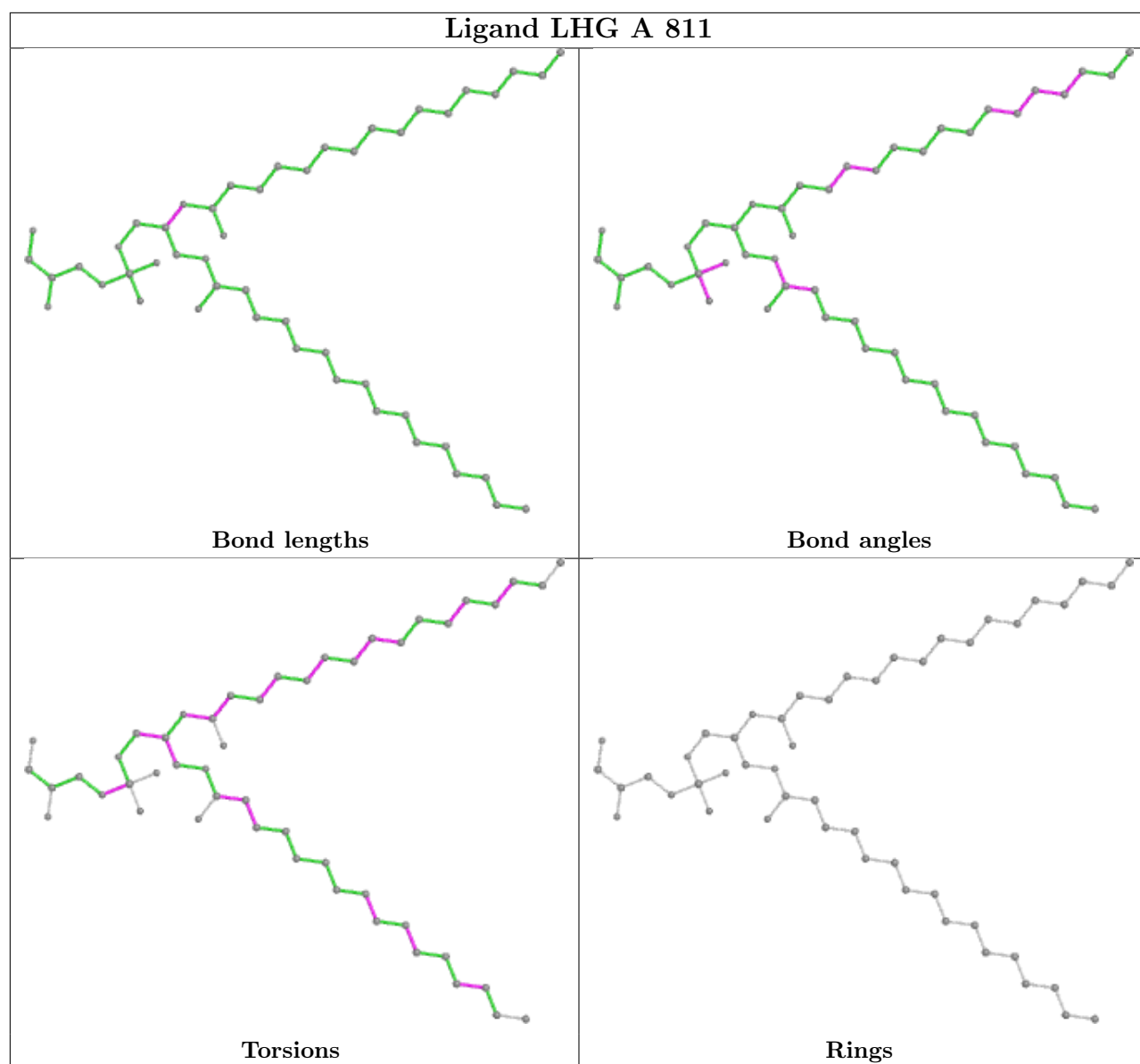
Bond angles

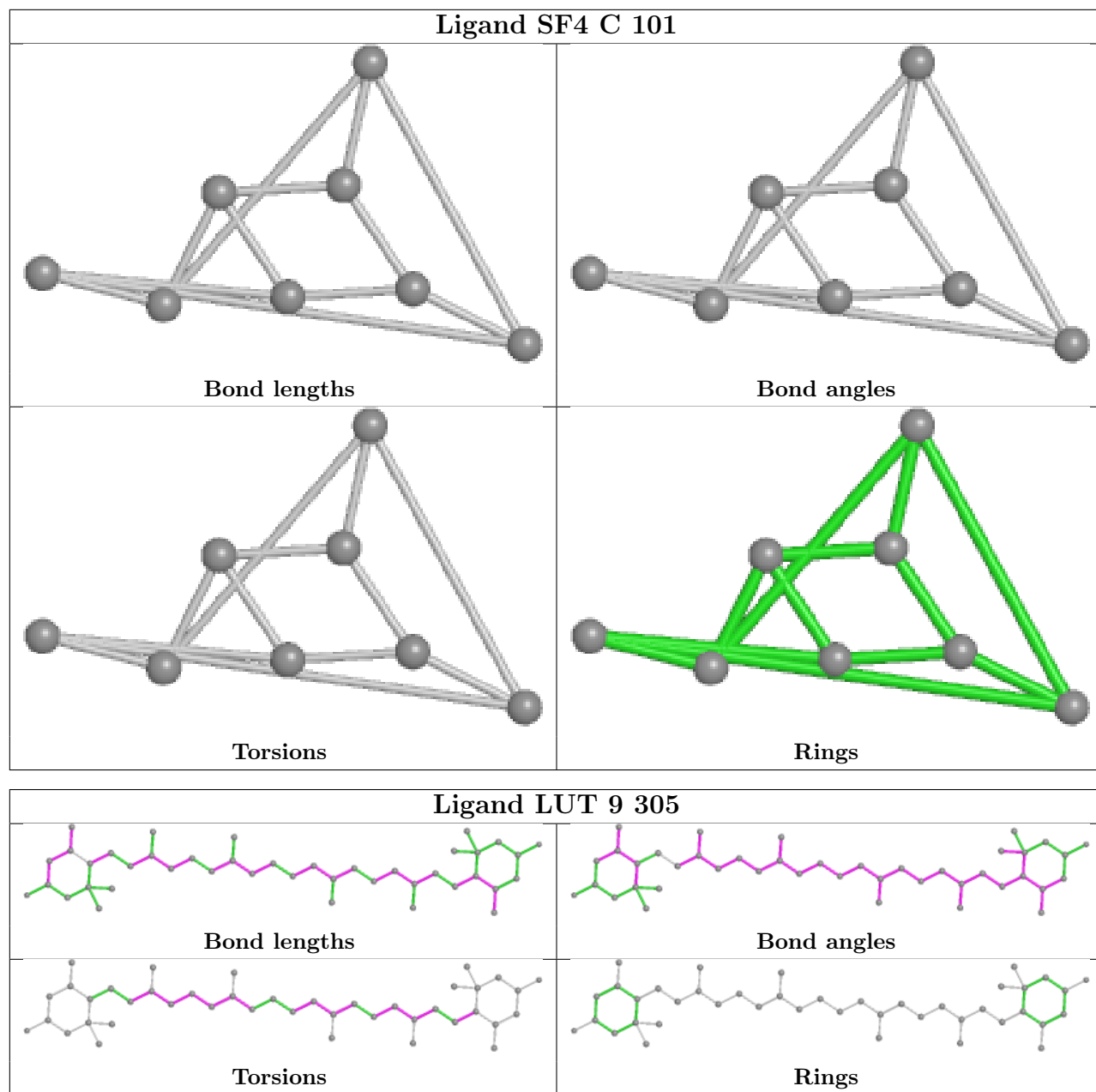


Torsions

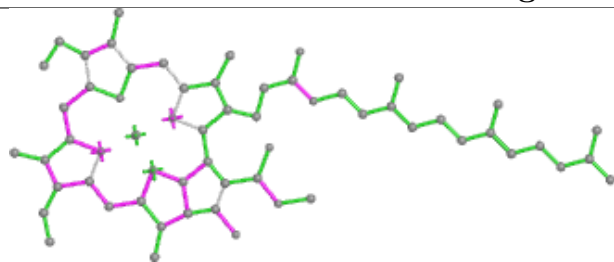


Rings

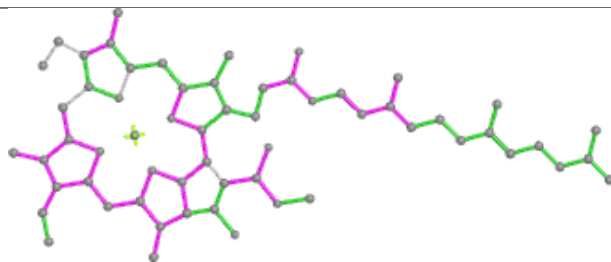




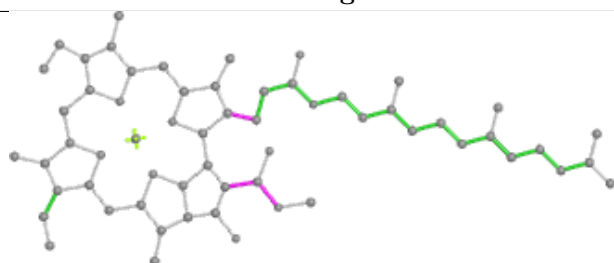
## Ligand CLA 7 309



Bond lengths



Bond angles

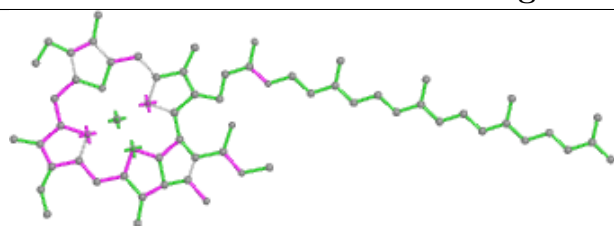


Torsions

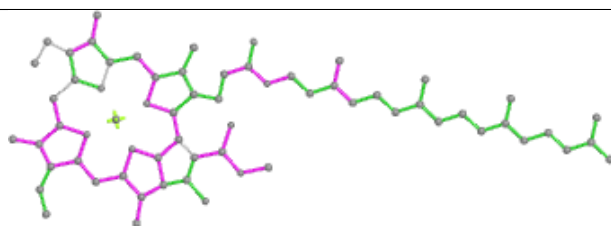


Rings

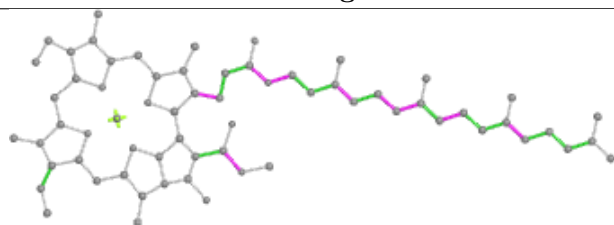
## Ligand CLA 3 309



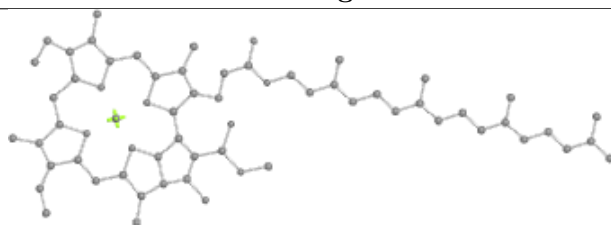
Bond lengths



Bond angles

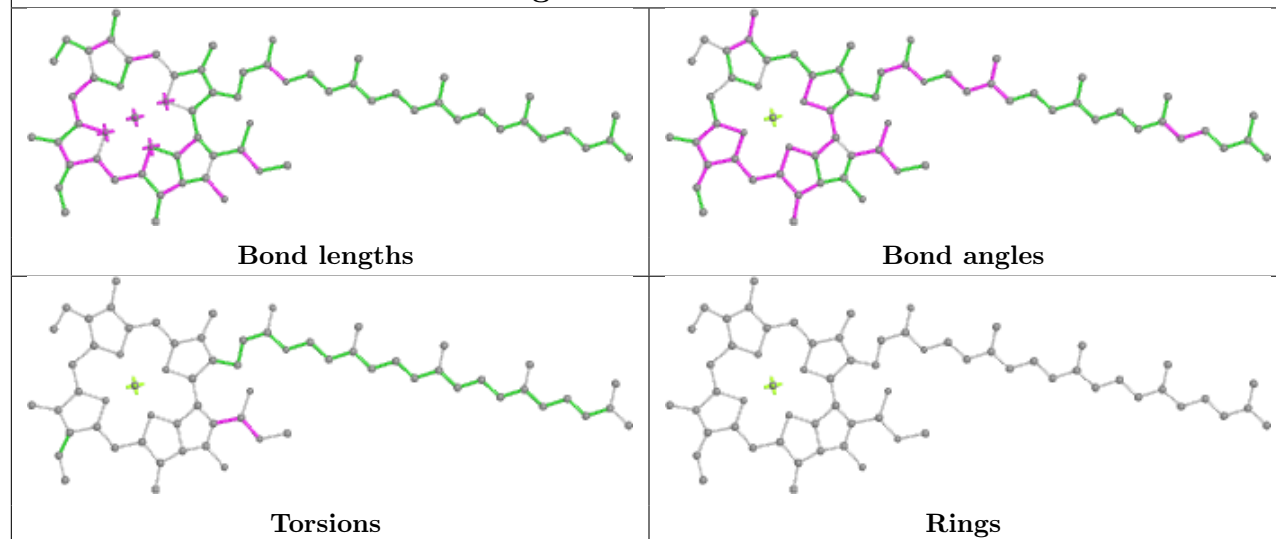


Torsions

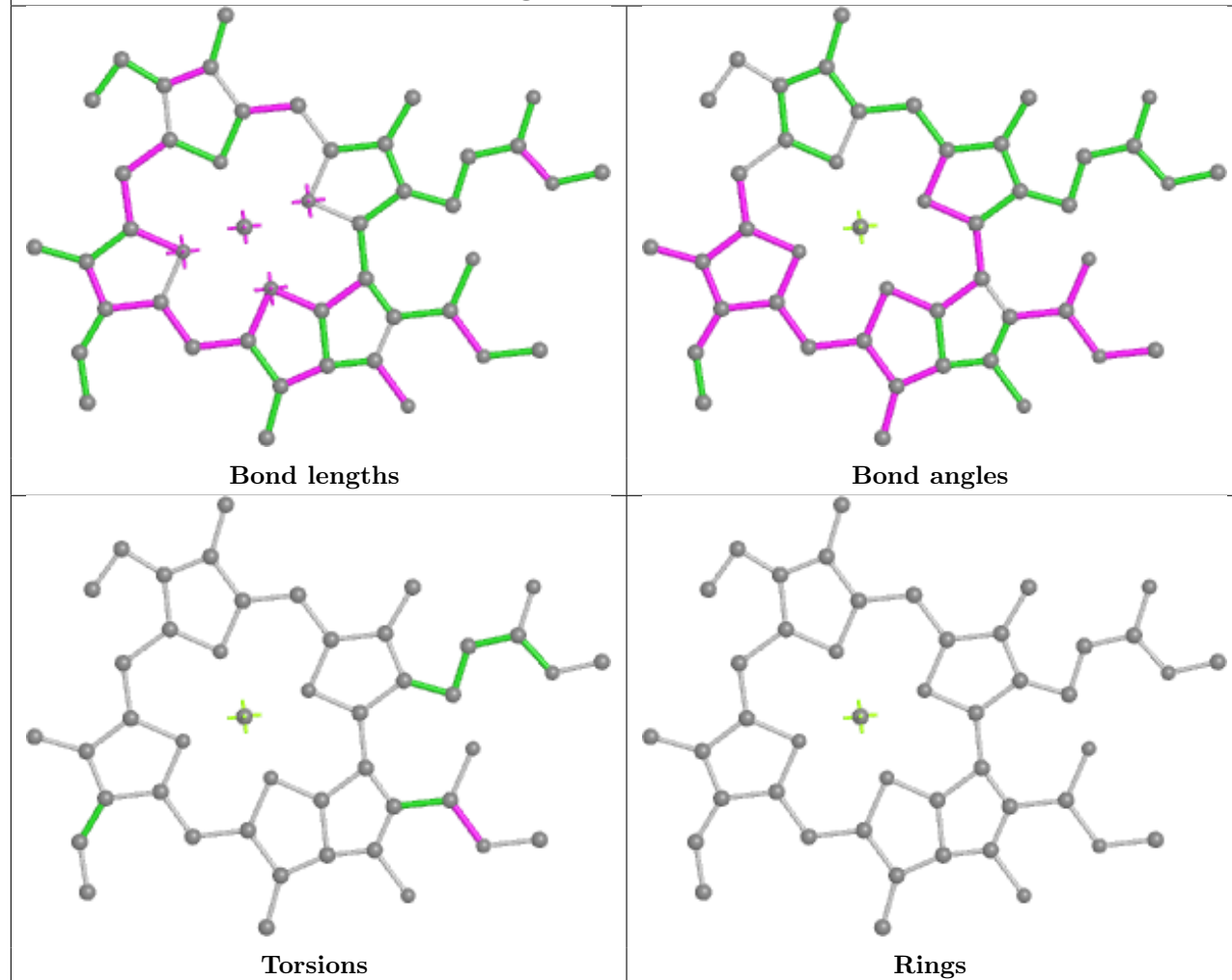


Rings

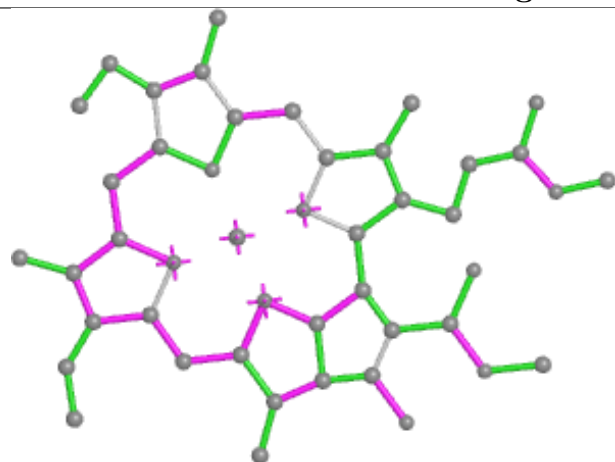
## Ligand CLA B 834



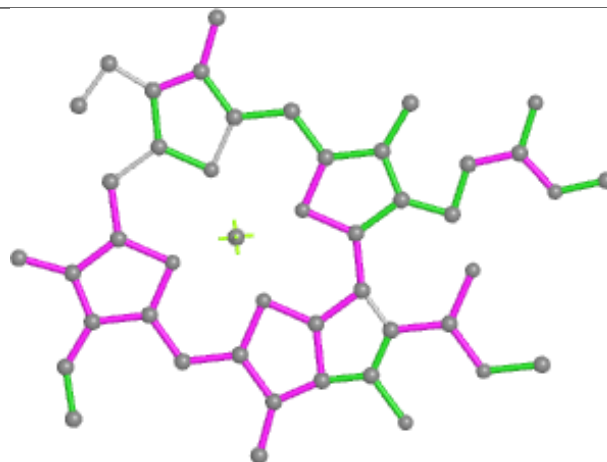
## Ligand CLA 5 308



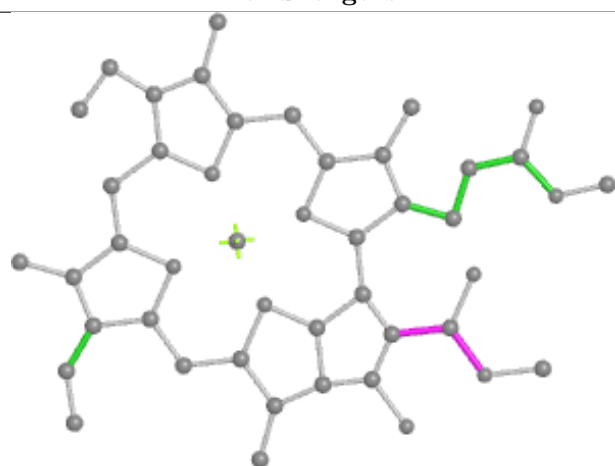
## Ligand CLA H 902



Bond lengths



Bond angles

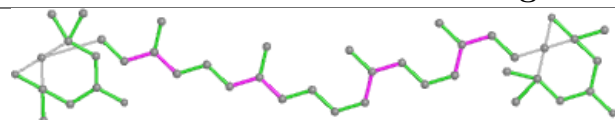


Torsions

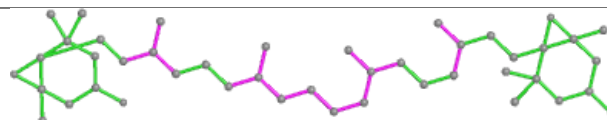


Rings

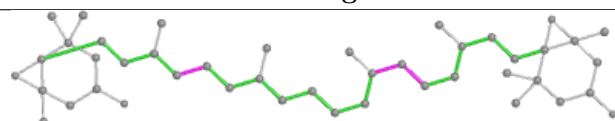
## Ligand XAT 7 306



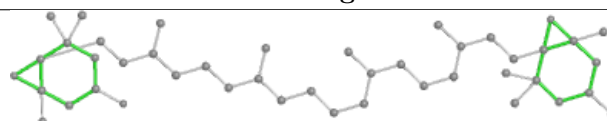
Bond lengths



Bond angles

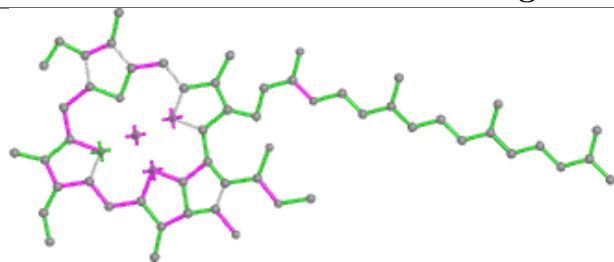


Torsions

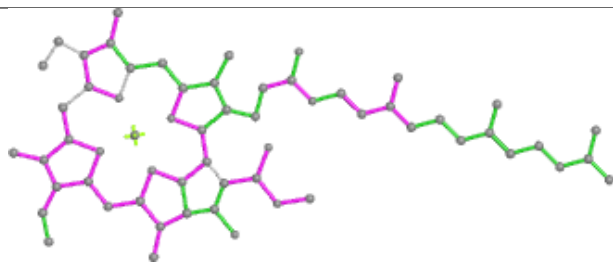


Rings

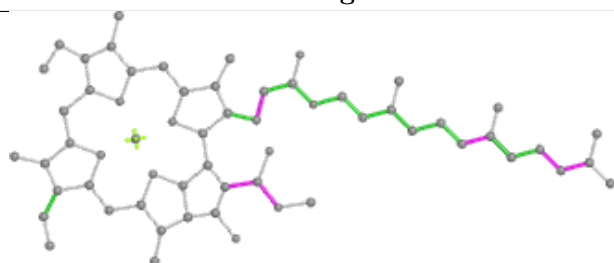
## Ligand CLA 9 314



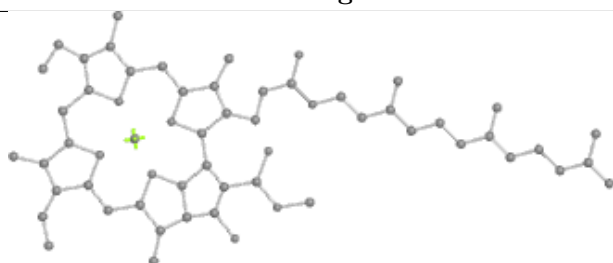
Bond lengths



Bond angles

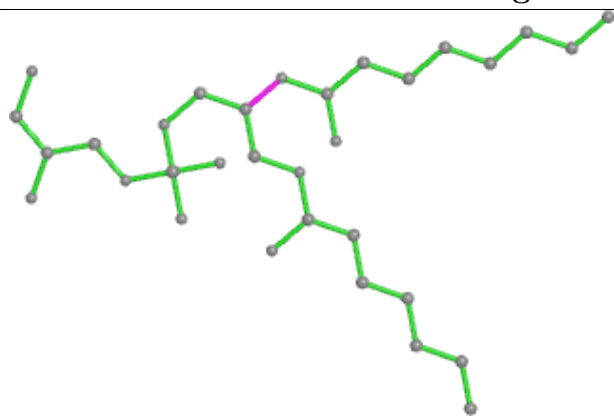


Torsions

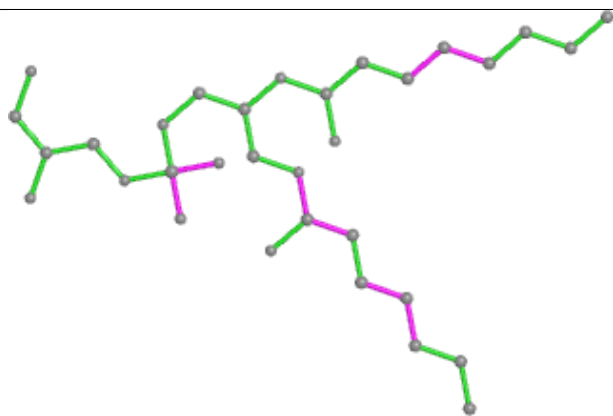


Rings

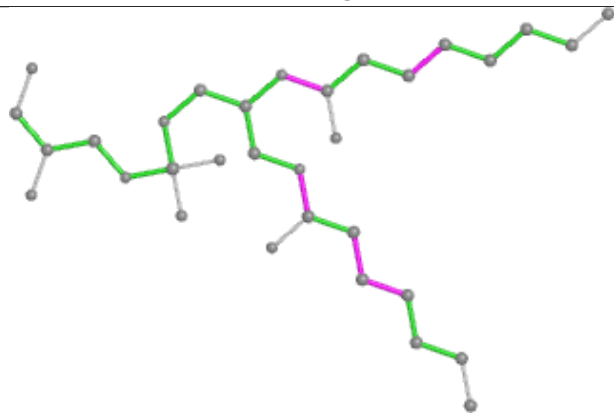
## Ligand LHG B 807



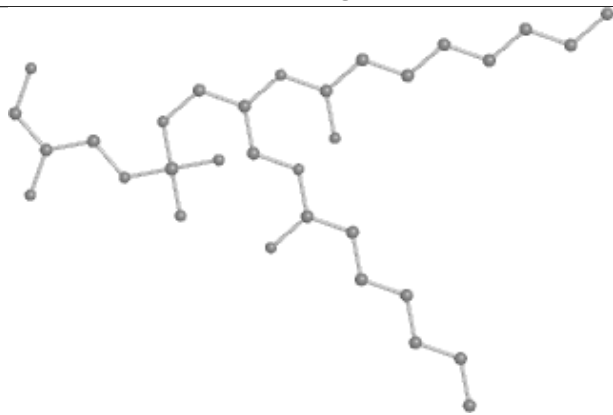
Bond lengths



Bond angles



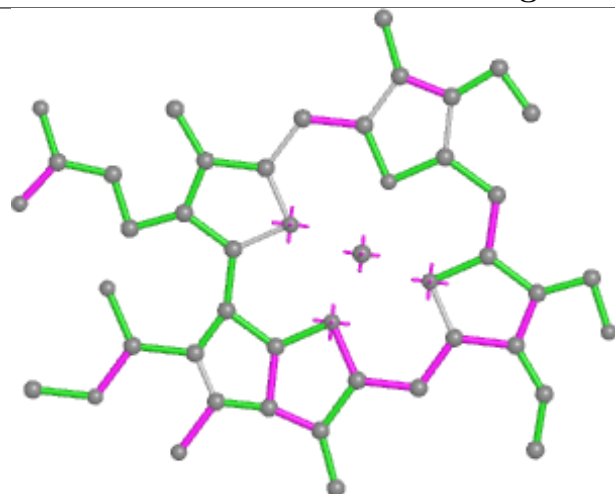
Torsions



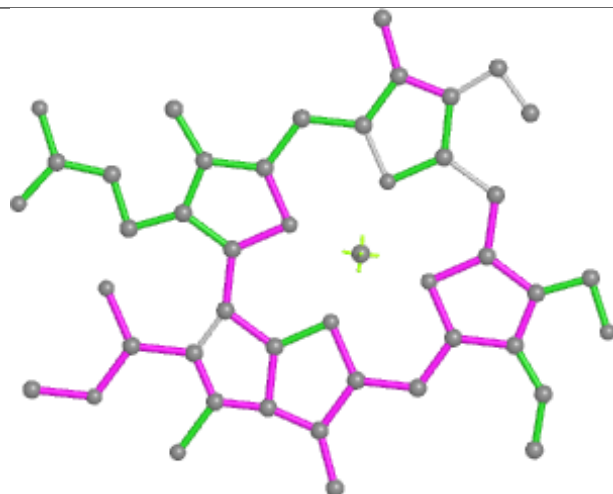
Rings



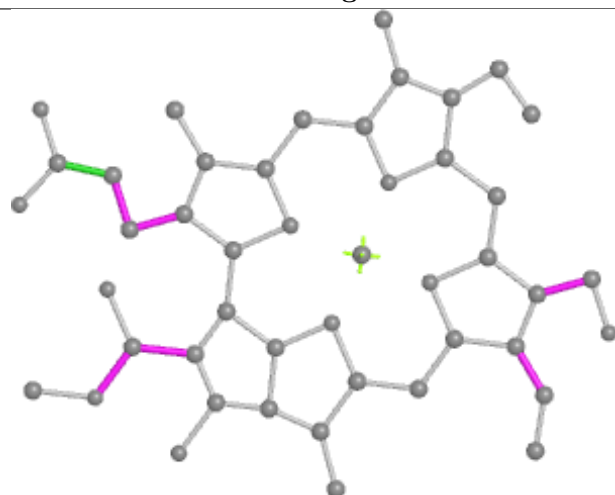
## Ligand CHL 4 317



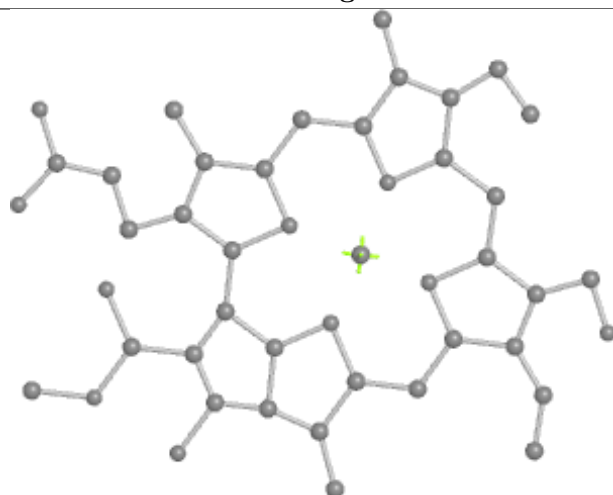
Bond lengths



Bond angles

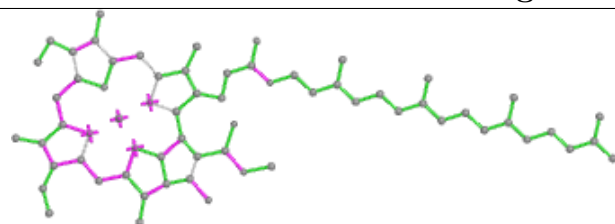


Torsions

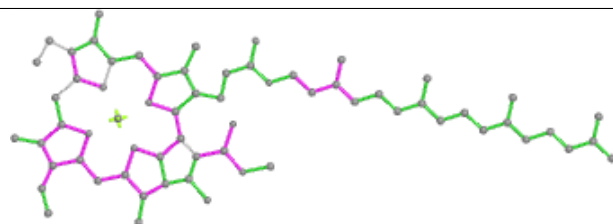


Rings

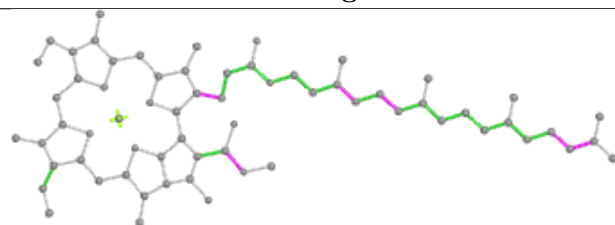
## Ligand CLA B 847



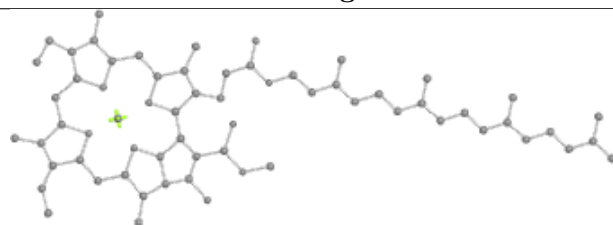
Bond lengths



Bond angles

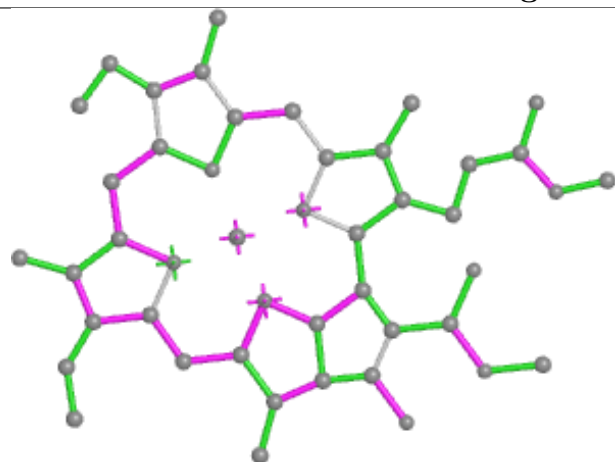


Torsions

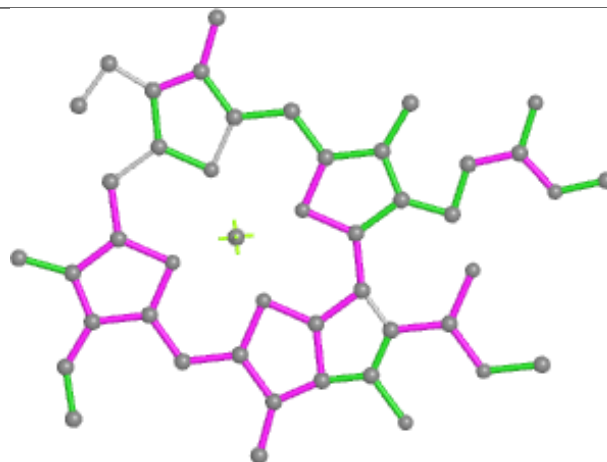


Rings

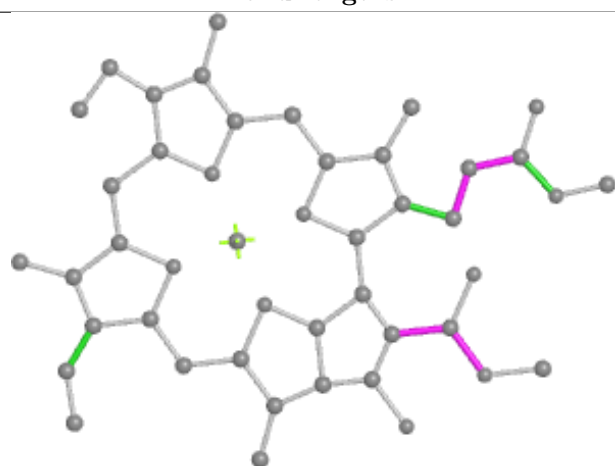
## Ligand CLA a 322



Bond lengths



Bond angles

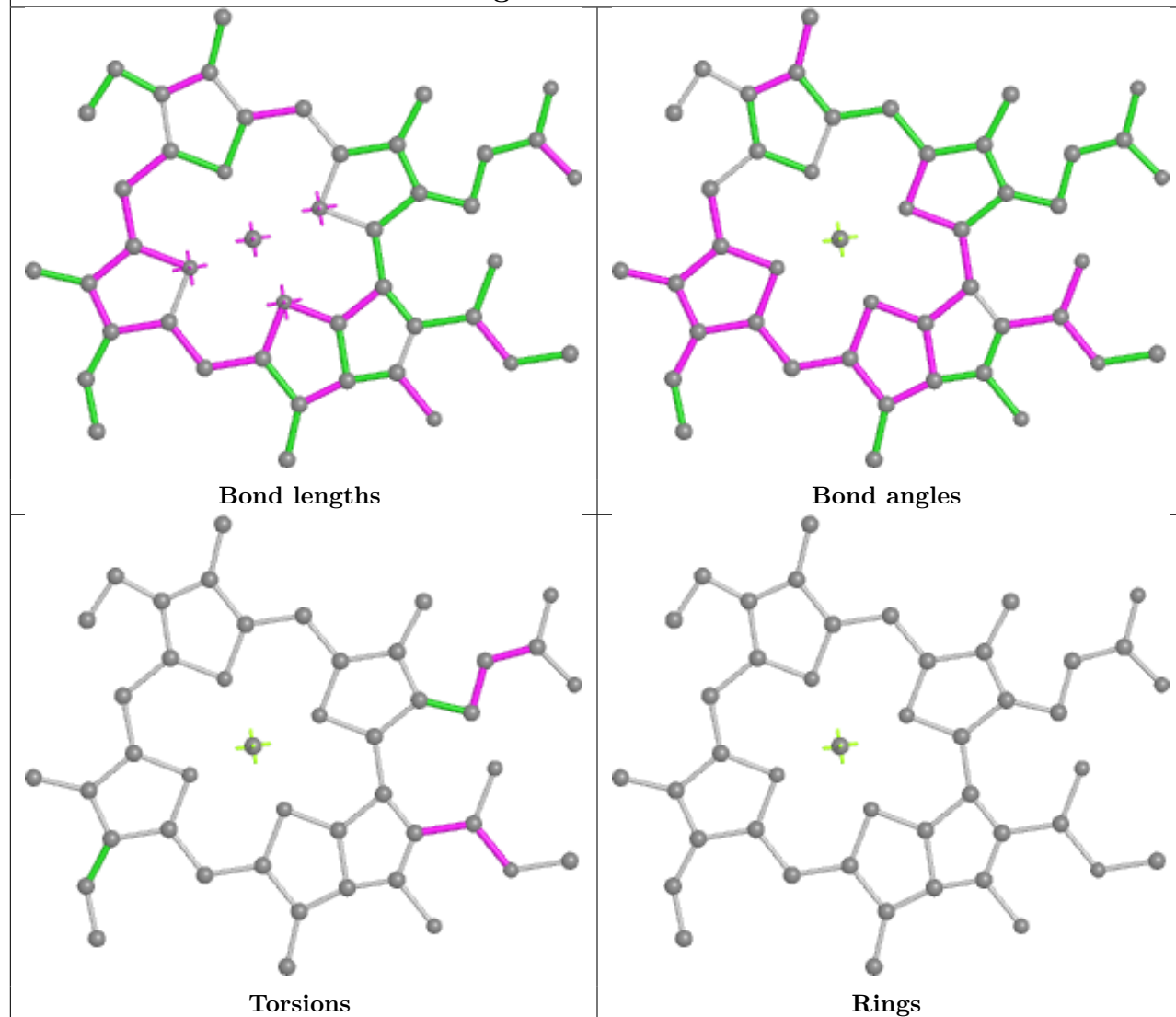


Torsions

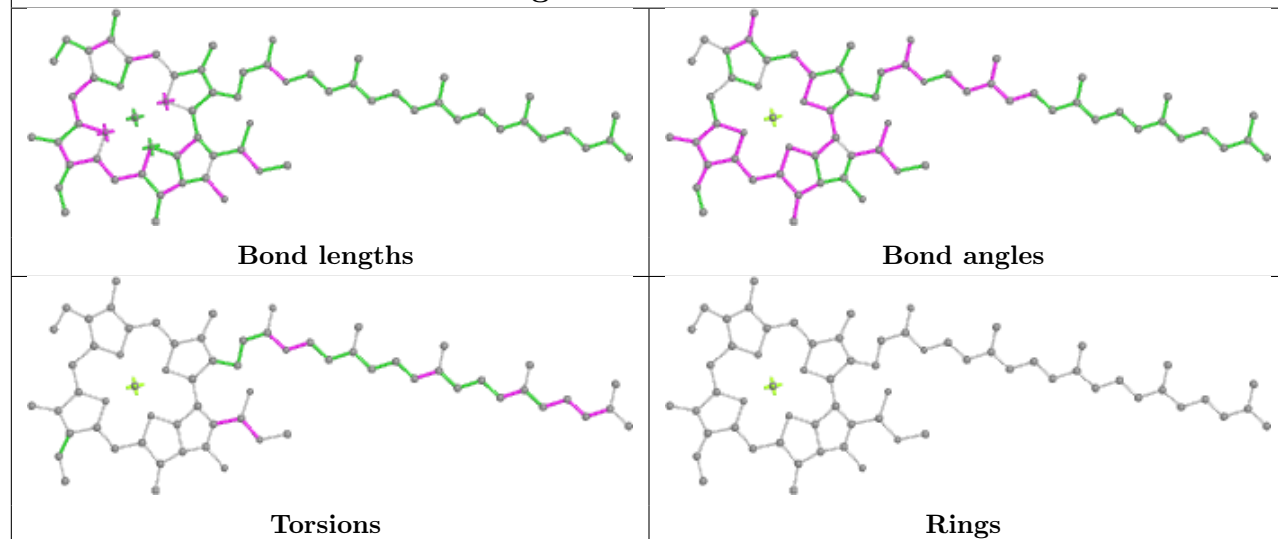


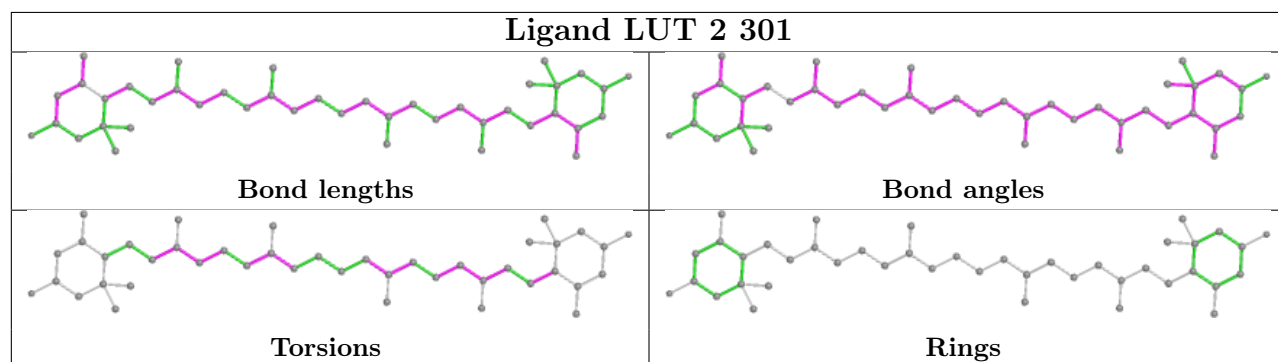
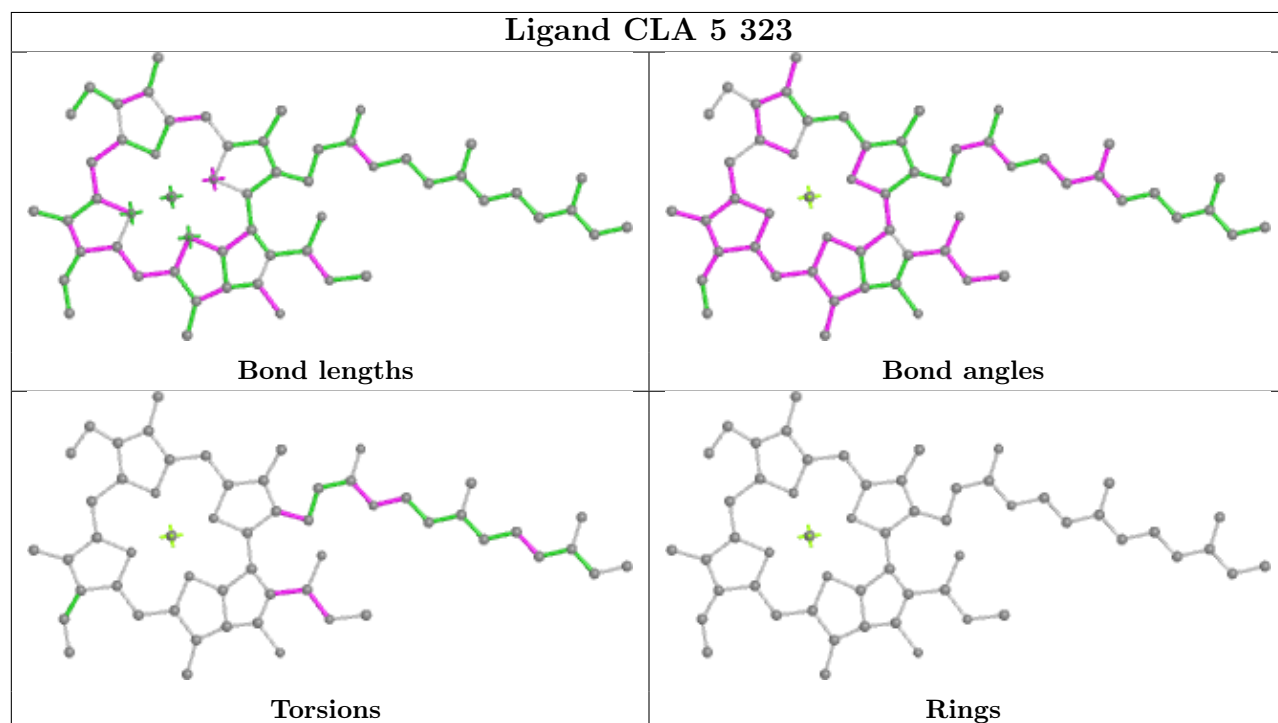
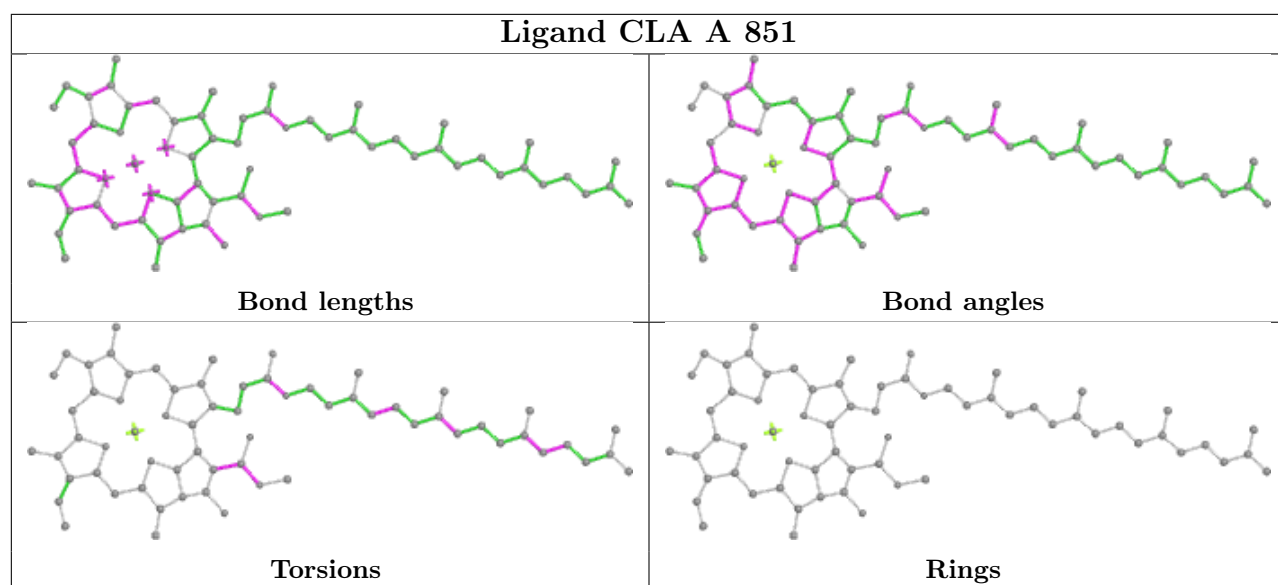
Rings

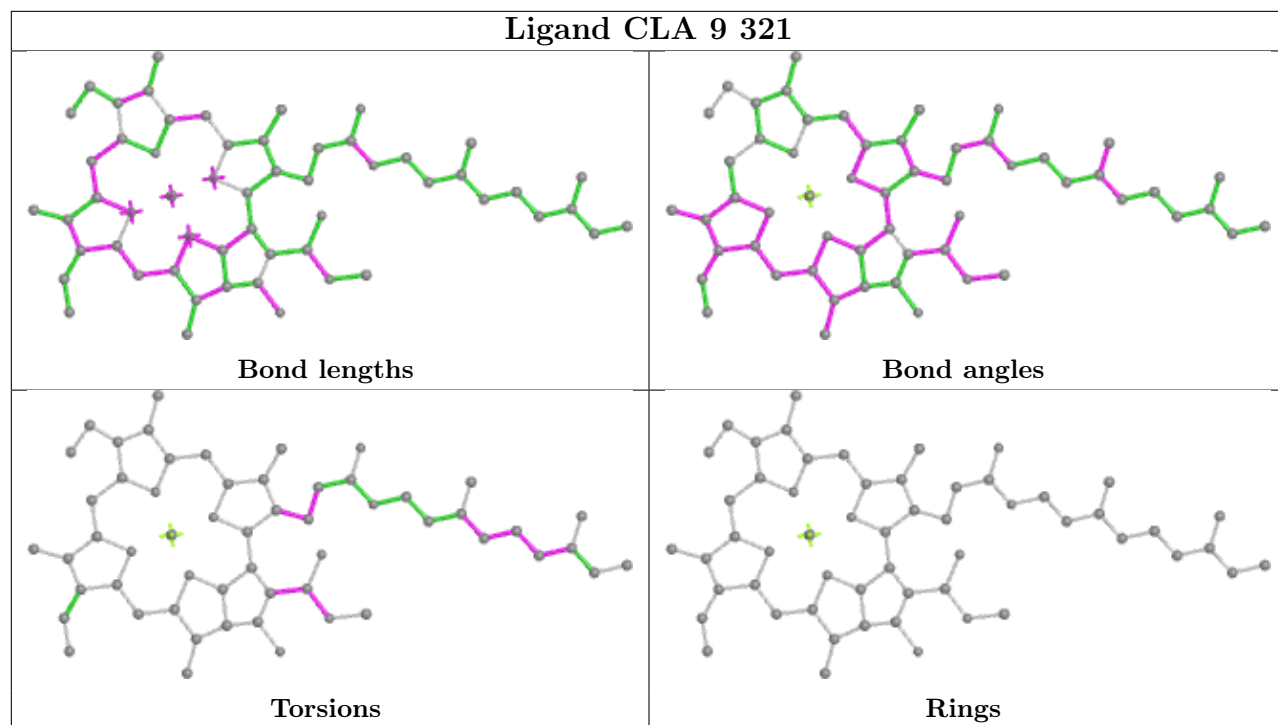
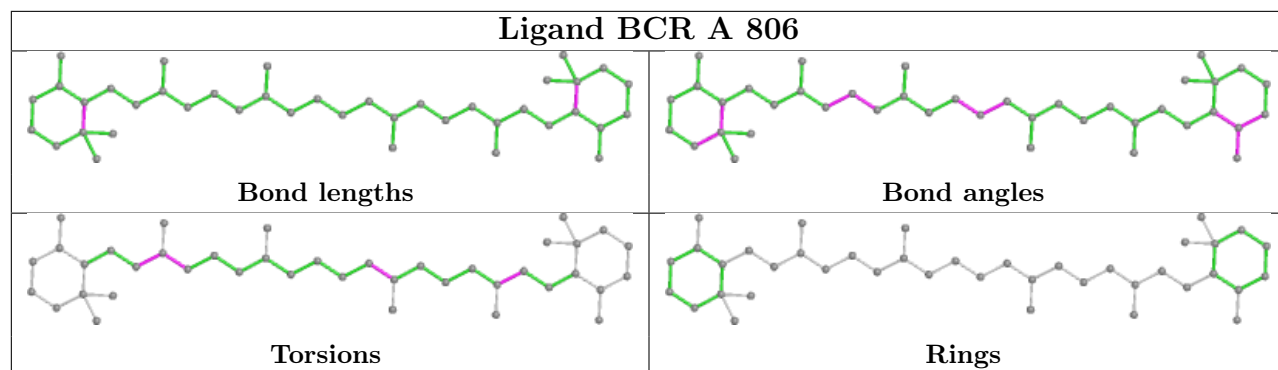
## Ligand CLA 2 311

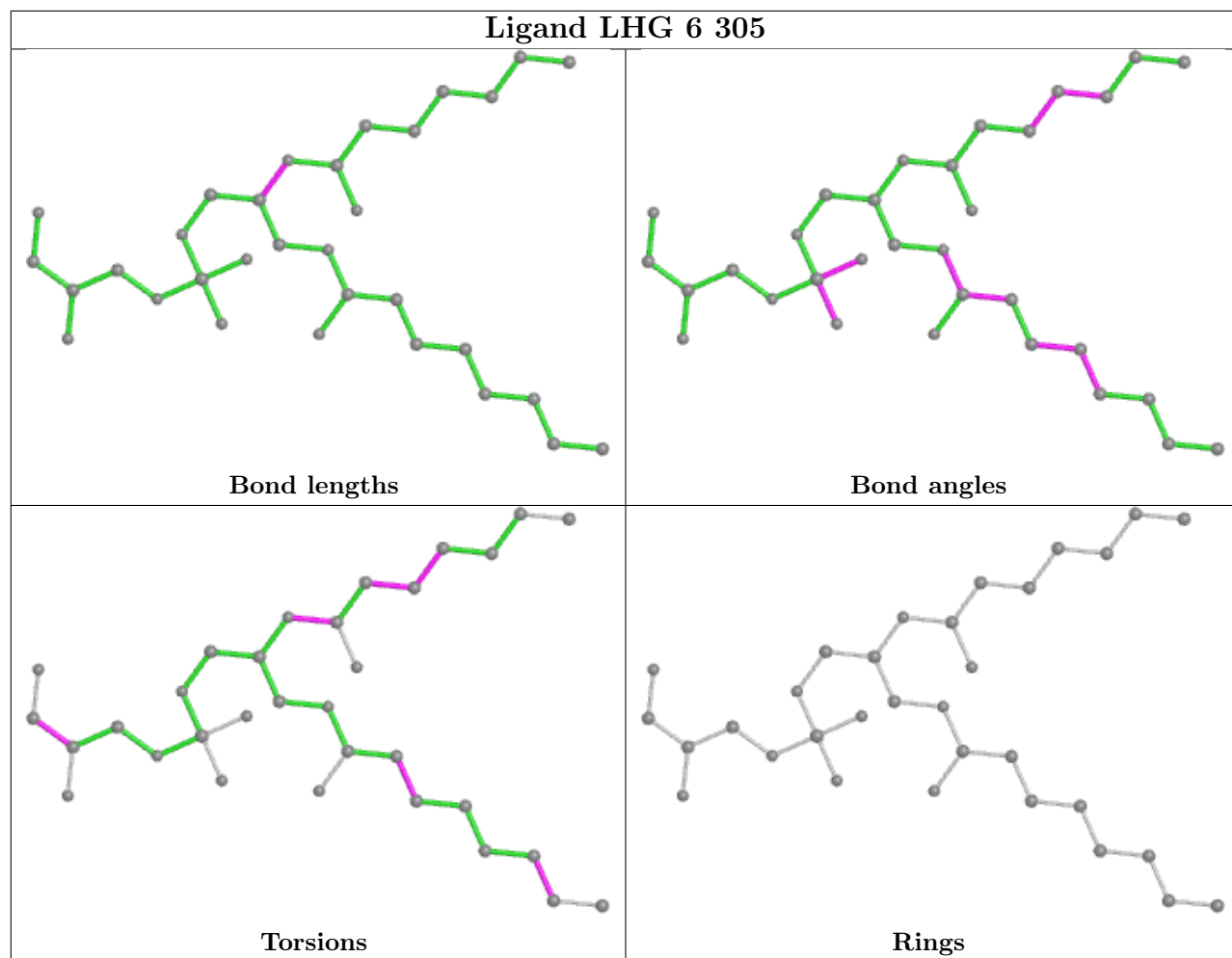


## Ligand CLA A 841

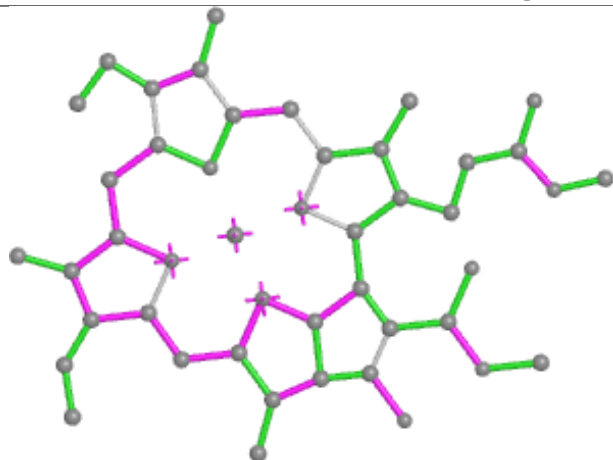




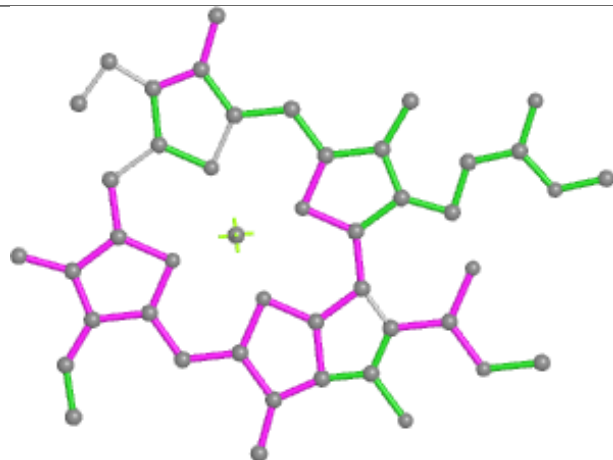




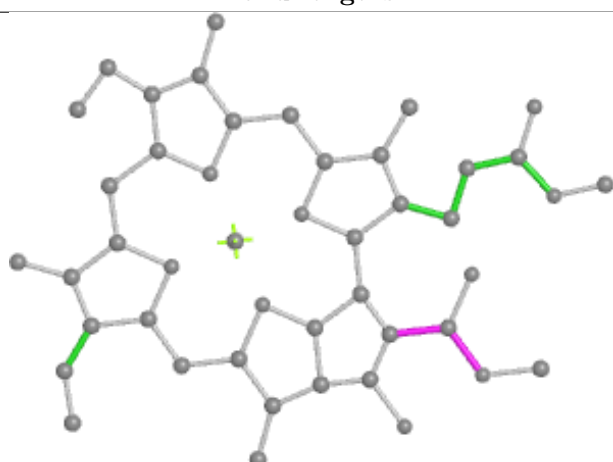
## Ligand CLA 6 315



Bond lengths



Bond angles

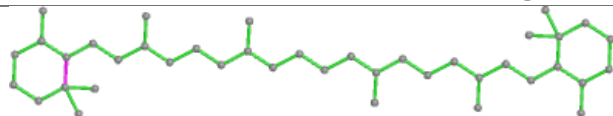


Torsions

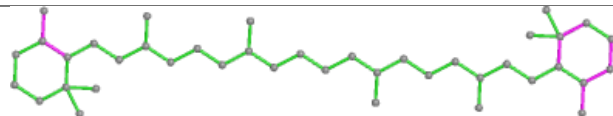


Rings

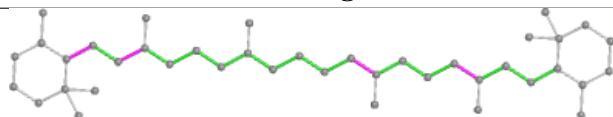
## Ligand BCR I 801



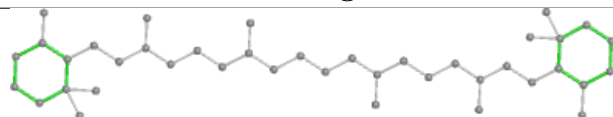
Bond lengths



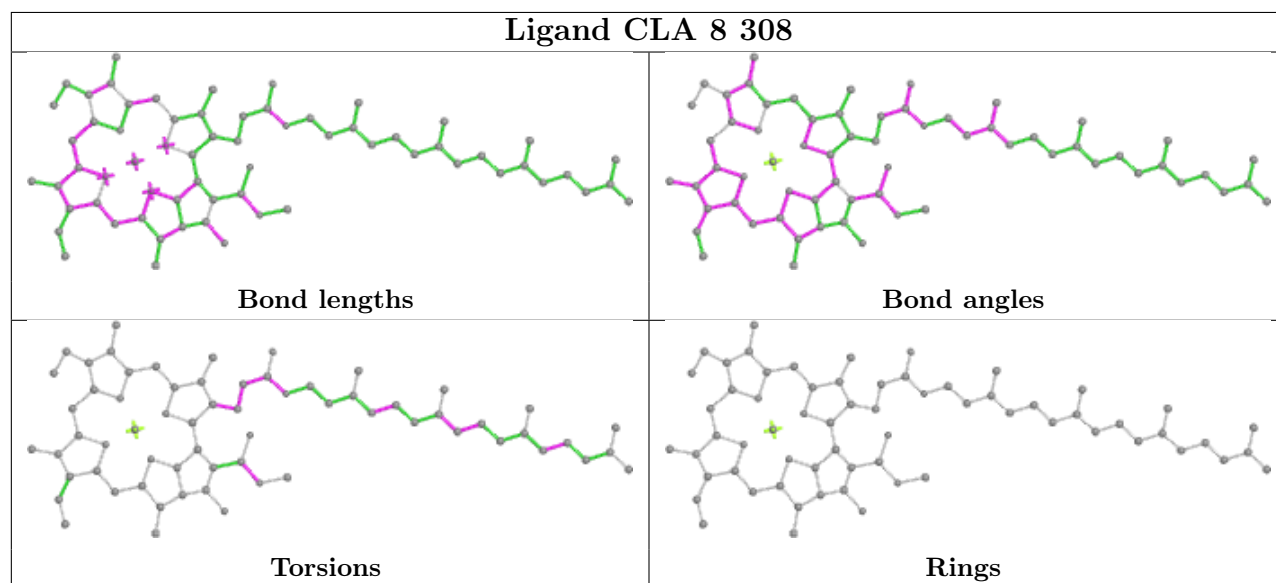
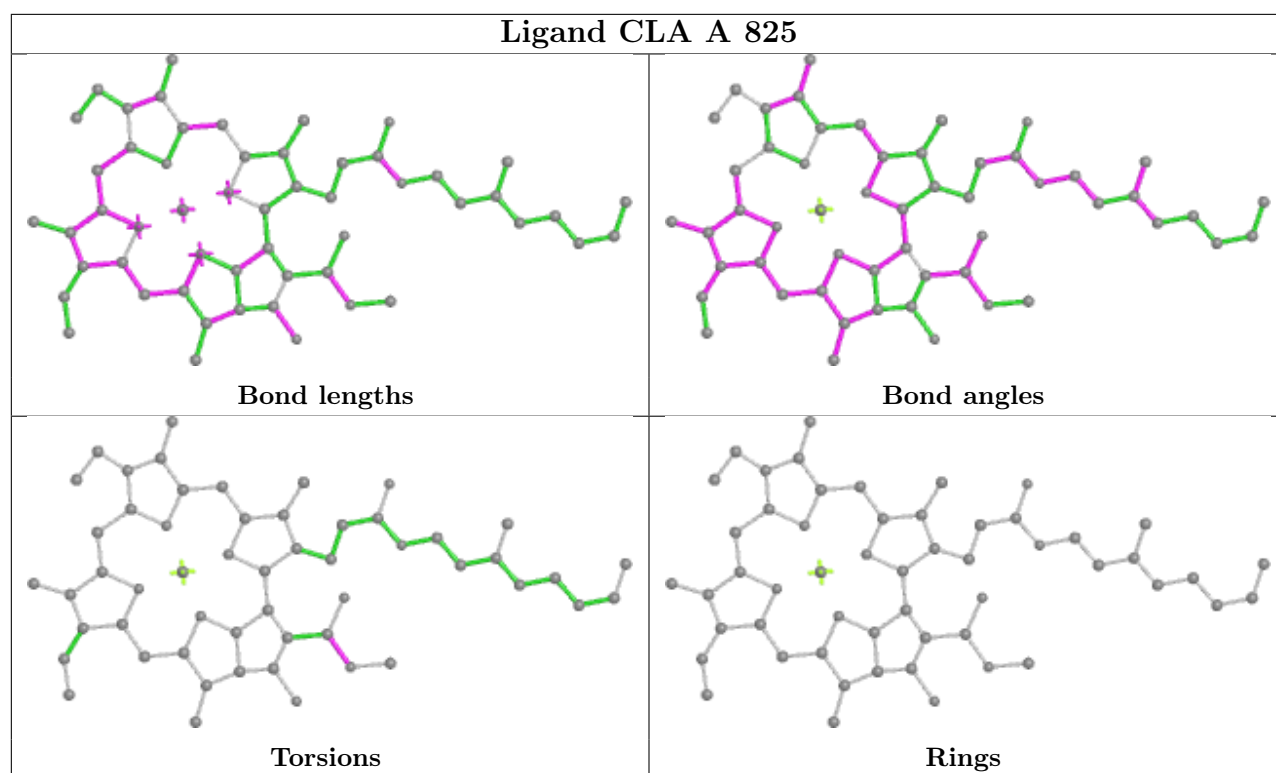
Bond angles



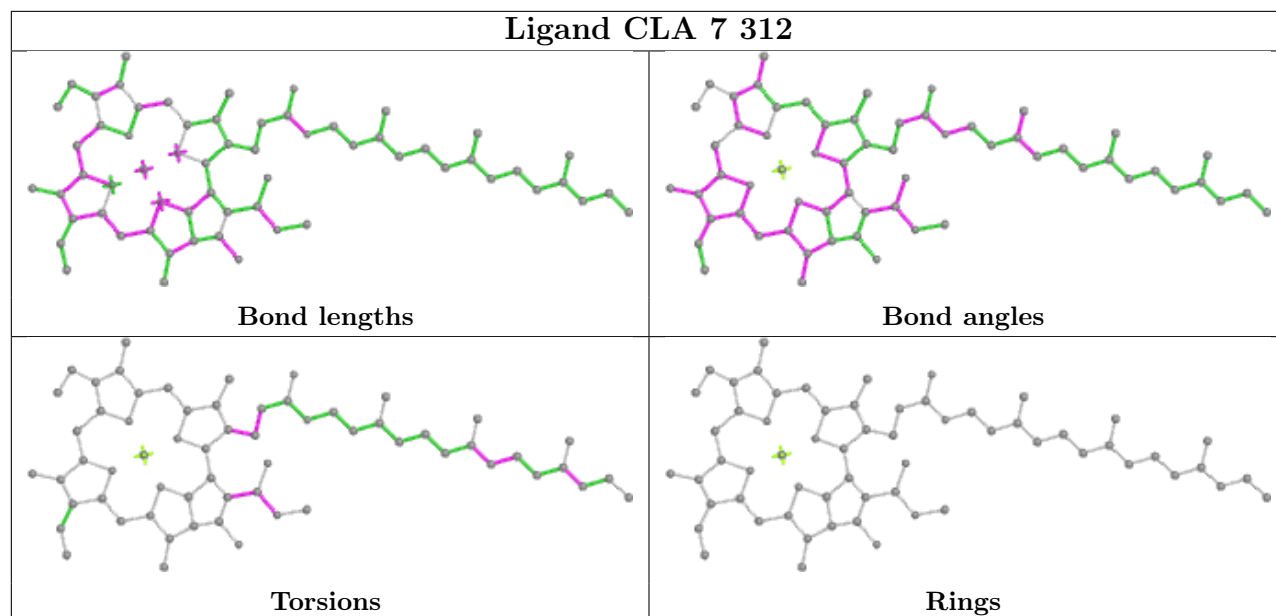
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

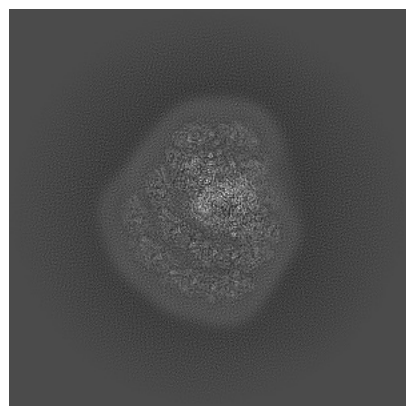
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62511. These allow visual inspection of the internal detail of the map and identification of artifacts.

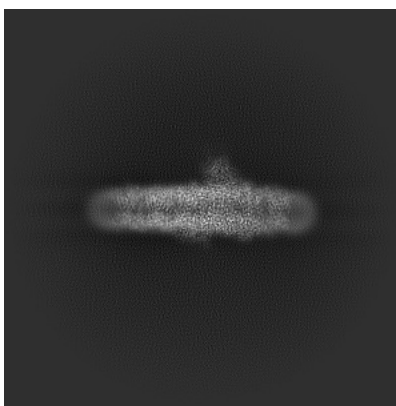
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

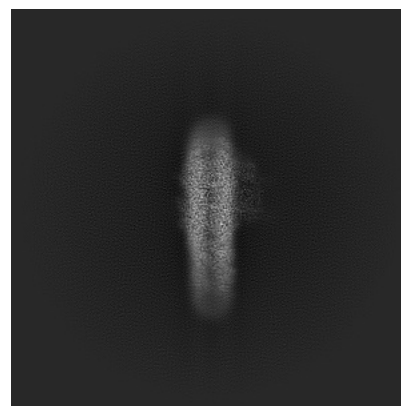
#### 6.1.1 Primary map



X

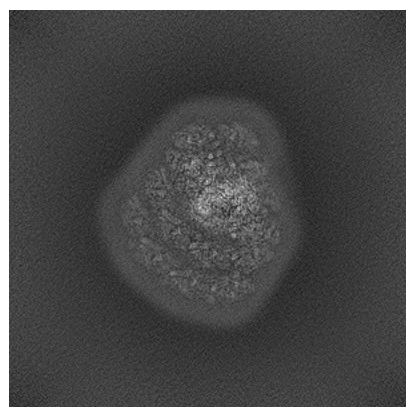


Y

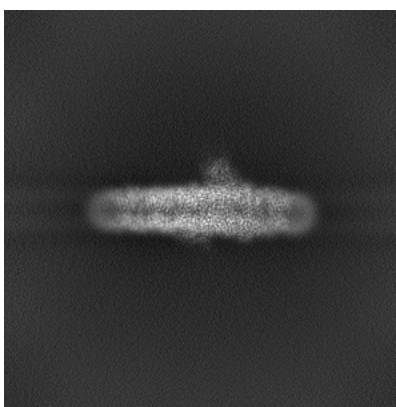


Z

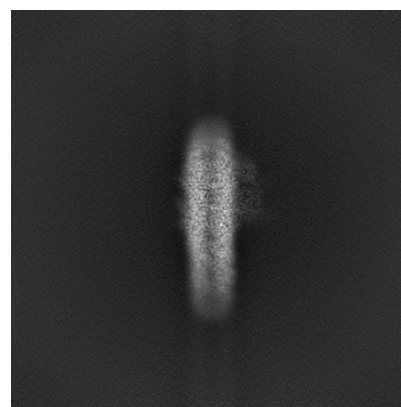
#### 6.1.2 Raw map



X



Y

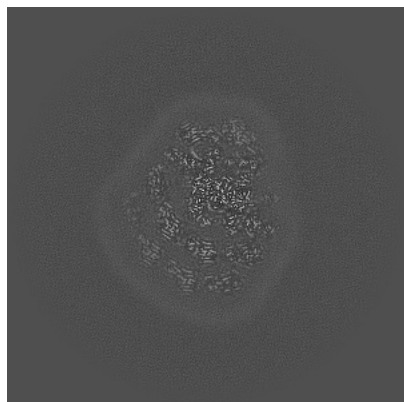


Z

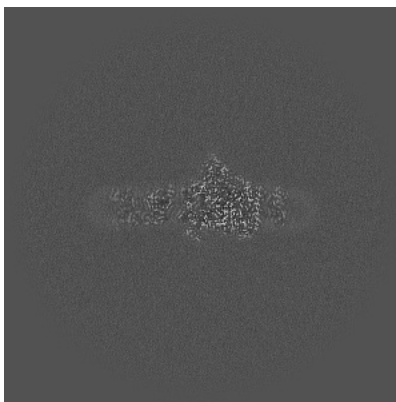
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

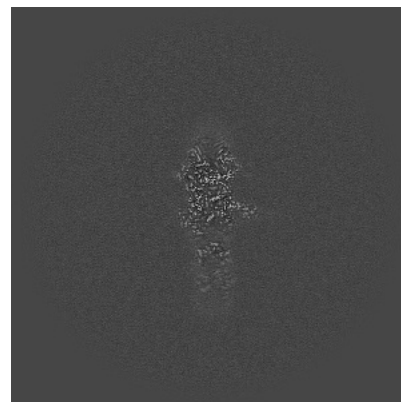
### 6.2.1 Primary map



X Index: 300

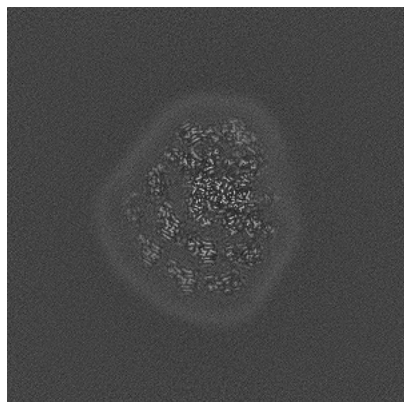


Y Index: 300

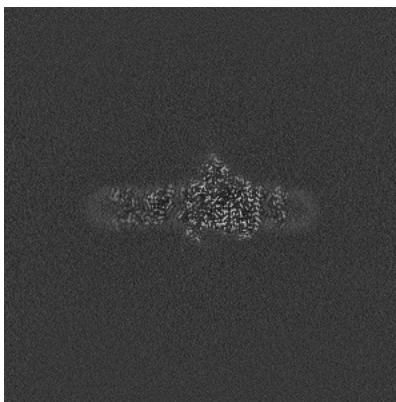


Z Index: 300

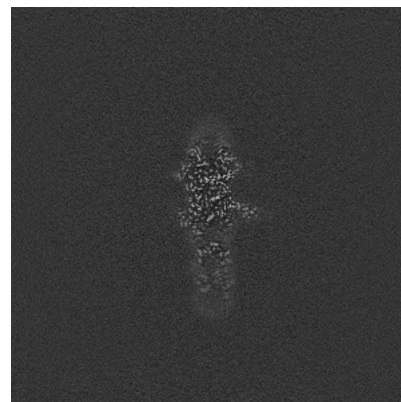
### 6.2.2 Raw map



X Index: 300



Y Index: 300

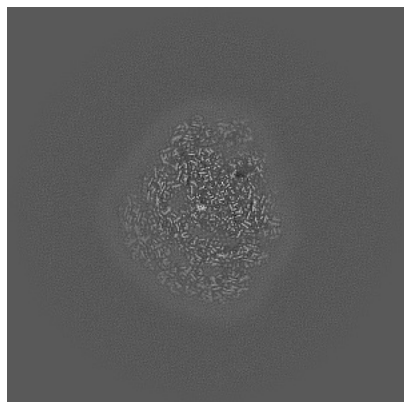


Z Index: 300

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

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

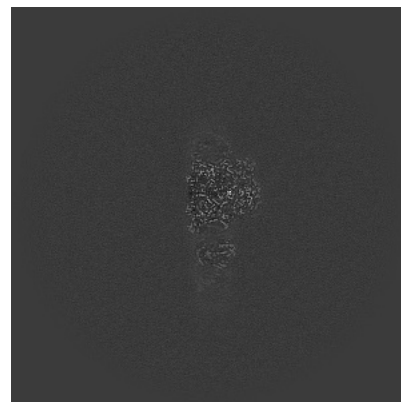
### 6.3.1 Primary map



X Index: 316

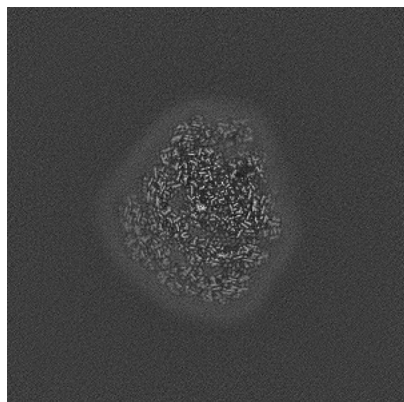


Y Index: 307

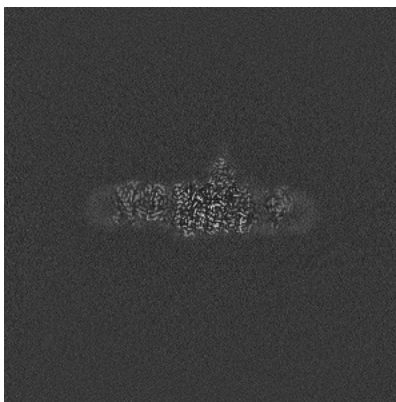


Z Index: 320

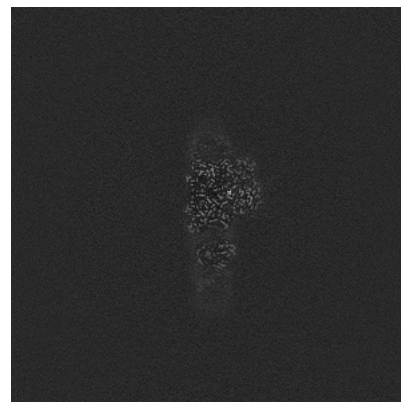
### 6.3.2 Raw map



X Index: 316



Y Index: 339



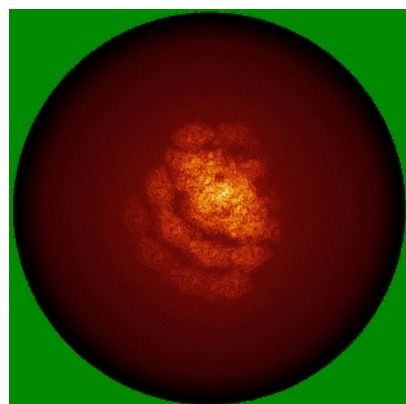
Z Index: 320

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

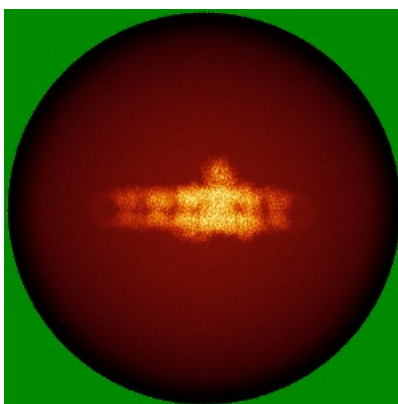


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

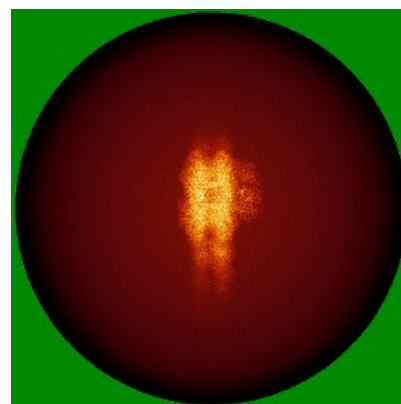
### 6.4.1 Primary map



X

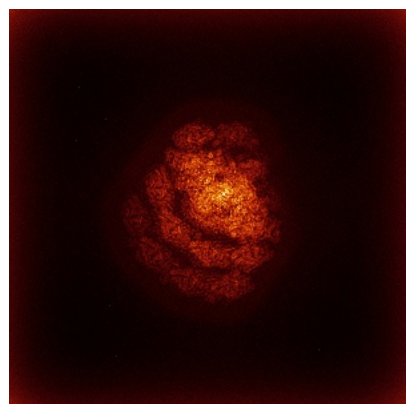


Y

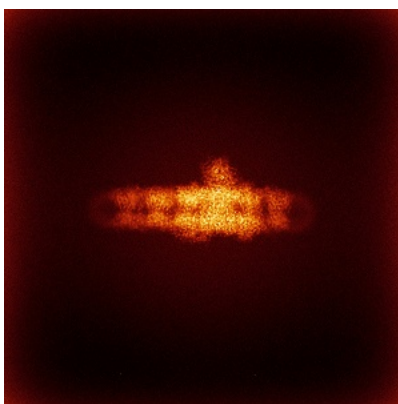


Z

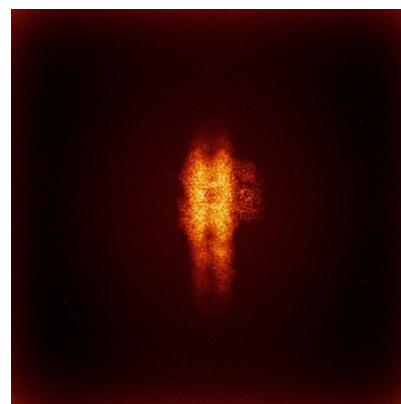
### 6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

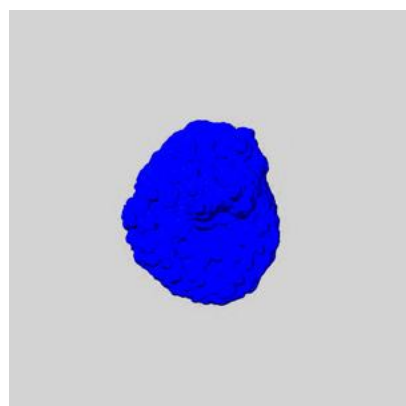
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

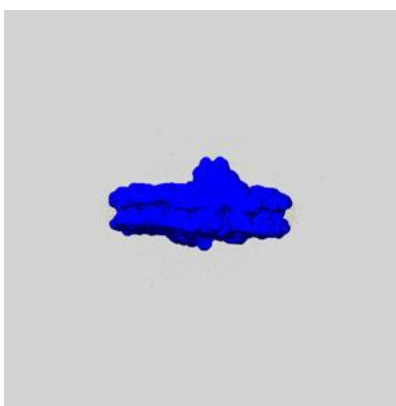
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

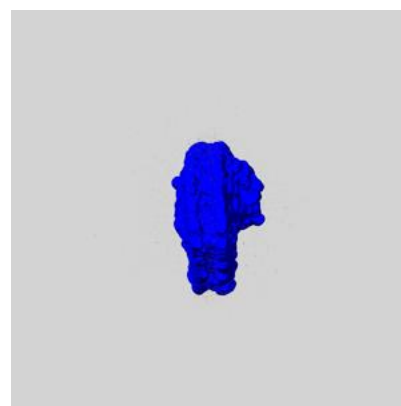
### 6.6.1 emd\_62511\_msk\_1.map [i](#)



X



Y

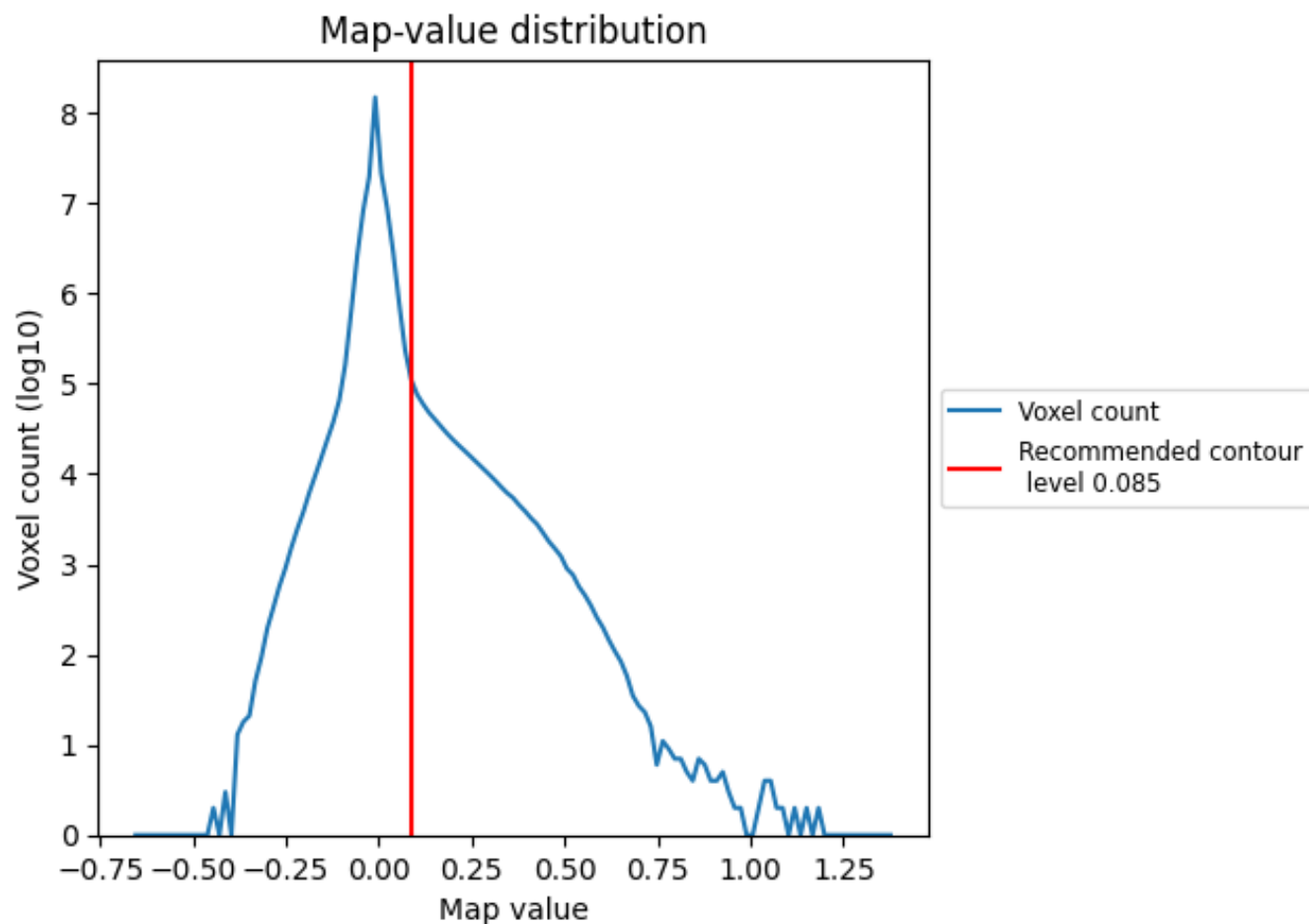


Z

## 7 Map analysis [i](#)

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

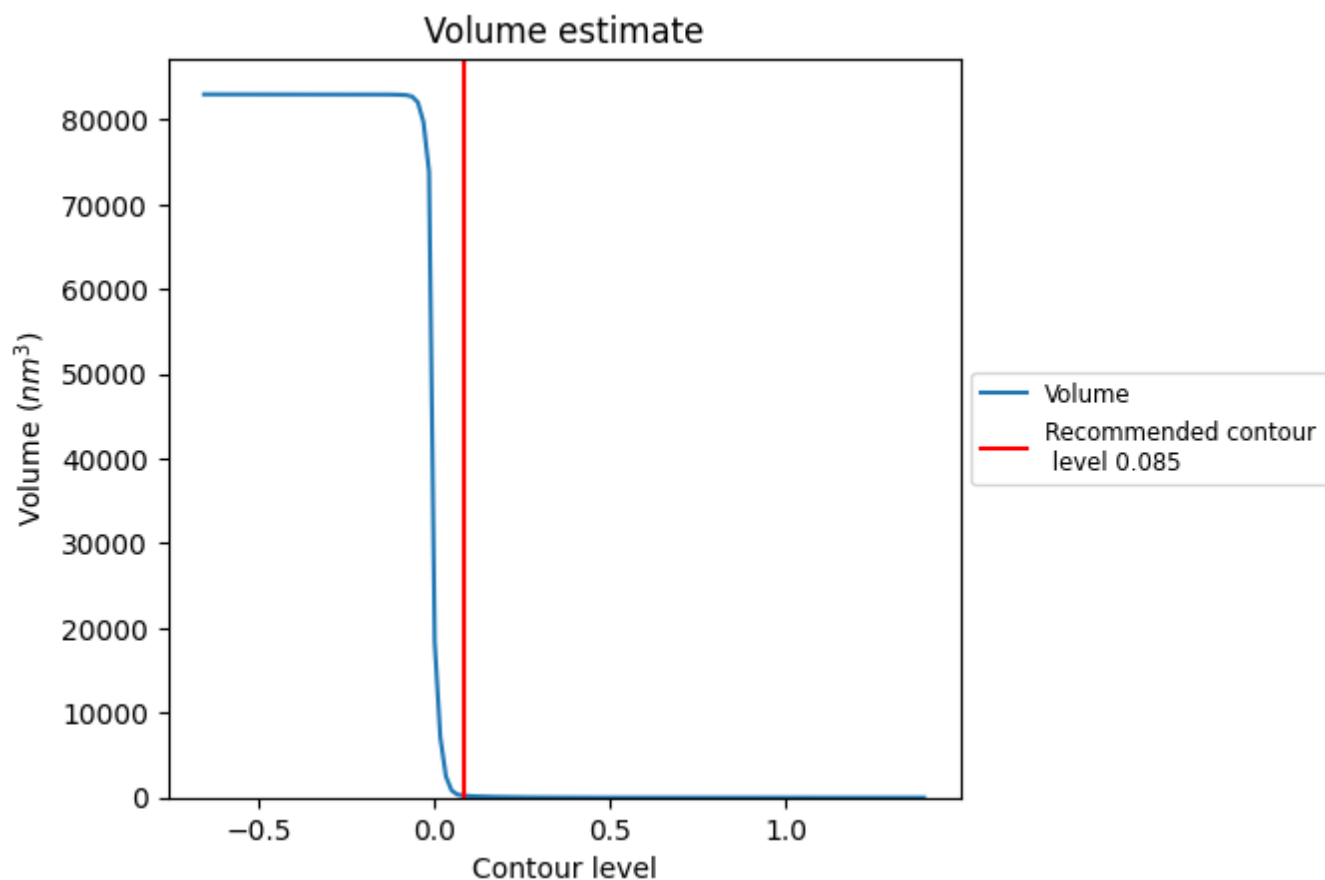
### 7.1 Map-value distribution [i](#)



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.



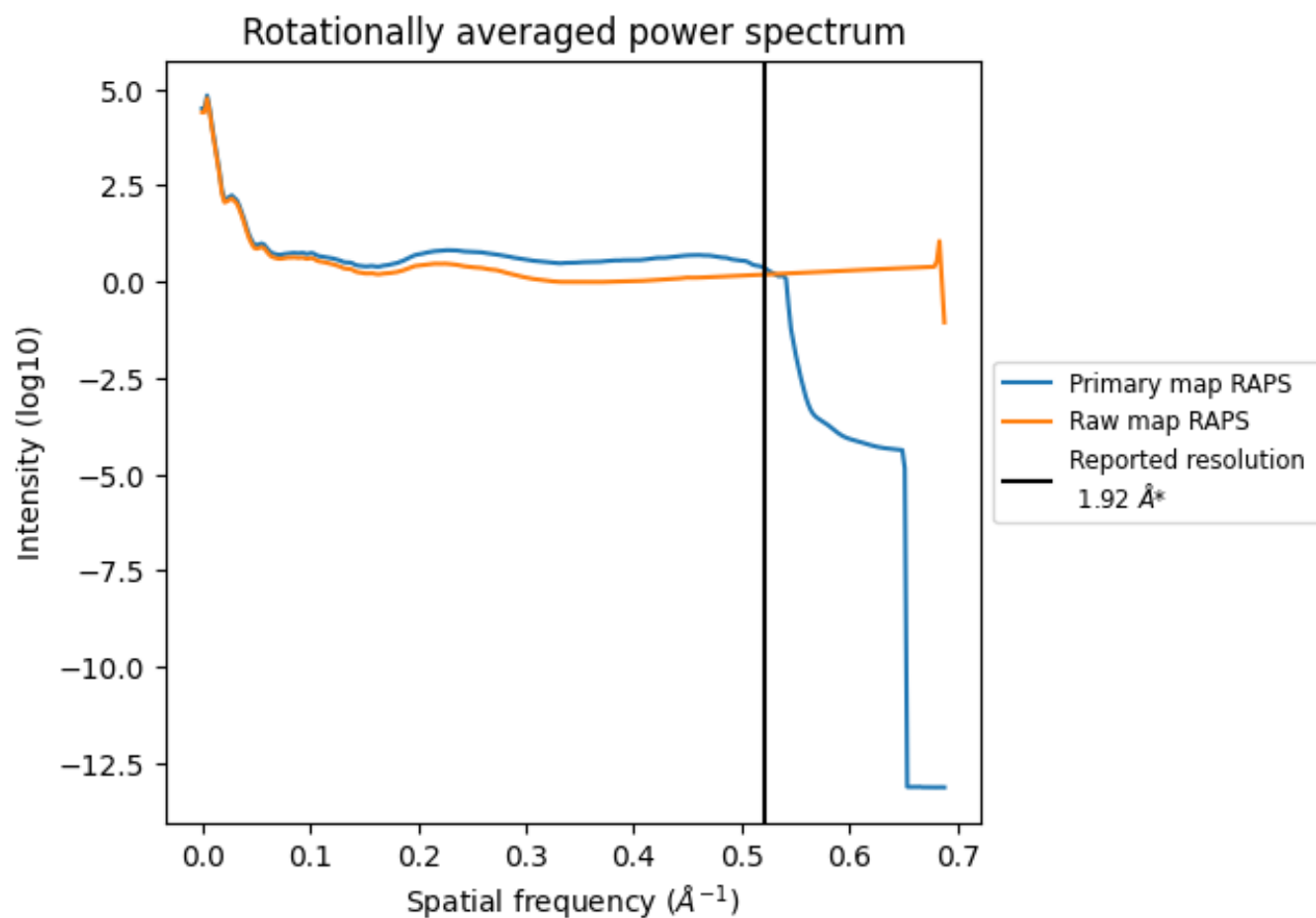
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227  $\text{nm}^3$ ; this corresponds to an approximate mass of 205 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 ⓘ

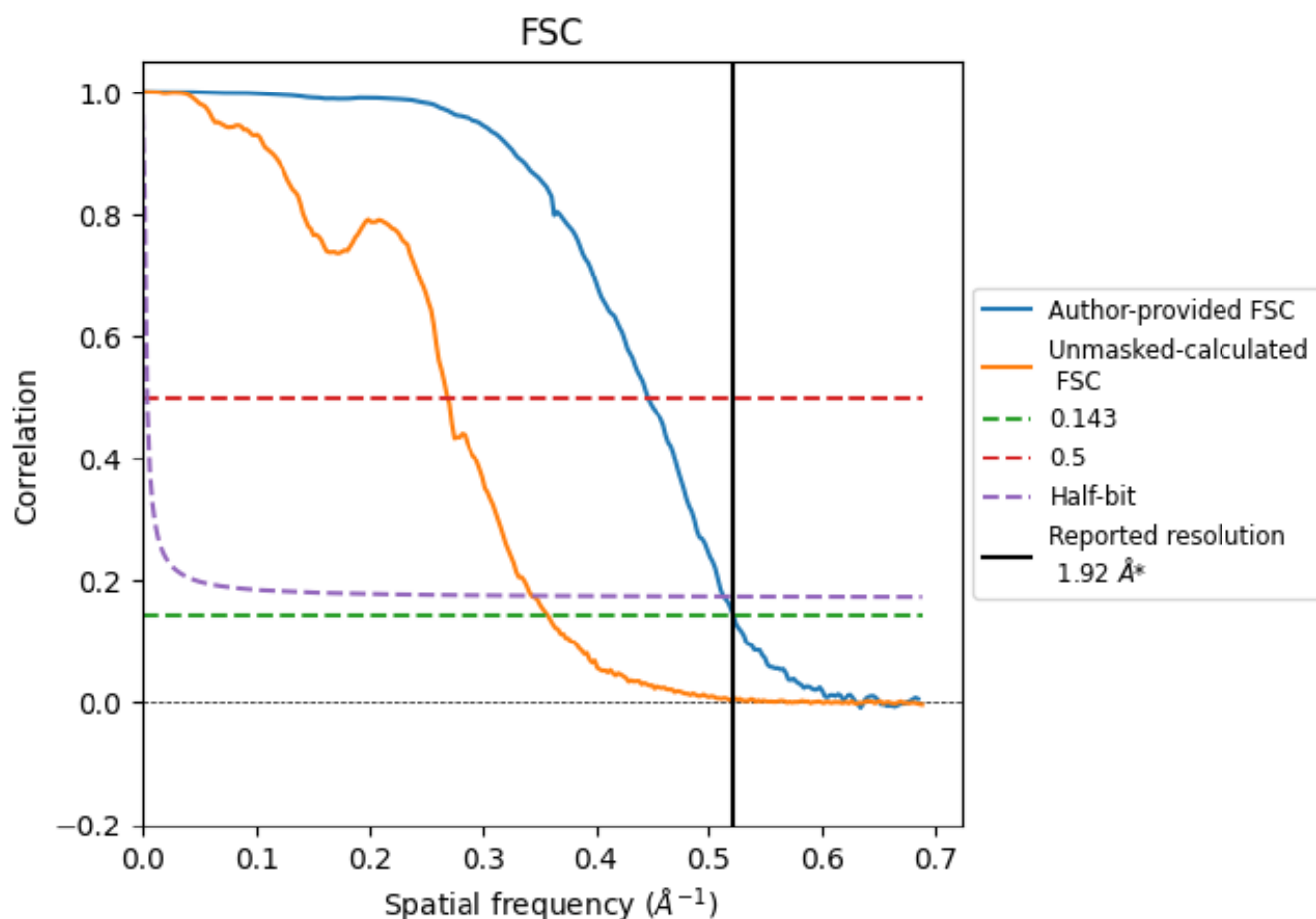


\*Reported resolution corresponds to spatial frequency of 0.521 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.521 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

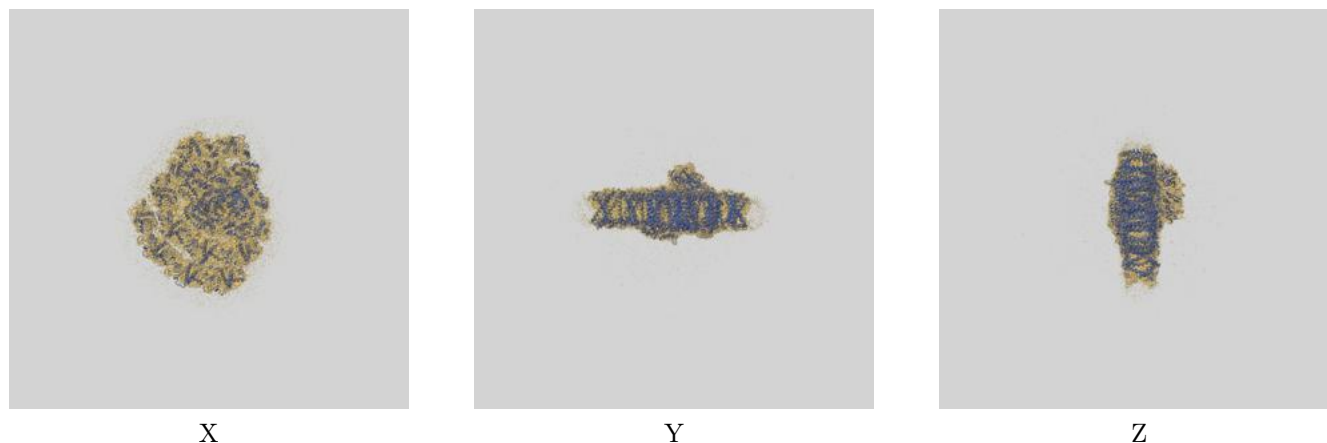
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 1.92                               | -    | -        |
| Author-provided FSC curve | 1.92                               | 2.24 | 1.95     |
| Unmasked-calculated*      | 2.79                               | 3.72 | 2.91     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 1.92 by more than 10 %

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

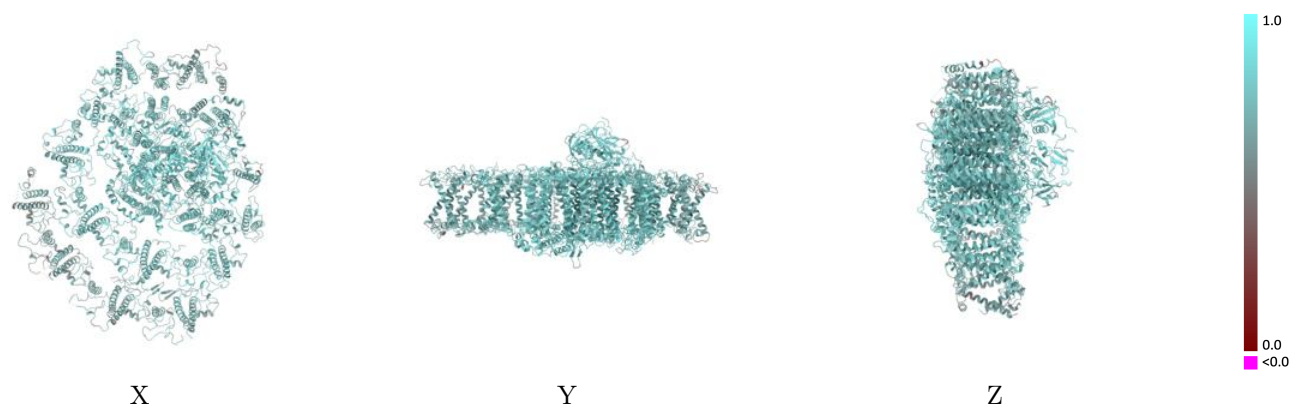
This section contains information regarding the fit between EMDB map EMD-62511 and PDB model 9KQP. Per-residue inclusion information can be found in [section 3](#) on [page 40](#).

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



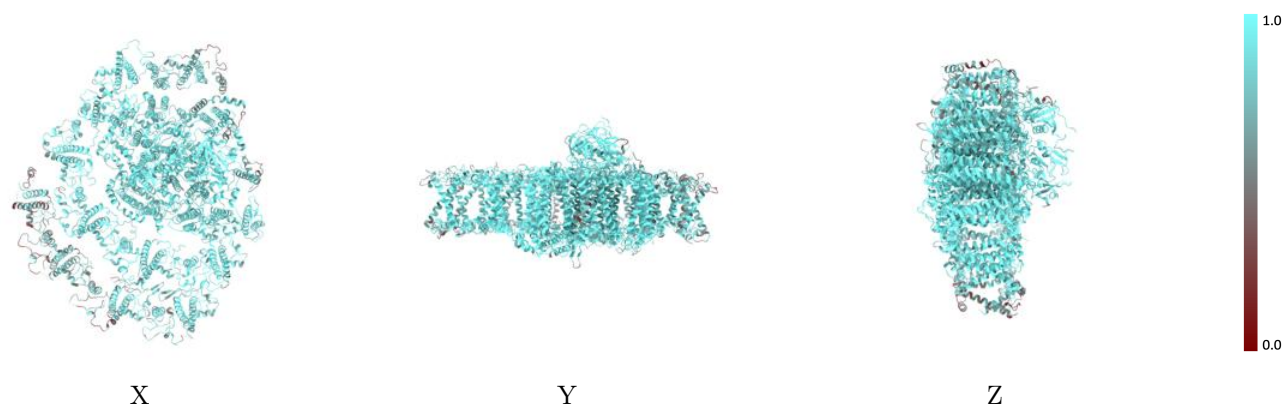
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



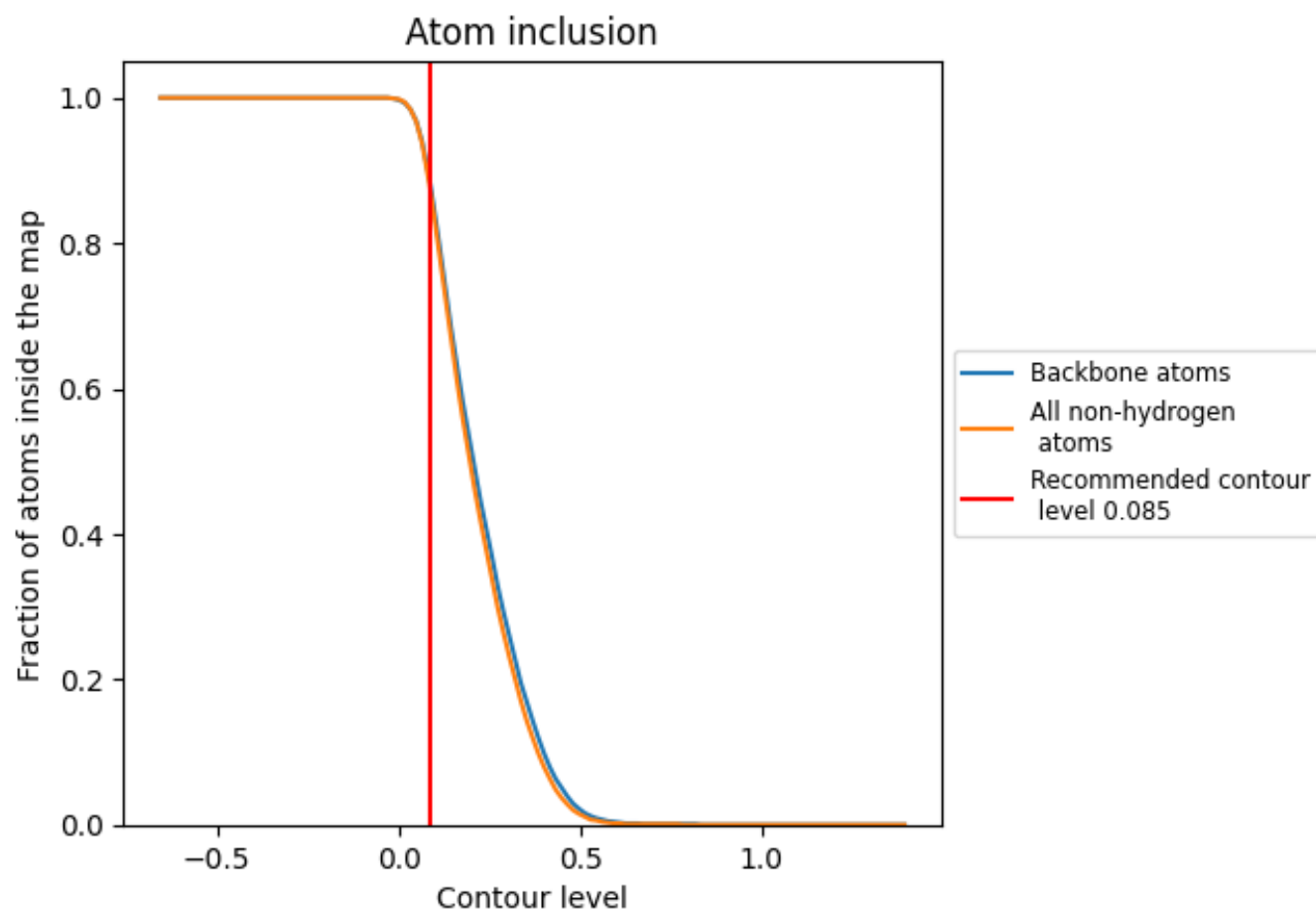
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.085) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8820 | <div><div></div></div> 0.7230 |
| 2     | <div><div></div></div> 0.7470 | <div><div></div></div> 0.6320 |
| 3     | <div><div></div></div> 0.9070 | <div><div></div></div> 0.7070 |
| 4     | <div><div></div></div> 0.6450 | <div><div></div></div> 0.5770 |
| 5     | <div><div></div></div> 0.7930 | <div><div></div></div> 0.6420 |
| 6     | <div><div></div></div> 0.7360 | <div><div></div></div> 0.6210 |
| 7     | <div><div></div></div> 0.9190 | <div><div></div></div> 0.7280 |
| 8     | <div><div></div></div> 0.9100 | <div><div></div></div> 0.7290 |
| 9     | <div><div></div></div> 0.8830 | <div><div></div></div> 0.6910 |
| A     | <div><div></div></div> 0.9650 | <div><div></div></div> 0.7910 |
| B     | <div><div></div></div> 0.9690 | <div><div></div></div> 0.7950 |
| C     | <div><div></div></div> 0.9920 | <div><div></div></div> 0.8120 |
| D     | <div><div></div></div> 0.9590 | <div><div></div></div> 0.7800 |
| E     | <div><div></div></div> 0.9200 | <div><div></div></div> 0.7700 |
| F     | <div><div></div></div> 0.9490 | <div><div></div></div> 0.7810 |
| G     | <div><div></div></div> 0.9090 | <div><div></div></div> 0.7300 |
| H     | <div><div></div></div> 0.7620 | <div><div></div></div> 0.6860 |
| I     | <div><div></div></div> 0.9760 | <div><div></div></div> 0.7770 |
| J     | <div><div></div></div> 0.9690 | <div><div></div></div> 0.7790 |
| K     | <div><div></div></div> 0.8840 | <div><div></div></div> 0.6980 |
| L     | <div><div></div></div> 0.9000 | <div><div></div></div> 0.7320 |
| M     | <div><div></div></div> 0.9530 | <div><div></div></div> 0.7720 |
| O     | <div><div></div></div> 0.6770 | <div><div></div></div> 0.6560 |
| a     | <div><div></div></div> 0.8890 | <div><div></div></div> 0.7080 |
| b     | <div><div></div></div> 0.5990 | <div><div></div></div> 0.5800 |

