



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:31 PM JST

PDB ID : 6L35 / pdb\_00006l35  
EMDB ID : EMD-0821  
Title : PSI-LHCI Supercomplex from *Physcometrella patens*  
Authors : Zhao, L.; Yan, Q.J.; Qin, X.C.  
Deposited on : 2019-10-09  
Resolution : 3.23 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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 : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

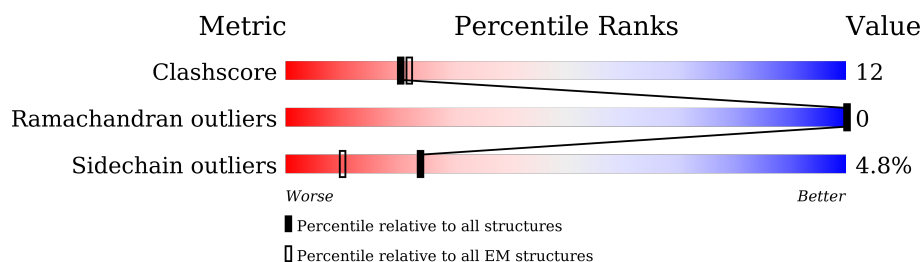
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.23 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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 742    | 77% 22% .        |
| 2   | B     | 733    | 77% 22% .        |
| 3   | C     | 80     | 70% 25% 5%       |
| 4   | D     | 141    | 83% 16% .        |
| 5   | E     | 62     | 71% 27% .        |
| 6   | F     | 159    | 74% 24% .        |
| 7   | G     | 98     | 68% 28% .        |
| 8   | H     | 90     | 79% 20% .        |
| 9   | I     | 34     | 68% 32%          |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 10  | J     | 41     |  78% 22%    |
| 11  | K     | 79     |  65% 30% 5% |
| 12  | L     | 159    |  73% 26% .  |
| 13  | M     | 29     |  72% 24% .  |
| 14  | 2     | 210    |  77% 20% .. |
| 15  | 6     | 192    |  69% 29% .  |
| 16  | 3     | 213    |  71% 28% .  |
| 17  | 5     | 205    |  63% 34% .. |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 18  | CLA  | 2     | 602 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 603 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 604 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 609 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 610 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 611 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 612 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 613 | X         | -        | -       | -                |
| 18  | CLA  | 2     | 614 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 602 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 603 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 604 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 606 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 607 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 609 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 610 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 611 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 612 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 613 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 614 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 615 | X         | -        | -       | -                |
| 18  | CLA  | 3     | 617 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 601 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 18  | CLA  | 5     | 602 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 603 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 604 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 609 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 610 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 611 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 612 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 613 | X         | -        | -       | -                |
| 18  | CLA  | 5     | 614 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 602 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 603 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 604 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 606 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 608 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 609 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 610 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 611 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 612 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 613 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 614 | X         | -        | -       | -                |
| 18  | CLA  | 6     | 616 | X         | -        | -       | -                |
| 18  | CLA  | A     | 801 | X         | -        | -       | -                |
| 18  | CLA  | A     | 802 | X         | -        | -       | -                |
| 18  | CLA  | A     | 803 | X         | -        | -       | -                |
| 18  | CLA  | A     | 804 | X         | -        | -       | -                |
| 18  | CLA  | A     | 805 | X         | -        | -       | -                |
| 18  | CLA  | A     | 806 | X         | -        | -       | -                |
| 18  | CLA  | A     | 807 | X         | -        | -       | -                |
| 18  | CLA  | A     | 808 | X         | -        | -       | -                |
| 18  | CLA  | A     | 809 | X         | -        | -       | -                |
| 18  | CLA  | A     | 810 | X         | -        | -       | -                |
| 18  | CLA  | A     | 811 | X         | -        | -       | -                |
| 18  | CLA  | A     | 812 | X         | -        | -       | -                |
| 18  | CLA  | A     | 813 | X         | -        | -       | -                |
| 18  | CLA  | A     | 814 | X         | -        | -       | -                |
| 18  | CLA  | A     | 815 | X         | -        | -       | -                |
| 18  | CLA  | A     | 816 | X         | -        | -       | -                |
| 18  | CLA  | A     | 817 | X         | -        | -       | -                |
| 18  | CLA  | A     | 818 | X         | -        | -       | -                |
| 18  | CLA  | A     | 819 | X         | -        | -       | -                |
| 18  | CLA  | A     | 820 | X         | -        | -       | -                |
| 18  | CLA  | A     | 821 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 18  | CLA  | A     | 822 | X         | -        | -       | -                |
| 18  | CLA  | A     | 823 | X         | -        | -       | -                |
| 18  | CLA  | A     | 824 | X         | -        | -       | -                |
| 18  | CLA  | A     | 825 | X         | -        | -       | -                |
| 18  | CLA  | A     | 826 | X         | -        | -       | -                |
| 18  | CLA  | A     | 827 | X         | -        | -       | -                |
| 18  | CLA  | A     | 828 | X         | -        | -       | -                |
| 18  | CLA  | A     | 829 | X         | -        | -       | -                |
| 18  | CLA  | A     | 830 | X         | -        | -       | -                |
| 18  | CLA  | A     | 831 | X         | -        | -       | -                |
| 18  | CLA  | A     | 832 | X         | -        | -       | -                |
| 18  | CLA  | A     | 833 | X         | -        | -       | -                |
| 18  | CLA  | A     | 834 | X         | -        | -       | -                |
| 18  | CLA  | A     | 835 | X         | -        | -       | -                |
| 18  | CLA  | A     | 836 | X         | -        | -       | -                |
| 18  | CLA  | A     | 837 | X         | -        | -       | -                |
| 18  | CLA  | A     | 838 | X         | -        | -       | -                |
| 18  | CLA  | A     | 839 | X         | -        | -       | -                |
| 18  | CLA  | A     | 840 | X         | -        | -       | -                |
| 18  | CLA  | A     | 841 | X         | -        | -       | -                |
| 18  | CLA  | A     | 842 | X         | -        | -       | -                |
| 18  | CLA  | A     | 843 | X         | -        | -       | -                |
| 18  | CLA  | A     | 845 | X         | -        | -       | -                |
| 18  | CLA  | A     | 854 | X         | -        | -       | -                |
| 18  | CLA  | B     | 802 | X         | -        | -       | -                |
| 18  | CLA  | B     | 803 | X         | -        | -       | -                |
| 18  | CLA  | B     | 804 | X         | -        | -       | -                |
| 18  | CLA  | B     | 805 | X         | -        | -       | -                |
| 18  | CLA  | B     | 806 | X         | -        | -       | -                |
| 18  | CLA  | B     | 807 | X         | -        | -       | -                |
| 18  | CLA  | B     | 808 | X         | -        | -       | -                |
| 18  | CLA  | B     | 809 | X         | -        | -       | -                |
| 18  | CLA  | B     | 810 | X         | -        | -       | -                |
| 18  | CLA  | B     | 811 | X         | -        | -       | -                |
| 18  | CLA  | B     | 812 | X         | -        | -       | -                |
| 18  | CLA  | B     | 813 | X         | -        | -       | -                |
| 18  | CLA  | B     | 814 | X         | -        | -       | -                |
| 18  | CLA  | B     | 815 | X         | -        | -       | -                |
| 18  | CLA  | B     | 816 | X         | -        | -       | -                |
| 18  | CLA  | B     | 817 | X         | -        | -       | -                |
| 18  | CLA  | B     | 818 | X         | -        | -       | -                |
| 18  | CLA  | B     | 819 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 18  | CLA  | B     | 820 | X         | -        | -       | -                |
| 18  | CLA  | B     | 821 | X         | -        | -       | -                |
| 18  | CLA  | B     | 822 | X         | -        | -       | -                |
| 18  | CLA  | B     | 823 | X         | -        | -       | -                |
| 18  | CLA  | B     | 824 | X         | -        | -       | -                |
| 18  | CLA  | B     | 825 | X         | -        | -       | -                |
| 18  | CLA  | B     | 826 | X         | -        | -       | -                |
| 18  | CLA  | B     | 827 | X         | -        | -       | -                |
| 18  | CLA  | B     | 828 | X         | -        | -       | -                |
| 18  | CLA  | B     | 829 | X         | -        | -       | -                |
| 18  | CLA  | B     | 830 | X         | -        | -       | -                |
| 18  | CLA  | B     | 831 | X         | -        | -       | -                |
| 18  | CLA  | B     | 832 | X         | -        | -       | -                |
| 18  | CLA  | B     | 833 | X         | -        | -       | -                |
| 18  | CLA  | B     | 834 | X         | -        | -       | -                |
| 18  | CLA  | B     | 835 | X         | -        | -       | -                |
| 18  | CLA  | B     | 836 | X         | -        | -       | -                |
| 18  | CLA  | B     | 837 | X         | -        | -       | -                |
| 18  | CLA  | B     | 838 | X         | -        | -       | -                |
| 18  | CLA  | B     | 839 | X         | -        | -       | -                |
| 18  | CLA  | B     | 840 | X         | -        | -       | -                |
| 18  | CLA  | B     | 841 | X         | -        | -       | -                |
| 18  | CLA  | F     | 301 | X         | -        | -       | -                |
| 18  | CLA  | F     | 303 | X         | -        | -       | -                |
| 18  | CLA  | F     | 304 | X         | -        | -       | -                |
| 18  | CLA  | F     | 305 | X         | -        | -       | -                |
| 18  | CLA  | G     | 201 | X         | -        | -       | -                |
| 18  | CLA  | G     | 203 | X         | -        | -       | -                |
| 18  | CLA  | G     | 204 | X         | -        | -       | -                |
| 18  | CLA  | J     | 101 | X         | -        | -       | -                |
| 18  | CLA  | K     | 201 | X         | -        | -       | -                |
| 18  | CLA  | K     | 203 | X         | -        | -       | -                |
| 18  | CLA  | K     | 204 | X         | -        | -       | -                |
| 18  | CLA  | K     | 206 | X         | -        | -       | -                |
| 18  | CLA  | L     | 302 | X         | -        | -       | -                |
| 18  | CLA  | L     | 303 | X         | -        | -       | -                |
| 18  | CLA  | L     | 304 | X         | -        | -       | -                |
| 22  | SF4  | C     | 101 | -         | -        | X       | -                |
| 22  | SF4  | C     | 102 | -         | -        | X       | -                |
| 25  | CHL  | 2     | 601 | X         | -        | -       | -                |
| 25  | CHL  | 2     | 606 | X         | -        | -       | -                |
| 25  | CHL  | 2     | 607 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 25  | CHL  | 2     | 608 | X         | -        | -       | -                |
| 25  | CHL  | 2     | 616 | X         | -        | -       | -                |
| 25  | CHL  | 3     | 608 | X         | -        | -       | -                |
| 25  | CHL  | 5     | 606 | X         | -        | -       | -                |
| 25  | CHL  | 5     | 607 | X         | -        | -       | -                |
| 25  | CHL  | 5     | 608 | X         | -        | -       | -                |
| 25  | CHL  | 5     | 615 | X         | -        | -       | -                |
| 25  | CHL  | 6     | 601 | X         | -        | -       | -                |
| 25  | CHL  | 6     | 607 | X         | -        | -       | -                |
| 27  | XAT  | 2     | 620 | -         | -        | X       | -                |
| 27  | XAT  | 5     | 620 | -         | -        | X       | -                |

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 34822 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     | 742      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5837  | 3827 | 993 | 998 | 19 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 733      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5849  | 3839 | 996 | 998 | 16 |         |       |

- 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     |
|     |       |          | 595   | 365 | 103 | 116 | 11 |         |       |

- Molecule 4 is a protein called Predicted protein PsaD.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 707 | 196 | 198 | 3 |         |       |

- Molecule 5 is a protein called PsaE.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | E     | 62       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 487   | 309 | 87 | 91 |         |       |

- Molecule 6 is a protein called PSI-F.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1226  | 793 | 209 | 221 | 3 |         |       |

- Molecule 7 is a protein called Predicted protein PsaG.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | G     | 98       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 749   | 483 | 128 | 138 |         |       |

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 445 | 117 | 130 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | I     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 266   | 181 | 35 | 48 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 325   | 222 | 48 | 54 | 1 |         |       |

- Molecule 11 is a protein called PsaK.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 11  | K     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 550   | 346 | 96 | 105 | 3 |         |       |

- Molecule 12 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1189  | 781 | 192 | 214 | 2 |         |       |

- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 13  | M     | 29       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 214   | 141 | 34 | 39 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | 2     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1595  | 1039 | 267 | 285 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | 6     | 192      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1473  | 961 | 247 | 264 | 1 |         |       |

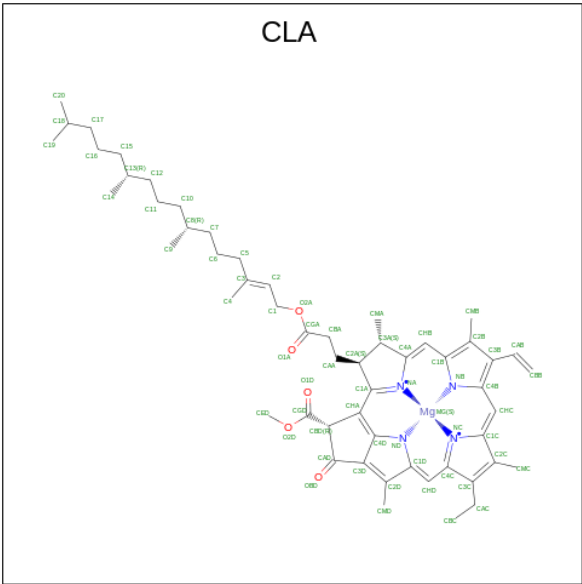
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 3     | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1644  | 1076 | 265 | 296 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | 5     | 202      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 1020 | 258 | 282 | 6 |         |       |

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 33 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 18  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 53    | 43 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | B     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | B     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | F     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | G     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | G     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | G     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | J     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | K     | 1        | Total<br>46 | C<br>36 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | K     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | K     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | L     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 2     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 2     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 2     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |

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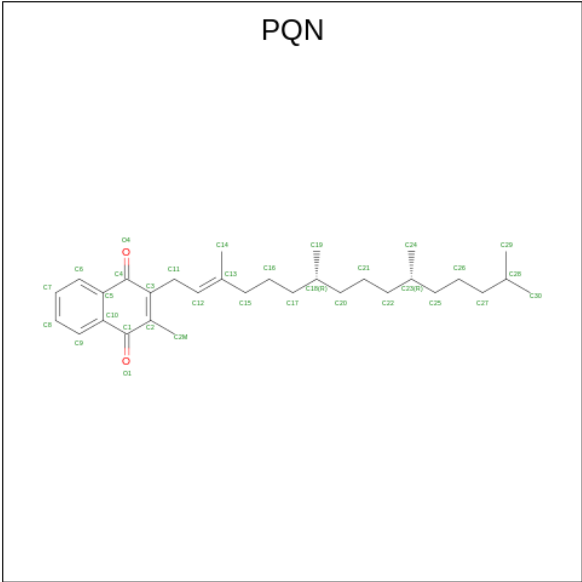
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 18  | 2     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 2     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 2     | 1        | Total<br>42 | C<br>34 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 6     | 1        | Total<br>44 | C<br>34 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 6     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 6     | 1        | Total<br>38 | C<br>30 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 6     | 1        | Total<br>43 | C<br>33 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>42 | C<br>32 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 18  | 3     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 3     | 1        | Total<br>40 | C<br>32 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 18  | 3     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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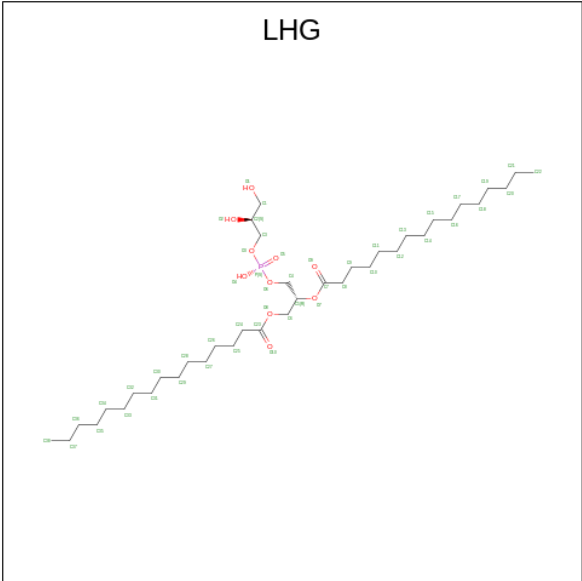
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 36    | 30 | 1  | 4 | 1 |         |
| 18  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 38    | 30 | 1  | 4 | 3 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 18  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 35 | 1  | 4 | 3 |         |

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 19  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 19  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



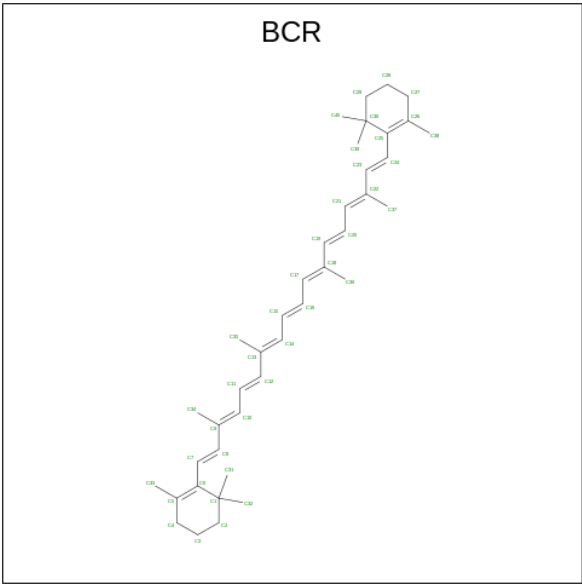
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 27    | 16 | 10 | 1 |         |
| 20  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 23    | 12 | 10 | 1 |         |
| 20  | 2     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 35    | 24 | 10 | 1 |         |
| 20  | 6     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 28    | 17 | 10 | 1 |         |
| 20  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 26 | 10 | 1 |         |

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

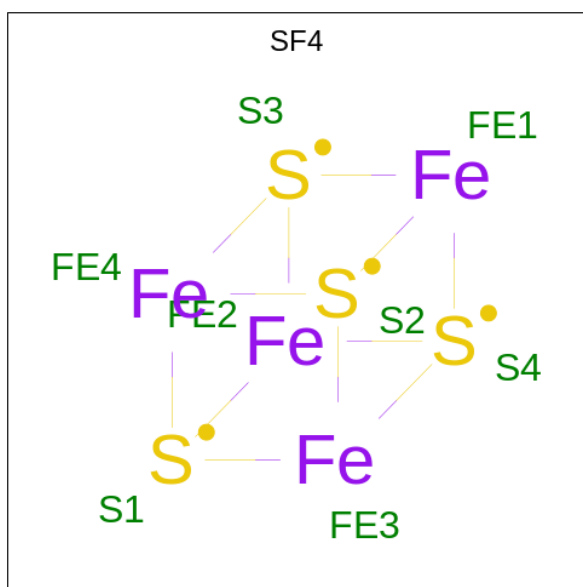
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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | B     | 1        | Total C<br>40 40 | 0       |
| 21  | F     | 1        | Total C<br>40 40 | 0       |
| 21  | G     | 1        | Total C<br>40 40 | 0       |
| 21  | I     | 1        | Total C<br>40 40 | 0       |
| 21  | J     | 1        | Total C<br>40 40 | 0       |
| 21  | J     | 1        | Total C<br>40 40 | 0       |
| 21  | K     | 1        | Total C<br>40 40 | 0       |
| 21  | K     | 1        | Total C<br>40 40 | 0       |
| 21  | L     | 1        | Total C<br>40 40 | 0       |
| 21  | L     | 1        | Total C<br>40 40 | 0       |
| 21  | 2     | 1        | Total C<br>40 40 | 0       |
| 21  | 3     | 1        | Total C<br>40 40 | 0       |
| 21  | 3     | 1        | Total C<br>40 40 | 0       |
| 21  | 5     | 1        | Total C<br>40 40 | 0       |

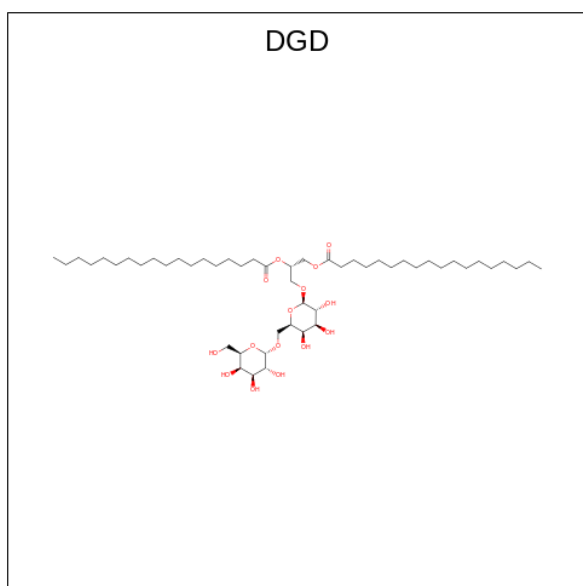
- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





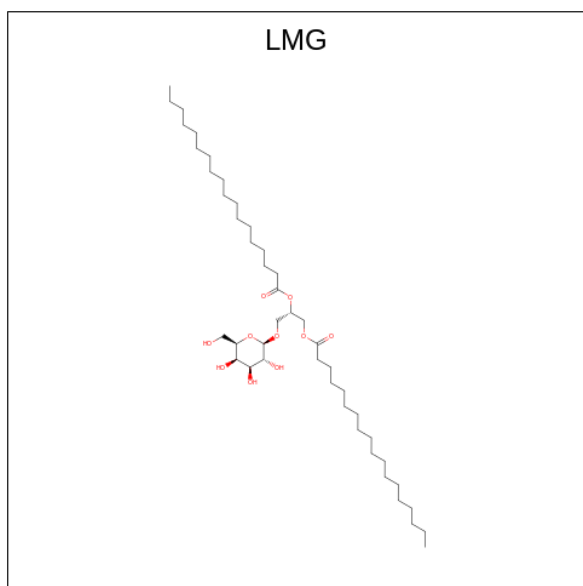
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 22  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 22  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 22  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



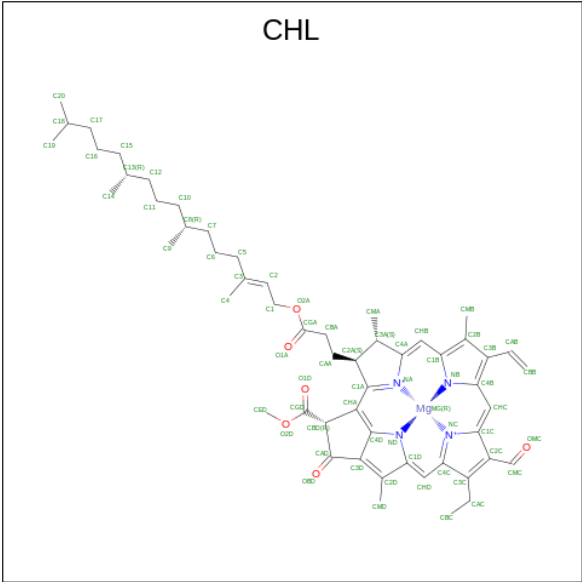
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 23  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 66    | 51 | 15 |         |

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



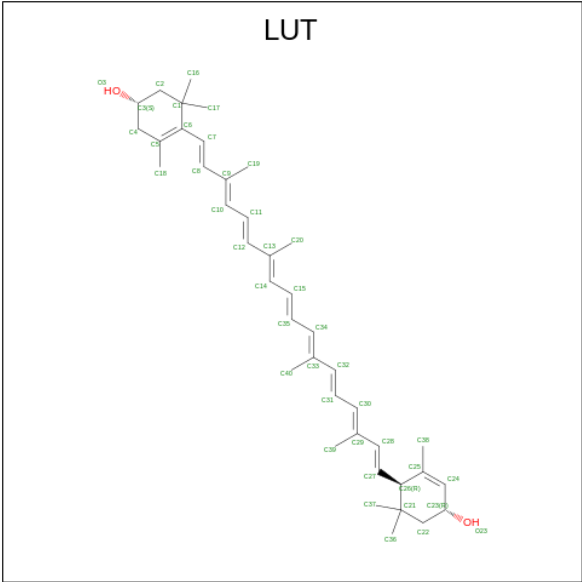
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 24  | J     | 1        | Total | C  | O  | 0       |
|     |       |          | 30    | 20 | 10 |         |
| 24  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 13    | 7  | 6  |         |
| 24  | 2     | 1        | Total | C  | O  | 0       |
|     |       |          | 13    | 7  | 6  |         |

- Molecule 25 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



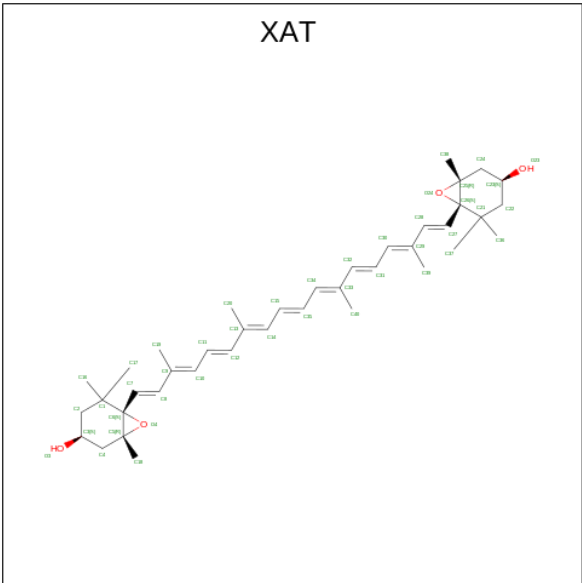
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 34 | 1  | 4 | 6 |         |
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 32 | 1  | 4 | 4 |         |
| 25  | 2     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 35 | 1  | 4 | 6 |         |
| 25  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 34 | 1  | 4 | 6 |         |
| 25  | 6     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 32 | 1  | 4 | 4 |         |
| 25  | 3     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 40    | 32 | 1  | 4 | 3 |         |
| 25  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 32 | 1  | 4 | 4 |         |
| 25  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 25  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 40 | 1  | 4 | 6 |         |
| 25  | 5     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26  | 2     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 26  | 6     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 26  | 3     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |
| 26  | 5     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 27 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 (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms       |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|
| 27  | 2     | 1        | Total<br>44 | C<br>40 | O<br>4 | 0       |
| 27  | 6     | 1        | Total<br>44 | C<br>40 | O<br>4 | 0       |
| 27  | 3     | 1        | Total<br>44 | C<br>40 | O<br>4 | 0       |
| 27  | 5     | 1        | Total<br>44 | C<br>40 | O<br>4 | 0       |




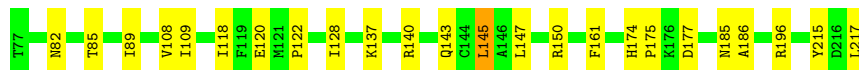
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  70% 25% 5%



- Molecule 4: Predicted protein PsaD

Chain D:  83% 16% .



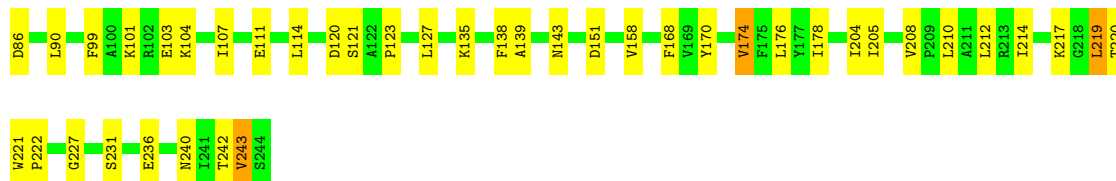
- Molecule 5: PsaE

Chain E:  71% 27% .



- Molecule 6: PSI-F

Chain F:  74% 24% .




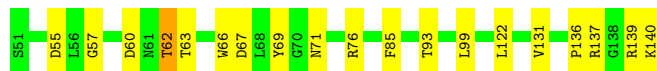
- Molecule 7: Predicted protein PsaG

Chain G:  68% 28% .



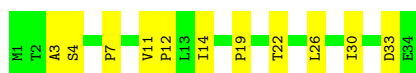
- Molecule 8: PsaH photosystem I reaction center subunit

Chain H:  79% 20% .



- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  68% 32%



- Molecule 10: Photosystem I reaction center subunit IX

Chain J: 78% 22%



- Molecule 11: PsaK

Chain K: 65% 30% 5%



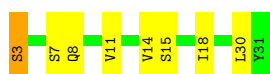
- Molecule 12: PSI subunit V

Chain L: 73% 26%



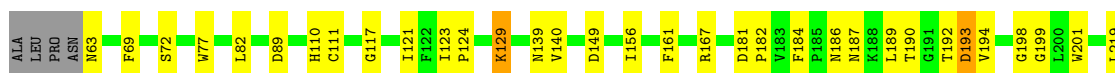
- Molecule 13: Photosystem I reaction center subunit XII

Chain M: 72% 24%



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

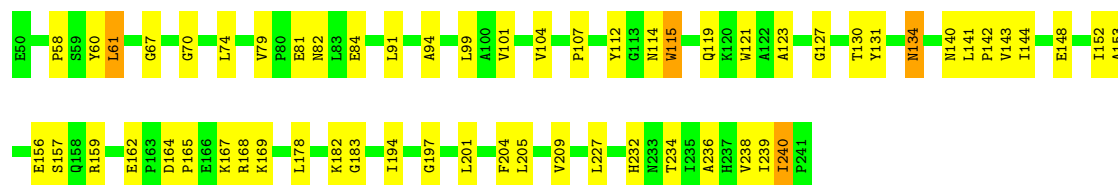
Chain 2: 77% 20%



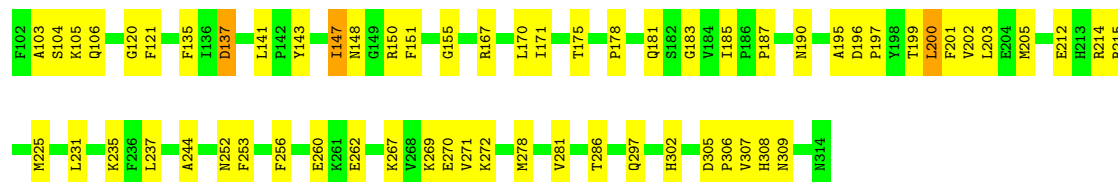
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 69% 29%

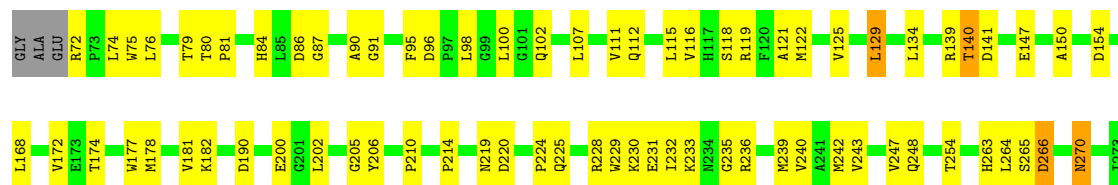




- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: 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             | 70288                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, BCR, PQN, LMG, XAT, CHL, LUT, LHG, SF4, DGD

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     | 0.26         | 0/6032      | 0.40        | 0/8227      |
| 2   | B     | 0.26         | 0/6063      | 0.41        | 0/8274      |
| 3   | C     | 0.27         | 0/605       | 0.45        | 0/821       |
| 4   | D     | 0.26         | 0/1132      | 0.45        | 0/1532      |
| 5   | E     | 0.27         | 0/498       | 0.44        | 0/677       |
| 6   | F     | 0.26         | 0/1251      | 0.43        | 0/1692      |
| 7   | G     | 0.25         | 0/767       | 0.46        | 0/1046      |
| 8   | H     | 0.25         | 0/710       | 0.42        | 0/961       |
| 9   | I     | 0.27         | 0/273       | 0.45        | 0/373       |
| 10  | J     | 0.26         | 0/334       | 0.39        | 0/457       |
| 11  | K     | 0.26         | 0/556       | 0.51        | 0/752       |
| 12  | L     | 0.26         | 0/1222      | 0.42        | 0/1671      |
| 13  | M     | 0.24         | 0/215       | 0.37        | 0/290       |
| 14  | 2     | 0.26         | 0/1646      | 0.41        | 0/2252      |
| 15  | 6     | 0.26         | 0/1522      | 0.40        | 0/2081      |
| 16  | 3     | 0.27         | 0/1695      | 0.43        | 0/2302      |
| 17  | 5     | 0.26         | 0/1614      | 0.45        | 0/2201      |
| All | All   | 0.26         | 0/26135     | 0.42        | 0/35609     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5837  | 0        | 5725     | 120     | 0            |
| 2   | B     | 5849  | 0        | 5623     | 133     | 0            |
| 3   | C     | 595   | 0        | 576      | 25      | 0            |
| 4   | D     | 1104  | 0        | 1112     | 15      | 0            |
| 5   | E     | 487   | 0        | 480      | 11      | 0            |
| 6   | F     | 1226  | 0        | 1269     | 27      | 0            |
| 7   | G     | 749   | 0        | 729      | 20      | 0            |
| 8   | H     | 693   | 0        | 672      | 16      | 0            |
| 9   | I     | 266   | 0        | 274      | 7       | 0            |
| 10  | J     | 325   | 0        | 341      | 9       | 0            |
| 11  | K     | 550   | 0        | 566      | 15      | 0            |
| 12  | L     | 1189  | 0        | 1200     | 29      | 0            |
| 13  | M     | 214   | 0        | 236      | 6       | 0            |
| 14  | 2     | 1595  | 0        | 1561     | 35      | 0            |
| 15  | 6     | 1473  | 0        | 1446     | 43      | 0            |
| 16  | 3     | 1644  | 0        | 1598     | 62      | 0            |
| 17  | 5     | 1566  | 0        | 1531     | 62      | 0            |
| 18  | 2     | 410   | 0        | 310      | 12      | 0            |
| 18  | 3     | 577   | 0        | 422      | 21      | 0            |
| 18  | 5     | 445   | 0        | 318      | 20      | 0            |
| 18  | 6     | 525   | 0        | 355      | 4       | 0            |
| 18  | A     | 2421  | 0        | 2229     | 103     | 0            |
| 18  | B     | 2093  | 0        | 1861     | 77      | 0            |
| 18  | F     | 176   | 0        | 128      | 5       | 0            |
| 18  | G     | 139   | 0        | 102      | 4       | 0            |
| 18  | J     | 42    | 0        | 31       | 1       | 0            |
| 18  | K     | 180   | 0        | 126      | 4       | 0            |
| 18  | L     | 132   | 0        | 97       | 7       | 0            |
| 19  | A     | 33    | 0        | 46       | 1       | 0            |
| 19  | B     | 33    | 0        | 46       | 5       | 0            |
| 20  | 2     | 35    | 0        | 40       | 3       | 0            |
| 20  | 5     | 37    | 0        | 44       | 5       | 0            |
| 20  | 6     | 28    | 0        | 26       | 1       | 0            |
| 20  | A     | 76    | 0        | 98       | 3       | 0            |
| 20  | B     | 23    | 0        | 16       | 1       | 0            |
| 21  | 2     | 40    | 0        | 56       | 5       | 0            |
| 21  | 3     | 80    | 0        | 112      | 8       | 0            |
| 21  | 5     | 40    | 0        | 56       | 2       | 0            |
| 21  | A     | 240   | 0        | 336      | 14      | 0            |
| 21  | B     | 280   | 0        | 392      | 16      | 0            |
| 21  | F     | 40    | 0        | 56       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21  | G     | 40    | 0        | 56       | 3       | 0            |
| 21  | I     | 40    | 0        | 56       | 2       | 0            |
| 21  | J     | 80    | 0        | 110      | 6       | 0            |
| 21  | K     | 80    | 0        | 112      | 5       | 0            |
| 21  | L     | 80    | 0        | 112      | 2       | 0            |
| 22  | A     | 8     | 0        | 0        | 0       | 0            |
| 22  | C     | 16    | 0        | 0        | 11      | 0            |
| 23  | B     | 66    | 0        | 96       | 4       | 0            |
| 24  | 2     | 26    | 0        | 22       | 0       | 0            |
| 24  | J     | 30    | 0        | 30       | 1       | 0            |
| 25  | 2     | 221   | 0        | 143      | 16      | 0            |
| 25  | 3     | 40    | 0        | 23       | 1       | 0            |
| 25  | 5     | 178   | 0        | 116      | 18      | 0            |
| 25  | 6     | 86    | 0        | 52       | 8       | 0            |
| 26  | 2     | 42    | 0        | 56       | 2       | 0            |
| 26  | 3     | 42    | 0        | 55       | 1       | 0            |
| 26  | 5     | 42    | 0        | 56       | 2       | 0            |
| 26  | 6     | 42    | 0        | 56       | 3       | 0            |
| 27  | 2     | 44    | 0        | 56       | 24      | 0            |
| 27  | 3     | 44    | 0        | 56       | 17      | 0            |
| 27  | 5     | 44    | 0        | 56       | 31      | 0            |
| 27  | 6     | 44    | 0        | 56       | 13      | 0            |
| All | All   | 34822 | 0        | 33617    | 814     | 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 12.

All (814) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:2:121:ILE:HD11 | 27:2:620:XAT:C17  | 1.25                     | 1.61              |
| 3:C:21:CYS:SG     | 22:C:101:SF4:FE2  | 1.20                     | 1.34              |
| 3:C:14:CYS:SG     | 22:C:102:SF4:S4   | 2.29                     | 1.29              |
| 14:2:121:ILE:CD1  | 27:2:620:XAT:H173 | 1.68                     | 1.22              |
| 3:C:21:CYS:SG     | 22:C:101:SF4:S1   | 2.38                     | 1.20              |
| 14:2:121:ILE:CD1  | 27:2:620:XAT:C17  | 2.19                     | 1.19              |
| 3:C:14:CYS:SG     | 22:C:102:SF4:FE3  | 1.33                     | 1.18              |
| 3:C:54:CYS:SG     | 22:C:101:SF4:S4   | 2.43                     | 1.16              |
| 25:2:606:CHL:HBB1 | 27:2:620:XAT:H182 | 1.26                     | 1.13              |
| 3:C:14:CYS:SG     | 22:C:102:SF4:S2   | 2.47                     | 1.12              |
| 3:C:54:CYS:SG     | 22:C:101:SF4:FE3  | 1.42                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:3:121:PHE:HE2  | 27:3:619:XAT:H383 | 1.14                     | 1.10              |
| 14:2:121:ILE:HD11 | 27:2:620:XAT:H172 | 1.41                     | 1.00              |
| 14:2:121:ILE:HD11 | 27:2:620:XAT:H173 | 1.02                     | 0.98              |
| 25:2:606:CHL:CBB  | 27:2:620:XAT:C18  | 2.41                     | 0.98              |
| 25:2:606:CHL:HBB1 | 27:2:620:XAT:C18  | 1.96                     | 0.95              |
| 25:5:607:CHL:C3B  | 27:5:620:XAT:H163 | 1.96                     | 0.95              |
| 14:2:121:ILE:HD11 | 27:2:620:XAT:H171 | 1.48                     | 0.93              |
| 14:2:121:ILE:CG1  | 27:2:620:XAT:H173 | 1.97                     | 0.92              |
| 16:3:121:PHE:CE2  | 27:3:619:XAT:H383 | 2.05                     | 0.92              |
| 25:2:606:CHL:CBB  | 27:2:620:XAT:H182 | 1.99                     | 0.89              |
| 3:C:58:CYS:SG     | 22:C:102:SF4:S2   | 2.73                     | 0.87              |
| 18:2:602:CLA:O1A  | 27:2:620:XAT:H241 | 1.76                     | 0.85              |
| 3:C:21:CYS:HG     | 22:C:101:SF4:FE2  | 0.83                     | 0.85              |
| 25:2:607:CHL:HMB3 | 27:2:620:XAT:H161 | 1.61                     | 0.82              |
| 25:5:607:CHL:HMB3 | 27:5:620:XAT:H171 | 1.61                     | 0.82              |
| 18:B:821:CLA:HMD2 | 21:B:843:BCR:HC7  | 1.61                     | 0.81              |
| 25:2:607:CHL:HMB3 | 27:2:620:XAT:C16  | 2.09                     | 0.81              |
| 25:5:607:CHL:HMB3 | 27:5:620:XAT:C17  | 2.11                     | 0.81              |
| 1:A:416:PRO:HG3   | 4:D:120:GLU:HB2   | 1.63                     | 0.80              |
| 18:2:602:CLA:HMC2 | 27:2:620:XAT:C31  | 2.13                     | 0.79              |
| 18:B:823:CLA:HAB  | 18:B:830:CLA:HMD2 | 1.64                     | 0.79              |
| 12:L:70:LEU:HD13  | 12:L:76:ILE:HB    | 1.65                     | 0.78              |
| 19:A:844:PQN:H172 | 21:B:801:BCR:H382 | 1.66                     | 0.78              |
| 16:3:121:PHE:HE2  | 27:3:619:XAT:C38  | 1.96                     | 0.77              |
| 17:5:118:SER:HB3  | 17:5:235:GLY:HA3  | 1.66                     | 0.77              |
| 25:2:616:CHL:HHB  | 25:2:616:CHL:HBB1 | 1.68                     | 0.76              |
| 1:A:196:ASN:ND2   | 1:A:306:GLY:O     | 2.19                     | 0.75              |
| 17:5:243:VAL:HG21 | 27:5:620:XAT:H401 | 1.67                     | 0.75              |
| 21:A:856:BCR:H312 | 10:J:31:ARG:HD3   | 1.68                     | 0.75              |
| 17:5:121:ALA:HB2  | 27:5:620:XAT:H202 | 1.67                     | 0.74              |
| 25:5:607:CHL:HAB  | 27:5:620:XAT:H161 | 1.69                     | 0.74              |
| 18:5:602:CLA:HMC2 | 27:5:620:XAT:C31  | 2.17                     | 0.74              |
| 10:J:40:PRO:HG2   | 21:J:103:BCR:H382 | 1.69                     | 0.73              |
| 2:B:292:ARG:NH1   | 7:G:92:GLY:O      | 2.21                     | 0.73              |
| 15:6:119:GLN:NE2  | 27:6:619:XAT:H21  | 2.04                     | 0.72              |
| 9:I:11:VAL:HA     | 9:I:14:ILE:HG22   | 1.70                     | 0.72              |
| 6:F:158:VAL:HG12  | 6:F:168:PHE:HB2   | 1.72                     | 0.72              |
| 17:5:243:VAL:HG21 | 27:5:620:XAT:C40  | 2.20                     | 0.71              |
| 14:2:240:GLN:HE21 | 14:2:251:ASN:HD22 | 1.37                     | 0.71              |
| 17:5:125:VAL:HG13 | 17:5:129:LEU:HD23 | 1.72                     | 0.71              |
| 18:A:810:CLA:HAB  | 18:B:833:CLA:HMD2 | 1.72                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:2:606:CHL:HAA1 | 21:2:621:BCR:H402 | 1.72                     | 0.70              |
| 25:5:607:CHL:CAB  | 27:5:620:XAT:C16  | 2.68                     | 0.70              |
| 14:2:111:CYS:HB2  | 14:2:227:GLY:HA3  | 1.72                     | 0.70              |
| 25:5:607:CHL:C3B  | 27:5:620:XAT:C16  | 2.71                     | 0.69              |
| 25:2:607:CHL:HHC  | 25:2:607:CHL:HBB1 | 1.74                     | 0.69              |
| 17:5:74:LEU:HD12  | 17:5:79:THR:HB    | 1.73                     | 0.69              |
| 1:A:732:LEU:HD12  | 18:A:842:CLA:HMA1 | 1.74                     | 0.69              |
| 14:2:219:LEU:HA   | 14:2:222:LYS:HD2  | 1.75                     | 0.68              |
| 18:B:819:CLA:HAA2 | 18:B:824:CLA:HBB1 | 1.75                     | 0.68              |
| 15:6:178:LEU:HD12 | 26:6:617:LUT:H222 | 1.77                     | 0.67              |
| 3:C:21:CYS:SG     | 22:C:101:SF4:S3   | 2.93                     | 0.67              |
| 17:5:95:PHE:CE2   | 27:5:620:XAT:H383 | 2.29                     | 0.67              |
| 18:5:602:CLA:HMC2 | 27:5:620:XAT:C32  | 2.24                     | 0.67              |
| 2:B:475:ASP:HA    | 2:B:479:SER:HB2   | 1.77                     | 0.67              |
| 20:2:622:LHG:HC42 | 21:3:620:BCR:HC32 | 1.77                     | 0.66              |
| 16:3:231:LEU:HG   | 21:3:620:BCR:H323 | 1.77                     | 0.66              |
| 3:C:54:CYS:SG     | 22:C:101:SF4:S1   | 2.94                     | 0.66              |
| 17:5:243:VAL:CG2  | 27:5:620:XAT:H401 | 2.24                     | 0.66              |
| 6:F:86:ASP:N      | 6:F:90:LEU:O      | 2.29                     | 0.66              |
| 25:5:608:CHL:HHC  | 25:5:608:CHL:HBB1 | 1.77                     | 0.66              |
| 25:2:606:CHL:CBB  | 27:2:620:XAT:H181 | 2.25                     | 0.65              |
| 16:3:167:ARG:HH12 | 16:3:297:GLN:HE22 | 1.44                     | 0.65              |
| 25:2:606:CHL:HBB2 | 27:2:620:XAT:C18  | 2.25                     | 0.65              |
| 15:6:234:THR:HG23 | 15:6:236:ALA:H    | 1.61                     | 0.65              |
| 16:3:212:GLU:OE2  | 16:3:215:ARG:NH1  | 2.29                     | 0.65              |
| 17:5:264:LEU:HD21 | 18:5:614:CLA:HMC3 | 1.78                     | 0.65              |
| 2:B:42:LEU:O      | 2:B:46:ILE:HG12   | 1.97                     | 0.65              |
| 18:A:823:CLA:HMD2 | 21:K:202:BCR:H24C | 1.79                     | 0.65              |
| 17:5:134:LEU:HB2  | 17:5:139:ARG:HB3  | 1.78                     | 0.64              |
| 3:C:58:CYS:SG     | 3:C:64:SER:OG     | 2.54                     | 0.64              |
| 18:G:201:CLA:HAC2 | 15:6:123:ALA:HB2  | 1.78                     | 0.64              |
| 15:6:201:LEU:HD22 | 27:6:619:XAT:C35  | 2.27                     | 0.64              |
| 1:A:739:TRP:NE1   | 18:A:829:CLA:O1A  | 2.28                     | 0.64              |
| 2:B:707:LEU:HD23  | 23:B:850:DGD:HA21 | 1.78                     | 0.64              |
| 2:B:65:LEU:HD11   | 21:B:845:BCR:H271 | 1.78                     | 0.64              |
| 11:K:69:ALA:O     | 11:K:80:ARG:NH2   | 2.32                     | 0.63              |
| 1:A:118:ILE:HG23  | 1:A:119:VAL:HG22  | 1.80                     | 0.63              |
| 15:6:156:GLU:OE1  | 15:6:159:ARG:NH2  | 2.30                     | 0.63              |
| 14:2:129:LYS:NZ   | 14:2:250:ASP:OD1  | 2.29                     | 0.63              |
| 15:6:162:GLU:O    | 15:6:168:ARG:NH2  | 2.32                     | 0.63              |
| 12:L:105:PRO:HA   | 12:L:108:ARG:HD3  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:2:622:LHG:HC82 | 21:3:620:BCR:HC42 | 1.80                     | 0.63              |
| 18:A:843:CLA:H172 | 18:L:303:CLA:HMC3 | 1.80                     | 0.62              |
| 2:B:721:TYR:HB2   | 18:B:802:CLA:HED2 | 1.81                     | 0.62              |
| 18:B:805:CLA:H93  | 18:B:813:CLA:H2   | 1.80                     | 0.62              |
| 15:6:130:THR:HG22 | 15:6:131:TYR:H    | 1.65                     | 0.62              |
| 25:6:607:CHL:C2B  | 27:6:619:XAT:H171 | 2.28                     | 0.62              |
| 6:F:217:LYS:HA    | 17:5:98:LEU:HD22  | 1.81                     | 0.62              |
| 1:A:57:ASP:OD2    | 1:A:347:HIS:NE2   | 2.30                     | 0.62              |
| 12:L:111:GLU:HG3  | 18:L:302:CLA:HMA3 | 1.82                     | 0.61              |
| 16:3:150:ARG:NH1  | 16:3:270:GLU:OE2  | 2.33                     | 0.61              |
| 17:5:95:PHE:HE2   | 27:5:620:XAT:H383 | 1.65                     | 0.61              |
| 16:3:281:VAL:HG21 | 27:3:619:XAT:H12  | 1.83                     | 0.61              |
| 17:5:206:TYR:HB3  | 18:5:610:CLA:HED2 | 1.83                     | 0.61              |
| 2:B:272:ASP:HB3   | 18:B:817:CLA:HMA1 | 1.83                     | 0.61              |
| 18:A:843:CLA:H143 | 21:L:301:BCR:H17C | 1.81                     | 0.61              |
| 12:L:70:LEU:HD12  | 12:L:70:LEU:H     | 1.66                     | 0.61              |
| 12:L:92:TYR:OH    | 18:L:303:CLA:O1A  | 2.19                     | 0.61              |
| 2:B:201:GLU:OE1   | 2:B:208:ARG:NH1   | 2.33                     | 0.60              |
| 2:B:694:LYS:NZ    | 18:B:839:CLA:O2D  | 2.29                     | 0.60              |
| 17:5:242:MET:HE2  | 27:5:620:XAT:H10  | 1.83                     | 0.60              |
| 18:A:834:CLA:HED3 | 18:A:843:CLA:H12  | 1.83                     | 0.60              |
| 20:B:851:LHG:HC11 | 15:6:82:ASN:HD22  | 1.65                     | 0.60              |
| 5:E:84:ARG:O      | 6:F:242:THR:OG1   | 2.19                     | 0.60              |
| 16:3:281:VAL:CG1  | 27:3:619:XAT:H14  | 2.31                     | 0.60              |
| 18:A:822:CLA:HMB2 | 18:A:826:CLA:HMA3 | 1.83                     | 0.60              |
| 2:B:342:GLY:HA2   | 2:B:345:THR:HG22  | 1.83                     | 0.60              |
| 2:B:729:THR:O     | 2:B:733:PHE:N     | 2.32                     | 0.60              |
| 4:D:89:ILE:HB     | 4:D:128:ILE:HG13  | 1.84                     | 0.60              |
| 15:6:84:GLU:OE2   | 15:6:169:LYS:NZ   | 2.34                     | 0.60              |
| 15:6:152:ILE:HG21 | 18:6:609:CLA:HMC3 | 1.82                     | 0.60              |
| 1:A:327:LYS:H     | 18:A:845:CLA:HBC2 | 1.67                     | 0.60              |
| 18:B:841:CLA:HMC3 | 18:6:603:CLA:H12  | 1.84                     | 0.60              |
| 6:F:120:ASP:OD1   | 6:F:120:ASP:N     | 2.35                     | 0.60              |
| 9:I:14:ILE:HD11   | 21:I:101:BCR:H333 | 1.84                     | 0.60              |
| 2:B:268:LEU:HB2   | 2:B:273:MET:HE3   | 1.84                     | 0.59              |
| 1:A:433:ALA:O     | 1:A:437:HIS:HD2   | 1.84                     | 0.59              |
| 18:B:806:CLA:H151 | 18:B:828:CLA:HBB2 | 1.83                     | 0.59              |
| 2:B:716:GLY:O     | 2:B:720:THR:HG22  | 2.03                     | 0.59              |
| 18:5:611:CLA:HBC3 | 20:5:622:LHG:HC62 | 1.83                     | 0.59              |
| 2:B:43:TYR:OH     | 2:B:169:LYS:NZ    | 2.35                     | 0.58              |
| 2:B:77:TRP:HA     | 2:B:84:VAL:HG11   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:167:TRP:CZ2   | 18:B:813:CLA:HAC2 | 2.38                     | 0.58              |
| 2:B:546:LEU:O     | 2:B:564:ARG:NH2   | 2.35                     | 0.58              |
| 14:2:190:THR:HG23 | 14:2:199:GLY:HA2  | 1.85                     | 0.58              |
| 15:6:201:LEU:HD22 | 27:6:619:XAT:C34  | 2.32                     | 0.58              |
| 4:D:120:GLU:O     | 4:D:150:ARG:NH1   | 2.36                     | 0.58              |
| 2:B:733:PHE:HE2   | 8:H:136:PRO:HD2   | 1.67                     | 0.58              |
| 25:5:607:CHL:C2B  | 27:5:620:XAT:H163 | 2.33                     | 0.58              |
| 1:A:44:THR:O      | 1:A:48:ASN:ND2    | 2.36                     | 0.58              |
| 2:B:415:LYS:HB2   | 2:B:539:LEU:HD13  | 1.84                     | 0.58              |
| 4:D:185:ASN:ND2   | 4:D:186:ALA:O     | 2.36                     | 0.58              |
| 16:3:178:PRO:HG2  | 16:3:181:GLN:HB2  | 1.84                     | 0.58              |
| 1:A:14:VAL:HG21   | 18:A:811:CLA:HED2 | 1.84                     | 0.58              |
| 2:B:85:ARG:HD3    | 8:H:139:ARG:HD3   | 1.85                     | 0.58              |
| 2:B:684:ARG:NE    | 12:L:77:GLY:O     | 2.36                     | 0.58              |
| 14:2:189:LEU:HD22 | 14:2:199:GLY:HA3  | 1.85                     | 0.58              |
| 17:5:119:ARG:NH1  | 25:5:608:CHL:OBD  | 2.30                     | 0.58              |
| 1:A:330:PHE:O     | 1:A:426:ARG:NH1   | 2.37                     | 0.58              |
| 16:3:195:ALA:HB3  | 16:3:200:LEU:HD13 | 1.85                     | 0.58              |
| 16:3:199:THR:HA   | 16:3:202:VAL:HG12 | 1.86                     | 0.58              |
| 18:A:814:CLA:HMB1 | 18:A:814:CLA:HBB1 | 1.84                     | 0.57              |
| 2:B:459:PHE:HD1   | 18:F:304:CLA:HMC2 | 1.69                     | 0.57              |
| 18:2:604:CLA:HBB1 | 18:2:604:CLA:HMB1 | 1.86                     | 0.57              |
| 25:6:607:CHL:C2B  | 27:6:619:XAT:C17  | 2.82                     | 0.57              |
| 1:A:676:PHE:CD1   | 21:A:852:BCR:H363 | 2.38                     | 0.57              |
| 19:B:842:PQN:H293 | 23:B:850:DGD:HAE2 | 1.85                     | 0.57              |
| 25:5:607:CHL:HAB  | 27:5:620:XAT:C16  | 2.31                     | 0.57              |
| 1:A:331:THR:OG1   | 20:A:847:LHG:O2   | 2.19                     | 0.57              |
| 1:A:698:SER:O     | 2:B:420:SER:OG    | 2.22                     | 0.57              |
| 2:B:435:GLY:HA3   | 18:B:833:CLA:HAB  | 1.87                     | 0.57              |
| 1:A:353:ASN:ND2   | 18:A:806:CLA:OBD  | 2.31                     | 0.57              |
| 1:A:471:ASP:O     | 1:A:475:GLN:NE2   | 2.38                     | 0.57              |
| 4:D:196:ARG:NH2   | 4:D:217:LEU:O     | 2.38                     | 0.57              |
| 16:3:281:VAL:HG13 | 27:3:619:XAT:H14  | 1.87                     | 0.57              |
| 1:A:118:ILE:HG12  | 1:A:119:VAL:HG13  | 1.86                     | 0.57              |
| 2:B:142:LEU:HA    | 2:B:145:VAL:HG12  | 1.86                     | 0.57              |
| 6:F:139:ALA:O     | 6:F:143:ASN:ND2   | 2.38                     | 0.57              |
| 18:A:803:CLA:HMB1 | 18:A:803:CLA:HBB1 | 1.86                     | 0.57              |
| 2:B:15:ASP:HB3    | 2:B:20:ARG:HB2    | 1.86                     | 0.57              |
| 4:D:174:HIS:HB3   | 4:D:175:PRO:HD3   | 1.86                     | 0.57              |
| 16:3:185:ILE:HG22 | 16:3:187:PRO:HD2  | 1.87                     | 0.57              |
| 18:A:809:CLA:HMC3 | 18:A:810:CLA:HMD2 | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:71:ARG:HH12  | 11:K:99:ASP:HB2   | 1.69                     | 0.57              |
| 16:3:148:ASN:ND2  | 18:3:609:CLA:OBD  | 2.37                     | 0.57              |
| 1:A:460:SER:HG    | 2:B:635:TYR:HD2   | 1.53                     | 0.57              |
| 1:A:503:THR:HG23  | 1:A:507:TRP:HE1   | 1.69                     | 0.57              |
| 1:A:687:SER:OG    | 1:A:688:GLY:N     | 2.38                     | 0.57              |
| 18:A:854:CLA:HAB  | 2:B:582:TRP:CH2   | 2.40                     | 0.57              |
| 1:A:12:ILE:HD12   | 18:A:811:CLA:HAA2 | 1.87                     | 0.56              |
| 21:J:103:BCR:H311 | 21:J:103:BCR:H342 | 1.87                     | 0.56              |
| 15:6:74:LEU:HD12  | 27:6:619:XAT:H221 | 1.86                     | 0.56              |
| 17:5:112:GLN:HE22 | 17:5:205:GLY:H    | 1.52                     | 0.56              |
| 1:A:687:SER:OG    | 1:A:692:TRP:NE1   | 2.36                     | 0.56              |
| 18:A:854:CLA:H42  | 2:B:438:VAL:HG22  | 1.87                     | 0.56              |
| 1:A:576:PRO:HD2   | 3:C:52:LYS:HG3    | 1.86                     | 0.56              |
| 6:F:208:VAL:HG21  | 24:J:104:LMG:H111 | 1.87                     | 0.56              |
| 18:3:604:CLA:HMB3 | 27:3:619:XAT:H162 | 1.88                     | 0.56              |
| 14:2:193:ASP:OD1  | 14:2:193:ASP:N    | 2.38                     | 0.56              |
| 1:A:522:LEU:HD11  | 1:A:616:VAL:HA    | 1.88                     | 0.56              |
| 17:5:210:PRO:HA   | 17:5:214:PRO:HA   | 1.87                     | 0.56              |
| 2:B:631:LEU:HD11  | 2:B:724:PHE:HA    | 1.88                     | 0.55              |
| 18:B:819:CLA:HMB2 | 18:B:824:CLA:HMA3 | 1.88                     | 0.55              |
| 1:A:72:SER:HB2    | 18:A:812:CLA:HMD3 | 1.88                     | 0.55              |
| 7:G:151:TYR:HE2   | 18:G:201:CLA:HED2 | 1.70                     | 0.55              |
| 13:M:14:VAL:O     | 13:M:18:ILE:HG12  | 2.05                     | 0.55              |
| 16:3:286:THR:HG21 | 18:3:613:CLA:HAC2 | 1.88                     | 0.55              |
| 1:A:600:ALA:O     | 1:A:604:VAL:HG23  | 2.06                     | 0.55              |
| 1:A:367:HIS:ND1   | 18:A:819:CLA:OBD  | 2.39                     | 0.55              |
| 16:3:121:PHE:CE2  | 27:3:619:XAT:C38  | 2.80                     | 0.55              |
| 21:A:848:BCR:H383 | 21:K:202:BCR:HC8  | 1.87                     | 0.55              |
| 2:B:351:HIS:ND1   | 18:B:817:CLA:OBD  | 2.39                     | 0.55              |
| 18:B:803:CLA:H143 | 21:B:848:BCR:H362 | 1.89                     | 0.55              |
| 15:6:201:LEU:HD22 | 27:6:619:XAT:C15  | 2.36                     | 0.55              |
| 8:H:67:ASP:HB2    | 12:L:172:PRO:HB2  | 1.88                     | 0.55              |
| 15:6:58:PRO:HD2   | 15:6:61:LEU:HB2   | 1.89                     | 0.55              |
| 17:5:266:ASP:O    | 17:5:270:ASN:ND2  | 2.40                     | 0.55              |
| 2:B:693:TRP:HE3   | 18:B:839:CLA:HMD3 | 1.72                     | 0.54              |
| 1:A:617:TRP:O     | 1:A:628:HIS:ND1   | 2.31                     | 0.54              |
| 18:B:815:CLA:HBB1 | 21:B:843:BCR:H382 | 1.90                     | 0.54              |
| 11:K:81:LYS:NZ    | 11:K:82:SER:O     | 2.39                     | 0.54              |
| 17:5:100:LEU:CD2  | 27:5:620:XAT:H373 | 2.37                     | 0.54              |
| 1:A:10:VAL:HG13   | 18:A:813:CLA:HED3 | 1.89                     | 0.54              |
| 1:A:359:SER:O     | 1:A:363:ILE:HG12  | 2.06                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:126:SER:OG    | 5:E:128:ASP:OD1   | 2.20                     | 0.54              |
| 14:2:192:THR:OG1  | 14:2:193:ASP:OD1  | 2.24                     | 0.54              |
| 3:C:60:THR:HG22   | 3:C:61:ASP:H      | 1.72                     | 0.54              |
| 11:K:81:LYS:H     | 11:K:90:ASP:HB3   | 1.73                     | 0.54              |
| 15:6:101:VAL:HG21 | 26:6:617:LUT:H12  | 1.90                     | 0.54              |
| 17:5:121:ALA:HB2  | 27:5:620:XAT:C20  | 2.36                     | 0.54              |
| 1:A:192:GLU:HG3   | 1:A:309:TYR:HB3   | 1.89                     | 0.54              |
| 11:K:105:ALA:HA   | 18:K:201:CLA:HBA2 | 1.90                     | 0.54              |
| 16:3:137:ASP:N    | 16:3:137:ASP:OD1  | 2.39                     | 0.54              |
| 1:A:576:PRO:HD3   | 2:B:561:GLY:HA2   | 1.90                     | 0.54              |
| 18:A:816:CLA:HBB1 | 18:A:816:CLA:HMB1 | 1.89                     | 0.54              |
| 4:D:140:ARG:HB2   | 4:D:143:GLN:HG3   | 1.90                     | 0.54              |
| 17:5:230:LYS:HD3  | 18:5:612:CLA:HBA1 | 1.88                     | 0.54              |
| 25:5:607:CHL:CMB  | 27:5:620:XAT:H171 | 2.37                     | 0.54              |
| 14:2:167:ARG:HA   | 18:5:601:CLA:HED1 | 1.91                     | 0.53              |
| 16:3:231:LEU:HD22 | 16:3:231:LEU:H    | 1.73                     | 0.53              |
| 21:J:103:BCR:H371 | 21:J:103:BCR:H383 | 1.90                     | 0.53              |
| 1:A:310:ARG:N     | 1:A:317:HIS:O     | 2.40                     | 0.53              |
| 2:B:527:LEU:O     | 2:B:531:THR:HG23  | 2.09                     | 0.53              |
| 6:F:107:ILE:O     | 6:F:111:GLU:HG2   | 2.08                     | 0.53              |
| 16:3:103:ALA:O    | 16:3:104:SER:OG   | 2.25                     | 0.53              |
| 2:B:364:ASP:OD1   | 8:H:139:ARG:NH2   | 2.32                     | 0.53              |
| 8:H:76:ARG:HG3    | 18:L:302:CLA:HMD3 | 1.91                     | 0.53              |
| 15:6:182:LYS:HG3  | 15:6:183:GLY:H    | 1.73                     | 0.53              |
| 1:A:476:LEU:HB2   | 1:A:528:THR:HG23  | 1.91                     | 0.53              |
| 2:B:174:ARG:HB2   | 18:B:813:CLA:HBC3 | 1.89                     | 0.53              |
| 18:B:832:CLA:HAB  | 18:B:833:CLA:HMB2 | 1.90                     | 0.53              |
| 7:G:85:ARG:NH2    | 7:G:123:GLY:O     | 2.38                     | 0.53              |
| 2:B:448:THR:OG1   | 2:B:448:THR:O     | 2.24                     | 0.53              |
| 6:F:101:LYS:HA    | 6:F:104:LYS:HG2   | 1.89                     | 0.53              |
| 12:L:185:LYS:O    | 12:L:188:THR:OG1  | 2.27                     | 0.53              |
| 16:3:200:LEU:HD21 | 18:3:606:CLA:HMD3 | 1.91                     | 0.53              |
| 1:A:138:THR:HG22  | 18:A:809:CLA:HMD1 | 1.91                     | 0.52              |
| 1:A:363:ILE:HD13  | 18:A:827:CLA:HED3 | 1.91                     | 0.52              |
| 3:C:24:ASP:OD1    | 3:C:44:ARG:NH2    | 2.41                     | 0.52              |
| 16:3:306:PRO:HG3  | 18:3:614:CLA:HMB3 | 1.91                     | 0.52              |
| 17:5:122:MET:HB3  | 26:5:619:LUT:H34  | 1.91                     | 0.52              |
| 18:A:805:CLA:HMB1 | 18:A:805:CLA:HBB1 | 1.91                     | 0.52              |
| 2:B:40:GLU:O      | 2:B:44:GLN:NE2    | 2.42                     | 0.52              |
| 2:B:405:ASP:OD1   | 2:B:410:ARG:NH2   | 2.42                     | 0.52              |
| 18:B:825:CLA:HMA1 | 21:B:847:BCR:H14C | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:60:VAL:O     | 11:K:64:THR:HG23  | 2.09                     | 0.52              |
| 2:B:294:ASN:HB2   | 7:G:111:GLU:HA    | 1.92                     | 0.52              |
| 14:2:193:ASP:OD2  | 14:2:220:ARG:NH2  | 2.41                     | 0.52              |
| 2:B:143:LEU:HD23  | 13:M:15:SER:HB2   | 1.90                     | 0.52              |
| 16:3:272:LYS:HD3  | 18:3:611:CLA:HMA3 | 1.91                     | 0.52              |
| 25:5:607:CHL:HMB3 | 27:5:620:XAT:H172 | 1.88                     | 0.52              |
| 4:D:108:VAL:HA    | 4:D:137:LYS:HA    | 1.90                     | 0.52              |
| 5:E:83:ARG:HB3    | 5:E:86:SER:HB2    | 1.92                     | 0.52              |
| 16:3:281:VAL:HG11 | 27:3:619:XAT:C14  | 2.40                     | 0.52              |
| 2:B:363:GLN:O     | 8:H:137:ARG:NH2   | 2.43                     | 0.52              |
| 16:3:196:ASP:OD1  | 16:3:197:PRO:HD2  | 2.10                     | 0.52              |
| 18:5:609:CLA:HBB1 | 18:5:609:CLA:HMB1 | 1.91                     | 0.52              |
| 14:2:263:THR:OG1  | 14:2:264:ILE:N    | 2.43                     | 0.52              |
| 1:A:393:TRP:HB3   | 18:A:829:CLA:HMC3 | 1.92                     | 0.52              |
| 1:A:541:ILE:O     | 1:A:545:VAL:HG23  | 2.10                     | 0.52              |
| 2:B:310:PRO:HD2   | 2:B:315:LEU:HD11  | 1.92                     | 0.52              |
| 2:B:339:ALA:HB2   | 21:B:847:BCR:H372 | 1.91                     | 0.52              |
| 18:A:841:CLA:HBB1 | 18:F:301:CLA:HMD1 | 1.92                     | 0.52              |
| 18:A:802:CLA:CGA  | 18:A:802:CLA:H3A  | 2.40                     | 0.52              |
| 18:B:834:CLA:HBA2 | 18:B:835:CLA:HMB3 | 1.91                     | 0.52              |
| 25:5:607:CHL:CMB  | 27:5:620:XAT:C17  | 2.86                     | 0.52              |
| 1:A:18:PRO:HG3    | 1:A:182:ALA:HB3   | 1.92                     | 0.51              |
| 1:A:52:ASP:OD2    | 20:A:846:LHG:O2   | 2.25                     | 0.51              |
| 18:A:832:CLA:HMA2 | 12:L:81:THR:HG21  | 1.92                     | 0.51              |
| 14:2:69:PHE:HD2   | 14:2:72:SER:HB2   | 1.75                     | 0.51              |
| 14:2:77:TRP:NE1   | 14:2:89:ASP:OD2   | 2.41                     | 0.51              |
| 2:B:284:PHE:HE1   | 18:B:819:CLA:HAB  | 1.75                     | 0.51              |
| 3:C:32:ASP:HA     | 3:C:37:SER:HA     | 1.92                     | 0.51              |
| 18:5:604:CLA:HMB1 | 18:5:604:CLA:HBB1 | 1.91                     | 0.51              |
| 18:A:809:CLA:HBB1 | 18:A:809:CLA:HMB1 | 1.92                     | 0.51              |
| 9:I:19:PRO:HA     | 9:I:22:THR:HG22   | 1.92                     | 0.51              |
| 18:B:833:CLA:O1A  | 10:J:30:ASN:ND2   | 2.36                     | 0.51              |
| 18:K:203:CLA:HED2 | 18:K:203:CLA:H2A  | 1.93                     | 0.51              |
| 1:A:60:THR:OG1    | 1:A:61:ASN:N      | 2.43                     | 0.51              |
| 6:F:212:LEU:HB3   | 18:F:305:CLA:HMD1 | 1.93                     | 0.51              |
| 9:I:7:PRO:O       | 9:I:11:VAL:HG13   | 2.11                     | 0.51              |
| 15:6:94:ALA:HB1   | 15:6:197:GLY:HA3  | 1.91                     | 0.51              |
| 2:B:418:ILE:HG23  | 18:B:838:CLA:HBB2 | 1.92                     | 0.51              |
| 18:B:825:CLA:HAA2 | 18:B:826:CLA:OBD  | 2.10                     | 0.51              |
| 17:5:233:LYS:HD3  | 20:5:622:LHG:HC42 | 1.91                     | 0.51              |
| 1:A:445:LEU:O     | 1:A:449:SER:OG    | 2.18                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:51:ILE:O     | 11:K:56:ASN:ND2   | 2.43                     | 0.51              |
| 2:B:69:ALA:HB2    | 2:B:135:LEU:HB2   | 1.93                     | 0.51              |
| 10:J:7:TYR:O      | 10:J:10:THR:OG1   | 2.18                     | 0.51              |
| 18:A:808:CLA:HMB3 | 18:A:809:CLA:H3A  | 1.93                     | 0.51              |
| 5:E:80:LYS:HB3    | 5:E:132:ALA:HB3   | 1.92                     | 0.51              |
| 20:2:622:LHG:HC91 | 20:2:622:LHG:H281 | 1.93                     | 0.51              |
| 16:3:269:LYS:HD3  | 18:3:612:CLA:HAA2 | 1.92                     | 0.51              |
| 1:A:54:HIS:CD2    | 18:A:806:CLA:HBB2 | 2.46                     | 0.50              |
| 21:L:305:BCR:H403 | 21:L:305:BCR:H23C | 1.92                     | 0.50              |
| 2:B:136:TYR:CZ    | 13:M:8:GLN:HB3    | 2.46                     | 0.50              |
| 18:B:836:CLA:HBB1 | 18:B:836:CLA:HMB1 | 1.93                     | 0.50              |
| 21:2:621:BCR:HC32 | 20:5:622:LHG:HC81 | 1.92                     | 0.50              |
| 12:L:118:TYR:HD1  | 12:L:210:ALA:HB2  | 1.76                     | 0.50              |
| 15:6:239:ILE:HG22 | 15:6:240:ILE:HG12 | 1.92                     | 0.50              |
| 15:6:91:LEU:HD12  | 15:6:169:LYS:HB2  | 1.93                     | 0.50              |
| 17:5:79:THR:OG1   | 17:5:80:THR:N     | 2.44                     | 0.50              |
| 17:5:200:GLU:HB2  | 17:5:202:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:358:GLY:O     | 1:A:362:ILE:HG12  | 2.12                     | 0.50              |
| 5:E:101:ALA:HB3   | 5:E:104:VAL:HG23  | 1.93                     | 0.50              |
| 1:A:337:GLY:HA3   | 1:A:421:ASN:HD22  | 1.75                     | 0.50              |
| 21:A:852:BCR:H362 | 18:A:854:CLA:H43  | 1.94                     | 0.50              |
| 14:2:167:ARG:HH12 | 14:2:182:PRO:HG3  | 1.76                     | 0.50              |
| 1:A:411:VAL:HG23  | 1:A:555:ALA:HB1   | 1.94                     | 0.50              |
| 2:B:90:ALA:HA     | 2:B:113:VAL:HG12  | 1.93                     | 0.50              |
| 2:B:276:HIS:HB2   | 18:B:817:CLA:C1B  | 2.42                     | 0.50              |
| 2:B:294:ASN:HD21  | 18:B:812:CLA:HMA2 | 1.76                     | 0.50              |
| 14:2:223:GLU:HB2  | 18:2:610:CLA:HMB3 | 1.93                     | 0.50              |
| 1:A:465:PRO:HA    | 1:A:468:MET:HG3   | 1.94                     | 0.49              |
| 1:A:571:PHE:CE1   | 1:A:585:SER:HB3   | 2.48                     | 0.49              |
| 2:B:101:VAL:HG13  | 2:B:112:PRO:HG3   | 1.95                     | 0.49              |
| 17:5:74:LEU:HD11  | 17:5:81:PRO:HB3   | 1.94                     | 0.49              |
| 17:5:100:LEU:HD22 | 27:5:620:XAT:H373 | 1.94                     | 0.49              |
| 2:B:477:LEU:HD21  | 18:B:835:CLA:HMC3 | 1.94                     | 0.49              |
| 21:B:843:BCR:HC8  | 7:G:135:LEU:HD13  | 1.94                     | 0.49              |
| 4:D:109:ILE:HG13  | 4:D:161:PHE:HB3   | 1.93                     | 0.49              |
| 1:A:427:VAL:HA    | 1:A:430:HIS:CE1   | 2.46                     | 0.49              |
| 1:A:656:VAL:O     | 1:A:659:SER:OG    | 2.25                     | 0.49              |
| 4:D:161:PHE:CZ    | 4:D:174:HIS:HB2   | 2.47                     | 0.49              |
| 15:6:61:LEU:HD12  | 15:6:70:GLY:HA2   | 1.93                     | 0.49              |
| 16:3:267:LYS:O    | 16:3:271:VAL:HG13 | 2.11                     | 0.49              |
| 2:B:388:ALA:O     | 2:B:392:ILE:HG13  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:11:VAL:HG22   | 9:I:12:PRO:HD3    | 1.93                     | 0.49              |
| 16:3:302:HIS:CG   | 18:3:613:CLA:HAA2 | 2.47                     | 0.49              |
| 1:A:40:PRO:HG3    | 6:F:204:ILE:HD13  | 1.95                     | 0.49              |
| 18:B:814:CLA:C1B  | 21:B:845:BCR:H20C | 2.42                     | 0.49              |
| 18:3:606:CLA:HMB1 | 18:3:609:CLA:HBC2 | 1.93                     | 0.49              |
| 17:5:225:GLN:O    | 17:5:229:TRP:HB2  | 2.13                     | 0.49              |
| 2:B:300:SER:HB3   | 7:G:91:GLN:HB2    | 1.93                     | 0.49              |
| 3:C:55:GLU:OE1    | 3:C:66:ARG:NH1    | 2.45                     | 0.49              |
| 12:L:171:ALA:HB3  | 12:L:183:ALA:HB1  | 1.94                     | 0.49              |
| 15:6:164:ASP:HB3  | 15:6:167:LYS:HB2  | 1.93                     | 0.49              |
| 12:L:121:VAL:HG11 | 12:L:210:ALA:HB1  | 1.94                     | 0.49              |
| 2:B:256:THR:OG1   | 2:B:257:PHE:N     | 2.46                     | 0.49              |
| 18:3:603:CLA:HMD2 | 18:3:609:CLA:C1D  | 2.43                     | 0.49              |
| 17:5:84:HIS:NE2   | 17:5:96:ASP:OD2   | 2.46                     | 0.49              |
| 17:5:86:ASP:OD1   | 17:5:87:GLY:N     | 2.43                     | 0.49              |
| 17:5:140:THR:HG22 | 17:5:141:ASP:H    | 1.78                     | 0.49              |
| 1:A:56:PHE:CD2    | 18:A:806:CLA:HMC2 | 2.47                     | 0.48              |
| 7:G:125:THR:OG1   | 7:G:126:ILE:N     | 2.46                     | 0.48              |
| 25:6:607:CHL:HHC  | 25:6:607:CHL:HBB1 | 1.94                     | 0.48              |
| 16:3:121:PHE:CE2  | 27:3:619:XAT:H242 | 2.48                     | 0.48              |
| 6:F:114:LEU:HA    | 6:F:127:LEU:HD13  | 1.95                     | 0.48              |
| 18:5:613:CLA:O2D  | 18:5:613:CLA:H2A  | 2.13                     | 0.48              |
| 1:A:43:THR:HG22   | 1:A:715:ARG:H     | 1.77                     | 0.48              |
| 2:B:292:ARG:HH21  | 2:B:296:GLY:HA2   | 1.78                     | 0.48              |
| 18:B:826:CLA:H92  | 18:B:826:CLA:H62  | 1.69                     | 0.48              |
| 17:5:224:PRO:HG2  | 17:5:228:ARG:HD2  | 1.94                     | 0.48              |
| 1:A:537:HIS:HE1   | 1:A:603:VAL:HG12  | 1.78                     | 0.48              |
| 2:B:733:PHE:HB3   | 8:H:137:ARG:HD3   | 1.94                     | 0.48              |
| 15:6:67:GLY:HA3   | 15:6:194:ILE:HG21 | 1.93                     | 0.48              |
| 1:A:422:ASN:HB3   | 1:A:426:ARG:HG3   | 1.95                     | 0.48              |
| 2:B:9:SER:O       | 2:B:13:SER:OG     | 2.32                     | 0.48              |
| 2:B:410:ARG:O     | 2:B:414:HIS:ND1   | 2.43                     | 0.48              |
| 18:A:833:CLA:HMB1 | 18:A:843:CLA:HAA2 | 1.94                     | 0.48              |
| 1:A:175:TRP:HB2   | 18:A:812:CLA:HMC3 | 1.96                     | 0.48              |
| 2:B:292:ARG:NE    | 2:B:296:GLY:O     | 2.34                     | 0.48              |
| 2:B:704:GLN:O     | 2:B:708:VAL:HG23  | 2.14                     | 0.48              |
| 15:6:205:LEU:O    | 15:6:209:VAL:HG23 | 2.14                     | 0.48              |
| 2:B:576:PHE:O     | 2:B:580:VAL:HG23  | 2.14                     | 0.48              |
| 18:B:816:CLA:H61  | 7:G:142:PHE:HD1   | 1.77                     | 0.48              |
| 12:L:164:LYS:HB3  | 12:L:167:GLU:HG2  | 1.96                     | 0.48              |
| 2:B:91:ILE:HD11   | 2:B:112:PRO:HB2   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:459:PHE:CD1   | 18:F:304:CLA:HMC2 | 2.47                     | 0.48              |
| 18:3:603:CLA:HMC2 | 27:3:619:XAT:C12  | 2.43                     | 0.48              |
| 18:5:602:CLA:CBB  | 27:5:620:XAT:H34  | 2.44                     | 0.48              |
| 1:A:317:HIS:NE2   | 18:A:824:CLA:OBD  | 2.46                     | 0.48              |
| 14:2:219:LEU:HD22 | 18:2:610:CLA:HMA1 | 1.94                     | 0.48              |
| 1:A:462:LEU:HG    | 18:B:809:CLA:HMC3 | 1.96                     | 0.47              |
| 25:2:606:CHL:HBB2 | 27:2:620:XAT:H181 | 1.92                     | 0.47              |
| 2:B:84:VAL:HG23   | 8:H:140:LYS:HG2   | 1.96                     | 0.47              |
| 8:H:62:THR:O      | 8:H:62:THR:OG1    | 2.29                     | 0.47              |
| 16:3:150:ARG:NH2  | 16:3:244:ALA:O    | 2.47                     | 0.47              |
| 1:A:444:PHE:HE2   | 18:A:839:CLA:HAB  | 1.78                     | 0.47              |
| 1:A:537:HIS:HB3   | 18:A:838:CLA:HAB  | 1.95                     | 0.47              |
| 18:A:808:CLA:HBB1 | 18:A:808:CLA:HMB1 | 1.97                     | 0.47              |
| 18:A:819:CLA:H3A  | 18:A:819:CLA:HBA2 | 1.50                     | 0.47              |
| 18:A:833:CLA:H3A  | 18:A:833:CLA:HBA2 | 1.55                     | 0.47              |
| 2:B:671:TRP:O     | 2:B:675:ILE:HG12  | 2.13                     | 0.47              |
| 18:B:815:CLA:H112 | 18:B:815:CLA:H91  | 1.68                     | 0.47              |
| 6:F:204:ILE:HG13  | 6:F:205:ILE:HG12  | 1.95                     | 0.47              |
| 14:2:181:ASP:OD2  | 14:2:187:ASN:ND2  | 2.47                     | 0.47              |
| 16:3:235:LYS:HB3  | 16:3:237:LEU:HD11 | 1.96                     | 0.47              |
| 2:B:15:ASP:OD1    | 2:B:17:THR:OG1    | 2.26                     | 0.47              |
| 6:F:227:GLY:O     | 6:F:231:SER:OG    | 2.24                     | 0.47              |
| 1:A:197:HIS:CD2   | 18:A:814:CLA:HMC2 | 2.49                     | 0.47              |
| 18:A:826:CLA:H141 | 18:A:826:CLA:H162 | 1.72                     | 0.47              |
| 18:B:816:CLA:CHD  | 18:B:817:CLA:HBB2 | 2.44                     | 0.47              |
| 7:G:61:THR:O      | 7:G:65:ILE:HG23   | 2.14                     | 0.47              |
| 17:5:72:ARG:NH1   | 17:5:86:ASP:O     | 2.38                     | 0.47              |
| 17:5:236:ARG:O    | 17:5:240:VAL:HG22 | 2.14                     | 0.47              |
| 2:B:364:ASP:OD2   | 2:B:367:THR:OG1   | 2.22                     | 0.47              |
| 18:B:807:CLA:H2   | 18:B:807:CLA:H62  | 1.73                     | 0.47              |
| 10:J:10:THR:HG22  | 10:J:12:PRO:HD2   | 1.97                     | 0.47              |
| 15:6:134:ASN:OD1  | 15:6:134:ASN:N    | 2.36                     | 0.47              |
| 25:6:601:CHL:HMA2 | 17:5:174:THR:HG21 | 1.97                     | 0.47              |
| 1:A:646:ARG:HA    | 1:A:650:TRP:HB3   | 1.96                     | 0.47              |
| 1:A:680:PHE:HZ    | 18:A:842:CLA:HBC2 | 1.78                     | 0.47              |
| 2:B:182:LEU:HD13  | 18:B:813:CLA:HHB  | 1.96                     | 0.47              |
| 18:B:839:CLA:HBB2 | 19:B:842:PQN:H141 | 1.97                     | 0.47              |
| 3:C:24:ASP:OD2    | 4:D:174:HIS:ND1   | 2.42                     | 0.47              |
| 15:6:60:TYR:HD2   | 15:6:61:LEU:HD23  | 1.80                     | 0.47              |
| 15:6:60:TYR:CD2   | 15:6:61:LEU:HD23  | 2.49                     | 0.47              |
| 16:3:141:LEU:HD13 | 18:3:602:CLA:H12  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:3:155:GLY:HA2  | 27:3:619:XAT:H181 | 1.97                     | 0.47              |
| 16:3:262:GLU:OE1  | 16:3:262:GLU:N    | 2.41                     | 0.47              |
| 1:A:511:ASP:OD1   | 1:A:511:ASP:N     | 2.48                     | 0.47              |
| 18:A:829:CLA:H92  | 18:A:829:CLA:H41  | 1.97                     | 0.47              |
| 6:F:210:LEU:O     | 6:F:214:ILE:HG13  | 2.15                     | 0.47              |
| 10:J:32:PHE:HE2   | 18:J:101:CLA:HMA3 | 1.79                     | 0.47              |
| 18:A:829:CLA:H162 | 18:A:829:CLA:H202 | 1.70                     | 0.47              |
| 18:A:829:CLA:H191 | 21:J:102:BCR:H19C | 1.96                     | 0.47              |
| 2:B:2:ALA:HA      | 2:B:7:LYS:HA      | 1.97                     | 0.47              |
| 4:D:145:LEU:HD23  | 4:D:145:LEU:HA    | 1.78                     | 0.47              |
| 13:M:3:SER:O      | 13:M:3:SER:OG     | 2.25                     | 0.47              |
| 14:2:184:PHE:O    | 14:2:186:ASN:N    | 2.42                     | 0.47              |
| 25:6:607:CHL:C1B  | 27:6:619:XAT:H172 | 2.45                     | 0.47              |
| 1:A:294:HIS:HE1   | 18:A:820:CLA:C1B  | 2.27                     | 0.47              |
| 18:A:814:CLA:HAA2 | 18:A:826:CLA:H52  | 1.96                     | 0.47              |
| 2:B:438:VAL:O     | 2:B:442:VAL:HG23  | 2.14                     | 0.47              |
| 18:B:805:CLA:HED1 | 18:B:829:CLA:HBB2 | 1.96                     | 0.47              |
| 12:L:111:GLU:HB2  | 18:L:302:CLA:HED1 | 1.97                     | 0.47              |
| 25:6:607:CHL:CMB  | 27:6:619:XAT:H171 | 2.44                     | 0.47              |
| 18:B:812:CLA:H3A  | 18:B:812:CLA:HBA2 | 1.43                     | 0.46              |
| 18:2:610:CLA:H3A  | 18:2:610:CLA:HBA2 | 1.49                     | 0.46              |
| 2:B:129:LEU:HD22  | 2:B:134:ASP:HB3   | 1.96                     | 0.46              |
| 16:3:183:GLY:H    | 16:3:190:ASN:HA   | 1.81                     | 0.46              |
| 18:A:831:CLA:H92  | 18:A:831:CLA:H61  | 1.75                     | 0.46              |
| 2:B:656:VAL:HG22  | 18:B:840:CLA:HMB3 | 1.97                     | 0.46              |
| 2:B:467:HIS:HD2   | 2:B:509:PHE:CZ    | 2.33                     | 0.46              |
| 19:B:842:PQN:H242 | 21:B:848:BCR:H17C | 1.97                     | 0.46              |
| 8:H:71:ASN:HD22   | 12:L:100:ARG:HG2  | 1.81                     | 0.46              |
| 11:K:107:ASP:OD1  | 11:K:107:ASP:N    | 2.48                     | 0.46              |
| 1:A:10:VAL:O      | 1:A:312:ASN:ND2   | 2.48                     | 0.46              |
| 18:B:828:CLA:H171 | 21:B:844:BCR:H352 | 1.97                     | 0.46              |
| 3:C:29:VAL:HG12   | 3:C:39:ILE:HG22   | 1.96                     | 0.46              |
| 17:5:112:GLN:NE2  | 17:5:205:GLY:H    | 2.13                     | 0.46              |
| 18:B:840:CLA:H2A  | 18:B:840:CLA:O1D  | 2.16                     | 0.46              |
| 8:H:60:ASP:HA     | 8:H:63:THR:HG22   | 1.97                     | 0.46              |
| 14:2:240:GLN:HE22 | 26:2:619:LUT:H24  | 1.81                     | 0.46              |
| 2:B:720:THR:HG23  | 18:B:802:CLA:O1D  | 2.15                     | 0.46              |
| 3:C:33:GLY:O      | 5:E:104:VAL:HA    | 2.16                     | 0.46              |
| 6:F:170:TYR:HB3   | 10:J:39:LEU:HD23  | 1.97                     | 0.46              |
| 18:2:604:CLA:H2A  | 18:2:604:CLA:O2D  | 2.15                     | 0.46              |
| 25:5:608:CHL:HBA2 | 18:5:610:CLA:HMD2 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:27:THR:HG23   | 23:B:850:DGD:HG31 | 1.96                     | 0.46              |
| 18:B:827:CLA:HBB1 | 18:B:827:CLA:HMB1 | 1.97                     | 0.46              |
| 6:F:135:LYS:HB2   | 6:F:135:LYS:HE3   | 1.71                     | 0.46              |
| 17:5:231:GLU:HG3  | 18:5:610:CLA:C1B  | 2.46                     | 0.46              |
| 1:A:275:PHE:CE2   | 18:A:837:CLA:HED1 | 2.51                     | 0.46              |
| 2:B:203:ARG:HG3   | 2:B:250:ALA:HB1   | 1.97                     | 0.46              |
| 15:6:201:LEU:CD2  | 27:6:619:XAT:C15  | 2.94                     | 0.46              |
| 18:A:806:CLA:H101 | 18:A:814:CLA:H43  | 1.97                     | 0.45              |
| 18:A:817:CLA:HMD2 | 16:3:187:PRO:HG3  | 1.98                     | 0.45              |
| 2:B:177:HIS:CG    | 18:B:813:CLA:HMC2 | 2.51                     | 0.45              |
| 2:B:309:THR:O     | 2:B:309:THR:OG1   | 2.34                     | 0.45              |
| 2:B:649:MET:O     | 2:B:652:PHE:HB3   | 2.16                     | 0.45              |
| 25:2:607:CHL:CMB  | 27:2:620:XAT:H161 | 2.38                     | 0.45              |
| 17:5:239:MET:SD   | 18:5:602:CLA:HBB1 | 2.56                     | 0.45              |
| 25:5:607:CHL:CAB  | 27:5:620:XAT:H161 | 2.34                     | 0.45              |
| 2:B:326:ILE:HD12  | 18:B:824:CLA:HMC2 | 1.98                     | 0.45              |
| 4:D:122:PRO:HD3   | 4:D:147:LEU:HD13  | 1.99                     | 0.45              |
| 7:G:85:ARG:NH2    | 7:G:128:ASP:OD2   | 2.49                     | 0.45              |
| 12:L:119:LEU:HD13 | 18:L:304:CLA:HBC2 | 1.99                     | 0.45              |
| 21:2:621:BCR:H24C | 21:2:621:BCR:H371 | 1.76                     | 0.45              |
| 2:B:442:VAL:HG21  | 18:B:833:CLA:HAC2 | 1.98                     | 0.45              |
| 4:D:118:ILE:HG12  | 4:D:128:ILE:HG22  | 1.99                     | 0.45              |
| 14:2:121:ILE:CD1  | 27:2:620:XAT:H172 | 2.17                     | 0.45              |
| 17:5:202:LEU:HG   | 17:5:206:TYR:HB2  | 1.97                     | 0.45              |
| 1:A:335:HIS:HB3   | 1:A:338:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:536:ILE:O     | 1:A:540:THR:HG23  | 2.16                     | 0.45              |
| 2:B:434:LEU:O     | 2:B:438:VAL:HG23  | 2.15                     | 0.45              |
| 18:B:815:CLA:H61  | 18:B:815:CLA:H41  | 1.64                     | 0.45              |
| 11:K:97:THR:OG1   | 11:K:98:GLY:N     | 2.50                     | 0.45              |
| 17:5:84:HIS:ND1   | 17:5:102:GLN:OE1  | 2.49                     | 0.45              |
| 1:A:48:ASN:HA     | 1:A:51:ALA:HB3    | 1.99                     | 0.45              |
| 1:A:147:ALA:HB2   | 1:A:375:PRO:HD2   | 1.99                     | 0.45              |
| 2:B:152:ALA:HB2   | 18:B:811:CLA:HBC2 | 1.99                     | 0.45              |
| 18:B:806:CLA:H2   | 18:B:806:CLA:H62  | 1.64                     | 0.45              |
| 14:2:230:ALA:O    | 14:2:234:VAL:HG12 | 2.17                     | 0.45              |
| 1:A:92:GLY:HA3    | 1:A:145:TRP:CH2   | 2.51                     | 0.45              |
| 18:A:818:CLA:H93  | 11:K:120:VAL:HG12 | 1.99                     | 0.45              |
| 2:B:569:ASP:OD1   | 2:B:574:ASP:HB3   | 2.15                     | 0.45              |
| 18:B:823:CLA:C4A  | 21:B:846:BCR:H16C | 2.47                     | 0.45              |
| 16:3:281:VAL:CG1  | 27:3:619:XAT:C14  | 2.95                     | 0.45              |
| 2:B:415:LYS:HZ1   | 6:F:243:VAL:HG21  | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:B:818:CLA:HBA2 | 18:B:818:CLA:H3A  | 1.43                     | 0.45              |
| 6:F:151:ASP:OD1   | 6:F:151:ASP:N     | 2.50                     | 0.45              |
| 1:A:13:MET:HB2    | 1:A:187:TRP:HB2   | 1.99                     | 0.45              |
| 18:B:825:CLA:HMB2 | 18:B:838:CLA:H3A  | 1.97                     | 0.45              |
| 18:6:603:CLA:HMD2 | 18:6:609:CLA:C1D  | 2.47                     | 0.45              |
| 16:3:105:LYS:HB3  | 16:3:120:GLY:O    | 2.16                     | 0.45              |
| 1:A:646:ARG:HB3   | 2:B:632:ILE:HD12  | 1.99                     | 0.45              |
| 2:B:75:GLU:OE2    | 2:B:132:ASN:ND2   | 2.50                     | 0.45              |
| 2:B:345:THR:HA    | 2:B:348:VAL:HG12  | 1.99                     | 0.45              |
| 27:6:619:XAT:H35  | 27:6:619:XAT:H401 | 1.64                     | 0.45              |
| 26:3:618:LUT:H31  | 26:3:618:LUT:H391 | 1.87                     | 0.45              |
| 27:5:620:XAT:H373 | 27:5:620:XAT:H23  | 1.81                     | 0.45              |
| 1:A:575:GLY:HA2   | 2:B:562:PRO:HD3   | 1.99                     | 0.45              |
| 1:A:735:ILE:HG21  | 18:A:829:CLA:HMC2 | 1.99                     | 0.45              |
| 18:B:809:CLA:H91  | 18:B:840:CLA:H12  | 1.98                     | 0.45              |
| 16:3:147:ILE:HD11 | 18:3:609:CLA:CAD  | 2.47                     | 0.45              |
| 16:3:281:VAL:HG11 | 27:3:619:XAT:C12  | 2.47                     | 0.45              |
| 17:5:112:GLN:O    | 17:5:116:VAL:HG22 | 2.17                     | 0.45              |
| 1:A:25:LYS:HB3    | 18:A:812:CLA:HAA2 | 2.00                     | 0.44              |
| 21:A:856:BCR:H20C | 21:A:856:BCR:H361 | 1.84                     | 0.44              |
| 21:G:205:BCR:H24C | 21:G:205:BCR:H371 | 1.78                     | 0.44              |
| 8:H:55:ASP:OD1    | 8:H:57:GLY:N      | 2.44                     | 0.44              |
| 1:A:147:ALA:HB1   | 18:A:820:CLA:HED1 | 1.98                     | 0.44              |
| 1:A:693:GLN:HE22  | 1:A:715:ARG:HA    | 1.82                     | 0.44              |
| 18:A:826:CLA:H62  | 18:A:826:CLA:H2   | 1.60                     | 0.44              |
| 18:A:835:CLA:O2D  | 18:A:835:CLA:H2A  | 2.17                     | 0.44              |
| 18:A:843:CLA:HMA2 | 2:B:685:THR:HG21  | 1.98                     | 0.44              |
| 7:G:99:VAL:HG22   | 7:G:103:ASP:HB2   | 1.99                     | 0.44              |
| 11:K:74:LEU:HD23  | 11:K:74:LEU:HA    | 1.76                     | 0.44              |
| 1:A:40:PRO:HB3    | 1:A:45:TRP:CE3    | 2.53                     | 0.44              |
| 18:A:827:CLA:HAB  | 21:A:851:BCR:H311 | 1.99                     | 0.44              |
| 18:B:821:CLA:H3A  | 18:B:822:CLA:H42  | 1.99                     | 0.44              |
| 12:L:138:GLU:N    | 12:L:138:GLU:OE1  | 2.50                     | 0.44              |
| 1:A:467:ASP:HB3   | 18:A:835:CLA:HED3 | 2.00                     | 0.44              |
| 2:B:65:LEU:HD12   | 2:B:142:LEU:HD12  | 1.99                     | 0.44              |
| 2:B:158:GLN:O     | 2:B:162:LYS:HG3   | 2.18                     | 0.44              |
| 2:B:348:VAL:HG21  | 18:B:828:CLA:HMD3 | 2.00                     | 0.44              |
| 18:B:813:CLA:H152 | 18:B:828:CLA:HMD2 | 2.00                     | 0.44              |
| 5:E:81:VAL:HG12   | 5:E:83:ARG:H      | 1.82                     | 0.44              |
| 21:F:302:BCR:H20C | 21:F:302:BCR:H361 | 1.84                     | 0.44              |
| 15:6:140:ASN:HB3  | 15:6:143:VAL:HG22 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:5:125:VAL:HG23 | 17:5:242:MET:HG2  | 1.99                     | 0.44              |
| 1:A:156:LEU:O     | 1:A:159:THR:HG22  | 2.18                     | 0.44              |
| 1:A:197:HIS:CE1   | 18:A:821:CLA:HMD2 | 2.52                     | 0.44              |
| 1:A:390:HIS:O     | 1:A:394:ILE:HG12  | 2.18                     | 0.44              |
| 8:H:69:TYR:OH     | 12:L:84:THR:O     | 2.36                     | 0.44              |
| 27:5:620:XAT:H401 | 27:5:620:XAT:H35  | 1.78                     | 0.44              |
| 27:5:620:XAT:H31  | 27:5:620:XAT:H391 | 1.85                     | 0.44              |
| 18:A:833:CLA:HMB1 | 18:A:833:CLA:HBB1 | 1.99                     | 0.44              |
| 2:B:299:HIS:HB3   | 2:B:304:ILE:HD11  | 1.98                     | 0.44              |
| 3:C:12:ILE:HG21   | 5:E:124:ASN:HD21  | 1.83                     | 0.44              |
| 14:2:123:ILE:HB   | 14:2:124:PRO:HD3  | 2.00                     | 0.44              |
| 25:5:607:CHL:HHC  | 25:5:607:CHL:HBB1 | 1.99                     | 0.44              |
| 18:A:809:CLA:H3A  | 18:A:809:CLA:HBA2 | 1.35                     | 0.44              |
| 18:A:820:CLA:H3A  | 18:A:820:CLA:HBA2 | 1.38                     | 0.44              |
| 18:A:824:CLA:O1D  | 18:A:824:CLA:H2A  | 2.18                     | 0.44              |
| 2:B:441:ASP:OD2   | 2:B:615:TYR:HB2   | 2.18                     | 0.44              |
| 16:3:214:ARG:HH21 | 16:3:237:LEU:HD13 | 1.82                     | 0.44              |
| 16:3:281:VAL:HG11 | 27:3:619:XAT:H14  | 1.98                     | 0.44              |
| 1:A:694:GLU:OE1   | 2:B:536:LYS:NZ    | 2.47                     | 0.44              |
| 21:A:848:BCR:H362 | 21:A:849:BCR:H21C | 2.00                     | 0.44              |
| 2:B:519:VAL:HG11  | 2:B:593:TYR:HB2   | 2.00                     | 0.44              |
| 6:F:174:VAL:O     | 6:F:178:ILE:HG13  | 2.18                     | 0.44              |
| 25:3:608:CHL:HHC  | 25:3:608:CHL:HBB1 | 1.99                     | 0.44              |
| 17:5:147:GLU:HA   | 17:5:150:ALA:HB3  | 2.00                     | 0.44              |
| 17:5:202:LEU:HD12 | 17:5:228:ARG:NH2  | 2.33                     | 0.44              |
| 1:A:44:THR:HG23   | 1:A:715:ARG:HB2   | 1.99                     | 0.43              |
| 18:A:801:CLA:H162 | 18:A:801:CLA:H122 | 1.73                     | 0.43              |
| 18:A:831:CLA:H62  | 18:A:831:CLA:H41  | 1.82                     | 0.43              |
| 2:B:48:ALA:HB3    | 13:M:30:LEU:HD21  | 2.00                     | 0.43              |
| 9:I:26:LEU:O      | 9:I:30:ILE:HG12   | 2.18                     | 0.43              |
| 15:6:107:PRO:O    | 15:6:112:TYR:N    | 2.50                     | 0.43              |
| 1:A:346:TRP:HB3   | 18:A:806:CLA:HAC1 | 2.00                     | 0.43              |
| 21:A:852:BCR:H20C | 21:A:852:BCR:H361 | 1.73                     | 0.43              |
| 21:A:856:BCR:H11C | 21:A:856:BCR:H341 | 1.91                     | 0.43              |
| 18:B:809:CLA:H121 | 18:B:809:CLA:H161 | 1.77                     | 0.43              |
| 25:6:601:CHL:HMC  | 20:6:620:LHG:HC41 | 2.00                     | 0.43              |
| 16:3:201:PHE:O    | 16:3:205:MET:HG2  | 2.17                     | 0.43              |
| 18:A:827:CLA:HAA2 | 18:A:828:CLA:OBD  | 2.18                     | 0.43              |
| 18:A:841:CLA:HED3 | 18:A:841:CLA:H2A  | 2.00                     | 0.43              |
| 21:A:848:BCR:H20C | 21:A:848:BCR:H361 | 1.77                     | 0.43              |
| 11:K:82:SER:OG    | 11:K:83:THR:N     | 2.50                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:2:619:LUT:H15  | 26:2:619:LUT:H201 | 1.67                     | 0.43              |
| 16:3:214:ARG:NH1  | 16:3:225:MET:SD   | 2.91                     | 0.43              |
| 1:A:294:HIS:HB2   | 18:A:819:CLA:C1B  | 2.48                     | 0.43              |
| 2:B:357:PRO:HG3   | 18:B:818:CLA:HBA1 | 2.00                     | 0.43              |
| 18:B:827:CLA:H3A  | 18:B:827:CLA:HBA2 | 1.43                     | 0.43              |
| 18:K:204:CLA:HMC2 | 21:K:207:BCR:HC8  | 2.00                     | 0.43              |
| 12:L:145:ALA:O    | 12:L:149:THR:HG22 | 2.17                     | 0.43              |
| 16:3:231:LEU:HD23 | 21:3:620:BCR:HC8  | 2.00                     | 0.43              |
| 1:A:550:LYS:HD3   | 2:B:670:TYR:CE1   | 2.54                     | 0.43              |
| 21:G:205:BCR:H20C | 21:G:205:BCR:H361 | 1.82                     | 0.43              |
| 12:L:70:LEU:HD11  | 12:L:78:GLY:N     | 2.33                     | 0.43              |
| 15:6:238:VAL:HG11 | 18:6:613:CLA:HMD1 | 2.00                     | 0.43              |
| 16:3:305:ASP:O    | 16:3:309:ASN:HB2  | 2.19                     | 0.43              |
| 1:A:147:ALA:O     | 1:A:218:SER:OG    | 2.37                     | 0.43              |
| 18:B:826:CLA:H112 | 18:B:826:CLA:H71  | 1.73                     | 0.43              |
| 15:6:165:PRO:HA   | 15:6:168:ARG:HB3  | 2.01                     | 0.43              |
| 1:A:572:PRO:HB3   | 1:A:719:ILE:HB    | 1.99                     | 0.43              |
| 18:A:832:CLA:HAB  | 18:A:840:CLA:HBB2 | 2.01                     | 0.43              |
| 2:B:516:ASP:OD2   | 2:B:593:TYR:OH    | 2.28                     | 0.43              |
| 3:C:23:THR:HB     | 3:C:25:VAL:HG23   | 2.00                     | 0.43              |
| 8:H:93:THR:O      | 12:L:193:ALA:HB1  | 2.19                     | 0.43              |
| 13:M:7:SER:O      | 13:M:11:VAL:HG23  | 2.19                     | 0.43              |
| 17:5:91:GLY:HA3   | 17:5:232:ILE:HD11 | 2.01                     | 0.43              |
| 17:5:219:ASN:OD1  | 17:5:219:ASN:N    | 2.47                     | 0.43              |
| 1:A:411:VAL:HG11  | 1:A:569:PHE:HB2   | 2.00                     | 0.43              |
| 18:B:835:CLA:HBA2 | 18:B:835:CLA:H3A  | 1.67                     | 0.43              |
| 5:E:108:VAL:O     | 5:E:124:ASN:HA    | 2.18                     | 0.43              |
| 18:G:204:CLA:H3A  | 18:G:204:CLA:HBA1 | 1.76                     | 0.43              |
| 16:3:306:PRO:HB2  | 18:3:614:CLA:HMA3 | 2.00                     | 0.43              |
| 2:B:404:LYS:HA    | 2:B:404:LYS:HD2   | 1.81                     | 0.43              |
| 2:B:658:ALA:HB3   | 18:B:803:CLA:HBB2 | 2.01                     | 0.43              |
| 18:B:840:CLA:H2   | 19:B:842:PQN:H252 | 2.00                     | 0.43              |
| 6:F:219:LEU:HD23  | 6:F:220:THR:HG23  | 2.01                     | 0.43              |
| 21:I:101:BCR:H20C | 21:I:101:BCR:H361 | 1.83                     | 0.43              |
| 12:L:156:THR:O    | 12:L:160:ILE:HG13 | 2.18                     | 0.43              |
| 14:2:117:GLY:HA3  | 27:2:620:XAT:H8   | 2.00                     | 0.43              |
| 25:2:601:CHL:HED3 | 16:3:225:MET:HE1  | 2.01                     | 0.43              |
| 21:B:843:BCR:H15C | 21:B:843:BCR:H351 | 1.87                     | 0.43              |
| 6:F:103:GLU:HG3   | 6:F:138:PHE:CG    | 2.54                     | 0.43              |
| 17:5:263:HIS:ND1  | 18:5:613:CLA:HAA2 | 2.34                     | 0.43              |
| 1:A:138:THR:HG21  | 1:A:743:LEU:HD21  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:A:805:CLA:HMA2 | 18:A:812:CLA:HMD2 | 2.01                     | 0.42              |
| 18:A:827:CLA:H51  | 18:A:838:CLA:H2   | 2.00                     | 0.42              |
| 2:B:428:PHE:CZ    | 21:J:103:BCR:HC21 | 2.54                     | 0.42              |
| 18:B:808:CLA:O1A  | 18:B:827:CLA:HBD  | 2.18                     | 0.42              |
| 18:B:823:CLA:HMA1 | 18:B:841:CLA:CGD  | 2.49                     | 0.42              |
| 21:B:848:BCR:H20C | 21:B:848:BCR:H361 | 1.81                     | 0.42              |
| 11:K:114:LEU:HD23 | 11:K:114:LEU:HA   | 1.87                     | 0.42              |
| 15:6:141:LEU:HB3  | 15:6:142:PRO:HD3  | 2.01                     | 0.42              |
| 16:3:272:LYS:HB3  | 18:3:611:CLA:O1D  | 2.19                     | 0.42              |
| 1:A:645:LEU:HD22  | 2:B:651:LEU:HD21  | 2.00                     | 0.42              |
| 18:A:812:CLA:H62  | 18:A:812:CLA:H92  | 1.86                     | 0.42              |
| 2:B:345:THR:HG23  | 2:B:379:ALA:HB2   | 2.00                     | 0.42              |
| 2:B:358:TYR:OH    | 18:B:828:CLA:OBD  | 2.24                     | 0.42              |
| 16:3:183:GLY:HA3  | 18:3:606:CLA:HBC1 | 2.01                     | 0.42              |
| 17:5:154:ASP:OD1  | 17:5:154:ASP:N    | 2.51                     | 0.42              |
| 1:A:65:GLU:N      | 1:A:65:GLU:OE1    | 2.53                     | 0.42              |
| 1:A:707:LYS:HE2   | 6:F:236:GLU:HG2   | 2.01                     | 0.42              |
| 2:B:194:LEU:HA    | 2:B:198:ALA:HB3   | 2.00                     | 0.42              |
| 18:2:602:CLA:H3A  | 18:2:602:CLA:HBA2 | 1.46                     | 0.42              |
| 17:5:177:TRP:O    | 17:5:181:VAL:HG12 | 2.19                     | 0.42              |
| 2:B:294:ASN:ND2   | 18:B:812:CLA:HMA2 | 2.34                     | 0.42              |
| 12:L:70:LEU:HA    | 12:L:80:GLU:HG3   | 2.02                     | 0.42              |
| 12:L:125:VAL:HG22 | 12:L:140:GLY:HA3  | 2.02                     | 0.42              |
| 27:2:620:XAT:H15  | 27:2:620:XAT:H201 | 1.83                     | 0.42              |
| 25:5:607:CHL:CAB  | 27:5:620:XAT:H163 | 2.38                     | 0.42              |
| 18:A:814:CLA:H111 | 18:A:814:CLA:H91  | 1.80                     | 0.42              |
| 18:A:814:CLA:H61  | 18:A:814:CLA:H101 | 1.76                     | 0.42              |
| 18:B:831:CLA:C1B  | 21:F:302:BCR:H11C | 2.50                     | 0.42              |
| 7:G:152:ASN:N     | 7:G:153:PRO:HD3   | 2.35                     | 0.42              |
| 8:H:69:TYR:CZ     | 12:L:93:LEU:HD13  | 2.54                     | 0.42              |
| 15:6:121:TRP:HB2  | 15:6:127:GLY:HA3  | 2.01                     | 0.42              |
| 17:5:214:PRO:HD2  | 26:5:619:LUT:H23  | 2.00                     | 0.42              |
| 1:A:504:SER:OG    | 1:A:506:THR:OG1   | 2.32                     | 0.42              |
| 18:A:854:CLA:H11  | 2:B:616:LEU:HD23  | 2.02                     | 0.42              |
| 2:B:160:LYS:HB2   | 2:B:160:LYS:HE3   | 1.80                     | 0.42              |
| 7:G:61:THR:HA     | 7:G:64:THR:HG22   | 2.02                     | 0.42              |
| 9:I:3:ALA:O       | 9:I:4:SER:OG      | 2.33                     | 0.42              |
| 12:L:128:GLY:H    | 12:L:131:ARG:HB3  | 1.84                     | 0.42              |
| 14:2:117:GLY:CA   | 27:2:620:XAT:H8   | 2.50                     | 0.42              |
| 15:6:99:LEU:HD23  | 15:6:99:LEU:HA    | 1.91                     | 0.42              |
| 16:3:278:MET:HG2  | 27:3:619:XAT:C15  | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:3:619:XAT:H15  | 27:3:619:XAT:H201 | 1.77                     | 0.42              |
| 18:5:602:CLA:HBB2 | 27:5:620:XAT:H34  | 2.01                     | 0.42              |
| 14:2:140:VAL:HG12 | 25:2:607:CHL:HED2 | 2.00                     | 0.42              |
| 25:6:607:CHL:HBB1 | 25:6:607:CHL:CHC  | 2.50                     | 0.42              |
| 17:5:265:SER:OG   | 17:5:266:ASP:OD1  | 2.34                     | 0.42              |
| 1:A:139:SER:OG    | 18:A:809:CLA:OBD  | 2.38                     | 0.42              |
| 1:A:513:VAL:HG23  | 1:A:520:ALA:HB3   | 2.02                     | 0.42              |
| 2:B:228:GLY:HA3   | 7:G:144:LEU:HD13  | 2.01                     | 0.42              |
| 5:E:107:PRO:HD2   | 5:E:127:PRO:HD3   | 2.01                     | 0.42              |
| 12:L:95:ASN:HB3   | 18:L:302:CLA:HAC1 | 2.01                     | 0.42              |
| 15:6:141:LEU:HA   | 15:6:144:ILE:HG22 | 2.02                     | 0.42              |
| 15:6:144:ILE:HA   | 15:6:144:ILE:HD12 | 1.82                     | 0.42              |
| 26:6:617:LUT:H15  | 26:6:617:LUT:H201 | 1.83                     | 0.42              |
| 18:A:854:CLA:H142 | 18:A:854:CLA:H112 | 1.81                     | 0.42              |
| 2:B:98:GLN:O      | 2:B:102:GLU:HG2   | 2.19                     | 0.42              |
| 2:B:466:ALA:HA    | 2:B:476:VAL:O     | 2.20                     | 0.42              |
| 2:B:548:PRO:HD2   | 3:C:62:PHE:CE1    | 2.54                     | 0.42              |
| 11:K:117:VAL:HG22 | 21:K:207:BCR:H313 | 2.01                     | 0.42              |
| 16:3:272:LYS:HB3  | 18:3:611:CLA:CGD  | 2.49                     | 0.42              |
| 17:5:90:ALA:HA    | 17:5:229:TRP:CD1  | 2.55                     | 0.42              |
| 1:A:262:PHE:HA    | 18:K:204:CLA:HBC3 | 2.02                     | 0.42              |
| 18:A:805:CLA:HAA1 | 18:A:812:CLA:H2   | 2.02                     | 0.42              |
| 7:G:144:LEU:HD23  | 7:G:144:LEU:HA    | 1.88                     | 0.42              |
| 15:6:115:TRP:O    | 15:6:119:GLN:NE2  | 2.53                     | 0.42              |
| 16:3:151:PHE:CE1  | 18:3:609:CLA:HBC3 | 2.55                     | 0.42              |
| 21:3:620:BCR:H371 | 21:3:620:BCR:H24C | 1.81                     | 0.42              |
| 17:5:263:HIS:HA   | 17:5:270:ASN:CG   | 2.40                     | 0.42              |
| 27:5:620:XAT:H30  | 27:5:620:XAT:H27  | 1.70                     | 0.42              |
| 21:5:621:BCR:H24C | 21:5:621:BCR:H371 | 1.84                     | 0.42              |
| 18:A:830:CLA:H161 | 18:A:830:CLA:H192 | 1.81                     | 0.41              |
| 2:B:31:PHE:O      | 2:B:37:MET:HG3    | 2.20                     | 0.41              |
| 2:B:172:GLU:HG3   | 7:G:94:PRO:HB3    | 2.02                     | 0.41              |
| 2:B:429:LEU:HB3   | 2:B:525:LEU:HB2   | 2.02                     | 0.41              |
| 18:2:604:CLA:HMB2 | 21:2:621:BCR:H392 | 2.02                     | 0.41              |
| 16:3:307:VAL:HG13 | 16:3:308:HIS:CD2  | 2.55                     | 0.41              |
| 18:3:609:CLA:HMB2 | 18:3:617:CLA:C4B  | 2.50                     | 0.41              |
| 21:5:621:BCR:H15C | 21:5:621:BCR:H351 | 1.93                     | 0.41              |
| 1:A:538:ALA:HB2   | 18:A:839:CLA:HMA1 | 2.01                     | 0.41              |
| 18:A:826:CLA:H192 | 18:A:826:CLA:H161 | 1.89                     | 0.41              |
| 2:B:616:LEU:HD12  | 2:B:616:LEU:HA    | 1.80                     | 0.41              |
| 2:B:733:PHE:CE2   | 8:H:136:PRO:HD2   | 2.52                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:176:LEU:HD23  | 6:F:176:LEU:HA    | 1.90                     | 0.41              |
| 6:F:221:TRP:CG    | 6:F:222:PRO:HD3   | 2.55                     | 0.41              |
| 7:G:113:THR:HA    | 7:G:116:LEU:HB2   | 2.02                     | 0.41              |
| 15:6:227:LEU:HD13 | 15:6:227:LEU:HA   | 1.89                     | 0.41              |
| 21:3:622:BCR:H361 | 21:3:622:BCR:H20C | 1.82                     | 0.41              |
| 17:5:107:LEU:O    | 17:5:111:VAL:HG23 | 2.19                     | 0.41              |
| 1:A:435:ILE:HG13  | 1:A:554:PHE:HE1   | 1.85                     | 0.41              |
| 18:A:829:CLA:H72  | 18:A:829:CLA:H111 | 1.60                     | 0.41              |
| 2:B:523:ILE:HG12  | 2:B:590:VAL:HG22  | 2.03                     | 0.41              |
| 18:B:813:CLA:H62  | 18:B:818:CLA:HBC3 | 2.02                     | 0.41              |
| 18:B:831:CLA:C1C  | 21:F:302:BCR:H15C | 2.51                     | 0.41              |
| 10:J:39:LEU:HD13  | 21:J:103:BCR:H20C | 2.01                     | 0.41              |
| 14:2:198:GLY:N    | 18:2:610:CLA:OBD  | 2.52                     | 0.41              |
| 27:2:620:XAT:H35  | 27:2:620:XAT:H401 | 1.85                     | 0.41              |
| 1:A:78:LEU:HD23   | 1:A:78:LEU:HA     | 1.91                     | 0.41              |
| 1:A:373:PRO:HG3   | 18:A:820:CLA:HBA1 | 2.02                     | 0.41              |
| 18:A:803:CLA:OBD  | 18:B:802:CLA:HMB3 | 2.19                     | 0.41              |
| 3:C:34:CYS:SG     | 3:C:35:LYS:N      | 2.90                     | 0.41              |
| 21:3:622:BCR:H403 | 21:3:622:BCR:H371 | 2.01                     | 0.41              |
| 17:5:75:TRP:CE2   | 17:5:76:LEU:HD22  | 2.55                     | 0.41              |
| 17:5:125:VAL:HG13 | 17:5:129:LEU:CD2  | 2.46                     | 0.41              |
| 17:5:129:LEU:HD13 | 17:5:129:LEU:HA   | 1.79                     | 0.41              |
| 1:A:138:THR:O     | 1:A:138:THR:OG1   | 2.38                     | 0.41              |
| 18:B:813:CLA:H102 | 18:B:813:CLA:H61  | 1.79                     | 0.41              |
| 6:F:158:VAL:O     | 6:F:158:VAL:HG23  | 2.21                     | 0.41              |
| 15:6:153:ALA:O    | 15:6:157:SER:OG   | 2.29                     | 0.41              |
| 16:3:148:ASN:ND2  | 18:3:609:CLA:HMD1 | 2.35                     | 0.41              |
| 17:5:263:HIS:HA   | 17:5:270:ASN:OD1  | 2.21                     | 0.41              |
| 1:A:591:PHE:CE1   | 1:A:727:VAL:HB    | 2.55                     | 0.41              |
| 18:A:827:CLA:HBB1 | 18:A:827:CLA:HMB1 | 2.03                     | 0.41              |
| 18:A:834:CLA:C3B  | 18:A:835:CLA:HMB2 | 2.51                     | 0.41              |
| 21:A:849:BCR:H11C | 21:A:849:BCR:H341 | 1.95                     | 0.41              |
| 2:B:373:THR:HG23  | 2:B:591:THR:HG21  | 2.03                     | 0.41              |
| 2:B:694:LYS:HE2   | 2:B:694:LYS:HB2   | 1.72                     | 0.41              |
| 3:C:6:LYS:HE3     | 4:D:215:TYR:HD1   | 1.85                     | 0.41              |
| 5:E:131:GLU:OE2   | 5:E:133:ALA:N     | 2.53                     | 0.41              |
| 21:F:302:BCR:H24C | 21:F:302:BCR:H371 | 1.88                     | 0.41              |
| 11:K:54:SER:HA    | 11:K:57:LEU:HB2   | 2.03                     | 0.41              |
| 16:3:143:TYR:O    | 16:3:147:ILE:HG23 | 2.21                     | 0.41              |
| 16:3:260:GLU:N    | 16:3:260:GLU:OE2  | 2.53                     | 0.41              |
| 17:5:115:LEU:HD23 | 17:5:115:LEU:HA   | 1.92                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:498:ASN:HB2   | 18:A:837:CLA:HED2 | 2.01                     | 0.41              |
| 1:A:530:ASP:HA    | 1:A:533:VAL:HG12  | 2.02                     | 0.41              |
| 1:A:582:CYS:HB3   | 2:B:667:TRP:HE3   | 1.86                     | 0.41              |
| 1:A:693:GLN:NE2   | 1:A:716:ALA:H     | 2.19                     | 0.41              |
| 21:A:850:BCR:H15C | 21:A:850:BCR:H351 | 1.89                     | 0.41              |
| 7:G:103:ASP:N     | 7:G:103:ASP:OD1   | 2.54                     | 0.41              |
| 16:3:106:GLN:OE1  | 16:3:106:GLN:N    | 2.48                     | 0.41              |
| 1:A:32:PHE:HZ     | 1:A:49:LEU:HD12   | 1.86                     | 0.41              |
| 1:A:77:GLN:NE2    | 1:A:81:ILE:HG13   | 2.36                     | 0.41              |
| 1:A:474:ILE:H     | 1:A:474:ILE:HG13  | 1.58                     | 0.41              |
| 1:A:537:HIS:CE1   | 1:A:603:VAL:HG12  | 2.55                     | 0.41              |
| 18:A:811:CLA:H2A  | 18:A:811:CLA:HED3 | 2.02                     | 0.41              |
| 18:A:812:CLA:H152 | 18:A:812:CLA:H18  | 1.69                     | 0.41              |
| 19:B:842:PQN:C29  | 23:B:850:DGD:HAE2 | 2.51                     | 0.41              |
| 12:L:116:HIS:HA   | 12:L:119:LEU:HD23 | 2.03                     | 0.41              |
| 21:2:621:BCR:H20C | 21:2:621:BCR:H361 | 1.91                     | 0.41              |
| 17:5:178:MET:HE3  | 17:5:182:LYS:HB2  | 2.03                     | 0.41              |
| 1:A:46:ILE:O      | 1:A:50:HIS:ND1    | 2.45                     | 0.41              |
| 1:A:393:TRP:CD1   | 18:A:829:CLA:HAB  | 2.55                     | 0.41              |
| 18:A:835:CLA:H161 | 18:A:835:CLA:H141 | 1.83                     | 0.41              |
| 21:A:856:BCR:H371 | 21:A:856:BCR:H24C | 1.82                     | 0.41              |
| 2:B:268:LEU:HD12  | 2:B:357:PRO:HA    | 2.02                     | 0.41              |
| 2:B:429:LEU:HD11  | 18:B:837:CLA:HMB3 | 2.02                     | 0.41              |
| 2:B:510:LEU:HD12  | 2:B:510:LEU:H     | 1.86                     | 0.41              |
| 21:G:205:BCR:H11C | 21:G:205:BCR:H341 | 1.94                     | 0.41              |
| 16:3:170:LEU:HG   | 16:3:171:ILE:HD13 | 2.03                     | 0.41              |
| 16:3:302:HIS:CD2  | 18:3:613:CLA:HAA2 | 2.56                     | 0.41              |
| 1:A:296:LEU:O     | 1:A:300:VAL:HG12  | 2.21                     | 0.41              |
| 18:A:821:CLA:HBB1 | 21:K:202:BCR:H14C | 2.03                     | 0.41              |
| 18:A:843:CLA:HMD2 | 21:B:848:BCR:H393 | 2.03                     | 0.41              |
| 7:G:96:GLN:HG2    | 7:G:101:HIS:ND1   | 2.36                     | 0.41              |
| 7:G:121:PRO:HG2   | 18:G:204:CLA:HBC2 | 2.02                     | 0.41              |
| 10:J:26:LEU:HD13  | 10:J:26:LEU:HA    | 1.92                     | 0.41              |
| 12:L:204:LEU:HD13 | 12:L:204:LEU:HA   | 1.90                     | 0.41              |
| 18:2:613:CLA:HHB  | 18:2:614:CLA:HBC3 | 2.02                     | 0.41              |
| 15:6:204:PHE:CZ   | 27:6:619:XAT:H10  | 2.56                     | 0.41              |
| 1:A:47:TRP:HE1    | 18:F:301:CLA:CBB  | 2.34                     | 0.40              |
| 1:A:455:HIS:CD2   | 1:A:459:MET:HG2   | 2.56                     | 0.40              |
| 18:A:829:CLA:HBB1 | 18:A:829:CLA:HMB1 | 2.02                     | 0.40              |
| 20:A:847:LHG:H242 | 20:A:847:LHG:H112 | 2.03                     | 0.40              |
| 2:B:574:ASP:N     | 2:B:574:ASP:OD1   | 2.54                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:121:SER:HB2   | 6:F:123:PRO:HD2   | 2.03                     | 0.40              |
| 25:2:606:CHL:HBA1 | 25:2:606:CHL:H3A  | 1.69                     | 0.40              |
| 25:5:608:CHL:HBB1 | 25:5:608:CHL:CHC  | 2.49                     | 0.40              |
| 1:A:426:ARG:O     | 1:A:430:HIS:ND1   | 2.53                     | 0.40              |
| 2:B:216:LEU:HD13  | 2:B:218:HIS:O     | 2.21                     | 0.40              |
| 14:2:156:ILE:HG12 | 18:5:614:CLA:HAA2 | 2.02                     | 0.40              |
| 17:5:230:LYS:HA   | 18:5:611:CLA:HED3 | 2.02                     | 0.40              |
| 18:A:802:CLA:HBA2 | 2:B:427:LEU:HD23  | 2.03                     | 0.40              |
| 18:A:854:CLA:H41  | 18:A:854:CLA:H62  | 1.64                     | 0.40              |
| 2:B:524:ALA:HB2   | 18:B:837:CLA:HMA1 | 2.02                     | 0.40              |
| 21:B:801:BCR:H11C | 21:B:801:BCR:H341 | 1.99                     | 0.40              |
| 18:B:809:CLA:H92  | 18:B:809:CLA:H62  | 1.94                     | 0.40              |
| 14:2:263:THR:HG21 | 16:3:199:THR:HB   | 2.03                     | 0.40              |
| 17:5:247:VAL:HG12 | 18:5:613:CLA:HMD3 | 2.03                     | 0.40              |
| 18:5:601:CLA:HBB1 | 20:5:622:LHG:H262 | 2.03                     | 0.40              |
| 21:A:852:BCR:H15C | 21:A:852:BCR:H351 | 1.89                     | 0.40              |
| 15:6:114:ASN:O    | 15:6:115:TRP:CD1  | 2.75                     | 0.40              |
| 27:6:619:XAT:H15  | 27:6:619:XAT:H201 | 1.93                     | 0.40              |
| 21:3:622:BCR:H15C | 21:3:622:BCR:H351 | 1.95                     | 0.40              |
| 18:A:820:CLA:O1A  | 18:A:830:CLA:HMD1 | 2.22                     | 0.40              |
| 18:A:839:CLA:H11  | 18:A:839:CLA:H51  | 1.92                     | 0.40              |
| 18:2:614:CLA:HAA2 | 16:3:203:LEU:HB2  | 2.03                     | 0.40              |
| 15:6:104:VAL:HG23 | 15:6:115:TRP:CB   | 2.52                     | 0.40              |
| 20:5:622:LHG:H281 | 20:5:622:LHG:H102 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 740/742 (100%) | 700 (95%) | 40 (5%) | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | B     | 731/733 (100%)  | 696 (95%)  | 35 (5%)  | 0        | 100         | 100 |
| 3   | C     | 78/80 (98%)     | 68 (87%)   | 10 (13%) | 0        | 100         | 100 |
| 4   | D     | 139/141 (99%)   | 133 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 5   | E     | 60/62 (97%)     | 56 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 6   | F     | 157/159 (99%)   | 149 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 7   | G     | 96/98 (98%)     | 90 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 8   | H     | 88/90 (98%)     | 84 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 9   | I     | 32/34 (94%)     | 29 (91%)   | 3 (9%)   | 0        | 100         | 100 |
| 10  | J     | 39/41 (95%)     | 39 (100%)  | 0        | 0        | 100         | 100 |
| 11  | K     | 77/79 (98%)     | 66 (86%)   | 11 (14%) | 0        | 100         | 100 |
| 12  | L     | 157/159 (99%)   | 146 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 13  | M     | 27/29 (93%)     | 27 (100%)  | 0        | 0        | 100         | 100 |
| 14  | 2     | 204/210 (97%)   | 192 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 15  | 6     | 190/192 (99%)   | 170 (90%)  | 20 (10%) | 0        | 100         | 100 |
| 16  | 3     | 211/213 (99%)   | 195 (92%)  | 16 (8%)  | 0        | 100         | 100 |
| 17  | 5     | 200/205 (98%)   | 173 (86%)  | 27 (14%) | 0        | 100         | 100 |
| All | All   | 3226/3267 (99%) | 3013 (93%) | 213 (7%) | 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     | 603/603 (100%) | 580 (96%) | 23 (4%)  | 28          | 58 |
| 2   | B     | 595/595 (100%) | 580 (98%) | 15 (2%)  | 42          | 68 |
| 3   | C     | 67/67 (100%)   | 63 (94%)  | 4 (6%)   | 16          | 45 |
| 4   | D     | 115/115 (100%) | 111 (96%) | 4 (4%)   | 31          | 60 |
| 5   | E     | 52/52 (100%)   | 49 (94%)  | 3 (6%)   | 17          | 46 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 6   | F     | 128/129 (99%)    | 123 (96%)  | 5 (4%)   | 27          | 57  |
| 7   | G     | 78/78 (100%)     | 68 (87%)   | 10 (13%) | 3           | 16  |
| 8   | H     | 72/73 (99%)      | 66 (92%)   | 6 (8%)   | 9           | 33  |
| 9   | I     | 30/30 (100%)     | 29 (97%)   | 1 (3%)   | 33          | 61  |
| 10  | J     | 35/35 (100%)     | 35 (100%)  | 0        | 100         | 100 |
| 11  | K     | 56/57 (98%)      | 46 (82%)   | 10 (18%) | 1           | 6   |
| 12  | L     | 121/122 (99%)    | 114 (94%)  | 7 (6%)   | 17          | 46  |
| 13  | M     | 24/24 (100%)     | 23 (96%)   | 1 (4%)   | 25          | 55  |
| 14  | 2     | 164/167 (98%)    | 153 (93%)  | 11 (7%)  | 13          | 41  |
| 15  | 6     | 148/148 (100%)   | 140 (95%)  | 8 (5%)   | 18          | 49  |
| 16  | 3     | 166/166 (100%)   | 158 (95%)  | 8 (5%)   | 21          | 52  |
| 17  | 5     | 162/164 (99%)    | 152 (94%)  | 10 (6%)  | 15          | 44  |
| All | All   | 2616/2625 (100%) | 2490 (95%) | 126 (5%) | 24          | 52  |

All (126) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | THR  |
| 1   | A     | 25  | LYS  |
| 1   | A     | 34  | ARG  |
| 1   | A     | 35  | THR  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 71  | PHE  |
| 1   | A     | 86  | SER  |
| 1   | A     | 96  | SER  |
| 1   | A     | 141 | PHE  |
| 1   | A     | 266 | TRP  |
| 1   | A     | 275 | PHE  |
| 1   | A     | 276 | ARG  |
| 1   | A     | 312 | ASN  |
| 1   | A     | 423 | LEU  |
| 1   | A     | 432 | ASP  |
| 1   | A     | 459 | MET  |
| 1   | A     | 470 | SER  |
| 1   | A     | 503 | THR  |
| 1   | A     | 519 | VAL  |
| 1   | A     | 522 | LEU  |
| 1   | A     | 530 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 638 | SER  |
| 1   | A     | 732 | LEU  |
| 2   | B     | 47  | PHE  |
| 2   | B     | 85  | ARG  |
| 2   | B     | 106 | ARG  |
| 2   | B     | 203 | ARG  |
| 2   | B     | 205 | GLU  |
| 2   | B     | 216 | LEU  |
| 2   | B     | 257 | PHE  |
| 2   | B     | 315 | LEU  |
| 2   | B     | 394 | PHE  |
| 2   | B     | 465 | SER  |
| 2   | B     | 576 | PHE  |
| 2   | B     | 577 | TYR  |
| 2   | B     | 677 | THR  |
| 2   | B     | 701 | SER  |
| 2   | B     | 703 | VAL  |
| 3   | C     | 23  | THR  |
| 3   | C     | 44  | ARG  |
| 3   | C     | 54  | CYS  |
| 3   | C     | 58  | CYS  |
| 4   | D     | 82  | ASN  |
| 4   | D     | 85  | THR  |
| 4   | D     | 145 | LEU  |
| 4   | D     | 177 | ASP  |
| 5   | E     | 91  | ASP  |
| 5   | E     | 113 | ASP  |
| 5   | E     | 126 | SER  |
| 6   | F     | 99  | PHE  |
| 6   | F     | 174 | VAL  |
| 6   | F     | 219 | LEU  |
| 6   | F     | 240 | ASN  |
| 6   | F     | 243 | VAL  |
| 7   | G     | 61  | THR  |
| 7   | G     | 63  | LEU  |
| 7   | G     | 65  | ILE  |
| 7   | G     | 72  | LEU  |
| 7   | G     | 73  | LEU  |
| 7   | G     | 96  | GLN  |
| 7   | G     | 102 | PHE  |
| 7   | G     | 106 | ASP  |
| 7   | G     | 117 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 125 | THR  |
| 8   | H     | 62  | THR  |
| 8   | H     | 66  | TRP  |
| 8   | H     | 85  | PHE  |
| 8   | H     | 99  | LEU  |
| 8   | H     | 122 | LEU  |
| 8   | H     | 131 | VAL  |
| 9   | I     | 33  | ASP  |
| 11  | K     | 54  | SER  |
| 11  | K     | 56  | ASN  |
| 11  | K     | 57  | LEU  |
| 11  | K     | 63  | THR  |
| 11  | K     | 77  | SER  |
| 11  | K     | 88  | LEU  |
| 11  | K     | 95  | LEU  |
| 11  | K     | 103 | PHE  |
| 11  | K     | 108 | THR  |
| 11  | K     | 114 | LEU  |
| 12  | L     | 70  | LEU  |
| 12  | L     | 71  | ASN  |
| 12  | L     | 127 | THR  |
| 12  | L     | 151 | LEU  |
| 12  | L     | 174 | LEU  |
| 12  | L     | 179 | ARG  |
| 12  | L     | 219 | LEU  |
| 13  | M     | 3   | SER  |
| 14  | 2     | 63  | ASN  |
| 14  | 2     | 82  | LEU  |
| 14  | 2     | 110 | HIS  |
| 14  | 2     | 129 | LYS  |
| 14  | 2     | 139 | ASN  |
| 14  | 2     | 149 | ASP  |
| 14  | 2     | 161 | PHE  |
| 14  | 2     | 193 | ASP  |
| 14  | 2     | 194 | VAL  |
| 14  | 2     | 201 | TRP  |
| 14  | 2     | 222 | LYS  |
| 15  | 6     | 61  | LEU  |
| 15  | 6     | 79  | VAL  |
| 15  | 6     | 81  | GLU  |
| 15  | 6     | 115 | TRP  |
| 15  | 6     | 134 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 6     | 148 | GLU  |
| 15  | 6     | 232 | HIS  |
| 15  | 6     | 240 | ILE  |
| 16  | 3     | 135 | PHE  |
| 16  | 3     | 137 | ASP  |
| 16  | 3     | 147 | ILE  |
| 16  | 3     | 175 | THR  |
| 16  | 3     | 200 | LEU  |
| 16  | 3     | 252 | ASN  |
| 16  | 3     | 253 | PHE  |
| 16  | 3     | 256 | PHE  |
| 17  | 5     | 129 | LEU  |
| 17  | 5     | 140 | THR  |
| 17  | 5     | 168 | LEU  |
| 17  | 5     | 172 | VAL  |
| 17  | 5     | 190 | ASP  |
| 17  | 5     | 220 | ASP  |
| 17  | 5     | 248 | GLN  |
| 17  | 5     | 254 | THR  |
| 17  | 5     | 266 | ASP  |
| 17  | 5     | 270 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 179 | HIS  |
| 1   | A     | 197 | HIS  |
| 1   | A     | 222 | ASN  |
| 1   | A     | 294 | HIS  |
| 1   | A     | 421 | ASN  |
| 1   | A     | 437 | HIS  |
| 1   | A     | 613 | GLN  |
| 1   | A     | 693 | GLN  |
| 2   | B     | 132 | ASN  |
| 2   | B     | 218 | HIS  |
| 2   | B     | 294 | ASN  |
| 2   | B     | 308 | HIS  |
| 2   | B     | 363 | GLN  |
| 2   | B     | 374 | HIS  |
| 2   | B     | 432 | HIS  |
| 2   | B     | 467 | HIS  |
| 2   | B     | 528 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 682 | HIS  |
| 3   | C     | 3   | HIS  |
| 4   | D     | 185 | ASN  |
| 5   | E     | 90  | ASN  |
| 5   | E     | 124 | ASN  |
| 6   | F     | 105 | GLN  |
| 7   | G     | 148 | ASN  |
| 7   | G     | 152 | ASN  |
| 8   | H     | 65  | ASN  |
| 8   | H     | 81  | GLN  |
| 8   | H     | 126 | ASN  |
| 8   | H     | 130 | GLN  |
| 10  | J     | 2   | GLN  |
| 12  | L     | 95  | ASN  |
| 14  | 2     | 110 | HIS  |
| 14  | 2     | 186 | ASN  |
| 14  | 2     | 187 | ASN  |
| 14  | 2     | 251 | ASN  |
| 14  | 2     | 261 | HIS  |
| 15  | 6     | 82  | ASN  |
| 15  | 6     | 226 | HIS  |
| 16  | 3     | 148 | ASN  |
| 16  | 3     | 297 | GLN  |
| 16  | 3     | 298 | ASN  |
| 16  | 3     | 308 | HIS  |
| 16  | 3     | 309 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

205 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 18  | CLA  | B     | 840 | -    | 65,73,73     | 1.48 | 6 (9%)      | 76,113,113  | 1.40 | 6 (7%)      |
| 18  | CLA  | B     | 832 | -    | 45,53,73     | 1.76 | 6 (13%)     | 52,89,113   | 1.62 | 9 (17%)     |
| 18  | CLA  | B     | 837 | -    | 46,54,73     | 1.75 | 7 (15%)     | 53,90,113   | 1.57 | 8 (15%)     |
| 18  | CLA  | G     | 204 | 7    | 43,52,73     | 1.83 | 6 (13%)     | 49,88,113   | 1.56 | 7 (14%)     |
| 18  | CLA  | B     | 825 | -    | 65,73,73     | 1.46 | 7 (10%)     | 76,113,113  | 1.39 | 8 (10%)     |
| 18  | CLA  | A     | 823 | 1    | 44,52,73     | 1.78 | 6 (13%)     | 51,88,113   | 1.66 | 6 (11%)     |
| 18  | CLA  | 6     | 603 | -    | 55,63,73     | 1.61 | 6 (10%)     | 64,101,113  | 1.49 | 8 (12%)     |
| 27  | XAT  | 5     | 620 | -    | 39,47,47     | 1.03 | 3 (7%)      | 54,74,74    | 2.76 | 21 (38%)    |
| 18  | CLA  | 5     | 611 | -    | 38,45,73     | 2.93 | 9 (23%)     | 41,76,113   | 1.45 | 8 (19%)     |
| 18  | CLA  | B     | 810 | -    | 46,54,73     | 1.74 | 6 (13%)     | 53,90,113   | 1.53 | 6 (11%)     |
| 19  | PQN  | A     | 844 | -    | 34,34,34     | 0.39 | 0           | 42,45,45    | 0.47 | 0           |
| 18  | CLA  | A     | 804 | -    | 65,73,73     | 1.46 | 7 (10%)     | 76,113,113  | 1.43 | 9 (11%)     |
| 18  | CLA  | A     | 819 | -    | 45,53,73     | 1.77 | 7 (15%)     | 52,89,113   | 1.62 | 7 (13%)     |
| 18  | CLA  | 2     | 612 | -    | 41,49,73     | 1.87 | 6 (14%)     | 47,84,113   | 1.62 | 7 (14%)     |
| 18  | CLA  | 6     | 602 | -    | 45,53,73     | 1.76 | 6 (13%)     | 52,89,113   | 1.62 | 7 (13%)     |
| 18  | CLA  | 6     | 613 | 15   | 45,53,73     | 1.79 | 6 (13%)     | 52,89,113   | 1.56 | 7 (13%)     |
| 18  | CLA  | A     | 820 | -    | 45,53,73     | 1.78 | 6 (13%)     | 52,89,113   | 1.60 | 7 (13%)     |
| 18  | CLA  | 3     | 602 | 16   | 60,68,73     | 1.54 | 5 (8%)      | 70,107,113  | 1.42 | 8 (11%)     |
| 25  | CHL  | 5     | 606 | -    | 41,49,74     | 2.24 | 13 (31%)    | 48,84,114   | 2.95 | 19 (39%)    |
| 21  | BCR  | B     | 846 | -    | 41,41,41     | 1.16 | 2 (4%)      | 56,56,56    | 1.23 | 6 (10%)     |
| 21  | BCR  | I     | 101 | -    | 41,41,41     | 1.13 | 2 (4%)      | 56,56,56    | 1.19 | 4 (7%)      |
| 18  | CLA  | B     | 819 | -    | 45,53,73     | 1.78 | 6 (13%)     | 52,89,113   | 1.61 | 8 (15%)     |
| 24  | LMG  | J     | 104 | -    | 30,30,55     | 0.94 | 0           | 38,38,63    | 1.27 | 5 (13%)     |
| 18  | CLA  | B     | 803 | -    | 65,73,73     | 1.47 | 7 (10%)     | 76,113,113  | 1.42 | 7 (9%)      |
| 20  | LHG  | A     | 847 | 18   | 26,26,48     | 0.83 | 1 (3%)      | 29,32,54    | 1.35 | 3 (10%)     |
| 18  | CLA  | A     | 839 | -    | 65,73,73     | 1.45 | 5 (7%)      | 76,113,113  | 1.41 | 8 (10%)     |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | LMG  | 2     | 618 | -    | 13,13,55     | 1.07 | 0        | 18,18,63    | 1.54 | 4 (22%)  |
| 18  | CLA  | B     | 802 | -    | 53,61,73     | 1.63 | 7 (13%)  | 61,98,113   | 1.42 | 8 (13%)  |
| 21  | BCR  | B     | 843 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 18  | CLA  | A     | 830 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.40 | 6 (7%)   |
| 18  | CLA  | A     | 831 | -    | 65,73,73     | 1.49 | 6 (9%)   | 76,113,113  | 1.44 | 7 (9%)   |
| 18  | CLA  | A     | 845 | 20   | 52,60,73     | 1.66 | 5 (9%)   | 60,97,113   | 1.52 | 8 (13%)  |
| 18  | CLA  | B     | 806 | 2    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.39 | 8 (10%)  |
| 18  | CLA  | A     | 801 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.33 | 7 (9%)   |
| 18  | CLA  | B     | 820 | -    | 43,51,73     | 1.77 | 6 (13%)  | 49,86,113   | 1.64 | 6 (12%)  |
| 18  | CLA  | B     | 827 | -    | 45,53,73     | 1.76 | 7 (15%)  | 52,89,113   | 1.61 | 8 (15%)  |
| 18  | CLA  | 2     | 609 | 14   | 55,63,73     | 1.60 | 6 (10%)  | 64,101,113  | 1.47 | 8 (12%)  |
| 18  | CLA  | 3     | 614 | -    | 39,48,73     | 1.89 | 6 (15%)  | 44,83,113   | 1.62 | 7 (15%)  |
| 25  | CHL  | 6     | 607 | 15   | 40,49,74     | 2.53 | 16 (40%) | 41,84,114   | 2.84 | 19 (46%) |
| 18  | CLA  | 3     | 615 | -    | 37,44,73     | 1.95 | 6 (16%)  | 42,77,113   | 1.59 | 6 (14%)  |
| 18  | CLA  | A     | 828 | -    | 46,54,73     | 1.73 | 7 (15%)  | 53,90,113   | 1.53 | 6 (11%)  |
| 18  | CLA  | 3     | 609 | -    | 45,53,73     | 1.75 | 6 (13%)  | 52,89,113   | 1.61 | 6 (11%)  |
| 18  | CLA  | 5     | 602 | -    | 45,53,73     | 1.82 | 6 (13%)  | 52,89,113   | 1.52 | 8 (15%)  |
| 18  | CLA  | 5     | 610 | -    | 55,63,73     | 1.61 | 6 (10%)  | 64,101,113  | 1.45 | 8 (12%)  |
| 27  | XAT  | 2     | 620 | -    | 39,47,47     | 1.01 | 2 (5%)   | 54,74,74    | 3.14 | 22 (40%) |
| 18  | CLA  | B     | 826 | -    | 65,73,73     | 1.46 | 7 (10%)  | 76,113,113  | 1.41 | 8 (10%)  |
| 18  | CLA  | 6     | 610 | 15   | 42,51,73     | 1.83 | 6 (14%)  | 48,87,113   | 1.61 | 7 (14%)  |
| 18  | CLA  | 5     | 613 | 17   | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.63 | 7 (13%)  |
| 18  | CLA  | A     | 826 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.43 | 7 (9%)   |
| 21  | BCR  | K     | 207 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.32 | 6 (10%)  |
| 18  | CLA  | B     | 814 | -    | 43,52,73     | 1.81 | 6 (13%)  | 49,88,113   | 1.61 | 7 (14%)  |
| 18  | CLA  | A     | 825 | -    | 55,63,73     | 1.62 | 6 (10%)  | 64,101,113  | 1.42 | 8 (12%)  |
| 18  | CLA  | A     | 821 | -    | 44,52,73     | 1.81 | 6 (13%)  | 51,88,113   | 1.58 | 7 (13%)  |
| 20  | LHG  | 5     | 622 | -    | 36,36,48     | 0.72 | 1 (2%)   | 39,42,54    | 1.25 | 4 (10%)  |
| 18  | CLA  | A     | 805 | -    | 55,63,73     | 1.56 | 7 (12%)  | 64,101,113  | 1.56 | 8 (12%)  |
| 21  | BCR  | A     | 851 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.26 | 9 (16%)  |
| 21  | BCR  | A     | 848 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.28 | 4 (7%)   |
| 18  | CLA  | A     | 824 | -    | 51,59,73     | 1.68 | 6 (11%)  | 59,96,113   | 1.52 | 6 (10%)  |
| 18  | CLA  | A     | 836 | -    | 50,58,73     | 1.69 | 6 (12%)  | 58,95,113   | 1.54 | 7 (12%)  |
| 18  | CLA  | 3     | 613 | -    | 53,62,73     | 1.66 | 6 (11%)  | 61,100,113  | 1.46 | 8 (13%)  |
| 18  | CLA  | J     | 101 | -    | 42,50,73     | 1.83 | 6 (14%)  | 48,85,113   | 1.57 | 6 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | CLA  | B     | 821 | -    | 46,54,73     | 1.75 | 5 (10%)  | 53,90,113   | 1.54 | 7 (13%)  |
| 18  | CLA  | A     | 854 | -    | 65,73,73     | 1.46 | 6 (9%)   | 76,113,113  | 1.38 | 9 (11%)  |
| 18  | CLA  | 5     | 614 | -    | 43,51,73     | 1.81 | 6 (13%)  | 49,86,113   | 1.59 | 7 (14%)  |
| 18  | CLA  | 2     | 613 | 14   | 45,53,73     | 1.79 | 5 (11%)  | 52,89,113   | 1.55 | 7 (13%)  |
| 18  | CLA  | A     | 811 | -    | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.62 | 7 (13%)  |
| 22  | SF4  | C     | 101 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 18  | CLA  | B     | 811 | -    | 54,62,73     | 1.68 | 7 (12%)  | 67,100,113  | 1.48 | 9 (13%)  |
| 21  | BCR  | A     | 850 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.20 | 6 (10%)  |
| 18  | CLA  | A     | 835 | -    | 65,73,73     | 1.48 | 7 (10%)  | 76,113,113  | 1.42 | 9 (11%)  |
| 18  | CLA  | 2     | 610 | 14   | 45,53,73     | 1.72 | 7 (15%)  | 52,89,113   | 1.59 | 6 (11%)  |
| 25  | CHL  | 5     | 607 | -    | 43,51,74     | 2.44 | 15 (34%) | 45,86,114   | 2.84 | 20 (44%) |
| 18  | CLA  | B     | 807 | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.41 | 9 (11%)  |
| 18  | CLA  | L     | 304 | -    | 42,50,73     | 1.80 | 6 (14%)  | 48,85,113   | 1.67 | 7 (14%)  |
| 18  | CLA  | 5     | 601 | 17   | 45,53,73     | 1.79 | 5 (11%)  | 52,89,113   | 1.56 | 7 (13%)  |
| 18  | CLA  | B     | 830 | -    | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.62 | 7 (13%)  |
| 18  | CLA  | A     | 842 | -    | 43,52,73     | 1.81 | 6 (13%)  | 49,88,113   | 1.56 | 7 (14%)  |
| 18  | CLA  | 3     | 607 | 16   | 39,48,73     | 1.93 | 7 (17%)  | 48,83,113   | 1.67 | 9 (18%)  |
| 18  | CLA  | B     | 815 | -    | 60,68,73     | 1.55 | 7 (11%)  | 70,107,113  | 1.39 | 7 (10%)  |
| 18  | CLA  | 2     | 611 | 20   | 41,50,73     | 1.85 | 6 (14%)  | 49,85,113   | 1.60 | 6 (12%)  |
| 18  | CLA  | A     | 827 | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.38 | 8 (10%)  |
| 21  | BCR  | 3     | 622 | -    | 41,41,41     | 1.11 | 2 (4%)   | 56,56,56    | 1.28 | 6 (10%)  |
| 18  | CLA  | 2     | 614 | -    | 42,50,73     | 1.82 | 6 (14%)  | 48,85,113   | 1.59 | 7 (14%)  |
| 22  | SF4  | A     | 853 | 1,2  | 0,12,12      | -    | -        | -           |      |          |
| 25  | CHL  | 2     | 608 | -    | 40,49,74     | 2.43 | 16 (40%) | 41,84,114   | 2.87 | 18 (43%) |
| 19  | PQN  | B     | 842 | -    | 34,34,34     | 0.40 | 0        | 42,45,45    | 0.45 | 0        |
| 18  | CLA  | A     | 816 | -    | 42,50,73     | 1.78 | 6 (14%)  | 48,85,113   | 1.69 | 7 (14%)  |
| 18  | CLA  | 3     | 606 | -    | 40,49,73     | 1.87 | 6 (15%)  | 45,84,113   | 1.61 | 6 (13%)  |
| 18  | CLA  | F     | 305 | -    | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.57 | 6 (11%)  |
| 18  | CLA  | B     | 836 | -    | 60,68,73     | 1.52 | 6 (10%)  | 70,107,113  | 1.44 | 7 (10%)  |
| 18  | CLA  | B     | 829 | -    | 45,53,73     | 1.81 | 6 (13%)  | 52,89,113   | 1.64 | 7 (13%)  |
| 18  | CLA  | 3     | 611 | -    | 39,48,73     | 1.90 | 6 (15%)  | 44,83,113   | 1.68 | 8 (18%)  |
| 18  | CLA  | 5     | 603 | -    | 43,52,73     | 1.82 | 6 (13%)  | 49,88,113   | 1.57 | 6 (12%)  |
| 18  | CLA  | A     | 843 | -    | 65,73,73     | 1.50 | 7 (10%)  | 76,113,113  | 1.37 | 9 (11%)  |
| 25  | CHL  | 6     | 601 | 15   | 44,53,74     | 2.38 | 16 (36%) | 46,89,114   | 2.73 | 17 (36%) |
| 18  | CLA  | A     | 802 | -    | 45,53,73     | 1.75 | 6 (13%)  | 52,89,113   | 1.63 | 6 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 21  | BCR  | B     | 845 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 21  | BCR  | B     | 801 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.17 | 4 (7%)   |
| 18  | CLA  | A     | 832 | -    | 41,49,73     | 1.81 | 6 (14%)  | 47,84,113   | 1.71 | 9 (19%)  |
| 18  | CLA  | B     | 841 | 20   | 65,73,73     | 1.49 | 6 (9%)   | 76,113,113  | 1.35 | 9 (11%)  |
| 18  | CLA  | A     | 818 | -    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.43 | 8 (10%)  |
| 18  | CLA  | K     | 201 | 11   | 46,54,73     | 1.84 | 7 (15%)  | 53,90,113   | 1.46 | 4 (7%)   |
| 21  | BCR  | 2     | 621 | -    | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 25  | CHL  | 3     | 608 | -    | 39,48,74     | 2.42 | 15 (38%) | 44,83,114   | 2.74 | 19 (43%) |
| 20  | LHG  | B     | 851 | 18   | 22,22,48     | 0.83 | 0        | 25,28,54    | 1.20 | 1 (4%)   |
| 18  | CLA  | 2     | 602 | -    | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.59 | 7 (13%)  |
| 26  | LUT  | 5     | 619 | -    | 42,43,43     | 7.28 | 26 (61%) | 51,60,60    | 3.85 | 19 (37%) |
| 18  | CLA  | A     | 806 | -    | 65,73,73     | 1.47 | 7 (10%)  | 76,113,113  | 1.40 | 7 (9%)   |
| 18  | CLA  | 3     | 612 | -    | 43,51,73     | 1.83 | 5 (11%)  | 49,86,113   | 1.56 | 6 (12%)  |
| 18  | CLA  | B     | 833 | -    | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.65 | 9 (17%)  |
| 18  | CLA  | A     | 837 | 1    | 45,53,73     | 1.79 | 5 (11%)  | 52,89,113   | 1.59 | 9 (17%)  |
| 18  | CLA  | B     | 805 | -    | 65,73,73     | 1.49 | 6 (9%)   | 76,113,113  | 1.38 | 8 (10%)  |
| 18  | CLA  | B     | 818 | -    | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.55 | 7 (13%)  |
| 21  | BCR  | J     | 103 | 2    | 41,41,41     | 1.15 | 3 (7%)   | 56,56,56    | 1.30 | 7 (12%)  |
| 20  | LHG  | A     | 846 | -    | 48,48,48     | 0.64 | 1 (2%)   | 51,54,54    | 1.27 | 6 (11%)  |
| 18  | CLA  | G     | 203 | -    | 50,58,73     | 1.70 | 6 (12%)  | 58,95,113   | 1.51 | 8 (13%)  |
| 18  | CLA  | A     | 815 | -    | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.57 | 8 (15%)  |
| 18  | CLA  | B     | 823 | -    | 45,53,73     | 1.76 | 7 (15%)  | 52,89,113   | 1.61 | 6 (11%)  |
| 25  | CHL  | 2     | 601 | 14   | 45,53,74     | 2.33 | 15 (33%) | 52,89,114   | 2.80 | 21 (40%) |
| 18  | CLA  | 5     | 604 | -    | 43,51,73     | 1.78 | 5 (11%)  | 48,86,113   | 1.66 | 7 (14%)  |
| 18  | CLA  | A     | 814 | -    | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.43 | 8 (10%)  |
| 18  | CLA  | A     | 838 | -    | 51,59,73     | 1.68 | 5 (9%)   | 59,96,113   | 1.48 | 8 (13%)  |
| 21  | BCR  | B     | 848 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 18  | CLA  | B     | 838 | -    | 47,55,73     | 1.72 | 6 (12%)  | 54,91,113   | 1.57 | 8 (14%)  |
| 18  | CLA  | A     | 813 | -    | 54,62,73     | 1.60 | 6 (11%)  | 62,99,113   | 1.48 | 6 (9%)   |
| 18  | CLA  | B     | 839 | -    | 40,49,73     | 1.86 | 6 (15%)  | 45,84,113   | 1.61 | 6 (13%)  |
| 26  | LUT  | 3     | 618 | 16   | 42,43,43     | 7.26 | 24 (57%) | 51,60,60    | 3.85 | 22 (43%) |
| 18  | CLA  | B     | 828 | -    | 65,73,73     | 1.49 | 7 (10%)  | 76,113,113  | 1.31 | 8 (10%)  |
| 18  | CLA  | L     | 303 | -    | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.58 | 7 (13%)  |
| 18  | CLA  | B     | 809 | -    | 65,73,73     | 1.47 | 6 (9%)   | 76,113,113  | 1.37 | 8 (10%)  |
| 21  | BCR  | K     | 202 | -    | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.28 | 6 (10%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CHL  | 2     | 616 | -     | 46,54,74     | 2.34 | 15 (32%) | 49,90,114   | 2.78 | 18 (36%) |
| 21  | BCR  | L     | 301 | -     | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 18  | CLA  | 5     | 612 | -     | 44,52,73     | 1.82 | 6 (13%)  | 51,88,113   | 1.59 | 7 (13%)  |
| 18  | CLA  | A     | 803 | -     | 65,73,73     | 1.49 | 6 (9%)   | 76,113,113  | 1.36 | 7 (9%)   |
| 18  | CLA  | A     | 833 | -     | 45,53,73     | 1.78 | 5 (11%)  | 52,89,113   | 1.63 | 7 (13%)  |
| 18  | CLA  | 6     | 611 | 20    | 37,46,73     | 2.01 | 7 (18%)  | 46,81,113   | 1.70 | 9 (19%)  |
| 21  | BCR  | F     | 302 | -     | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.21 | 6 (10%)  |
| 18  | CLA  | A     | 829 | -     | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.42 | 9 (11%)  |
| 18  | CLA  | K     | 206 | 11    | 45,53,73     | 1.80 | 6 (13%)  | 52,89,113   | 1.54 | 7 (13%)  |
| 21  | BCR  | B     | 847 | -     | 41,41,41     | 1.14 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 21  | BCR  | 3     | 620 | -     | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.25 | 6 (10%)  |
| 21  | BCR  | A     | 856 | -     | 41,41,41     | 1.15 | 2 (4%)   | 56,56,56    | 1.33 | 7 (12%)  |
| 18  | CLA  | 3     | 610 | -     | 41,49,73     | 1.82 | 7 (17%)  | 47,84,113   | 1.67 | 8 (17%)  |
| 18  | CLA  | B     | 831 | -     | 49,57,73     | 1.69 | 6 (12%)  | 55,93,113   | 1.53 | 6 (10%)  |
| 18  | CLA  | F     | 303 | -     | 45,53,73     | 1.78 | 5 (11%)  | 52,89,113   | 1.55 | 8 (15%)  |
| 22  | SF4  | C     | 102 | 3     | 0,12,12      | -    | -        | -           | -    | -        |
| 18  | CLA  | B     | 834 | -     | 45,53,73     | 1.80 | 6 (13%)  | 52,89,113   | 1.57 | 7 (13%)  |
| 25  | CHL  | 2     | 607 | -     | 43,51,74     | 2.37 | 15 (34%) | 45,86,114   | 2.85 | 20 (44%) |
| 18  | CLA  | A     | 808 | -     | 45,53,73     | 1.76 | 6 (13%)  | 52,89,113   | 1.63 | 8 (15%)  |
| 18  | CLA  | 6     | 606 | -     | 39,48,73     | 1.87 | 6 (15%)  | 45,82,113   | 1.75 | 9 (20%)  |
| 25  | CHL  | 5     | 608 | -     | 51,59,74     | 2.16 | 16 (31%) | 55,96,114   | 2.69 | 20 (36%) |
| 18  | CLA  | 6     | 612 | -     | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.57 | 7 (13%)  |
| 18  | CLA  | B     | 816 | -     | 53,62,73     | 1.64 | 6 (11%)  | 61,100,113  | 1.42 | 6 (9%)   |
| 18  | CLA  | 6     | 604 | -     | 49,57,73     | 1.70 | 6 (12%)  | 55,93,113   | 1.53 | 8 (14%)  |
| 20  | LHG  | 2     | 622 | 14,18 | 34,34,48     | 0.72 | 0        | 37,40,54    | 1.27 | 4 (10%)  |
| 18  | CLA  | B     | 822 | -     | 55,63,73     | 1.60 | 6 (10%)  | 64,101,113  | 1.49 | 8 (12%)  |
| 25  | CHL  | 2     | 606 | 14    | 46,54,74     | 2.28 | 15 (32%) | 49,90,114   | 2.87 | 18 (36%) |
| 18  | CLA  | A     | 840 | -     | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.55 | 6 (11%)  |
| 18  | CLA  | A     | 834 | -     | 65,73,73     | 1.49 | 6 (9%)   | 76,113,113  | 1.35 | 7 (9%)   |
| 21  | BCR  | J     | 102 | -     | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.27 | 6 (10%)  |
| 18  | CLA  | 5     | 609 | 17    | 43,51,73     | 1.79 | 6 (13%)  | 48,86,113   | 1.64 | 6 (12%)  |
| 18  | CLA  | K     | 203 | -     | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.57 | 7 (13%)  |
| 18  | CLA  | A     | 841 | -     | 65,73,73     | 1.48 | 7 (10%)  | 76,113,113  | 1.38 | 9 (11%)  |
| 18  | CLA  | 6     | 608 | -     | 43,52,73     | 1.83 | 6 (13%)  | 49,88,113   | 1.56 | 6 (12%)  |
| 24  | LMG  | 2     | 617 | -     | 13,13,55     | 1.01 | 0        | 18,18,63    | 1.55 | 4 (22%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CHL  | 5     | 615 | 17    | 43,51,74     | 2.31 | 15 (34%) | 45,86,114   | 2.89 | 20 (44%) |
| 18  | CLA  | K     | 204 | -     | 44,52,73     | 1.84 | 6 (13%)  | 55,88,113   | 1.65 | 8 (14%)  |
| 18  | CLA  | A     | 817 | -     | 39,48,73     | 1.86 | 6 (15%)  | 44,83,113   | 1.68 | 8 (18%)  |
| 18  | CLA  | F     | 304 | -     | 41,49,73     | 1.83 | 6 (14%)  | 47,84,113   | 1.67 | 7 (14%)  |
| 18  | CLA  | B     | 824 | -     | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.59 | 8 (15%)  |
| 18  | CLA  | 2     | 603 | -     | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.57 | 6 (11%)  |
| 18  | CLA  | A     | 809 | 1     | 45,53,73     | 1.73 | 6 (13%)  | 52,89,113   | 1.65 | 8 (15%)  |
| 21  | BCR  | G     | 205 | -     | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.23 | 6 (10%)  |
| 21  | BCR  | A     | 849 | -     | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.21 | 6 (10%)  |
| 18  | CLA  | A     | 822 | -     | 43,51,73     | 1.87 | 7 (16%)  | 54,87,113   | 1.65 | 8 (14%)  |
| 18  | CLA  | 6     | 609 | -     | 40,48,73     | 1.91 | 7 (17%)  | 50,83,113   | 1.70 | 10 (20%) |
| 18  | CLA  | B     | 817 | -     | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.58 | 6 (11%)  |
| 18  | CLA  | 3     | 603 | -     | 55,63,73     | 1.63 | 7 (12%)  | 64,101,113  | 1.43 | 6 (9%)   |
| 18  | CLA  | G     | 201 | -     | 45,53,73     | 1.80 | 5 (11%)  | 52,89,113   | 1.56 | 7 (13%)  |
| 18  | CLA  | A     | 807 | 1     | 43,52,73     | 1.80 | 6 (13%)  | 49,88,113   | 1.57 | 6 (12%)  |
| 18  | CLA  | 3     | 617 | -     | 39,48,73     | 1.88 | 6 (15%)  | 44,83,113   | 1.69 | 8 (18%)  |
| 27  | XAT  | 3     | 619 | -     | 39,47,47     | 0.98 | 2 (5%)   | 54,74,74    | 2.74 | 20 (37%) |
| 18  | CLA  | B     | 813 | -     | 65,73,73     | 1.45 | 7 (10%)  | 76,113,113  | 1.47 | 10 (13%) |
| 18  | CLA  | 6     | 614 | -     | 37,46,73     | 2.00 | 6 (16%)  | 46,81,113   | 1.69 | 11 (23%) |
| 18  | CLA  | B     | 835 | -     | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.57 | 7 (13%)  |
| 21  | BCR  | L     | 305 | -     | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.28 | 9 (16%)  |
| 27  | XAT  | 6     | 619 | -     | 39,47,47     | 0.98 | 2 (5%)   | 54,74,74    | 3.10 | 21 (38%) |
| 18  | CLA  | 2     | 604 | -     | 50,58,73     | 1.65 | 6 (12%)  | 58,95,113   | 1.64 | 8 (13%)  |
| 18  | CLA  | B     | 804 | -     | 45,53,73     | 1.76 | 6 (13%)  | 52,89,113   | 1.64 | 7 (13%)  |
| 18  | CLA  | B     | 812 | -     | 45,53,73     | 1.77 | 5 (11%)  | 52,89,113   | 1.63 | 7 (13%)  |
| 18  | CLA  | L     | 302 | -     | 45,53,73     | 1.78 | 6 (13%)  | 52,89,113   | 1.61 | 7 (13%)  |
| 21  | BCR  | B     | 844 | -     | 41,41,41     | 1.10 | 2 (4%)   | 56,56,56    | 1.18 | 4 (7%)   |
| 18  | CLA  | A     | 810 | 1     | 45,53,73     | 1.79 | 6 (13%)  | 52,89,113   | 1.59 | 7 (13%)  |
| 18  | CLA  | 3     | 604 | -     | 41,50,73     | 1.92 | 7 (17%)  | 51,86,113   | 1.63 | 9 (17%)  |
| 18  | CLA  | 6     | 616 | 15    | 43,51,73     | 1.91 | 6 (13%)  | 54,87,113   | 1.66 | 8 (14%)  |
| 21  | BCR  | A     | 852 | -     | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.18 | 6 (10%)  |
| 23  | DGD  | B     | 850 | -     | 67,67,67     | 0.86 | 2 (2%)   | 81,81,81    | 1.44 | 11 (13%) |
| 18  | CLA  | B     | 808 | -     | 50,58,73     | 1.67 | 7 (14%)  | 58,95,113   | 1.55 | 9 (15%)  |
| 18  | CLA  | F     | 301 | -     | 45,53,73     | 1.77 | 6 (13%)  | 52,89,113   | 1.56 | 6 (11%)  |
| 20  | LHG  | 6     | 620 | 18,15 | 27,27,48     | 0.80 | 1 (3%)   | 30,33,54    | 1.25 | 2 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 26  | LUT  | 6     | 617 | -    | 42,43,43     | 7.20 | 25 (59%) | 51,60,60    | 3.87 | 19 (37%) |
| 21  | BCR  | 5     | 621 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.24 | 5 (8%)   |
| 26  | LUT  | 2     | 619 | -    | 42,43,43     | 7.18 | 25 (59%) | 51,60,60    | 4.12 | 21 (41%) |
| 18  | CLA  | A     | 812 | -    | 65,73,73     | 1.50 | 6 (9%)   | 76,113,113  | 1.36 | 8 (10%)  |

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   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 18  | CLA  | B     | 840 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 18  | CLA  | B     | 832 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | CLA  | B     | 837 | -    | 1/1/11/20 | 4/15/93/115   | -       |
| 18  | CLA  | G     | 204 | 7    | 1/1/11/20 | 4/11/89/115   | -       |
| 18  | CLA  | B     | 825 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 18  | CLA  | A     | 823 | 1    | 1/1/11/20 | 5/11/89/115   | -       |
| 18  | CLA  | 6     | 603 | -    | 1/1/13/20 | 13/25/103/115 | -       |
| 27  | XAT  | 5     | 620 | -    | -         | 3/31/93/93    | 0/4/4/4 |
| 18  | CLA  | 5     | 611 | -    | 1/1/7/20  | 5/10/70/115   | -       |
| 18  | CLA  | B     | 810 | -    | 1/1/11/20 | 9/15/93/115   | -       |
| 19  | PQN  | A     | 844 | -    | -         | 8/23/43/43    | 0/2/2/2 |
| 18  | CLA  | A     | 804 | -    | 1/1/15/20 | 9/37/115/115  | -       |
| 18  | CLA  | A     | 819 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | CLA  | 2     | 612 | -    | 1/1/10/20 | 0/8/86/115    | -       |
| 18  | CLA  | 6     | 602 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 18  | CLA  | 6     | 613 | 15   | 1/1/11/20 | 7/13/91/115   | -       |
| 18  | CLA  | A     | 820 | -    | 1/1/11/20 | 4/13/91/115   | -       |
| 18  | CLA  | 3     | 602 | 16   | 1/1/14/20 | 9/31/109/115  | -       |
| 25  | CHL  | 5     | 606 | -    | 3/3/15/26 | 2/10/106/137  | -       |
| 21  | BCR  | B     | 846 | -    | -         | 17/29/63/63   | 0/2/2/2 |
| 21  | BCR  | I     | 101 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 18  | CLA  | B     | 819 | -    | 1/1/11/20 | 3/13/91/115   | -       |
| 24  | LMG  | J     | 104 | -    | -         | 12/25/45/70   | 0/1/1/1 |
| 18  | CLA  | B     | 803 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 20  | LHG  | A     | 847 | 18   | -         | 19/31/31/53   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 18  | CLA  | A     | 839 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 24  | LMG  | 2     | 618 | -    | -         | 2/4/24/70     | 0/1/1/1 |
| 18  | CLA  | B     | 802 | -    | 1/1/12/20 | 3/23/101/115  | -       |
| 21  | BCR  | B     | 843 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 830 | -    | 1/1/15/20 | 5/37/115/115  | -       |
| 18  | CLA  | A     | 831 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 18  | CLA  | A     | 845 | 20   | 1/1/12/20 | 10/22/100/115 | -       |
| 18  | CLA  | B     | 806 | 2    | 1/1/15/20 | 19/37/115/115 | -       |
| 18  | CLA  | A     | 801 | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 18  | CLA  | B     | 820 | -    | 1/1/10/20 | 1/11/89/115   | -       |
| 18  | CLA  | B     | 827 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | 2     | 609 | 14   | 1/1/13/20 | 11/25/103/115 | -       |
| 18  | CLA  | 3     | 614 | -    | 1/1/10/20 | 1/6/84/115    | -       |
| 25  | CHL  | 6     | 607 | 15   | 3/3/15/26 | 2/8/106/137   | -       |
| 18  | CLA  | 3     | 615 | -    | 1/1/8/20  | 0/0/74/115    | -       |
| 18  | CLA  | A     | 828 | -    | 1/1/11/20 | 7/15/93/115   | -       |
| 18  | CLA  | 3     | 609 | -    | 1/1/11/20 | 1/13/91/115   | -       |
| 18  | CLA  | 5     | 602 | -    | 1/1/11/20 | 3/13/91/115   | -       |
| 18  | CLA  | 5     | 610 | -    | 1/1/13/20 | 3/25/103/115  | -       |
| 27  | XAT  | 2     | 620 | -    | -         | 3/31/93/93    | 0/4/4/4 |
| 18  | CLA  | B     | 826 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 18  | CLA  | 6     | 610 | 15   | 1/1/11/20 | 1/9/87/115    | -       |
| 18  | CLA  | 5     | 613 | 17   | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | A     | 826 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 21  | BCR  | K     | 207 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 18  | CLA  | B     | 814 | -    | 1/1/11/20 | 1/11/89/115   | -       |
| 18  | CLA  | A     | 825 | -    | 1/1/13/20 | 9/25/103/115  | -       |
| 18  | CLA  | A     | 821 | -    | 1/1/11/20 | 6/11/89/115   | -       |
| 20  | LHG  | 5     | 622 | -    | -         | 19/41/41/53   | -       |
| 18  | CLA  | A     | 805 | -    | 1/1/13/20 | 10/25/103/115 | -       |
| 21  | BCR  | A     | 851 | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 21  | BCR  | A     | 848 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 824 | -    | 1/1/12/20 | 9/21/99/115   | -       |
| 18  | CLA  | A     | 836 | -    | 1/1/12/20 | 0/19/97/115   | -       |
| 18  | CLA  | 3     | 613 | -    | 1/1/13/20 | 7/23/101/115  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 18  | CLA  | J     | 101 | -    | 1/1/10/20 | 5/10/88/115   | -       |
| 18  | CLA  | B     | 821 | -    | 1/1/11/20 | 7/15/93/115   | -       |
| 18  | CLA  | A     | 854 | -    | 1/1/15/20 | 15/37/115/115 | -       |
| 18  | CLA  | 5     | 614 | -    | 1/1/10/20 | 7/11/89/115   | -       |
| 18  | CLA  | 2     | 613 | 14   | 1/1/11/20 | 6/13/91/115   | -       |
| 18  | CLA  | A     | 811 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 22  | SF4  | C     | 101 | 3    | -         | -             | 0/6/5/5 |
| 18  | CLA  | B     | 811 | -    | 1/1/13/20 | 9/25/101/115  | -       |
| 21  | BCR  | A     | 850 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 835 | -    | 1/1/15/20 | 7/37/115/115  | -       |
| 18  | CLA  | 2     | 610 | 14   | 1/1/11/20 | 4/13/91/115   | -       |
| 25  | CHL  | 5     | 607 | -    | 3/3/15/26 | 4/12/110/137  | -       |
| 18  | CLA  | B     | 807 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 18  | CLA  | L     | 304 | -    | 1/1/10/20 | 2/10/88/115   | -       |
| 18  | CLA  | 5     | 601 | 17   | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | CLA  | B     | 830 | -    | 1/1/11/20 | 1/13/91/115   | -       |
| 18  | CLA  | A     | 842 | -    | 1/1/11/20 | 3/11/89/115   | -       |
| 18  | CLA  | 3     | 607 | 16   | 1/1/10/20 | 1/8/84/115    | -       |
| 18  | CLA  | B     | 815 | -    | 1/1/14/20 | 11/31/109/115 | -       |
| 18  | CLA  | 2     | 611 | 20   | 1/1/10/20 | 0/7/85/115    | -       |
| 18  | CLA  | A     | 827 | -    | 1/1/15/20 | 12/37/115/115 | -       |
| 21  | BCR  | 3     | 622 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 18  | CLA  | 2     | 614 | -    | 1/1/10/20 | 2/10/88/115   | -       |
| 22  | SF4  | A     | 853 | 1,2  | -         | -             | 0/6/5/5 |
| 25  | CHL  | 2     | 608 | -    | 3/3/15/26 | 1/8/106/137   | -       |
| 19  | PQN  | B     | 842 | -    | -         | 9/23/43/43    | 0/2/2/2 |
| 18  | CLA  | A     | 816 | -    | 1/1/10/20 | 4/10/88/115   | -       |
| 18  | CLA  | 3     | 606 | -    | 1/1/10/20 | 0/8/86/115    | -       |
| 18  | CLA  | F     | 305 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | B     | 836 | -    | 1/1/14/20 | 7/31/109/115  | -       |
| 18  | CLA  | B     | 829 | -    | 1/1/11/20 | 0/13/91/115   | -       |
| 18  | CLA  | 3     | 611 | -    | 1/1/10/20 | 2/6/84/115    | -       |
| 18  | CLA  | 5     | 603 | -    | 1/1/11/20 | 4/11/89/115   | -       |
| 18  | CLA  | A     | 843 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 25  | CHL  | 6     | 601 | 15   | 3/3/16/26 | 3/13/111/137  | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 18  | CLA  | A     | 802 | -    | 1/1/11/20 | 7/13/91/115   | -       |
| 21  | BCR  | B     | 845 | -    | -         | 19/29/63/63   | 0/2/2/2 |
| 21  | BCR  | B     | 801 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 832 | -    | 1/1/10/20 | 6/8/86/115    | -       |
| 18  | CLA  | B     | 841 | 20   | 1/1/15/20 | 14/37/115/115 | -       |
| 18  | CLA  | A     | 818 | -    | 1/1/15/20 | 18/37/115/115 | -       |
| 18  | CLA  | K     | 201 | 11   | 1/1/11/20 | 7/15/93/115   | -       |
| 25  | CHL  | 3     | 608 | -    | 3/3/15/26 | 2/6/104/137   | -       |
| 21  | BCR  | 2     | 621 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 20  | LHG  | B     | 851 | 18   | -         | 10/26/26/53   | -       |
| 18  | CLA  | 2     | 602 | -    | 1/1/11/20 | 6/13/91/115   | -       |
| 26  | LUT  | 5     | 619 | -    | -         | 8/29/67/67    | 0/2/2/2 |
| 18  | CLA  | A     | 806 | -    | 1/1/15/20 | 14/37/115/115 | -       |
| 18  | CLA  | 3     | 612 | -    | 1/1/10/20 | 2/11/89/115   | -       |
| 18  | CLA  | B     | 833 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 18  | CLA  | A     | 837 | 1    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | CLA  | B     | 805 | -    | 1/1/15/20 | 11/37/115/115 | -       |
| 18  | CLA  | B     | 818 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 21  | BCR  | J     | 103 | 2    | -         | 23/29/63/63   | 0/2/2/2 |
| 20  | LHG  | A     | 846 | -    | -         | 24/53/53/53   | -       |
| 18  | CLA  | G     | 203 | -    | 1/1/12/20 | 7/19/97/115   | -       |
| 18  | CLA  | A     | 815 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | B     | 823 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 25  | CHL  | 2     | 601 | 14   | 3/3/16/26 | 8/15/111/137  | -       |
| 18  | CLA  | 5     | 604 | -    | 1/1/10/20 | 5/9/88/115    | -       |
| 18  | CLA  | A     | 814 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 18  | CLA  | A     | 838 | -    | 1/1/12/20 | 3/21/99/115   | -       |
| 21  | BCR  | B     | 848 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 18  | CLA  | B     | 838 | -    | 1/1/11/20 | 2/16/94/115   | -       |
| 18  | CLA  | A     | 813 | -    | 1/1/12/20 | 3/24/102/115  | -       |
| 18  | CLA  | B     | 839 | -    | 1/1/10/20 | 0/8/86/115    | -       |
| 26  | LUT  | 3     | 618 | 16   | -         | 7/29/67/67    | 0/2/2/2 |
| 18  | CLA  | B     | 828 | -    | 1/1/15/20 | 10/37/115/115 | -       |
| 18  | CLA  | L     | 303 | -    | 1/1/11/20 | 0/13/91/115   | -       |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 18  | CLA  | B     | 809 | -     | 1/1/15/20 | 9/37/115/115  | -       |
| 25  | CHL  | 2     | 616 | -     | 3/3/16/26 | 6/15/113/137  | -       |
| 21  | BCR  | K     | 202 | -     | -         | 8/29/63/63    | 0/2/2/2 |
| 21  | BCR  | L     | 301 | -     | -         | 10/29/63/63   | 0/2/2/2 |
| 18  | CLA  | 5     | 612 | -     | 1/1/11/20 | 5/11/89/115   | -       |
| 18  | CLA  | A     | 803 | -     | 1/1/15/20 | 7/37/115/115  | -       |
| 18  | CLA  | A     | 833 | -     | 1/1/11/20 | 7/13/91/115   | -       |
| 18  | CLA  | 6     | 611 | 20    | 1/1/10/20 | 1/4/80/115    | -       |
| 21  | BCR  | F     | 302 | -     | -         | 14/29/63/63   | 0/2/2/2 |
| 18  | CLA  | A     | 829 | -     | 1/1/15/20 | 20/37/115/115 | -       |
| 18  | CLA  | K     | 206 | 11    | 1/1/11/20 | 5/13/91/115   | -       |
| 21  | BCR  | B     | 847 | -     | -         | 2/29/63/63    | 0/2/2/2 |
| 21  | BCR  | 3     | 620 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 21  | BCR  | A     | 856 | -     | -         | 7/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 3     | 610 | -     | 1/1/10/20 | 3/8/86/115    | -       |
| 18  | CLA  | B     | 831 | -     | 1/1/11/20 | 7/18/96/115   | -       |
| 18  | CLA  | F     | 303 | -     | 1/1/11/20 | 4/13/91/115   | -       |
| 22  | SF4  | C     | 102 | 3     | -         | -             | 0/6/5/5 |
| 18  | CLA  | B     | 834 | -     | 1/1/11/20 | 5/13/91/115   | -       |
| 25  | CHL  | 2     | 607 | -     | 3/3/15/26 | 3/12/110/137  | -       |
| 18  | CLA  | A     | 808 | -     | 1/1/11/20 | 3/13/91/115   | -       |
| 18  | CLA  | 6     | 606 | -     | 1/1/9/20  | 3/8/82/115    | -       |
| 25  | CHL  | 5     | 608 | -     | 3/3/17/26 | 8/21/119/137  | -       |
| 18  | CLA  | 6     | 612 | -     | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | CLA  | B     | 816 | -     | 1/1/13/20 | 3/23/101/115  | -       |
| 18  | CLA  | 6     | 604 | -     | 1/1/11/20 | 8/18/96/115   | -       |
| 20  | LHG  | 2     | 622 | 14,18 | -         | 23/39/39/53   | -       |
| 18  | CLA  | B     | 822 | -     | 1/1/13/20 | 8/25/103/115  | -       |
| 25  | CHL  | 2     | 606 | 14    | 3/3/16/26 | 5/15/113/137  | -       |
| 18  | CLA  | A     | 840 | -     | 1/1/11/20 | 4/13/91/115   | -       |
| 18  | CLA  | A     | 834 | -     | 1/1/15/20 | 12/37/115/115 | -       |
| 21  | BCR  | J     | 102 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 18  | CLA  | 5     | 609 | 17    | 1/1/10/20 | 6/9/87/115    | -       |
| 18  | CLA  | K     | 203 | -     | 1/1/11/20 | 4/13/91/115   | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 18  | CLA  | A     | 841 | -    | 1/1/15/20 | 13/37/115/115 | -       |
| 18  | CLA  | 6     | 608 | -    | 1/1/11/20 | 3/11/89/115   | -       |
| 25  | CHL  | 5     | 615 | 17   | 3/3/15/26 | 3/12/110/137  | -       |
| 24  | LMG  | 2     | 617 | -    | -         | 4/4/24/70     | 0/1/1/1 |
| 18  | CLA  | K     | 204 | -    | 1/1/11/20 | 5/13/89/115   | -       |
| 18  | CLA  | A     | 817 | -    | 1/1/10/20 | 0/6/84/115    | -       |
| 18  | CLA  | F     | 304 | -    | 1/1/10/20 | 2/8/86/115    | -       |
| 18  | CLA  | B     | 824 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | CLA  | 2     | 603 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | A     | 809 | 1    | 1/1/11/20 | 5/13/91/115   | -       |
| 21  | BCR  | G     | 205 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 21  | BCR  | A     | 849 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 822 | -    | 1/1/11/20 | 2/11/87/115   | -       |
| 18  | CLA  | 6     | 609 | -    | 1/1/10/20 | 3/8/84/115    | -       |
| 18  | CLA  | B     | 817 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 18  | CLA  | 3     | 603 | -    | 1/1/13/20 | 6/25/103/115  | -       |
| 18  | CLA  | G     | 201 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | A     | 807 | 1    | 1/1/11/20 | 4/11/89/115   | -       |
| 18  | CLA  | 3     | 617 | -    | 1/1/10/20 | 2/6/84/115    | -       |
| 27  | XAT  | 3     | 619 | -    | -         | 0/31/93/93    | 0/4/4/4 |
| 18  | CLA  | B     | 813 | -    | 1/1/15/20 | 16/37/115/115 | -       |
| 18  | CLA  | 6     | 614 | -    | 1/1/10/20 | 2/4/80/115    | -       |
| 18  | CLA  | B     | 835 | -    | 1/1/11/20 | 8/13/91/115   | -       |
| 21  | BCR  | L     | 305 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 27  | XAT  | 6     | 619 | -    | -         | 1/31/93/93    | 0/4/4/4 |
| 18  | CLA  | 2     | 604 | -    | 1/1/12/20 | 7/19/97/115   | -       |
| 18  | CLA  | B     | 804 | -    | 1/1/11/20 | 5/13/91/115   | -       |
| 18  | CLA  | B     | 812 | -    | 1/1/11/20 | 3/13/91/115   | -       |
| 18  | CLA  | L     | 302 | -    | 1/1/11/20 | 2/13/91/115   | -       |
| 21  | BCR  | B     | 844 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 18  | CLA  | A     | 810 | 1    | 1/1/11/20 | 4/13/91/115   | -       |
| 18  | CLA  | 3     | 604 | -    | 1/1/11/20 | 0/9/85/115    | -       |
| 18  | CLA  | 6     | 616 | 15   | 1/1/11/20 | 4/11/87/115   | -       |
| 21  | BCR  | A     | 852 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 23  | DGD  | B     | 850 | -    | -         | 29/55/95/95   | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link  | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|-------|-----------|---------------|---------|
| 18  | CLA  | B     | 808 | -     | 1/1/12/20 | 2/19/97/115   | -       |
| 18  | CLA  | F     | 301 | -     | 1/1/11/20 | 3/13/91/115   | -       |
| 20  | LHG  | 6     | 620 | 18,15 | -         | 17/32/32/53   | -       |
| 26  | LUT  | 6     | 617 | -     | -         | 12/29/67/67   | 0/2/2/2 |
| 21  | BCR  | 5     | 621 | -     | -         | 9/29/63/63    | 0/2/2/2 |
| 26  | LUT  | 2     | 619 | -     | -         | 7/29/67/67    | 0/2/2/2 |
| 18  | CLA  | A     | 812 | -     | 1/1/15/20 | 11/37/115/115 | -       |

All (1235) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | 5     | 619 | LUT  | C34-C33 | 20.14 | 1.62        | 1.35     |
| 26  | 3     | 618 | LUT  | C34-C33 | 19.98 | 1.62        | 1.35     |
| 26  | 2     | 619 | LUT  | C34-C33 | 19.80 | 1.62        | 1.35     |
| 26  | 6     | 617 | LUT  | C34-C33 | 19.76 | 1.62        | 1.35     |
| 26  | 5     | 619 | LUT  | C14-C13 | 16.75 | 1.58        | 1.35     |
| 26  | 2     | 619 | LUT  | C14-C13 | 16.50 | 1.57        | 1.35     |
| 26  | 3     | 618 | LUT  | C24-C25 | 16.50 | 1.53        | 1.33     |
| 26  | 3     | 618 | LUT  | C14-C13 | 16.48 | 1.57        | 1.35     |
| 26  | 3     | 618 | LUT  | C10-C9  | 16.46 | 1.57        | 1.35     |
| 26  | 5     | 619 | LUT  | C24-C25 | 16.45 | 1.53        | 1.33     |
| 26  | 6     | 617 | LUT  | C14-C13 | 16.40 | 1.57        | 1.35     |
| 26  | 5     | 619 | LUT  | C10-C9  | 16.40 | 1.57        | 1.35     |
| 26  | 6     | 617 | LUT  | C24-C25 | 16.38 | 1.53        | 1.33     |
| 26  | 2     | 619 | LUT  | C24-C25 | 16.23 | 1.53        | 1.33     |
| 26  | 2     | 619 | LUT  | C10-C9  | 16.22 | 1.57        | 1.35     |
| 26  | 6     | 617 | LUT  | C10-C9  | 16.15 | 1.57        | 1.35     |
| 26  | 5     | 619 | LUT  | C30-C29 | 15.72 | 1.56        | 1.35     |
| 26  | 3     | 618 | LUT  | C30-C29 | 15.70 | 1.56        | 1.35     |
| 26  | 2     | 619 | LUT  | C30-C29 | 15.50 | 1.56        | 1.35     |
| 26  | 6     | 617 | LUT  | C30-C29 | 15.48 | 1.56        | 1.35     |
| 18  | 5     | 611 | CLA  | C1A-NA  | 12.34 | 1.40        | 1.29     |
| 26  | 6     | 617 | LUT  | C5-C6   | 11.69 | 1.54        | 1.34     |
| 26  | 3     | 618 | LUT  | C5-C6   | 11.59 | 1.54        | 1.34     |
| 26  | 5     | 619 | LUT  | C5-C6   | 11.52 | 1.54        | 1.34     |
| 26  | 2     | 619 | LUT  | C5-C6   | 10.90 | 1.53        | 1.34     |
| 26  | 5     | 619 | LUT  | C28-C27 | 10.63 | 1.57        | 1.32     |
| 26  | 3     | 618 | LUT  | C28-C27 | 10.61 | 1.57        | 1.32     |
| 26  | 2     | 619 | LUT  | C28-C27 | 10.55 | 1.57        | 1.32     |
| 26  | 6     | 617 | LUT  | C28-C27 | 10.52 | 1.57        | 1.32     |
| 26  | 3     | 618 | LUT  | C11-C12 | 9.25  | 1.58        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 26  | 5     | 619 | LUT  | C11-C12 | 9.21 | 1.58        | 1.34     |
| 26  | 2     | 619 | LUT  | C11-C12 | 9.08 | 1.58        | 1.34     |
| 26  | 6     | 617 | LUT  | C11-C12 | 9.03 | 1.57        | 1.34     |
| 26  | 5     | 619 | LUT  | C35-C15 | 8.95 | 1.59        | 1.36     |
| 26  | 3     | 618 | LUT  | C35-C15 | 8.87 | 1.59        | 1.36     |
| 26  | 2     | 619 | LUT  | C35-C15 | 8.80 | 1.58        | 1.36     |
| 26  | 6     | 617 | LUT  | C35-C15 | 8.76 | 1.58        | 1.36     |
| 26  | 5     | 619 | LUT  | C31-C32 | 8.13 | 1.55        | 1.34     |
| 26  | 3     | 618 | LUT  | C31-C32 | 8.13 | 1.55        | 1.34     |
| 26  | 2     | 619 | LUT  | C31-C32 | 8.04 | 1.55        | 1.34     |
| 26  | 6     | 617 | LUT  | C31-C32 | 8.01 | 1.55        | 1.34     |
| 18  | K     | 201 | CLA  | C4B-NB  | 7.94 | 1.42        | 1.35     |
| 26  | 3     | 618 | LUT  | C8-C7   | 7.73 | 1.56        | 1.33     |
| 18  | 3     | 612 | CLA  | C4B-NB  | 7.69 | 1.42        | 1.35     |
| 26  | 5     | 619 | LUT  | C8-C7   | 7.68 | 1.56        | 1.33     |
| 18  | 5     | 602 | CLA  | C4B-NB  | 7.64 | 1.42        | 1.35     |
| 26  | 2     | 619 | LUT  | C8-C7   | 7.63 | 1.56        | 1.33     |
| 18  | 6     | 616 | CLA  | C4B-NB  | 7.63 | 1.42        | 1.35     |
| 18  | 2     | 612 | CLA  | C4B-NB  | 7.59 | 1.42        | 1.35     |
| 26  | 6     | 617 | LUT  | C8-C7   | 7.58 | 1.56        | 1.33     |
| 18  | 6     | 613 | CLA  | C4B-NB  | 7.56 | 1.42        | 1.35     |
| 18  | 6     | 611 | CLA  | C4B-NB  | 7.55 | 1.41        | 1.35     |
| 18  | B     | 834 | CLA  | C4B-NB  | 7.55 | 1.41        | 1.35     |
| 18  | A     | 837 | CLA  | C4B-NB  | 7.52 | 1.41        | 1.35     |
| 18  | K     | 206 | CLA  | C4B-NB  | 7.52 | 1.41        | 1.35     |
| 18  | 3     | 613 | CLA  | C4B-NB  | 7.52 | 1.41        | 1.35     |
| 18  | A     | 840 | CLA  | C4B-NB  | 7.51 | 1.41        | 1.35     |
| 18  | G     | 201 | CLA  | C4B-NB  | 7.51 | 1.41        | 1.35     |
| 18  | 5     | 614 | CLA  | C4B-NB  | 7.51 | 1.41        | 1.35     |
| 18  | A     | 812 | CLA  | C4B-NB  | 7.50 | 1.41        | 1.35     |
| 18  | K     | 203 | CLA  | C4B-NB  | 7.50 | 1.41        | 1.35     |
| 18  | L     | 302 | CLA  | C4B-NB  | 7.50 | 1.41        | 1.35     |
| 18  | F     | 305 | CLA  | C4B-NB  | 7.49 | 1.41        | 1.35     |
| 18  | A     | 810 | CLA  | C4B-NB  | 7.49 | 1.41        | 1.35     |
| 18  | 5     | 601 | CLA  | C4B-NB  | 7.48 | 1.41        | 1.35     |
| 18  | 6     | 612 | CLA  | C4B-NB  | 7.48 | 1.41        | 1.35     |
| 18  | B     | 824 | CLA  | C4B-NB  | 7.48 | 1.41        | 1.35     |
| 18  | B     | 829 | CLA  | C4B-NB  | 7.48 | 1.41        | 1.35     |
| 18  | 5     | 612 | CLA  | C4B-NB  | 7.48 | 1.41        | 1.35     |
| 18  | B     | 835 | CLA  | C4B-NB  | 7.47 | 1.41        | 1.35     |
| 18  | A     | 831 | CLA  | C4B-NB  | 7.47 | 1.41        | 1.35     |
| 18  | 3     | 611 | CLA  | C4B-NB  | 7.46 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 18  | B     | 837 | CLA  | C4B-NB | 7.46 | 1.41        | 1.35     |
| 18  | 3     | 603 | CLA  | C4B-NB | 7.46 | 1.41        | 1.35     |
| 18  | 5     | 613 | CLA  | C4B-NB | 7.46 | 1.41        | 1.35     |
| 18  | 2     | 613 | CLA  | C4B-NB | 7.46 | 1.41        | 1.35     |
| 18  | 3     | 615 | CLA  | C4B-NB | 7.46 | 1.41        | 1.35     |
| 18  | A     | 824 | CLA  | C4B-NB | 7.45 | 1.41        | 1.35     |
| 18  | 3     | 607 | CLA  | C4B-NB | 7.45 | 1.41        | 1.35     |
| 18  | J     | 101 | CLA  | C4B-NB | 7.45 | 1.41        | 1.35     |
| 18  | 3     | 614 | CLA  | C4B-NB | 7.45 | 1.41        | 1.35     |
| 18  | B     | 818 | CLA  | C4B-NB | 7.44 | 1.41        | 1.35     |
| 18  | 3     | 617 | CLA  | C4B-NB | 7.44 | 1.41        | 1.35     |
| 18  | A     | 833 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | B     | 811 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | G     | 203 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | A     | 803 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | A     | 836 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | 2     | 614 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | 6     | 614 | CLA  | C4B-NB | 7.43 | 1.41        | 1.35     |
| 18  | A     | 819 | CLA  | C4B-NB | 7.42 | 1.41        | 1.35     |
| 18  | B     | 841 | CLA  | C4B-NB | 7.42 | 1.41        | 1.35     |
| 18  | 6     | 608 | CLA  | C4B-NB | 7.42 | 1.41        | 1.35     |
| 18  | B     | 815 | CLA  | C4B-NB | 7.42 | 1.41        | 1.35     |
| 18  | B     | 828 | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 18  | 6     | 606 | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 18  | A     | 845 | CLA  | C4B-NB | 7.41 | 1.41        | 1.35     |
| 18  | B     | 805 | CLA  | C4B-NB | 7.40 | 1.41        | 1.35     |
| 18  | G     | 204 | CLA  | C4B-NB | 7.40 | 1.41        | 1.35     |
| 18  | 5     | 611 | CLA  | C4B-NB | 7.39 | 1.41        | 1.35     |
| 18  | A     | 842 | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 18  | B     | 821 | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 18  | B     | 838 | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 18  | 2     | 603 | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 18  | 2     | 611 | CLA  | C4B-NB | 7.38 | 1.41        | 1.35     |
| 18  | A     | 825 | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |
| 18  | B     | 840 | CLA  | C4B-NB | 7.37 | 1.41        | 1.35     |
| 18  | A     | 834 | CLA  | C4B-NB | 7.36 | 1.41        | 1.35     |
| 18  | L     | 304 | CLA  | C4B-NB | 7.36 | 1.41        | 1.35     |
| 18  | A     | 820 | CLA  | C4B-NB | 7.36 | 1.41        | 1.35     |
| 18  | 6     | 604 | CLA  | C4B-NB | 7.36 | 1.41        | 1.35     |
| 18  | B     | 831 | CLA  | C4B-NB | 7.36 | 1.41        | 1.35     |
| 18  | A     | 843 | CLA  | C4B-NB | 7.35 | 1.41        | 1.35     |
| 18  | F     | 303 | CLA  | C4B-NB | 7.35 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 18  | A     | 811 | CLA  | C4B-NB | 7.34 | 1.41        | 1.35     |
| 18  | A     | 838 | CLA  | C4B-NB | 7.34 | 1.41        | 1.35     |
| 18  | B     | 809 | CLA  | C4B-NB | 7.34 | 1.41        | 1.35     |
| 18  | 6     | 609 | CLA  | C4B-NB | 7.33 | 1.41        | 1.35     |
| 18  | 3     | 604 | CLA  | C4B-NB | 7.33 | 1.41        | 1.35     |
| 18  | F     | 304 | CLA  | C4B-NB | 7.33 | 1.41        | 1.35     |
| 18  | 5     | 610 | CLA  | C4B-NB | 7.33 | 1.41        | 1.35     |
| 18  | B     | 812 | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 18  | B     | 839 | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 18  | 5     | 603 | CLA  | C4B-NB | 7.32 | 1.41        | 1.35     |
| 18  | B     | 804 | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 18  | B     | 816 | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 18  | A     | 821 | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 18  | B     | 832 | CLA  | C4B-NB | 7.31 | 1.41        | 1.35     |
| 18  | 3     | 606 | CLA  | C4B-NB | 7.30 | 1.41        | 1.35     |
| 18  | 6     | 603 | CLA  | C4B-NB | 7.30 | 1.41        | 1.35     |
| 18  | B     | 808 | CLA  | C4B-NB | 7.30 | 1.41        | 1.35     |
| 18  | 5     | 609 | CLA  | C4B-NB | 7.30 | 1.41        | 1.35     |
| 18  | B     | 819 | CLA  | C4B-NB | 7.29 | 1.41        | 1.35     |
| 18  | B     | 814 | CLA  | C4B-NB | 7.29 | 1.41        | 1.35     |
| 18  | A     | 808 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | 3     | 610 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | B     | 830 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | A     | 823 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | B     | 833 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | 2     | 604 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | 2     | 602 | CLA  | C4B-NB | 7.28 | 1.41        | 1.35     |
| 18  | F     | 301 | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 18  | A     | 818 | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 18  | A     | 822 | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 18  | B     | 822 | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 18  | A     | 835 | CLA  | C4B-NB | 7.27 | 1.41        | 1.35     |
| 18  | B     | 810 | CLA  | C4B-NB | 7.26 | 1.41        | 1.35     |
| 18  | A     | 832 | CLA  | C4B-NB | 7.26 | 1.41        | 1.35     |
| 18  | B     | 807 | CLA  | C4B-NB | 7.26 | 1.41        | 1.35     |
| 18  | 5     | 604 | CLA  | C4B-NB | 7.26 | 1.41        | 1.35     |
| 18  | A     | 827 | CLA  | C4B-NB | 7.25 | 1.41        | 1.35     |
| 18  | K     | 204 | CLA  | C4B-NB | 7.25 | 1.41        | 1.35     |
| 18  | A     | 841 | CLA  | C4B-NB | 7.24 | 1.41        | 1.35     |
| 18  | B     | 817 | CLA  | C4B-NB | 7.24 | 1.41        | 1.35     |
| 18  | 3     | 602 | CLA  | C4B-NB | 7.23 | 1.41        | 1.35     |
| 18  | B     | 825 | CLA  | C4B-NB | 7.23 | 1.41        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | A     | 807 | CLA  | C4B-NB  | 7.22  | 1.41        | 1.35     |
| 18  | 3     | 609 | CLA  | C4B-NB  | 7.21  | 1.41        | 1.35     |
| 18  | B     | 802 | CLA  | C4B-NB  | 7.21  | 1.41        | 1.35     |
| 18  | L     | 303 | CLA  | C4B-NB  | 7.21  | 1.41        | 1.35     |
| 18  | B     | 806 | CLA  | C4B-NB  | 7.20  | 1.41        | 1.35     |
| 18  | A     | 815 | CLA  | C4B-NB  | 7.19  | 1.41        | 1.35     |
| 18  | 2     | 609 | CLA  | C4B-NB  | 7.19  | 1.41        | 1.35     |
| 18  | A     | 806 | CLA  | C4B-NB  | 7.18  | 1.41        | 1.35     |
| 18  | A     | 817 | CLA  | C4B-NB  | 7.18  | 1.41        | 1.35     |
| 18  | B     | 820 | CLA  | C4B-NB  | 7.18  | 1.41        | 1.35     |
| 18  | B     | 827 | CLA  | C4B-NB  | 7.18  | 1.41        | 1.35     |
| 18  | 6     | 610 | CLA  | C4B-NB  | 7.18  | 1.41        | 1.35     |
| 18  | 6     | 602 | CLA  | C4B-NB  | 7.18  | 1.41        | 1.35     |
| 18  | A     | 804 | CLA  | C4B-NB  | 7.17  | 1.41        | 1.35     |
| 18  | A     | 813 | CLA  | C4B-NB  | 7.17  | 1.41        | 1.35     |
| 18  | A     | 816 | CLA  | C4B-NB  | 7.16  | 1.41        | 1.35     |
| 18  | A     | 839 | CLA  | C4B-NB  | 7.16  | 1.41        | 1.35     |
| 18  | A     | 830 | CLA  | C4B-NB  | 7.14  | 1.41        | 1.35     |
| 18  | A     | 802 | CLA  | C4B-NB  | 7.14  | 1.41        | 1.35     |
| 18  | A     | 854 | CLA  | C4B-NB  | 7.14  | 1.41        | 1.35     |
| 18  | B     | 836 | CLA  | C4B-NB  | 7.13  | 1.41        | 1.35     |
| 18  | B     | 803 | CLA  | C4B-NB  | 7.12  | 1.41        | 1.35     |
| 18  | B     | 823 | CLA  | C4B-NB  | 7.12  | 1.41        | 1.35     |
| 18  | B     | 826 | CLA  | C4B-NB  | 7.10  | 1.41        | 1.35     |
| 18  | A     | 828 | CLA  | C4B-NB  | 7.10  | 1.41        | 1.35     |
| 18  | A     | 826 | CLA  | C4B-NB  | 7.08  | 1.41        | 1.35     |
| 18  | A     | 801 | CLA  | C4B-NB  | 7.07  | 1.41        | 1.35     |
| 18  | A     | 809 | CLA  | C4B-NB  | 7.07  | 1.41        | 1.35     |
| 18  | A     | 829 | CLA  | C4B-NB  | 7.03  | 1.41        | 1.35     |
| 18  | A     | 814 | CLA  | C4B-NB  | 7.02  | 1.41        | 1.35     |
| 18  | A     | 805 | CLA  | C4B-NB  | 7.01  | 1.41        | 1.35     |
| 18  | B     | 813 | CLA  | C4B-NB  | 6.95  | 1.41        | 1.35     |
| 18  | 2     | 610 | CLA  | C4B-NB  | 6.95  | 1.41        | 1.35     |
| 26  | 6     | 617 | LUT  | C12-C13 | -6.14 | 1.32        | 1.45     |
| 26  | 2     | 619 | LUT  | C12-C13 | -6.05 | 1.32        | 1.45     |
| 26  | 5     | 619 | LUT  | C12-C13 | -6.00 | 1.33        | 1.45     |
| 26  | 6     | 617 | LUT  | C32-C33 | -6.00 | 1.33        | 1.45     |
| 26  | 2     | 619 | LUT  | C32-C33 | -5.99 | 1.33        | 1.45     |
| 26  | 5     | 619 | LUT  | C32-C33 | -5.86 | 1.33        | 1.45     |
| 26  | 3     | 618 | LUT  | C32-C33 | -5.83 | 1.33        | 1.45     |
| 26  | 3     | 618 | LUT  | C12-C13 | -5.76 | 1.33        | 1.45     |
| 25  | 5     | 607 | CHL  | CHC-C1C | 5.27  | 1.48        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 5     | 607 | CHL  | C3B-C2B | 5.22  | 1.47        | 1.40     |
| 25  | 6     | 607 | CHL  | CHC-C1C | 5.22  | 1.48        | 1.35     |
| 25  | 6     | 607 | CHL  | C3B-C2B | 5.22  | 1.47        | 1.40     |
| 25  | 5     | 607 | CHL  | O2D-CGD | 5.19  | 1.45        | 1.33     |
| 25  | 5     | 615 | CHL  | O2D-CGD | 5.19  | 1.45        | 1.33     |
| 25  | 2     | 608 | CHL  | CHC-C1C | 5.17  | 1.48        | 1.35     |
| 25  | 2     | 616 | CHL  | O2D-CGD | 5.16  | 1.45        | 1.33     |
| 25  | 2     | 607 | CHL  | O2D-CGD | 5.14  | 1.45        | 1.33     |
| 25  | 2     | 601 | CHL  | CHC-C1C | 5.13  | 1.48        | 1.35     |
| 18  | 5     | 611 | CLA  | CHB-C4A | 5.12  | 1.38        | 1.34     |
| 25  | 2     | 606 | CHL  | O2D-CGD | 5.12  | 1.45        | 1.33     |
| 25  | 5     | 606 | CHL  | O2D-CGD | 5.11  | 1.45        | 1.33     |
| 25  | 2     | 601 | CHL  | O2D-CGD | 5.09  | 1.45        | 1.33     |
| 25  | 6     | 601 | CHL  | CHC-C1C | 5.06  | 1.47        | 1.35     |
| 25  | 5     | 608 | CHL  | O2D-CGD | 5.05  | 1.45        | 1.33     |
| 25  | 2     | 607 | CHL  | CHC-C1C | 5.03  | 1.47        | 1.35     |
| 25  | 2     | 607 | CHL  | C3B-C2B | 4.99  | 1.47        | 1.40     |
| 25  | 2     | 616 | CHL  | CHC-C1C | 4.97  | 1.47        | 1.35     |
| 25  | 5     | 615 | CHL  | CHC-C1C | 4.96  | 1.47        | 1.35     |
| 25  | 5     | 606 | CHL  | CHC-C1C | 4.90  | 1.47        | 1.35     |
| 25  | 5     | 608 | CHL  | CHC-C1C | 4.89  | 1.47        | 1.35     |
| 25  | 6     | 601 | CHL  | C3B-C2B | 4.88  | 1.47        | 1.40     |
| 25  | 6     | 607 | CHL  | C2C-C3C | 4.87  | 1.47        | 1.36     |
| 25  | 6     | 607 | CHL  | CHD-C1D | 4.87  | 1.47        | 1.38     |
| 25  | 2     | 616 | CHL  | C3B-C2B | 4.86  | 1.47        | 1.40     |
| 25  | 2     | 606 | CHL  | CHC-C1C | 4.86  | 1.47        | 1.35     |
| 25  | 5     | 607 | CHL  | C2C-C3C | 4.83  | 1.47        | 1.36     |
| 25  | 6     | 607 | CHL  | C3D-C4D | -4.82 | 1.33        | 1.44     |
| 25  | 2     | 601 | CHL  | C2C-C3C | 4.81  | 1.47        | 1.36     |
| 25  | 3     | 608 | CHL  | CHC-C1C | 4.80  | 1.47        | 1.35     |
| 25  | 2     | 608 | CHL  | C3D-C4D | -4.79 | 1.33        | 1.44     |
| 25  | 6     | 601 | CHL  | C3D-C4D | -4.78 | 1.33        | 1.44     |
| 25  | 5     | 615 | CHL  | C3B-C2B | 4.77  | 1.47        | 1.40     |
| 25  | 3     | 608 | CHL  | C3D-C4D | -4.77 | 1.33        | 1.44     |
| 25  | 5     | 607 | CHL  | C3D-C4D | -4.77 | 1.33        | 1.44     |
| 25  | 5     | 607 | CHL  | CHD-C1D | 4.75  | 1.47        | 1.38     |
| 25  | 2     | 607 | CHL  | C3D-C4D | -4.75 | 1.33        | 1.44     |
| 25  | 2     | 601 | CHL  | C3D-C4D | -4.73 | 1.33        | 1.44     |
| 25  | 3     | 608 | CHL  | C3B-C2B | 4.72  | 1.46        | 1.40     |
| 25  | 5     | 608 | CHL  | C3B-C2B | 4.72  | 1.46        | 1.40     |
| 25  | 5     | 615 | CHL  | C3D-C4D | -4.70 | 1.33        | 1.44     |
| 25  | 2     | 607 | CHL  | C2C-C3C | 4.68  | 1.46        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 5     | 608 | CHL  | C3D-C4D | -4.68 | 1.33        | 1.44     |
| 25  | 2     | 607 | CHL  | CHD-C1D | 4.66  | 1.47        | 1.38     |
| 25  | 2     | 616 | CHL  | C3D-C4D | -4.65 | 1.33        | 1.44     |
| 25  | 6     | 607 | CHL  | O2D-CGD | 4.65  | 1.45        | 1.30     |
| 25  | 2     | 608 | CHL  | O2D-CGD | 4.64  | 1.45        | 1.30     |
| 25  | 6     | 601 | CHL  | C2C-C3C | 4.64  | 1.46        | 1.36     |
| 25  | 5     | 606 | CHL  | C3D-C4D | -4.63 | 1.33        | 1.44     |
| 25  | 2     | 601 | CHL  | CHD-C1D | 4.63  | 1.47        | 1.38     |
| 25  | 5     | 606 | CHL  | C2C-C3C | 4.62  | 1.46        | 1.37     |
| 25  | 2     | 606 | CHL  | C3D-C4D | -4.61 | 1.33        | 1.44     |
| 25  | 3     | 608 | CHL  | O2D-CGD | 4.60  | 1.45        | 1.30     |
| 25  | 3     | 608 | CHL  | C3C-C2C | 4.59  | 1.46        | 1.36     |
| 25  | 2     | 608 | CHL  | C3B-C2B | 4.58  | 1.46        | 1.40     |
| 25  | 2     | 608 | CHL  | C2C-C3C | 4.57  | 1.46        | 1.36     |
| 25  | 5     | 615 | CHL  | C2C-C3C | 4.57  | 1.46        | 1.36     |
| 25  | 2     | 606 | CHL  | C3B-C2B | 4.56  | 1.46        | 1.40     |
| 25  | 6     | 601 | CHL  | O2D-CGD | 4.56  | 1.45        | 1.30     |
| 25  | 2     | 616 | CHL  | C2C-C3C | 4.55  | 1.46        | 1.36     |
| 25  | 2     | 608 | CHL  | CHD-C1D | 4.55  | 1.47        | 1.38     |
| 25  | 2     | 606 | CHL  | C2C-C3C | 4.54  | 1.46        | 1.36     |
| 25  | 6     | 601 | CHL  | O2A-CGA | 4.52  | 1.45        | 1.30     |
| 25  | 6     | 601 | CHL  | CHD-C1D | 4.52  | 1.47        | 1.38     |
| 25  | 2     | 616 | CHL  | CHD-C1D | 4.51  | 1.47        | 1.38     |
| 25  | 2     | 601 | CHL  | O2A-CGA | 4.48  | 1.45        | 1.30     |
| 25  | 5     | 608 | CHL  | C2C-C3C | 4.48  | 1.46        | 1.36     |
| 25  | 2     | 616 | CHL  | O2A-CGA | 4.47  | 1.45        | 1.30     |
| 25  | 2     | 606 | CHL  | O2A-CGA | 4.45  | 1.45        | 1.30     |
| 25  | 5     | 606 | CHL  | CHD-C1D | 4.44  | 1.47        | 1.38     |
| 25  | 5     | 615 | CHL  | CHD-C1D | 4.42  | 1.47        | 1.38     |
| 25  | 3     | 608 | CHL  | CHD-C1D | 4.37  | 1.46        | 1.38     |
| 25  | 5     | 607 | CHL  | CHD-C4C | 4.30  | 1.49        | 1.39     |
| 25  | 2     | 606 | CHL  | CHD-C1D | 4.28  | 1.46        | 1.38     |
| 25  | 5     | 608 | CHL  | O2A-CGA | 4.25  | 1.45        | 1.33     |
| 25  | 6     | 607 | CHL  | CHD-C4C | 4.23  | 1.48        | 1.39     |
| 18  | K     | 201 | CLA  | C1D-ND  | 4.22  | 1.43        | 1.37     |
| 25  | 2     | 601 | CHL  | CHD-C4C | 4.17  | 1.48        | 1.39     |
| 25  | 5     | 608 | CHL  | CHD-C1D | 4.17  | 1.46        | 1.38     |
| 26  | 6     | 617 | LUT  | C28-C29 | -4.16 | 1.37        | 1.45     |
| 26  | 2     | 619 | LUT  | C8-C9   | -4.16 | 1.37        | 1.45     |
| 25  | 2     | 607 | CHL  | CHD-C4C | 4.13  | 1.48        | 1.39     |
| 25  | 2     | 608 | CHL  | CHD-C4C | 4.13  | 1.48        | 1.39     |
| 26  | 6     | 617 | LUT  | C8-C9   | -4.13 | 1.37        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | 5     | 619 | LUT  | C11-C10 | 4.11  | 1.56        | 1.43     |
| 26  | 3     | 618 | LUT  | C11-C10 | 4.10  | 1.56        | 1.43     |
| 26  | 2     | 619 | LUT  | C28-C29 | -4.09 | 1.37        | 1.45     |
| 26  | 5     | 619 | LUT  | C28-C29 | -4.09 | 1.37        | 1.45     |
| 25  | 6     | 601 | CHL  | CHD-C4C | 4.09  | 1.48        | 1.39     |
| 26  | 2     | 619 | LUT  | C11-C10 | 4.08  | 1.56        | 1.43     |
| 26  | 3     | 618 | LUT  | C28-C29 | -4.07 | 1.37        | 1.45     |
| 26  | 5     | 619 | LUT  | C8-C9   | -4.07 | 1.37        | 1.45     |
| 25  | 2     | 616 | CHL  | CHD-C4C | 4.05  | 1.48        | 1.39     |
| 26  | 3     | 618 | LUT  | C8-C9   | -4.04 | 1.37        | 1.45     |
| 25  | 3     | 608 | CHL  | CHD-C4C | 4.03  | 1.48        | 1.39     |
| 25  | 5     | 615 | CHL  | CHD-C4C | 4.01  | 1.48        | 1.39     |
| 26  | 6     | 617 | LUT  | C11-C10 | 4.00  | 1.55        | 1.43     |
| 25  | 5     | 606 | CHL  | CHD-C4C | 3.98  | 1.48        | 1.39     |
| 18  | 3     | 611 | CLA  | C1D-ND  | 3.95  | 1.42        | 1.37     |
| 18  | 6     | 616 | CLA  | C1D-ND  | 3.94  | 1.42        | 1.37     |
| 18  | B     | 805 | CLA  | C1D-ND  | 3.92  | 1.42        | 1.37     |
| 25  | 2     | 606 | CHL  | CHD-C4C | 3.90  | 1.48        | 1.39     |
| 18  | A     | 801 | CLA  | C1D-ND  | 3.89  | 1.42        | 1.37     |
| 18  | 3     | 604 | CLA  | C1D-ND  | 3.89  | 1.42        | 1.37     |
| 18  | 5     | 610 | CLA  | C1D-ND  | 3.88  | 1.42        | 1.37     |
| 18  | 5     | 614 | CLA  | C1D-ND  | 3.87  | 1.42        | 1.37     |
| 18  | 6     | 609 | CLA  | C1D-ND  | 3.86  | 1.42        | 1.37     |
| 18  | 3     | 612 | CLA  | C1D-ND  | 3.86  | 1.42        | 1.37     |
| 18  | 3     | 613 | CLA  | C1D-ND  | 3.86  | 1.42        | 1.37     |
| 18  | 3     | 615 | CLA  | C1D-ND  | 3.85  | 1.42        | 1.37     |
| 18  | K     | 206 | CLA  | C1D-ND  | 3.85  | 1.42        | 1.37     |
| 25  | 5     | 608 | CHL  | CHD-C4C | 3.84  | 1.48        | 1.39     |
| 18  | 6     | 614 | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 18  | 2     | 612 | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 18  | 5     | 613 | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 18  | A     | 825 | CLA  | C1D-ND  | 3.84  | 1.42        | 1.37     |
| 18  | B     | 822 | CLA  | C1D-ND  | 3.83  | 1.42        | 1.37     |
| 18  | K     | 204 | CLA  | C1D-ND  | 3.82  | 1.42        | 1.37     |
| 18  | 3     | 606 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 18  | B     | 830 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 18  | 5     | 611 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 18  | 3     | 602 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 18  | G     | 201 | CLA  | C1D-ND  | 3.81  | 1.42        | 1.37     |
| 18  | 5     | 609 | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |
| 18  | B     | 806 | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |
| 18  | A     | 816 | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 6     | 604 | CLA  | C1D-ND  | 3.80  | 1.42        | 1.37     |
| 18  | A     | 821 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 18  | K     | 203 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 18  | 6     | 603 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 18  | G     | 204 | CLA  | C1D-ND  | 3.79  | 1.42        | 1.37     |
| 18  | B     | 821 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 18  | J     | 101 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 18  | 5     | 612 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 18  | 2     | 604 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 18  | 3     | 610 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 18  | A     | 835 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 21  | 5     | 621 | BCR  | C1-C6   | -3.78 | 1.48        | 1.53     |
| 18  | 2     | 611 | CLA  | C1D-ND  | 3.78  | 1.42        | 1.37     |
| 18  | 5     | 604 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 18  | B     | 812 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 18  | 6     | 606 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 18  | B     | 802 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 18  | 6     | 610 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 18  | 5     | 602 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 18  | A     | 845 | CLA  | C1D-ND  | 3.77  | 1.42        | 1.37     |
| 25  | 5     | 607 | CHL  | OBD-CAD | 3.76  | 1.29        | 1.22     |
| 18  | A     | 815 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | G     | 203 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | F     | 304 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | 3     | 603 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | 2     | 609 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | B     | 827 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | A     | 808 | CLA  | C1D-ND  | 3.76  | 1.42        | 1.37     |
| 18  | B     | 817 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | B     | 824 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | A     | 832 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | B     | 835 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | L     | 302 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | 6     | 608 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | B     | 837 | CLA  | C1D-ND  | 3.75  | 1.42        | 1.37     |
| 18  | L     | 304 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 18  | A     | 843 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 18  | B     | 811 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 18  | A     | 837 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 18  | A     | 834 | CLA  | C1D-ND  | 3.74  | 1.42        | 1.37     |
| 18  | B     | 834 | CLA  | C1D-ND  | 3.73  | 1.42        | 1.37     |
| 18  | 6     | 612 | CLA  | C1D-ND  | 3.73  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 18  | B     | 829 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | A     | 838 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | A     | 826 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | B     | 836 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | 2     | 613 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | A     | 811 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | A     | 828 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | B     | 841 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | A     | 806 | CLA  | C1D-ND  | 3.73 | 1.42        | 1.37     |
| 18  | A     | 822 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 18  | A     | 841 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 25  | 2     | 606 | CHL  | OBD-CAD | 3.72 | 1.28        | 1.22     |
| 18  | 5     | 603 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 18  | L     | 303 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 18  | 5     | 601 | CLA  | C1D-ND  | 3.72 | 1.42        | 1.37     |
| 18  | A     | 831 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | 6     | 602 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | A     | 804 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | B     | 807 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | 3     | 609 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | B     | 818 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | 2     | 614 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | A     | 824 | CLA  | C1D-ND  | 3.71 | 1.42        | 1.37     |
| 18  | B     | 816 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | 3     | 614 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | A     | 814 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | 6     | 611 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | 3     | 617 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | A     | 818 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 25  | 5     | 615 | CHL  | OBD-CAD | 3.70 | 1.28        | 1.22     |
| 18  | A     | 812 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | A     | 810 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | A     | 817 | CLA  | C1D-ND  | 3.70 | 1.42        | 1.37     |
| 18  | B     | 814 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | A     | 833 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | B     | 819 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | B     | 838 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | F     | 303 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | F     | 305 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | F     | 301 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | B     | 839 | CLA  | C1D-ND  | 3.69 | 1.42        | 1.37     |
| 18  | A     | 840 | CLA  | C1D-ND  | 3.68 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 2     | 603 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 18  | A     | 836 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 18  | B     | 804 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 18  | B     | 803 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 18  | 2     | 602 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 18  | B     | 831 | CLA  | C1D-ND  | 3.68  | 1.42        | 1.37     |
| 18  | A     | 809 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 18  | 3     | 607 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 25  | 2     | 616 | CHL  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 25  | 5     | 606 | CHL  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 18  | B     | 810 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 18  | A     | 854 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 18  | B     | 808 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 18  | B     | 833 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 25  | 6     | 607 | CHL  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 18  | A     | 820 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 18  | B     | 820 | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 25  | 6     | 601 | CHL  | OBD-CAD | 3.67  | 1.28        | 1.22     |
| 18  | A     | 807 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 25  | 2     | 601 | CHL  | OBD-CAD | 3.66  | 1.28        | 1.22     |
| 18  | A     | 839 | CLA  | C1D-ND  | 3.66  | 1.42        | 1.37     |
| 26  | 2     | 619 | LUT  | C26-C27 | 3.66  | 1.55        | 1.50     |
| 18  | B     | 815 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 18  | A     | 813 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 18  | B     | 825 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 18  | 6     | 613 | CLA  | C1D-ND  | 3.65  | 1.42        | 1.37     |
| 18  | A     | 829 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 18  | A     | 803 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 18  | A     | 827 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 18  | B     | 826 | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 18  | A     | 842 | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 18  | B     | 823 | CLA  | C1D-ND  | 3.63  | 1.42        | 1.37     |
| 18  | B     | 828 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 18  | A     | 822 | CLA  | CAB-C3B | -3.62 | 1.44        | 1.51     |
| 18  | A     | 830 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 18  | A     | 823 | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 18  | 5     | 611 | CLA  | CAB-C3B | -3.62 | 1.44        | 1.51     |
| 18  | B     | 813 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 18  | A     | 819 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 18  | B     | 840 | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 25  | 2     | 607 | CHL  | OBD-CAD | 3.60  | 1.28        | 1.22     |
| 26  | 5     | 619 | LUT  | C26-C27 | 3.60  | 1.55        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 6     | 611 | CLA  | CAB-C3B | -3.59 | 1.44        | 1.51     |
| 18  | K     | 204 | CLA  | CAB-C3B | -3.59 | 1.44        | 1.51     |
| 25  | 3     | 608 | CHL  | OBD-CAD | 3.58  | 1.28        | 1.22     |
| 18  | B     | 832 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 21  | A     | 852 | BCR  | C1-C6   | -3.58 | 1.48        | 1.53     |
| 18  | B     | 809 | CLA  | C1D-ND  | 3.58  | 1.42        | 1.37     |
| 18  | A     | 805 | CLA  | C1D-ND  | 3.57  | 1.42        | 1.37     |
| 21  | A     | 849 | BCR  | C1-C6   | -3.57 | 1.48        | 1.53     |
| 18  | 6     | 609 | CLA  | CAB-C3B | -3.57 | 1.44        | 1.51     |
| 21  | B     | 848 | BCR  | C1-C6   | -3.56 | 1.48        | 1.53     |
| 18  | B     | 811 | CLA  | CAB-C3B | -3.55 | 1.44        | 1.51     |
| 18  | 3     | 607 | CLA  | CAB-C3B | -3.55 | 1.44        | 1.51     |
| 18  | 6     | 616 | CLA  | CAB-C3B | -3.55 | 1.44        | 1.51     |
| 25  | 5     | 608 | CHL  | OBD-CAD | 3.54  | 1.28        | 1.22     |
| 18  | 3     | 604 | CLA  | CAB-C3B | -3.54 | 1.44        | 1.51     |
| 25  | 2     | 608 | CHL  | OBD-CAD | 3.53  | 1.28        | 1.22     |
| 21  | B     | 843 | BCR  | C1-C6   | -3.53 | 1.48        | 1.53     |
| 21  | A     | 850 | BCR  | C1-C6   | -3.53 | 1.48        | 1.53     |
| 21  | A     | 851 | BCR  | C30-C25 | -3.53 | 1.48        | 1.53     |
| 18  | A     | 802 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 18  | 6     | 614 | CLA  | CAB-C3B | -3.52 | 1.44        | 1.51     |
| 21  | J     | 102 | BCR  | C30-C25 | -3.51 | 1.48        | 1.53     |
| 25  | 2     | 608 | CHL  | C3A-C2A | -3.51 | 1.51        | 1.54     |
| 21  | K     | 202 | BCR  | C1-C6   | -3.51 | 1.48        | 1.53     |
| 21  | B     | 847 | BCR  | C1-C6   | -3.51 | 1.48        | 1.53     |
| 21  | G     | 205 | BCR  | C1-C6   | -3.51 | 1.48        | 1.53     |
| 18  | 2     | 610 | CLA  | C1D-ND  | 3.50  | 1.42        | 1.37     |
| 25  | 3     | 608 | CHL  | C3A-C2A | -3.49 | 1.51        | 1.54     |
| 21  | B     | 801 | BCR  | C1-C6   | -3.48 | 1.49        | 1.53     |
| 21  | L     | 301 | BCR  | C1-C6   | -3.45 | 1.49        | 1.53     |
| 21  | B     | 845 | BCR  | C1-C6   | -3.45 | 1.49        | 1.53     |
| 21  | B     | 846 | BCR  | C1-C6   | -3.44 | 1.49        | 1.53     |
| 21  | 2     | 621 | BCR  | C1-C6   | -3.42 | 1.49        | 1.53     |
| 26  | 3     | 618 | LUT  | C26-C27 | 3.42  | 1.55        | 1.50     |
| 26  | 6     | 617 | LUT  | C26-C27 | 3.41  | 1.55        | 1.50     |
| 21  | L     | 305 | BCR  | C1-C6   | -3.41 | 1.49        | 1.53     |
| 26  | 5     | 619 | LUT  | C15-C14 | 3.36  | 1.53        | 1.43     |
| 21  | B     | 843 | BCR  | C30-C25 | -3.36 | 1.49        | 1.53     |
| 21  | B     | 845 | BCR  | C30-C25 | -3.34 | 1.49        | 1.53     |
| 21  | K     | 207 | BCR  | C1-C6   | -3.33 | 1.49        | 1.53     |
| 26  | 3     | 618 | LUT  | C15-C14 | 3.32  | 1.53        | 1.43     |
| 21  | A     | 851 | BCR  | C1-C6   | -3.31 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | B     | 846 | BCR  | C30-C25 | -3.31 | 1.49        | 1.53     |
| 21  | 2     | 621 | BCR  | C30-C25 | -3.30 | 1.49        | 1.53     |
| 21  | J     | 103 | BCR  | C1-C6   | -3.27 | 1.49        | 1.53     |
| 25  | 5     | 607 | CHL  | C3D-C2D | 3.27  | 1.48        | 1.39     |
| 18  | A     | 823 | CLA  | CHC-C1C | 3.26  | 1.43        | 1.35     |
| 26  | 2     | 619 | LUT  | C15-C14 | 3.26  | 1.53        | 1.43     |
| 21  | F     | 302 | BCR  | C1-C6   | -3.26 | 1.49        | 1.53     |
| 21  | A     | 856 | BCR  | C1-C6   | -3.23 | 1.49        | 1.53     |
| 26  | 6     | 617 | LUT  | C15-C14 | 3.23  | 1.53        | 1.43     |
| 21  | A     | 849 | BCR  | C30-C25 | -3.22 | 1.49        | 1.53     |
| 21  | A     | 848 | BCR  | C1-C6   | -3.21 | 1.49        | 1.53     |
| 18  | A     | 811 | CLA  | CHC-C1C | 3.20  | 1.43        | 1.35     |
| 18  | 5     | 610 | CLA  | CHC-C1C | 3.20  | 1.43        | 1.35     |
| 21  | J     | 102 | BCR  | C1-C6   | -3.20 | 1.49        | 1.53     |
| 18  | B     | 836 | CLA  | CHC-C1C | 3.19  | 1.43        | 1.35     |
| 18  | 6     | 611 | CLA  | CHC-C1C | 3.19  | 1.43        | 1.35     |
| 18  | A     | 833 | CLA  | CHC-C1C | 3.19  | 1.43        | 1.35     |
| 18  | A     | 827 | CLA  | CHC-C1C | 3.19  | 1.43        | 1.35     |
| 18  | 2     | 611 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 18  | 5     | 609 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 18  | 3     | 617 | CLA  | CHC-C1C | 3.18  | 1.43        | 1.35     |
| 21  | 3     | 620 | BCR  | C1-C6   | -3.17 | 1.49        | 1.53     |
| 18  | A     | 812 | CLA  | CHC-C1C | 3.17  | 1.43        | 1.35     |
| 21  | I     | 101 | BCR  | C1-C6   | -3.17 | 1.49        | 1.53     |
| 18  | G     | 204 | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 18  | F     | 301 | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 18  | 3     | 610 | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 25  | 6     | 607 | CHL  | C3D-C2D | 3.16  | 1.47        | 1.39     |
| 18  | B     | 804 | CLA  | CHC-C1C | 3.16  | 1.43        | 1.35     |
| 18  | A     | 820 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | 6     | 614 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | A     | 808 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | F     | 303 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | A     | 836 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 26  | 5     | 619 | LUT  | C7-C6   | 3.15  | 1.56        | 1.45     |
| 18  | 5     | 602 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | A     | 805 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | B     | 824 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | 5     | 614 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | A     | 825 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | A     | 854 | CLA  | CHC-C1C | 3.15  | 1.43        | 1.35     |
| 18  | A     | 802 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 5     | 611 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | 6     | 616 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | L     | 302 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 25  | 2     | 601 | CHL  | C3D-C2D | 3.14  | 1.47        | 1.39     |
| 18  | B     | 806 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | B     | 839 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 21  | A     | 852 | BCR  | C30-C25 | -3.14 | 1.49        | 1.53     |
| 18  | A     | 822 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | 3     | 607 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | 5     | 612 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | 5     | 604 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | A     | 806 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | A     | 828 | CLA  | CHC-C1C | 3.14  | 1.43        | 1.35     |
| 18  | B     | 803 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 18  | A     | 827 | CLA  | C4D-ND  | -3.13 | 1.33        | 1.37     |
| 18  | A     | 809 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | 2     | 602 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | 2     | 604 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | 2     | 612 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | B     | 811 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | A     | 829 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | B     | 816 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | A     | 824 | CLA  | CHC-C1C | 3.13  | 1.43        | 1.35     |
| 18  | A     | 807 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 814 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 837 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 823 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | K     | 203 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | 2     | 614 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 830 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 834 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | 3     | 612 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 833 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | B     | 820 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | 2     | 610 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | 3     | 609 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | 6     | 602 | CLA  | CHC-C1C | 3.12  | 1.43        | 1.35     |
| 18  | A     | 832 | CLA  | CHC-C1C | 3.11  | 1.43        | 1.35     |
| 18  | 6     | 604 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | A     | 806 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 18  | 5     | 601 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | A     | 819 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | A     | 817 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | 2     | 609 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | 6     | 613 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | A     | 841 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | L     | 304 | CLA  | CHC-C1C | 3.11  | 1.42        | 1.35     |
| 18  | B     | 832 | CLA  | C4D-ND  | -3.11 | 1.33        | 1.37     |
| 21  | K     | 207 | BCR  | C30-C25 | -3.11 | 1.49        | 1.53     |
| 18  | B     | 812 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | 6     | 612 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | A     | 821 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | 5     | 603 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 26  | 3     | 618 | LUT  | C7-C6   | 3.10  | 1.56        | 1.45     |
| 18  | B     | 832 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | B     | 838 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | A     | 815 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | B     | 822 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | 6     | 610 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | A     | 828 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 18  | 3     | 615 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | B     | 815 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | 2     | 613 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | B     | 828 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | 5     | 611 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 18  | B     | 840 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | B     | 841 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | 6     | 608 | CLA  | CHC-C1C | 3.10  | 1.42        | 1.35     |
| 18  | B     | 826 | CLA  | C4D-ND  | -3.10 | 1.33        | 1.37     |
| 18  | F     | 304 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | B     | 831 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | B     | 813 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | A     | 818 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | 6     | 609 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | B     | 827 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | J     | 101 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | K     | 206 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | A     | 816 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | B     | 803 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | A     | 838 | CLA  | C4D-ND  | -3.09 | 1.33        | 1.37     |
| 18  | A     | 838 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | A     | 839 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | L     | 303 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | 3     | 604 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | A     | 814 | CLA  | CHC-C1C | 3.09  | 1.42        | 1.35     |
| 18  | 2     | 603 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 18  | 5     | 613 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | A     | 804 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | A     | 842 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | B     | 808 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 25  | 2     | 607 | CHL  | C1D-C2D | 3.08  | 1.51        | 1.45     |
| 18  | G     | 201 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | 3     | 614 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | B     | 802 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | L     | 303 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 18  | 3     | 602 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | 3     | 606 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | B     | 823 | CLA  | C4D-ND  | -3.08 | 1.33        | 1.37     |
| 18  | A     | 835 | CLA  | CHC-C1C | 3.08  | 1.42        | 1.35     |
| 18  | A     | 810 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | B     | 825 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | A     | 813 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 21  | A     | 856 | BCR  | C30-C25 | -3.07 | 1.49        | 1.53     |
| 18  | B     | 819 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 18  | A     | 801 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 25  | 5     | 607 | CHL  | C1D-C2D | 3.07  | 1.51        | 1.45     |
| 18  | B     | 838 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 18  | B     | 825 | CLA  | C4D-ND  | -3.07 | 1.33        | 1.37     |
| 18  | A     | 845 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | K     | 204 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | 3     | 611 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | A     | 803 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | A     | 840 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | A     | 826 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | B     | 805 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 18  | 6     | 603 | CLA  | CHC-C1C | 3.07  | 1.42        | 1.35     |
| 26  | 6     | 617 | LUT  | C7-C6   | 3.07  | 1.56        | 1.45     |
| 18  | 6     | 606 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 21  | L     | 301 | BCR  | C30-C25 | -3.06 | 1.49        | 1.53     |
| 18  | B     | 836 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 18  | B     | 835 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 25  | 2     | 607 | CHL  | C3D-C2D | 3.06  | 1.47        | 1.39     |
| 18  | A     | 839 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 21  | 3     | 622 | BCR  | C1-C6   | -3.06 | 1.49        | 1.53     |
| 18  | B     | 807 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | 3     | 613 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | 3     | 618 | LUT  | C23-C24 | 3.06  | 1.54        | 1.50     |
| 18  | B     | 806 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 18  | A     | 837 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | A     | 830 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | B     | 819 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | F     | 305 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | B     | 810 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | B     | 826 | CLA  | CHC-C1C | 3.06  | 1.42        | 1.35     |
| 18  | 6     | 602 | CLA  | C4D-ND  | -3.06 | 1.33        | 1.37     |
| 18  | A     | 814 | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 18  | 2     | 603 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 18  | B     | 818 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 25  | 2     | 608 | CHL  | C1D-C2D | 3.05  | 1.51        | 1.45     |
| 18  | B     | 817 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 21  | B     | 801 | BCR  | C30-C25 | -3.05 | 1.49        | 1.53     |
| 18  | 3     | 603 | CLA  | CHC-C1C | 3.05  | 1.42        | 1.35     |
| 18  | A     | 819 | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 18  | A     | 803 | CLA  | C4D-ND  | -3.05 | 1.33        | 1.37     |
| 21  | B     | 844 | BCR  | C1-C6   | -3.04 | 1.49        | 1.53     |
| 18  | G     | 203 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 18  | B     | 829 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 18  | B     | 821 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 18  | A     | 831 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 18  | A     | 843 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 25  | 2     | 601 | CHL  | C1D-C2D | 3.04  | 1.51        | 1.45     |
| 18  | B     | 839 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 18  | 5     | 603 | CLA  | CHC-C1C | 3.04  | 1.42        | 1.35     |
| 21  | A     | 850 | BCR  | C30-C25 | -3.04 | 1.49        | 1.53     |
| 18  | B     | 827 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 18  | 3     | 602 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 18  | A     | 833 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 18  | A     | 830 | CLA  | C4D-ND  | -3.04 | 1.33        | 1.37     |
| 25  | 6     | 601 | CHL  | C3D-C2D | 3.04  | 1.47        | 1.39     |
| 21  | B     | 844 | BCR  | C30-C25 | -3.03 | 1.49        | 1.53     |
| 18  | K     | 204 | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 18  | B     | 813 | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 18  | B     | 814 | CLA  | C4D-ND  | -3.03 | 1.33        | 1.37     |
| 18  | A     | 834 | CLA  | CHC-C1C | 3.03  | 1.42        | 1.35     |
| 18  | A     | 807 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 18  | B     | 818 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 18  | 2     | 614 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 25  | 5     | 615 | CHL  | C1D-C2D | 3.02  | 1.51        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 6     | 607 | CHL  | C1D-C2D | 3.02  | 1.51        | 1.45     |
| 18  | B     | 817 | CLA  | C4D-ND  | -3.02 | 1.33        | 1.37     |
| 18  | A     | 813 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | 2     | 602 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | A     | 842 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | 2     | 613 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | 3     | 606 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | A     | 808 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | 5     | 601 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | 2     | 612 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 18  | A     | 804 | CLA  | C4D-ND  | -3.01 | 1.33        | 1.37     |
| 25  | 2     | 616 | CHL  | C3D-C2D | 3.01  | 1.47        | 1.39     |
| 18  | B     | 809 | CLA  | CHC-C1C | 3.00  | 1.42        | 1.35     |
| 18  | A     | 812 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 18  | G     | 201 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 18  | G     | 203 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 18  | F     | 304 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 18  | A     | 837 | CLA  | C4D-ND  | -3.00 | 1.33        | 1.37     |
| 18  | 2     | 609 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | 3     | 615 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | A     | 836 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | B     | 841 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | A     | 834 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | A     | 817 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | A     | 831 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | A     | 815 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | A     | 820 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | B     | 830 | CLA  | C4D-ND  | -2.99 | 1.33        | 1.37     |
| 18  | B     | 807 | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 25  | 3     | 608 | CHL  | C1D-C2D | 2.98  | 1.51        | 1.45     |
| 18  | A     | 801 | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 25  | 6     | 601 | CHL  | C1D-C2D | 2.98  | 1.51        | 1.45     |
| 21  | 3     | 622 | BCR  | C30-C25 | -2.98 | 1.49        | 1.53     |
| 25  | 5     | 606 | CHL  | C1D-C2D | 2.98  | 1.51        | 1.45     |
| 26  | 2     | 619 | LUT  | C7-C6   | 2.98  | 1.55        | 1.45     |
| 18  | B     | 833 | CLA  | C4D-ND  | -2.98 | 1.33        | 1.37     |
| 25  | 2     | 608 | CHL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 25  | 5     | 615 | CHL  | C3D-C2D | 2.97  | 1.47        | 1.39     |
| 18  | 6     | 604 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | B     | 835 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | 2     | 611 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | B     | 831 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | A     | 822 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 21  | F     | 302 | BCR  | C30-C25 | -2.97 | 1.49        | 1.53     |
| 25  | 6     | 607 | CHL  | C3A-C2A | -2.97 | 1.51        | 1.54     |
| 21  | I     | 101 | BCR  | C30-C25 | -2.97 | 1.49        | 1.53     |
| 18  | B     | 810 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | A     | 802 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | B     | 805 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | 5     | 610 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | B     | 812 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | B     | 828 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | A     | 829 | CLA  | C4D-ND  | -2.97 | 1.33        | 1.37     |
| 18  | A     | 811 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 18  | B     | 816 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 18  | A     | 810 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 18  | 6     | 609 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 18  | 6     | 603 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 18  | A     | 805 | CLA  | C4D-ND  | -2.96 | 1.33        | 1.37     |
| 18  | 5     | 602 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 18  | 3     | 604 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 21  | B     | 847 | BCR  | C30-C25 | -2.95 | 1.49        | 1.53     |
| 18  | A     | 840 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 18  | A     | 826 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 18  | J     | 101 | CLA  | C4D-ND  | -2.95 | 1.33        | 1.37     |
| 25  | 2     | 616 | CHL  | C1D-C2D | 2.95  | 1.51        | 1.45     |
| 18  | B     | 840 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 25  | 5     | 606 | CHL  | C3D-C2D | 2.94  | 1.47        | 1.39     |
| 18  | 6     | 613 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 18  | B     | 802 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 18  | B     | 837 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 18  | G     | 204 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 18  | B     | 821 | CLA  | C4D-ND  | -2.94 | 1.33        | 1.37     |
| 18  | 3     | 614 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 18  | A     | 841 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 18  | A     | 843 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 18  | F     | 301 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 18  | 3     | 610 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 18  | A     | 823 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 26  | 3     | 618 | LUT  | C18-C5  | 2.93  | 1.55        | 1.50     |
| 18  | L     | 304 | CLA  | C4D-ND  | -2.93 | 1.33        | 1.37     |
| 18  | 6     | 610 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 18  | A     | 818 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 18  | B     | 834 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 3     | 607 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 26  | 5     | 619 | LUT  | C18-C5  | 2.92  | 1.55        | 1.50     |
| 25  | 2     | 606 | CHL  | C1D-C2D | 2.92  | 1.51        | 1.45     |
| 18  | A     | 809 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 18  | B     | 820 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 18  | 3     | 613 | CLA  | C4D-ND  | -2.92 | 1.33        | 1.37     |
| 18  | F     | 303 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | A     | 816 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | B     | 811 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | 6     | 608 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 25  | 5     | 607 | CHL  | MG-NA   | -2.91 | 1.99        | 2.06     |
| 18  | B     | 815 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | 3     | 612 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 25  | 3     | 608 | CHL  | C3D-C2D | 2.91  | 1.47        | 1.39     |
| 18  | A     | 821 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | A     | 832 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | 6     | 611 | CLA  | C4D-ND  | -2.91 | 1.33        | 1.37     |
| 18  | A     | 825 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | B     | 809 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | F     | 305 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | K     | 203 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | B     | 808 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | 6     | 612 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | 5     | 612 | CLA  | C4D-ND  | -2.90 | 1.33        | 1.37     |
| 18  | L     | 302 | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 18  | 5     | 604 | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 18  | B     | 822 | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 18  | 3     | 603 | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 18  | A     | 845 | CLA  | C4D-ND  | -2.89 | 1.33        | 1.37     |
| 18  | 3     | 611 | CLA  | C4D-ND  | -2.88 | 1.33        | 1.37     |
| 21  | G     | 205 | BCR  | C30-C25 | -2.88 | 1.49        | 1.53     |
| 18  | K     | 201 | CLA  | CHC-C1C | 2.88  | 1.42        | 1.35     |
| 18  | B     | 829 | CLA  | CMB-C2B | -2.88 | 1.45        | 1.51     |
| 18  | B     | 804 | CLA  | C4D-ND  | -2.87 | 1.33        | 1.37     |
| 18  | K     | 206 | CLA  | C4D-ND  | -2.87 | 1.33        | 1.37     |
| 18  | 5     | 614 | CLA  | C4D-ND  | -2.87 | 1.33        | 1.37     |
| 18  | 5     | 609 | CLA  | C4D-ND  | -2.87 | 1.33        | 1.37     |
| 18  | 3     | 617 | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 21  | K     | 202 | BCR  | C30-C25 | -2.86 | 1.49        | 1.53     |
| 18  | 6     | 614 | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 18  | B     | 829 | CLA  | C4D-ND  | -2.86 | 1.33        | 1.37     |
| 18  | A     | 854 | CLA  | C4D-ND  | -2.85 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | B     | 824 | CLA  | C4D-ND  | -2.85 | 1.33        | 1.37     |
| 21  | 5     | 621 | BCR  | C30-C25 | -2.85 | 1.49        | 1.53     |
| 26  | 2     | 619 | LUT  | C18-C5  | 2.85  | 1.55        | 1.50     |
| 21  | 3     | 620 | BCR  | C30-C25 | -2.85 | 1.49        | 1.53     |
| 18  | A     | 835 | CLA  | C4D-ND  | -2.85 | 1.33        | 1.37     |
| 25  | 5     | 608 | CHL  | C3D-C2D | 2.85  | 1.46        | 1.39     |
| 26  | 6     | 617 | LUT  | C23-C24 | 2.84  | 1.54        | 1.50     |
| 25  | 2     | 606 | CHL  | C3D-C2D | 2.83  | 1.46        | 1.39     |
| 18  | 5     | 613 | CLA  | C4D-ND  | -2.83 | 1.33        | 1.37     |
| 26  | 6     | 617 | LUT  | C18-C5  | 2.82  | 1.55        | 1.50     |
| 18  | 3     | 609 | CLA  | C4D-ND  | -2.81 | 1.33        | 1.37     |
| 18  | A     | 824 | CLA  | C4D-ND  | -2.80 | 1.33        | 1.37     |
| 18  | 6     | 616 | CLA  | C4D-ND  | -2.79 | 1.33        | 1.37     |
| 25  | 6     | 607 | CHL  | MG-NA   | -2.79 | 1.99        | 2.06     |
| 21  | A     | 848 | BCR  | C30-C25 | -2.79 | 1.49        | 1.53     |
| 26  | 5     | 619 | LUT  | C31-C30 | 2.75  | 1.52        | 1.43     |
| 18  | 2     | 604 | CLA  | C4D-ND  | -2.75 | 1.33        | 1.37     |
| 26  | 3     | 618 | LUT  | C31-C30 | 2.75  | 1.52        | 1.43     |
| 26  | 5     | 619 | LUT  | C23-C24 | 2.73  | 1.54        | 1.50     |
| 26  | 2     | 619 | LUT  | C23-C24 | 2.73  | 1.54        | 1.50     |
| 26  | 5     | 619 | LUT  | C19-C9  | 2.72  | 1.56        | 1.50     |
| 26  | 6     | 617 | LUT  | C19-C9  | 2.71  | 1.56        | 1.50     |
| 18  | 2     | 610 | CLA  | C4D-ND  | -2.70 | 1.34        | 1.37     |
| 26  | 2     | 619 | LUT  | C19-C9  | 2.70  | 1.56        | 1.50     |
| 25  | 2     | 601 | CHL  | MG-NA   | -2.70 | 1.99        | 2.06     |
| 26  | 3     | 618 | LUT  | C19-C9  | 2.69  | 1.56        | 1.50     |
| 21  | B     | 848 | BCR  | C30-C25 | -2.69 | 1.50        | 1.53     |
| 21  | J     | 103 | BCR  | C30-C25 | -2.69 | 1.50        | 1.53     |
| 18  | B     | 833 | CLA  | CMB-C2B | -2.69 | 1.46        | 1.51     |
| 26  | 2     | 619 | LUT  | C31-C30 | 2.68  | 1.51        | 1.43     |
| 18  | A     | 831 | CLA  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 25  | 2     | 607 | CHL  | MG-NA   | -2.66 | 2.00        | 2.06     |
| 21  | L     | 305 | BCR  | C30-C25 | -2.66 | 1.50        | 1.53     |
| 25  | 5     | 608 | CHL  | C1D-C2D | 2.66  | 1.50        | 1.45     |
| 26  | 6     | 617 | LUT  | C31-C30 | 2.65  | 1.51        | 1.43     |
| 18  | B     | 819 | CLA  | CMB-C2B | -2.65 | 1.46        | 1.51     |
| 18  | B     | 818 | CLA  | CMB-C2B | -2.64 | 1.46        | 1.51     |
| 18  | 6     | 606 | CLA  | C4D-ND  | -2.62 | 1.34        | 1.37     |
| 18  | A     | 843 | CLA  | CMB-C2B | -2.62 | 1.46        | 1.51     |
| 18  | B     | 834 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 18  | A     | 822 | CLA  | CMB-C2B | -2.59 | 1.46        | 1.51     |
| 25  | 5     | 607 | CHL  | C4B-CHC | 2.59  | 1.48        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 6     | 607 | CHL  | C4B-CHC | 2.57  | 1.48        | 1.41     |
| 18  | A     | 820 | CLA  | CMB-C2B | -2.57 | 1.46        | 1.51     |
| 18  | 5     | 602 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 18  | B     | 828 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 18  | A     | 802 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 18  | 6     | 604 | CLA  | CMB-C2B | -2.56 | 1.46        | 1.51     |
| 18  | 3     | 606 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 18  | B     | 824 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 18  | B     | 840 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 18  | B     | 837 | CLA  | CMB-C2B | -2.55 | 1.46        | 1.51     |
| 18  | K     | 201 | CLA  | C4D-ND  | -2.55 | 1.34        | 1.37     |
| 18  | B     | 808 | CLA  | CMB-C2B | -2.54 | 1.46        | 1.51     |
| 25  | 2     | 607 | CHL  | C4B-CHC | 2.53  | 1.48        | 1.41     |
| 18  | B     | 830 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 18  | A     | 836 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 18  | B     | 809 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 18  | B     | 839 | CLA  | CMB-C2B | -2.53 | 1.46        | 1.51     |
| 18  | B     | 817 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 23  | B     | 850 | DGD  | O2G-C2G | -2.52 | 1.40        | 1.46     |
| 18  | 2     | 613 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 18  | 2     | 612 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 18  | 3     | 603 | CLA  | CMB-C2B | -2.52 | 1.46        | 1.51     |
| 18  | A     | 810 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | 5     | 612 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | B     | 807 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | A     | 840 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | A     | 845 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | 5     | 611 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | A     | 830 | CLA  | CMB-C2B | -2.51 | 1.46        | 1.51     |
| 18  | B     | 822 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | 6     | 611 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | A     | 837 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | A     | 815 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | B     | 831 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | A     | 838 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | 5     | 603 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | A     | 807 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | F     | 303 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | G     | 204 | CLA  | CMB-C2B | -2.50 | 1.46        | 1.51     |
| 18  | B     | 805 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | 3     | 604 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | A     | 801 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 2     | 609 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 25  | 6     | 601 | CHL  | MG-NA   | -2.49 | 2.00        | 2.06     |
| 18  | G     | 203 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | 2     | 603 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | 3     | 609 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | A     | 825 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | B     | 841 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | A     | 834 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | B     | 821 | CLA  | CMB-C2B | -2.49 | 1.46        | 1.51     |
| 18  | A     | 812 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | A     | 811 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | B     | 811 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | B     | 814 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | A     | 819 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | A     | 821 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | B     | 826 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | A     | 824 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | 6     | 602 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 23  | B     | 850 | DGD  | O1G-C1G | -2.48 | 1.39        | 1.45     |
| 18  | 3     | 607 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | K     | 206 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | 6     | 609 | CLA  | CMB-C2B | -2.48 | 1.46        | 1.51     |
| 18  | B     | 815 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | A     | 841 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | B     | 812 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 6     | 612 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | B     | 825 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 5     | 613 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | A     | 835 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | B     | 835 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 6     | 610 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | K     | 203 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 2     | 614 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | A     | 828 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 3     | 602 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 5     | 610 | CLA  | CMB-C2B | -2.47 | 1.46        | 1.51     |
| 18  | 5     | 601 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | A     | 832 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | A     | 833 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | B     | 816 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | 6     | 608 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | A     | 842 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 2     | 602 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | 6     | 613 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | 6     | 606 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | A     | 829 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | 3     | 614 | CLA  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 18  | 3     | 615 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 26  | 6     | 617 | LUT  | C39-C29 | 2.45  | 1.55        | 1.50     |
| 18  | B     | 802 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | F     | 301 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | A     | 809 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | B     | 836 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | A     | 808 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | A     | 839 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | K     | 204 | CLA  | CMB-C2B | -2.45 | 1.46        | 1.51     |
| 18  | A     | 826 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 25  | 6     | 607 | CHL  | C4C-C3C | 2.44  | 1.49        | 1.45     |
| 18  | B     | 804 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | 3     | 612 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | A     | 818 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | B     | 810 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | A     | 803 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 27  | 3     | 619 | XAT  | O4-C5   | -2.44 | 1.42        | 1.46     |
| 18  | B     | 832 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | A     | 813 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | B     | 803 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | B     | 820 | CLA  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 18  | L     | 303 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | G     | 201 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | L     | 302 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | A     | 827 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | 6     | 616 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | F     | 304 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | B     | 827 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | 2     | 611 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | 3     | 613 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | B     | 806 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | 5     | 614 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | A     | 804 | CLA  | CMB-C2B | -2.43 | 1.46        | 1.51     |
| 18  | B     | 823 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 18  | A     | 816 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |
| 25  | 6     | 607 | CHL  | C1B-CHB | 2.42  | 1.47        | 1.41     |
| 18  | 3     | 610 | CLA  | CMB-C2B | -2.42 | 1.46        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 6     | 614 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 18  | B     | 838 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 25  | 3     | 608 | CHL  | MG-NA   | -2.41 | 2.00        | 2.06     |
| 25  | 2     | 608 | CHL  | MG-NA   | -2.41 | 2.00        | 2.06     |
| 18  | B     | 813 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 18  | A     | 806 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 18  | A     | 814 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 18  | 6     | 603 | CLA  | CMB-C2B | -2.41 | 1.46        | 1.51     |
| 26  | 5     | 619 | LUT  | C39-C29 | 2.40  | 1.55        | 1.50     |
| 25  | 2     | 616 | CHL  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 18  | A     | 805 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 18  | K     | 201 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 26  | 2     | 619 | LUT  | C39-C29 | 2.40  | 1.55        | 1.50     |
| 25  | 2     | 608 | CHL  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 25  | 2     | 601 | CHL  | C4B-CHC | 2.40  | 1.47        | 1.41     |
| 18  | J     | 101 | CLA  | CMB-C2B | -2.40 | 1.46        | 1.51     |
| 18  | 5     | 609 | CLA  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 18  | A     | 854 | CLA  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 26  | 3     | 618 | LUT  | C39-C29 | 2.39  | 1.55        | 1.50     |
| 25  | 2     | 607 | CHL  | C4C-C3C | 2.39  | 1.49        | 1.45     |
| 25  | 5     | 607 | CHL  | C1B-CHB | 2.39  | 1.47        | 1.41     |
| 25  | 2     | 616 | CHL  | MG-NA   | -2.39 | 2.00        | 2.06     |
| 18  | F     | 305 | CLA  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 18  | 3     | 617 | CLA  | CMB-C2B | -2.39 | 1.46        | 1.51     |
| 18  | 3     | 611 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 20  | 5     | 622 | LHG  | O7-C5   | -2.38 | 1.40        | 1.46     |
| 18  | A     | 817 | CLA  | CMB-C2B | -2.38 | 1.46        | 1.51     |
| 18  | L     | 304 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 18  | A     | 823 | CLA  | CMB-C2B | -2.37 | 1.46        | 1.51     |
| 25  | 5     | 615 | CHL  | C4C-C3C | 2.37  | 1.49        | 1.45     |
| 25  | 2     | 616 | CHL  | C4C-C3C | 2.36  | 1.49        | 1.45     |
| 18  | 2     | 604 | CLA  | CMB-C2B | -2.36 | 1.46        | 1.51     |
| 20  | A     | 846 | LHG  | O7-C5   | -2.36 | 1.40        | 1.46     |
| 25  | 5     | 615 | CHL  | C4B-CHC | 2.35  | 1.47        | 1.41     |
| 25  | 5     | 608 | CHL  | C4B-CHC | 2.35  | 1.47        | 1.41     |
| 25  | 6     | 601 | CHL  | C4B-CHC | 2.35  | 1.47        | 1.41     |
| 25  | 2     | 601 | CHL  | C1B-CHB | 2.35  | 1.47        | 1.41     |
| 27  | 3     | 619 | XAT  | O24-C25 | -2.35 | 1.42        | 1.46     |
| 27  | 2     | 620 | XAT  | O24-C25 | -2.34 | 1.42        | 1.46     |
| 18  | 5     | 604 | CLA  | CMB-C2B | -2.33 | 1.46        | 1.51     |
| 25  | 5     | 607 | CHL  | C4C-C3C | 2.33  | 1.49        | 1.45     |
| 25  | 5     | 606 | CHL  | C4C-C3C | 2.33  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 3     | 608 | CHL  | C4B-CHC | 2.32  | 1.47        | 1.41     |
| 18  | K     | 201 | CLA  | C1B-NB  | 2.31  | 1.37        | 1.35     |
| 25  | 5     | 606 | CHL  | C4B-CHC | 2.29  | 1.47        | 1.41     |
| 25  | 2     | 606 | CHL  | C4B-CHC | 2.28  | 1.47        | 1.41     |
| 25  | 3     | 608 | CHL  | C1B-CHB | 2.27  | 1.47        | 1.41     |
| 18  | F     | 305 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 25  | 2     | 608 | CHL  | C4C-C3C | 2.27  | 1.49        | 1.45     |
| 21  | J     | 103 | BCR  | C33-C5  | -2.27 | 1.47        | 1.50     |
| 20  | 6     | 620 | LHG  | O7-C5   | -2.26 | 1.40        | 1.46     |
| 27  | 5     | 620 | XAT  | C22-C21 | -2.26 | 1.51        | 1.54     |
| 25  | 2     | 607 | CHL  | C1B-CHB | 2.24  | 1.47        | 1.41     |
| 27  | 5     | 620 | XAT  | O24-C25 | -2.24 | 1.43        | 1.46     |
| 25  | 6     | 601 | CHL  | C4C-C3C | 2.24  | 1.48        | 1.45     |
| 18  | B     | 829 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 25  | 5     | 607 | CHL  | C1D-ND  | -2.23 | 1.35        | 1.37     |
| 25  | 2     | 606 | CHL  | C4C-C3C | 2.22  | 1.48        | 1.45     |
| 25  | 5     | 606 | CHL  | MG-NA   | -2.21 | 2.01        | 2.06     |
| 25  | 6     | 607 | CHL  | C1D-ND  | -2.21 | 1.35        | 1.37     |
| 25  | 2     | 608 | CHL  | C1B-CHB | 2.21  | 1.47        | 1.41     |
| 18  | B     | 803 | CLA  | CMC-C2C | -2.20 | 1.46        | 1.50     |
| 25  | 2     | 616 | CHL  | C1B-CHB | 2.19  | 1.47        | 1.41     |
| 25  | 5     | 615 | CHL  | MG-NA   | -2.19 | 2.01        | 2.06     |
| 25  | 2     | 601 | CHL  | C4C-C3C | 2.18  | 1.48        | 1.45     |
| 20  | A     | 847 | LHG  | O7-C5   | -2.18 | 1.41        | 1.46     |
| 25  | 5     | 608 | CHL  | C1B-CHB | 2.17  | 1.47        | 1.41     |
| 18  | B     | 839 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 18  | A     | 843 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 18  | B     | 824 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 25  | 5     | 615 | CHL  | C1B-CHB | 2.16  | 1.47        | 1.41     |
| 18  | B     | 828 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 18  | A     | 824 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 25  | 5     | 608 | CHL  | MG-NA   | -2.15 | 2.01        | 2.06     |
| 25  | 2     | 601 | CHL  | C1D-ND  | -2.15 | 1.35        | 1.37     |
| 18  | A     | 827 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 27  | 5     | 620 | XAT  | O4-C5   | -2.15 | 1.43        | 1.46     |
| 25  | 5     | 608 | CHL  | C1D-ND  | -2.14 | 1.35        | 1.37     |
| 18  | B     | 810 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 27  | 6     | 619 | XAT  | O4-C5   | -2.13 | 1.43        | 1.46     |
| 25  | 5     | 606 | CHL  | C1B-CHB | 2.13  | 1.46        | 1.41     |
| 26  | 2     | 619 | LUT  | C38-C25 | 2.13  | 1.54        | 1.50     |
| 18  | B     | 823 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 18  | B     | 820 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | 6     | 601 | CHL  | C1B-CHB | 2.12  | 1.46        | 1.41     |
| 18  | 3     | 603 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 25  | 3     | 608 | CHL  | C4C-C3C | 2.12  | 1.48        | 1.45     |
| 18  | A     | 810 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 18  | 6     | 608 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 18  | B     | 828 | CLA  | C3B-C2B | -2.12 | 1.37        | 1.40     |
| 27  | 6     | 619 | XAT  | O24-C25 | -2.12 | 1.43        | 1.46     |
| 18  | A     | 807 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 18  | A     | 812 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 18  | A     | 822 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 18  | 5     | 610 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 26  | 6     | 617 | LUT  | C38-C25 | 2.10  | 1.54        | 1.50     |
| 25  | 6     | 601 | CHL  | C1D-ND  | -2.10 | 1.35        | 1.37     |
| 18  | 3     | 606 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 18  | 2     | 610 | CLA  | CMB-C2B | -2.10 | 1.47        | 1.51     |
| 18  | A     | 818 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 18  | 6     | 610 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | B     | 802 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | B     | 815 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | 5     | 614 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | 3     | 613 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | A     | 813 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | B     | 823 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 18  | B     | 830 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | A     | 814 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 18  | B     | 808 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | A     | 840 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | B     | 813 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 18  | B     | 819 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | B     | 816 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | L     | 304 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | A     | 806 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 18  | 2     | 609 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 25  | 2     | 606 | CHL  | MG-NA   | -2.07 | 2.01        | 2.06     |
| 18  | B     | 806 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | B     | 804 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | 2     | 603 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | B     | 837 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | K     | 201 | CLA  | C3B-C2B | -2.07 | 1.37        | 1.40     |
| 18  | A     | 825 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | A     | 809 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | A     | 821 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | A     | 836 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 18  | 5     | 602 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | A     | 805 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | B     | 818 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | A     | 802 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | B     | 840 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | A     | 854 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | B     | 802 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 18  | L     | 302 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | 2     | 604 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | B     | 803 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | B     | 808 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 18  | 6     | 613 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | 5     | 603 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | 6     | 609 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | A     | 814 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | 3     | 617 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | B     | 805 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | A     | 820 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 18  | F     | 301 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | 5     | 611 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | 6     | 602 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | 6     | 603 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | 3     | 615 | CLA  | CBD-CAD | 2.05  | 1.56        | 1.51     |
| 18  | 2     | 614 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | 6     | 606 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 26  | 5     | 619 | LUT  | C38-C25 | 2.05  | 1.54        | 1.50     |
| 18  | A     | 818 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | A     | 826 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | 6     | 612 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | B     | 838 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 25  | 2     | 608 | CHL  | C1D-ND  | -2.05 | 1.35        | 1.37     |
| 18  | A     | 804 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | A     | 830 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | B     | 835 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | A     | 843 | CLA  | C3B-C2B | -2.05 | 1.37        | 1.40     |
| 18  | A     | 828 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 18  | 2     | 602 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | A     | 831 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | B     | 834 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | A     | 828 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | A     | 803 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | 2     | 612 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | G     | 204 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | L     | 303 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | B     | 831 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | 6     | 611 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 25  | 2     | 607 | CHL  | C1D-ND  | -2.04 | 1.35        | 1.37     |
| 25  | 5     | 608 | CHL  | C4C-C3C | 2.04  | 1.48        | 1.45     |
| 18  | B     | 841 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 18  | A     | 801 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 813 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 826 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | A     | 819 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 811 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 807 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | 3     | 610 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 27  | 2     | 620 | XAT  | O4-C5   | -2.03 | 1.43        | 1.46     |
| 18  | B     | 826 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 18  | 2     | 611 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 833 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 822 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 25  | 2     | 606 | CHL  | C1B-CHB | 2.03  | 1.46        | 1.41     |
| 18  | A     | 832 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | A     | 811 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | B     | 825 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 18  | A     | 842 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | K     | 206 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | 3     | 603 | CLA  | C3B-C2B | -2.02 | 1.37        | 1.40     |
| 18  | A     | 815 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | A     | 823 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | 3     | 604 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | B     | 814 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | 3     | 607 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | A     | 834 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | K     | 203 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | 2     | 610 | CLA  | C3B-CAB | -2.02 | 1.43        | 1.47     |
| 26  | 5     | 619 | LUT  | C40-C33 | 2.02  | 1.55        | 1.50     |
| 18  | A     | 829 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | A     | 816 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 18  | 2     | 610 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | A     | 835 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | A     | 841 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | 5     | 609 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | A     | 808 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | F     | 304 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 25  | 5     | 615 | CHL  | C1D-ND  | -2.01 | 1.35        | 1.37     |
| 18  | A     | 806 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | A     | 835 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | 6     | 604 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | 3     | 609 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | A     | 819 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | J     | 101 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | A     | 841 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | B     | 809 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | 3     | 614 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | A     | 817 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | G     | 203 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | A     | 804 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | B     | 825 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | B     | 815 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | B     | 827 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | B     | 832 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | B     | 837 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 18  | B     | 817 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 18  | B     | 827 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 18  | 5     | 612 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 18  | A     | 805 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 18  | A     | 829 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 18  | 5     | 613 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 18  | B     | 836 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 18  | 3     | 610 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 18  | 3     | 611 | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |

All (1658) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 26  | 2     | 619 | LUT  | C18-C5-C6   | -14.02 | 108.78      | 124.53   |
| 26  | 5     | 619 | LUT  | C18-C5-C6   | -12.36 | 110.65      | 124.53   |
| 26  | 6     | 617 | LUT  | C18-C5-C6   | -12.10 | 110.94      | 124.53   |
| 26  | 2     | 619 | LUT  | C15-C14-C13 | -11.96 | 110.24      | 127.31   |
| 26  | 3     | 618 | LUT  | C18-C5-C6   | -11.81 | 111.26      | 124.53   |
| 26  | 3     | 618 | LUT  | C15-C14-C13 | -11.59 | 110.77      | 127.31   |
| 26  | 2     | 619 | LUT  | C11-C10-C9  | -11.19 | 111.34      | 127.31   |
| 26  | 5     | 619 | LUT  | C15-C14-C13 | -10.86 | 111.82      | 127.31   |
| 26  | 6     | 617 | LUT  | C15-C14-C13 | -10.76 | 111.96      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 27  | 6     | 619 | XAT  | O24-C25-C24 | 10.74  | 121.45      | 113.38   |
| 26  | 3     | 618 | LUT  | C11-C10-C9  | -10.09 | 112.90      | 127.31   |
| 26  | 6     | 617 | LUT  | C11-C10-C9  | -9.89  | 113.19      | 127.31   |
| 27  | 2     | 620 | XAT  | C18-C5-C6   | -9.89  | 105.69      | 122.26   |
| 26  | 5     | 619 | LUT  | C31-C30-C29 | -9.85  | 113.26      | 127.31   |
| 26  | 6     | 617 | LUT  | C31-C30-C29 | -9.74  | 113.40      | 127.31   |
| 27  | 2     | 620 | XAT  | O24-C25-C24 | 9.73   | 120.69      | 113.38   |
| 26  | 5     | 619 | LUT  | C11-C10-C9  | -9.60  | 113.62      | 127.31   |
| 26  | 3     | 618 | LUT  | C31-C30-C29 | -9.37  | 113.93      | 127.31   |
| 27  | 2     | 620 | XAT  | O4-C5-C18   | 9.33   | 126.23      | 115.06   |
| 25  | 2     | 606 | CHL  | CMD-C2D-C1D | 8.40   | 139.52      | 124.71   |
| 25  | 5     | 606 | CHL  | CMD-C2D-C1D | 8.30   | 139.33      | 124.71   |
| 26  | 2     | 619 | LUT  | C31-C30-C29 | -8.29  | 115.48      | 127.31   |
| 25  | 3     | 608 | CHL  | CMD-C2D-C1D | 8.29   | 139.32      | 124.71   |
| 25  | 2     | 608 | CHL  | CMD-C2D-C1D | 8.26   | 139.26      | 124.71   |
| 25  | 5     | 615 | CHL  | CMD-C2D-C1D | 8.24   | 139.24      | 124.71   |
| 25  | 2     | 616 | CHL  | CMD-C2D-C1D | 8.22   | 139.19      | 124.71   |
| 25  | 2     | 607 | CHL  | CMD-C2D-C1D | 8.14   | 139.05      | 124.71   |
| 25  | 6     | 601 | CHL  | CMD-C2D-C1D | 8.11   | 139.01      | 124.71   |
| 25  | 5     | 608 | CHL  | CMD-C2D-C1D | 8.09   | 138.97      | 124.71   |
| 25  | 2     | 601 | CHL  | CMD-C2D-C1D | 8.05   | 138.90      | 124.71   |
| 25  | 6     | 607 | CHL  | CMD-C2D-C1D | 8.05   | 138.89      | 124.71   |
| 25  | 5     | 607 | CHL  | CMD-C2D-C1D | 7.93   | 138.68      | 124.71   |
| 27  | 5     | 620 | XAT  | O24-C25-C24 | 7.76   | 119.21      | 113.38   |
| 25  | 2     | 606 | CHL  | C2C-C3C-C4C | -7.44  | 101.19      | 106.49   |
| 25  | 2     | 601 | CHL  | CHD-C1D-ND  | -7.44  | 117.62      | 124.45   |
| 25  | 5     | 607 | CHL  | CHD-C1D-ND  | -7.36  | 117.69      | 124.45   |
| 25  | 5     | 615 | CHL  | C2C-C3C-C4C | -7.28  | 101.30      | 106.49   |
| 25  | 2     | 607 | CHL  | C2C-C3C-C4C | -7.25  | 101.32      | 106.49   |
| 25  | 6     | 607 | CHL  | CHD-C1D-ND  | -7.22  | 117.82      | 124.45   |
| 25  | 5     | 606 | CHL  | C2C-C3C-C4C | -7.21  | 101.13      | 106.49   |
| 25  | 5     | 608 | CHL  | C2C-C3C-C4C | -7.21  | 101.35      | 106.49   |
| 27  | 6     | 619 | XAT  | C26-C27-C28 | -7.18  | 110.80      | 125.99   |
| 25  | 6     | 601 | CHL  | C2C-C3C-C4C | -7.15  | 101.39      | 106.49   |
| 25  | 6     | 607 | CHL  | C2C-C3C-C4C | -7.13  | 101.41      | 106.49   |
| 18  | K     | 201 | CLA  | C4A-NA-C1A  | 7.12   | 109.91      | 106.71   |
| 18  | A     | 845 | CLA  | C4A-NA-C1A  | 7.10   | 109.90      | 106.71   |
| 18  | B     | 804 | CLA  | C4A-NA-C1A  | 7.09   | 109.89      | 106.71   |
| 25  | 2     | 616 | CHL  | C2C-C3C-C4C | -7.08  | 101.44      | 106.49   |
| 25  | 2     | 608 | CHL  | C2C-C3C-C4C | -7.06  | 101.45      | 106.49   |
| 25  | 2     | 607 | CHL  | CHD-C1D-ND  | -7.03  | 117.99      | 124.45   |
| 27  | 5     | 620 | XAT  | C18-C5-C6   | -7.03  | 110.48      | 122.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | 5     | 619 | LUT  | C38-C25-C24 | -7.03 | 108.52      | 123.56   |
| 27  | 5     | 620 | XAT  | C27-C28-C29 | -7.03 | 114.62      | 125.53   |
| 18  | 3     | 611 | CLA  | C4A-NA-C1A  | 6.99  | 109.85      | 106.71   |
| 26  | 6     | 617 | LUT  | C38-C25-C24 | -6.96 | 108.68      | 123.56   |
| 26  | 2     | 619 | LUT  | C38-C25-C24 | -6.95 | 108.69      | 123.56   |
| 27  | 3     | 619 | XAT  | C38-C25-C26 | -6.91 | 110.68      | 122.26   |
| 18  | 2     | 604 | CLA  | C4A-NA-C1A  | 6.90  | 109.81      | 106.71   |
| 25  | 5     | 606 | CHL  | C1B-C2B-C3B | -6.90 | 100.50      | 106.92   |
| 25  | 2     | 601 | CHL  | C2C-C3C-C4C | -6.90 | 101.57      | 106.49   |
| 25  | 5     | 607 | CHL  | C2C-C3C-C4C | -6.88 | 101.58      | 106.49   |
| 18  | K     | 204 | CLA  | C4A-NA-C1A  | 6.87  | 109.80      | 106.71   |
| 25  | 2     | 608 | CHL  | CHD-C1D-ND  | -6.86 | 118.15      | 124.45   |
| 25  | 6     | 601 | CHL  | CHD-C1D-ND  | -6.85 | 118.16      | 124.45   |
| 18  | B     | 803 | CLA  | C4A-NA-C1A  | 6.82  | 109.77      | 106.71   |
| 18  | 5     | 613 | CLA  | C4A-NA-C1A  | 6.82  | 109.77      | 106.71   |
| 18  | A     | 839 | CLA  | C4A-NA-C1A  | 6.81  | 109.77      | 106.71   |
| 18  | A     | 810 | CLA  | C4A-NA-C1A  | 6.80  | 109.76      | 106.71   |
| 18  | B     | 837 | CLA  | C4A-NA-C1A  | 6.80  | 109.76      | 106.71   |
| 18  | F     | 304 | CLA  | C4A-NA-C1A  | 6.79  | 109.76      | 106.71   |
| 18  | A     | 805 | CLA  | C4A-NA-C1A  | 6.78  | 109.75      | 106.71   |
| 18  | 5     | 604 | CLA  | C4A-NA-C1A  | 6.77  | 109.75      | 106.71   |
| 18  | L     | 303 | CLA  | C4A-NA-C1A  | 6.75  | 109.74      | 106.71   |
| 18  | A     | 818 | CLA  | C4A-NA-C1A  | 6.74  | 109.73      | 106.71   |
| 18  | B     | 808 | CLA  | C4A-NA-C1A  | 6.72  | 109.73      | 106.71   |
| 25  | 3     | 608 | CHL  | CHD-C1D-ND  | -6.72 | 118.28      | 124.45   |
| 18  | A     | 831 | CLA  | C4A-NA-C1A  | 6.70  | 109.72      | 106.71   |
| 25  | 2     | 601 | CHL  | C1B-C2B-C3B | -6.70 | 100.69      | 106.92   |
| 18  | A     | 819 | CLA  | C4A-NA-C1A  | 6.68  | 109.71      | 106.71   |
| 18  | B     | 826 | CLA  | C4A-NA-C1A  | 6.68  | 109.71      | 106.71   |
| 18  | 6     | 603 | CLA  | C4A-NA-C1A  | 6.68  | 109.71      | 106.71   |
| 18  | A     | 816 | CLA  | C4A-NA-C1A  | 6.67  | 109.70      | 106.71   |
| 18  | A     | 830 | CLA  | C4A-NA-C1A  | 6.67  | 109.70      | 106.71   |
| 18  | L     | 302 | CLA  | C4A-NA-C1A  | 6.67  | 109.70      | 106.71   |
| 18  | A     | 822 | CLA  | C4A-NA-C1A  | 6.66  | 109.70      | 106.71   |
| 18  | A     | 841 | CLA  | C4A-NA-C1A  | 6.66  | 109.70      | 106.71   |
| 18  | B     | 812 | CLA  | C4A-NA-C1A  | 6.65  | 109.70      | 106.71   |
| 18  | K     | 203 | CLA  | C4A-NA-C1A  | 6.65  | 109.70      | 106.71   |
| 18  | A     | 804 | CLA  | C4A-NA-C1A  | 6.64  | 109.69      | 106.71   |
| 18  | 6     | 613 | CLA  | C4A-NA-C1A  | 6.64  | 109.69      | 106.71   |
| 18  | G     | 201 | CLA  | C4A-NA-C1A  | 6.63  | 109.69      | 106.71   |
| 18  | 3     | 612 | CLA  | C4A-NA-C1A  | 6.63  | 109.69      | 106.71   |
| 26  | 3     | 618 | LUT  | C38-C25-C24 | -6.62 | 109.40      | 123.56   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 18  | B     | 822 | CLA  | C4A-NA-C1A | 6.62  | 109.68      | 106.71   |
| 18  | B     | 814 | CLA  | C4A-NA-C1A | 6.61  | 109.68      | 106.71   |
| 18  | A     | 812 | CLA  | C4A-NA-C1A | 6.60  | 109.67      | 106.71   |
| 18  | 3     | 607 | CLA  | C4A-NA-C1A | 6.60  | 109.67      | 106.71   |
| 18  | B     | 832 | CLA  | C4A-NA-C1A | 6.60  | 109.67      | 106.71   |
| 18  | 5     | 614 | CLA  | C4A-NA-C1A | 6.60  | 109.67      | 106.71   |
| 18  | A     | 802 | CLA  | C4A-NA-C1A | 6.59  | 109.67      | 106.71   |
| 18  | B     | 815 | CLA  | C4A-NA-C1A | 6.58  | 109.67      | 106.71   |
| 18  | A     | 835 | CLA  | C4A-NA-C1A | 6.58  | 109.66      | 106.71   |
| 18  | 3     | 602 | CLA  | C4A-NA-C1A | 6.58  | 109.66      | 106.71   |
| 25  | 5     | 615 | CHL  | CHD-C1D-ND | -6.57 | 118.41      | 124.45   |
| 18  | 6     | 612 | CLA  | C4A-NA-C1A | 6.57  | 109.66      | 106.71   |
| 18  | B     | 819 | CLA  | C4A-NA-C1A | 6.56  | 109.66      | 106.71   |
| 18  | 2     | 614 | CLA  | C4A-NA-C1A | 6.56  | 109.66      | 106.71   |
| 18  | K     | 206 | CLA  | C4A-NA-C1A | 6.56  | 109.66      | 106.71   |
| 18  | B     | 807 | CLA  | C4A-NA-C1A | 6.56  | 109.65      | 106.71   |
| 18  | 2     | 602 | CLA  | C4A-NA-C1A | 6.55  | 109.65      | 106.71   |
| 18  | 6     | 616 | CLA  | C4A-NA-C1A | 6.55  | 109.65      | 106.71   |
| 18  | A     | 842 | CLA  | C4A-NA-C1A | 6.54  | 109.65      | 106.71   |
| 18  | A     | 823 | CLA  | C4A-NA-C1A | 6.54  | 109.65      | 106.71   |
| 18  | B     | 831 | CLA  | C4A-NA-C1A | 6.54  | 109.65      | 106.71   |
| 18  | B     | 820 | CLA  | C4A-NA-C1A | 6.53  | 109.64      | 106.71   |
| 18  | 5     | 612 | CLA  | C4A-NA-C1A | 6.53  | 109.64      | 106.71   |
| 18  | 3     | 603 | CLA  | C4A-NA-C1A | 6.53  | 109.64      | 106.71   |
| 25  | 2     | 616 | CHL  | CHD-C1D-ND | -6.53 | 118.46      | 124.45   |
| 18  | 2     | 613 | CLA  | C4A-NA-C1A | 6.52  | 109.64      | 106.71   |
| 18  | A     | 832 | CLA  | C4A-NA-C1A | 6.51  | 109.64      | 106.71   |
| 18  | B     | 825 | CLA  | C4A-NA-C1A | 6.51  | 109.64      | 106.71   |
| 18  | B     | 818 | CLA  | C4A-NA-C1A | 6.51  | 109.63      | 106.71   |
| 18  | A     | 809 | CLA  | C4A-NA-C1A | 6.51  | 109.63      | 106.71   |
| 18  | B     | 817 | CLA  | C4A-NA-C1A | 6.51  | 109.63      | 106.71   |
| 18  | B     | 834 | CLA  | C4A-NA-C1A | 6.51  | 109.63      | 106.71   |
| 18  | F     | 303 | CLA  | C4A-NA-C1A | 6.51  | 109.63      | 106.71   |
| 18  | 2     | 603 | CLA  | C4A-NA-C1A | 6.51  | 109.63      | 106.71   |
| 27  | 3     | 619 | XAT  | C18-C5-C6  | -6.50 | 111.36      | 122.26   |
| 18  | L     | 304 | CLA  | C4A-NA-C1A | 6.50  | 109.63      | 106.71   |
| 18  | 6     | 608 | CLA  | C4A-NA-C1A | 6.50  | 109.63      | 106.71   |
| 18  | B     | 829 | CLA  | C4A-NA-C1A | 6.49  | 109.63      | 106.71   |
| 18  | A     | 817 | CLA  | C4A-NA-C1A | 6.49  | 109.62      | 106.71   |
| 18  | A     | 813 | CLA  | C4A-NA-C1A | 6.49  | 109.62      | 106.71   |
| 18  | B     | 806 | CLA  | C4A-NA-C1A | 6.49  | 109.62      | 106.71   |
| 18  | A     | 815 | CLA  | C4A-NA-C1A | 6.49  | 109.62      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 3     | 609 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 18  | 5     | 609 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 18  | A     | 824 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 18  | A     | 836 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 18  | F     | 305 | CLA  | C4A-NA-C1A  | 6.48  | 109.62      | 106.71   |
| 27  | 5     | 620 | XAT  | O4-C5-C4    | 6.47  | 118.24      | 113.38   |
| 18  | A     | 808 | CLA  | C4A-NA-C1A  | 6.47  | 109.61      | 106.71   |
| 26  | 2     | 619 | LUT  | C1-C6-C5    | -6.47 | 113.50      | 122.61   |
| 18  | A     | 837 | CLA  | C4A-NA-C1A  | 6.46  | 109.61      | 106.71   |
| 18  | A     | 807 | CLA  | C4A-NA-C1A  | 6.46  | 109.61      | 106.71   |
| 18  | B     | 835 | CLA  | C4A-NA-C1A  | 6.46  | 109.61      | 106.71   |
| 18  | F     | 301 | CLA  | C4A-NA-C1A  | 6.46  | 109.61      | 106.71   |
| 18  | 3     | 614 | CLA  | C4A-NA-C1A  | 6.46  | 109.61      | 106.71   |
| 18  | 3     | 606 | CLA  | C4A-NA-C1A  | 6.44  | 109.60      | 106.71   |
| 18  | B     | 839 | CLA  | C4A-NA-C1A  | 6.44  | 109.60      | 106.71   |
| 18  | 6     | 609 | CLA  | C4A-NA-C1A  | 6.43  | 109.60      | 106.71   |
| 18  | 5     | 601 | CLA  | C4A-NA-C1A  | 6.42  | 109.59      | 106.71   |
| 25  | 5     | 606 | CHL  | CHD-C1D-ND  | -6.41 | 118.56      | 124.45   |
| 18  | A     | 829 | CLA  | C4A-NA-C1A  | 6.41  | 109.59      | 106.71   |
| 18  | B     | 830 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 18  | B     | 810 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 18  | 6     | 604 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 18  | 5     | 603 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 18  | B     | 805 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 18  | B     | 827 | CLA  | C4A-NA-C1A  | 6.40  | 109.58      | 106.71   |
| 25  | 2     | 606 | CHL  | CHD-C1D-ND  | -6.40 | 118.58      | 124.45   |
| 18  | G     | 204 | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 18  | 6     | 606 | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 18  | 2     | 612 | CLA  | C4A-NA-C1A  | 6.39  | 109.58      | 106.71   |
| 18  | B     | 821 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 18  | A     | 834 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 18  | 2     | 609 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 18  | 5     | 610 | CLA  | C4A-NA-C1A  | 6.37  | 109.57      | 106.71   |
| 18  | 2     | 611 | CLA  | C4A-NA-C1A  | 6.36  | 109.57      | 106.71   |
| 18  | A     | 806 | CLA  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 27  | 6     | 619 | XAT  | C35-C34-C33 | -6.36 | 118.24      | 127.31   |
| 18  | A     | 833 | CLA  | C4A-NA-C1A  | 6.36  | 109.56      | 106.71   |
| 18  | B     | 809 | CLA  | C4A-NA-C1A  | 6.35  | 109.56      | 106.71   |
| 18  | B     | 840 | CLA  | C4A-NA-C1A  | 6.34  | 109.56      | 106.71   |
| 18  | 3     | 613 | CLA  | C4A-NA-C1A  | 6.34  | 109.56      | 106.71   |
| 18  | A     | 826 | CLA  | C4A-NA-C1A  | 6.34  | 109.56      | 106.71   |
| 18  | 3     | 610 | CLA  | C4A-NA-C1A  | 6.33  | 109.55      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 838 | CLA  | C4A-NA-C1A  | 6.32  | 109.55      | 106.71   |
| 18  | B     | 823 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 18  | G     | 203 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 18  | J     | 101 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 18  | B     | 824 | CLA  | C4A-NA-C1A  | 6.30  | 109.54      | 106.71   |
| 18  | A     | 811 | CLA  | C4A-NA-C1A  | 6.29  | 109.54      | 106.71   |
| 18  | A     | 814 | CLA  | C4A-NA-C1A  | 6.29  | 109.53      | 106.71   |
| 18  | B     | 838 | CLA  | C4A-NA-C1A  | 6.28  | 109.53      | 106.71   |
| 18  | A     | 828 | CLA  | C4A-NA-C1A  | 6.27  | 109.53      | 106.71   |
| 18  | 6     | 610 | CLA  | C4A-NA-C1A  | 6.27  | 109.53      | 106.71   |
| 25  | 5     | 608 | CHL  | CHD-C1D-ND  | -6.27 | 118.69      | 124.45   |
| 18  | A     | 821 | CLA  | C4A-NA-C1A  | 6.27  | 109.52      | 106.71   |
| 18  | 6     | 611 | CLA  | C4A-NA-C1A  | 6.26  | 109.52      | 106.71   |
| 18  | 6     | 602 | CLA  | C4A-NA-C1A  | 6.26  | 109.52      | 106.71   |
| 18  | A     | 843 | CLA  | C4A-NA-C1A  | 6.26  | 109.52      | 106.71   |
| 18  | A     | 840 | CLA  | C4A-NA-C1A  | 6.25  | 109.52      | 106.71   |
| 18  | 3     | 604 | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |
| 18  | B     | 816 | CLA  | C4A-NA-C1A  | 6.24  | 109.51      | 106.71   |
| 18  | A     | 827 | CLA  | C4A-NA-C1A  | 6.23  | 109.51      | 106.71   |
| 18  | B     | 841 | CLA  | C4A-NA-C1A  | 6.23  | 109.51      | 106.71   |
| 18  | 3     | 617 | CLA  | C4A-NA-C1A  | 6.22  | 109.50      | 106.71   |
| 18  | B     | 802 | CLA  | C4A-NA-C1A  | 6.22  | 109.50      | 106.71   |
| 18  | B     | 811 | CLA  | C4A-NA-C1A  | 6.21  | 109.50      | 106.71   |
| 18  | 3     | 615 | CLA  | C4A-NA-C1A  | 6.21  | 109.50      | 106.71   |
| 18  | 5     | 602 | CLA  | C4A-NA-C1A  | 6.20  | 109.49      | 106.71   |
| 18  | B     | 836 | CLA  | C4A-NA-C1A  | 6.18  | 109.49      | 106.71   |
| 27  | 6     | 619 | XAT  | C18-C5-C6   | -6.15 | 111.95      | 122.26   |
| 18  | B     | 828 | CLA  | C4A-NA-C1A  | 6.14  | 109.47      | 106.71   |
| 18  | A     | 825 | CLA  | C4A-NA-C1A  | 6.13  | 109.46      | 106.71   |
| 27  | 6     | 619 | XAT  | C6-C7-C8    | -6.13 | 113.04      | 125.99   |
| 18  | A     | 801 | CLA  | C4A-NA-C1A  | 6.11  | 109.45      | 106.71   |
| 26  | 5     | 619 | LUT  | C8-C7-C6    | -6.11 | 110.04      | 127.20   |
| 18  | A     | 820 | CLA  | C4A-NA-C1A  | 6.10  | 109.45      | 106.71   |
| 27  | 3     | 619 | XAT  | C6-C7-C8    | -6.09 | 113.11      | 125.99   |
| 26  | 2     | 619 | LUT  | C7-C6-C5    | -6.06 | 106.77      | 121.46   |
| 18  | B     | 813 | CLA  | C4A-NA-C1A  | 6.06  | 109.43      | 106.71   |
| 27  | 6     | 619 | XAT  | C38-C25-C26 | -6.01 | 112.19      | 122.26   |
| 18  | A     | 854 | CLA  | C4A-NA-C1A  | 5.93  | 109.37      | 106.71   |
| 18  | B     | 833 | CLA  | C4A-NA-C1A  | 5.91  | 109.36      | 106.71   |
| 27  | 2     | 620 | XAT  | C38-C25-C26 | -5.83 | 112.49      | 122.26   |
| 26  | 6     | 617 | LUT  | C35-C15-C14 | -5.82 | 111.55      | 123.47   |
| 18  | 2     | 610 | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 6     | 614 | CLA  | C4A-NA-C1A  | 5.77  | 109.30      | 106.71   |
| 26  | 3     | 618 | LUT  | C1-C6-C5    | -5.68 | 114.61      | 122.61   |
| 18  | A     | 803 | CLA  | C4A-NA-C1A  | 5.64  | 109.24      | 106.71   |
| 26  | 3     | 618 | LUT  | C8-C7-C6    | -5.63 | 111.39      | 127.20   |
| 27  | 2     | 620 | XAT  | C26-C27-C28 | -5.44 | 114.50      | 125.99   |
| 26  | 5     | 619 | LUT  | C1-C6-C5    | -5.42 | 114.98      | 122.61   |
| 27  | 3     | 619 | XAT  | O4-C5-C18   | 5.42  | 121.55      | 115.06   |
| 27  | 3     | 619 | XAT  | O24-C25-C24 | 5.27  | 117.34      | 113.38   |
| 26  | 2     | 619 | LUT  | C8-C7-C6    | -5.25 | 112.45      | 127.20   |
| 25  | 2     | 606 | CHL  | C3C-C4C-NC  | 5.21  | 116.41      | 110.57   |
| 26  | 6     | 617 | LUT  | C8-C7-C6    | -5.18 | 112.66      | 127.20   |
| 26  | 6     | 617 | LUT  | C35-C34-C33 | -5.14 | 119.97      | 127.31   |
| 25  | 2     | 601 | CHL  | O2D-CGD-CBD | 5.14  | 120.40      | 111.27   |
| 25  | 2     | 616 | CHL  | O2D-CGD-CBD | 5.12  | 120.37      | 111.27   |
| 26  | 6     | 617 | LUT  | C7-C6-C5    | -5.10 | 109.11      | 121.46   |
| 25  | 5     | 608 | CHL  | C3C-C4C-NC  | 5.08  | 116.27      | 110.57   |
| 25  | 5     | 606 | CHL  | O2D-CGD-CBD | 5.08  | 120.29      | 111.27   |
| 25  | 5     | 606 | CHL  | C3C-C4C-NC  | 5.04  | 116.07      | 110.57   |
| 26  | 2     | 619 | LUT  | C30-C31-C32 | -5.03 | 107.51      | 123.22   |
| 25  | 2     | 607 | CHL  | O2D-CGD-CBD | 4.99  | 120.13      | 111.27   |
| 26  | 3     | 618 | LUT  | C35-C15-C14 | -4.94 | 113.36      | 123.47   |
| 25  | 5     | 607 | CHL  | C1B-CHB-C4A | -4.92 | 120.38      | 130.12   |
| 26  | 2     | 619 | LUT  | C7-C8-C9    | -4.86 | 118.89      | 126.23   |
| 25  | 5     | 615 | CHL  | C3C-C4C-NC  | 4.85  | 116.01      | 110.57   |
| 27  | 5     | 620 | XAT  | O4-C5-C18   | 4.83  | 120.85      | 115.06   |
| 26  | 5     | 619 | LUT  | C35-C15-C14 | -4.75 | 113.75      | 123.47   |
| 27  | 3     | 619 | XAT  | O24-C25-C38 | 4.70  | 120.69      | 115.06   |
| 27  | 6     | 619 | XAT  | O4-C5-C18   | 4.70  | 120.68      | 115.06   |
| 27  | 5     | 620 | XAT  | C35-C34-C33 | -4.66 | 120.66      | 127.31   |
| 25  | 3     | 608 | CHL  | C2C-C1C-NC  | 4.66  | 114.34      | 109.97   |
| 25  | 5     | 607 | CHL  | O2D-CGD-CBD | 4.65  | 119.54      | 111.27   |
| 25  | 2     | 606 | CHL  | C3D-C2D-C1D | -4.64 | 99.49       | 105.83   |
| 25  | 5     | 608 | CHL  | C3D-C2D-C1D | -4.60 | 99.55       | 105.83   |
| 25  | 5     | 615 | CHL  | O2D-CGD-CBD | 4.60  | 119.45      | 111.27   |
| 26  | 2     | 619 | LUT  | C35-C15-C14 | -4.59 | 114.08      | 123.47   |
| 25  | 3     | 608 | CHL  | C3D-C2D-C1D | -4.54 | 99.63       | 105.83   |
| 27  | 6     | 619 | XAT  | O4-C5-C4    | 4.54  | 116.79      | 113.38   |
| 25  | 2     | 616 | CHL  | C3C-C4C-NC  | 4.53  | 115.65      | 110.57   |
| 25  | 5     | 606 | CHL  | C3D-C2D-C1D | -4.52 | 99.66       | 105.83   |
| 25  | 5     | 615 | CHL  | C3D-C2D-C1D | -4.51 | 99.68       | 105.83   |
| 25  | 2     | 616 | CHL  | C3D-C2D-C1D | -4.50 | 99.70       | 105.83   |
| 25  | 3     | 608 | CHL  | C3C-C4C-NC  | 4.48  | 115.60      | 110.57   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 2     | 608 | CHL  | C3D-C2D-C1D | -4.47 | 99.73       | 105.83   |
| 25  | 6     | 601 | CHL  | C3C-C4C-NC  | 4.47  | 115.58      | 110.57   |
| 25  | 6     | 601 | CHL  | C3D-C2D-C1D | -4.44 | 99.77       | 105.83   |
| 25  | 2     | 608 | CHL  | C3C-C4C-NC  | 4.40  | 115.51      | 110.57   |
| 18  | A     | 814 | CLA  | CMB-C2B-C1B | -4.40 | 121.70      | 128.46   |
| 25  | 6     | 607 | CHL  | C1B-CHB-C4A | -4.40 | 121.40      | 130.12   |
| 27  | 3     | 619 | XAT  | C26-C27-C28 | -4.39 | 116.70      | 125.99   |
| 25  | 2     | 601 | CHL  | C3D-C2D-C1D | -4.37 | 99.86       | 105.83   |
| 18  | 5     | 609 | CLA  | CMB-C2B-C1B | -4.37 | 121.75      | 128.46   |
| 27  | 3     | 619 | XAT  | C18-C5-C4   | 4.37  | 119.19      | 114.28   |
| 27  | 5     | 620 | XAT  | C6-C7-C8    | -4.35 | 116.79      | 125.99   |
| 25  | 2     | 606 | CHL  | O2D-CGD-CBD | 4.35  | 119.00      | 111.27   |
| 18  | B     | 833 | CLA  | CMB-C2B-C1B | -4.35 | 121.78      | 128.46   |
| 18  | A     | 833 | CLA  | CMB-C2B-C1B | -4.35 | 121.78      | 128.46   |
| 25  | 2     | 607 | CHL  | C3D-C2D-C1D | -4.34 | 99.90       | 105.83   |
| 26  | 6     | 617 | LUT  | C10-C11-C12 | -4.33 | 109.71      | 123.22   |
| 25  | 5     | 607 | CHL  | C3D-C2D-C1D | -4.33 | 99.93       | 105.83   |
| 18  | 2     | 604 | CLA  | CMB-C2B-C1B | -4.31 | 121.83      | 128.46   |
| 26  | 5     | 619 | LUT  | C35-C34-C33 | -4.31 | 121.16      | 127.31   |
| 18  | A     | 809 | CLA  | CMB-C2B-C1B | -4.31 | 121.84      | 128.46   |
| 25  | 2     | 606 | CHL  | CHD-C4C-C3C | -4.31 | 118.51      | 124.84   |
| 25  | 2     | 607 | CHL  | C3C-C4C-NC  | 4.30  | 115.39      | 110.57   |
| 26  | 6     | 617 | LUT  | C30-C31-C32 | -4.29 | 109.82      | 123.22   |
| 18  | A     | 816 | CLA  | CMB-C2B-C1B | -4.29 | 121.88      | 128.46   |
| 20  | 2     | 622 | LHG  | O4-P-O5     | 4.28  | 133.39      | 112.24   |
| 18  | 2     | 610 | CLA  | CMB-C2B-C1B | -4.28 | 121.89      | 128.46   |
| 20  | 6     | 620 | LHG  | O4-P-O5     | 4.26  | 133.31      | 112.24   |
| 18  | A     | 805 | CLA  | CMB-C2B-C1B | -4.26 | 121.92      | 128.46   |
| 18  | B     | 836 | CLA  | CMB-C2B-C1B | -4.25 | 121.94      | 128.46   |
| 25  | 5     | 608 | CHL  | CHD-C4C-C3C | -4.23 | 118.63      | 124.84   |
| 25  | 5     | 607 | CHL  | C4A-NA-C1A  | 4.22  | 108.60      | 106.71   |
| 26  | 6     | 617 | LUT  | C7-C8-C9    | -4.22 | 119.86      | 126.23   |
| 20  | A     | 846 | LHG  | O4-P-O5     | 4.21  | 133.06      | 112.24   |
| 18  | A     | 806 | CLA  | CMB-C2B-C1B | -4.21 | 122.00      | 128.46   |
| 25  | 5     | 608 | CHL  | O2D-CGD-CBD | 4.20  | 118.74      | 111.27   |
| 18  | B     | 813 | CLA  | CMB-C2B-C1B | -4.20 | 122.00      | 128.46   |
| 18  | A     | 811 | CLA  | CMB-C2B-C1B | -4.20 | 122.01      | 128.46   |
| 18  | 5     | 604 | CLA  | CMB-C2B-C1B | -4.19 | 122.03      | 128.46   |
| 20  | A     | 847 | LHG  | O4-P-O5     | 4.19  | 132.94      | 112.24   |
| 18  | A     | 808 | CLA  | CMB-C2B-C1B | -4.18 | 122.04      | 128.46   |
| 20  | B     | 851 | LHG  | O4-P-O5     | 4.18  | 132.91      | 112.24   |
| 20  | 5     | 622 | LHG  | O4-P-O5     | 4.18  | 132.89      | 112.24   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 827 | CLA  | CMB-C2B-C1B | -4.17 | 122.05      | 128.46   |
| 26  | 5     | 619 | LUT  | C7-C6-C5    | -4.17 | 111.36      | 121.46   |
| 18  | A     | 823 | CLA  | CMB-C2B-C1B | -4.16 | 122.07      | 128.46   |
| 18  | A     | 831 | CLA  | CMB-C2B-C1B | -4.16 | 122.07      | 128.46   |
| 18  | A     | 803 | CLA  | CMB-C2B-C1B | -4.15 | 122.08      | 128.46   |
| 18  | A     | 826 | CLA  | CMB-C2B-C1B | -4.15 | 122.08      | 128.46   |
| 25  | 2     | 601 | CHL  | C3C-C4C-NC  | 4.15  | 115.22      | 110.57   |
| 18  | L     | 304 | CLA  | CMB-C2B-C1B | -4.15 | 122.09      | 128.46   |
| 18  | A     | 827 | CLA  | CMB-C2B-C1B | -4.15 | 122.09      | 128.46   |
| 26  | 3     | 618 | LUT  | C30-C31-C32 | -4.13 | 110.32      | 123.22   |
| 18  | A     | 802 | CLA  | CMB-C2B-C1B | -4.13 | 122.12      | 128.46   |
| 26  | 3     | 618 | LUT  | C35-C34-C33 | -4.13 | 121.42      | 127.31   |
| 18  | A     | 819 | CLA  | CMB-C2B-C1B | -4.11 | 122.15      | 128.46   |
| 18  | A     | 829 | CLA  | CMB-C2B-C1B | -4.11 | 122.15      | 128.46   |
| 18  | A     | 839 | CLA  | CMB-C2B-C1B | -4.10 | 122.16      | 128.46   |
| 25  | 2     | 606 | CHL  | C2D-C1D-ND  | 4.09  | 113.12      | 110.10   |
| 26  | 3     | 618 | LUT  | C7-C6-C5    | -4.08 | 111.58      | 121.46   |
| 27  | 3     | 619 | XAT  | C15-C14-C13 | -4.07 | 121.51      | 127.31   |
| 25  | 2     | 607 | CHL  | C1B-CHB-C4A | -4.06 | 122.07      | 130.12   |
| 27  | 2     | 620 | XAT  | C35-C34-C33 | -4.06 | 121.51      | 127.31   |
| 18  | A     | 818 | CLA  | CMB-C2B-C1B | -4.05 | 122.24      | 128.46   |
| 18  | B     | 829 | CLA  | CMB-C2B-C1B | -4.04 | 122.25      | 128.46   |
| 18  | 3     | 617 | CLA  | CMB-C2B-C1B | -4.04 | 122.26      | 128.46   |
| 25  | 6     | 607 | CHL  | C3C-C4C-NC  | 4.03  | 115.09      | 110.57   |
| 18  | B     | 830 | CLA  | CMB-C2B-C1B | -4.02 | 122.29      | 128.46   |
| 25  | 6     | 607 | CHL  | C3D-C2D-C1D | -4.01 | 100.36      | 105.83   |
| 18  | A     | 830 | CLA  | CMB-C2B-C1B | -3.99 | 122.32      | 128.46   |
| 26  | 6     | 617 | LUT  | C1-C6-C5    | -3.99 | 117.00      | 122.61   |
| 18  | 3     | 609 | CLA  | CMB-C2B-C1B | -3.99 | 122.34      | 128.46   |
| 18  | A     | 804 | CLA  | CMB-C2B-C1B | -3.97 | 122.36      | 128.46   |
| 18  | B     | 820 | CLA  | CMB-C2B-C1B | -3.97 | 122.36      | 128.46   |
| 23  | B     | 850 | DGD  | O3G-C3G-C2G | -3.96 | 101.33      | 110.90   |
| 18  | B     | 832 | CLA  | CMB-C2B-C1B | -3.96 | 122.38      | 128.46   |
| 18  | 6     | 610 | CLA  | CMB-C2B-C1B | -3.96 | 122.38      | 128.46   |
| 18  | B     | 823 | CLA  | CMB-C2B-C1B | -3.95 | 122.39      | 128.46   |
| 26  | 5     | 619 | LUT  | C30-C31-C32 | -3.95 | 110.90      | 123.22   |
| 27  | 3     | 619 | XAT  | C5-C4-C3    | -3.93 | 104.97      | 112.75   |
| 18  | B     | 819 | CLA  | CMB-C2B-C1B | -3.93 | 122.42      | 128.46   |
| 18  | B     | 838 | CLA  | CMB-C2B-C1B | -3.93 | 122.43      | 128.46   |
| 25  | 5     | 608 | CHL  | C2D-C1D-ND  | 3.93  | 113.00      | 110.10   |
| 18  | L     | 302 | CLA  | CMB-C2B-C1B | -3.91 | 122.46      | 128.46   |
| 18  | 3     | 610 | CLA  | CMB-C2B-C1B | -3.91 | 122.46      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 812 | CLA  | CMB-C2B-C1B | -3.88 | 122.50      | 128.46   |
| 18  | A     | 854 | CLA  | CMB-C2B-C1B | -3.88 | 122.50      | 128.46   |
| 25  | 5     | 607 | CHL  | C3C-C4C-NC  | 3.88  | 114.92      | 110.57   |
| 18  | B     | 825 | CLA  | CMB-C2B-C1B | -3.88 | 122.50      | 128.46   |
| 27  | 2     | 620 | XAT  | C7-C8-C9    | -3.87 | 119.52      | 125.53   |
| 27  | 2     | 620 | XAT  | C18-C5-C4   | 3.87  | 118.63      | 114.28   |
| 18  | A     | 820 | CLA  | CMB-C2B-C1B | -3.87 | 122.52      | 128.46   |
| 18  | B     | 806 | CLA  | CMB-C2B-C1B | -3.87 | 122.52      | 128.46   |
| 25  | 2     | 606 | CHL  | C1D-ND-C4D  | -3.86 | 103.59      | 106.33   |
| 18  | A     | 832 | CLA  | CMB-C2B-C1B | -3.86 | 122.54      | 128.46   |
| 27  | 5     | 620 | XAT  | C24-C23-C22 | -3.86 | 103.33      | 110.77   |
| 18  | A     | 807 | CLA  | CMB-C2B-C1B | -3.85 | 122.54      | 128.46   |
| 18  | B     | 804 | CLA  | CMB-C2B-C1B | -3.85 | 122.54      | 128.46   |
| 18  | B     | 814 | CLA  | CMB-C2B-C1B | -3.85 | 122.55      | 128.46   |
| 18  | B     | 826 | CLA  | CMB-C2B-C1B | -3.83 | 122.58      | 128.46   |
| 18  | B     | 822 | CLA  | CMB-C2B-C1B | -3.83 | 122.58      | 128.46   |
| 18  | 6     | 602 | CLA  | CMB-C2B-C1B | -3.82 | 122.59      | 128.46   |
| 27  | 6     | 619 | XAT  | C5-C4-C3    | -3.82 | 105.20      | 112.75   |
| 27  | 5     | 620 | XAT  | C31-C30-C29 | -3.81 | 121.87      | 127.31   |
| 25  | 5     | 615 | CHL  | CHD-C4C-C3C | -3.80 | 119.25      | 124.84   |
| 25  | 2     | 616 | CHL  | C1B-CHB-C4A | -3.80 | 122.59      | 130.12   |
| 18  | 2     | 611 | CLA  | CMB-C2B-C1B | -3.80 | 122.63      | 128.46   |
| 27  | 3     | 619 | XAT  | C24-C23-C22 | -3.79 | 103.45      | 110.77   |
| 25  | 5     | 606 | CHL  | CHD-C4C-C3C | -3.78 | 119.07      | 124.98   |
| 18  | B     | 803 | CLA  | CMB-C2B-C1B | -3.77 | 122.66      | 128.46   |
| 18  | A     | 836 | CLA  | CMB-C2B-C1B | -3.77 | 122.67      | 128.46   |
| 25  | 2     | 616 | CHL  | CAC-C3C-C4C | 3.76  | 129.69      | 124.81   |
| 18  | A     | 814 | CLA  | CMB-C2B-C3B | 3.76  | 131.71      | 124.68   |
| 27  | 6     | 619 | XAT  | C18-C5-C4   | 3.75  | 118.50      | 114.28   |
| 27  | 3     | 619 | XAT  | C38-C25-C24 | 3.74  | 118.49      | 114.28   |
| 18  | 3     | 606 | CLA  | CMB-C2B-C1B | -3.74 | 122.72      | 128.46   |
| 18  | B     | 809 | CLA  | CMB-C2B-C1B | -3.73 | 122.73      | 128.46   |
| 21  | K     | 207 | BCR  | C2-C1-C6    | 3.72  | 116.21      | 110.48   |
| 18  | B     | 807 | CLA  | CMB-C2B-C1B | -3.72 | 122.75      | 128.46   |
| 18  | 6     | 609 | CLA  | CAB-C3B-C4B | -3.72 | 122.75      | 128.46   |
| 18  | 6     | 616 | CLA  | CAB-C3B-C4B | -3.71 | 122.76      | 128.46   |
| 18  | A     | 813 | CLA  | CMB-C2B-C1B | -3.70 | 122.77      | 128.46   |
| 25  | 2     | 606 | CHL  | C3B-C4B-NB  | 3.70  | 114.00      | 109.21   |
| 18  | F     | 305 | CLA  | CMB-C2B-C1B | -3.70 | 122.78      | 128.46   |
| 18  | A     | 837 | CLA  | CMB-C2B-C1B | -3.69 | 122.79      | 128.46   |
| 18  | 5     | 611 | CLA  | CAB-C3B-C4B | -3.69 | 122.79      | 128.46   |
| 18  | 6     | 606 | CLA  | CBD-CHA-C1A | 3.69  | 132.85      | 128.50   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 5     | 609 | CLA  | CMB-C2B-C3B | 3.69  | 131.57      | 124.68   |
| 21  | A     | 848 | BCR  | C2-C1-C6    | 3.68  | 116.15      | 110.48   |
| 26  | 3     | 618 | LUT  | C7-C8-C9    | -3.67 | 120.68      | 126.23   |
| 18  | A     | 817 | CLA  | CMB-C2B-C1B | -3.67 | 122.82      | 128.46   |
| 21  | A     | 856 | BCR  | C2-C1-C6    | 3.67  | 116.13      | 110.48   |
| 18  | A     | 828 | CLA  | CMB-C2B-C1B | -3.67 | 122.83      | 128.46   |
| 26  | 5     | 619 | LUT  | C10-C11-C12 | -3.67 | 111.78      | 123.22   |
| 18  | 6     | 614 | CLA  | CAB-C3B-C4B | -3.64 | 122.87      | 128.46   |
| 18  | A     | 805 | CLA  | CMB-C2B-C3B | 3.64  | 131.49      | 124.68   |
| 25  | 5     | 615 | CHL  | CAC-C3C-C4C | 3.64  | 129.53      | 124.81   |
| 18  | A     | 809 | CLA  | CMB-C2B-C3B | 3.62  | 131.44      | 124.68   |
| 18  | A     | 816 | CLA  | CMB-C2B-C3B | 3.61  | 131.44      | 124.68   |
| 18  | 2     | 602 | CLA  | CMB-C2B-C1B | -3.61 | 122.91      | 128.46   |
| 18  | B     | 835 | CLA  | CMB-C2B-C1B | -3.61 | 122.91      | 128.46   |
| 27  | 6     | 619 | XAT  | C28-C29-C30 | -3.61 | 113.40      | 118.94   |
| 25  | 5     | 606 | CHL  | C2D-C1D-ND  | 3.61  | 112.76      | 110.10   |
| 25  | 2     | 607 | CHL  | CAC-C3C-C4C | 3.61  | 129.49      | 124.81   |
| 18  | K     | 204 | CLA  | CAB-C3B-C4B | -3.60 | 122.93      | 128.46   |
| 18  | A     | 803 | CLA  | CMB-C2B-C3B | 3.60  | 131.41      | 124.68   |
| 18  | 3     | 602 | CLA  | CMB-C2B-C1B | -3.60 | 122.94      | 128.46   |
| 18  | 6     | 603 | CLA  | CMB-C2B-C1B | -3.59 | 122.94      | 128.46   |
| 18  | 3     | 607 | CLA  | CAB-C3B-C4B | -3.59 | 122.94      | 128.46   |
| 18  | 2     | 604 | CLA  | CMB-C2B-C3B | 3.59  | 131.40      | 124.68   |
| 27  | 2     | 620 | XAT  | C5-C4-C3    | -3.59 | 105.64      | 112.75   |
| 25  | 3     | 608 | CHL  | C4C-C3C-C2C | -3.59 | 101.67      | 106.90   |
| 18  | B     | 831 | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 18  | B     | 839 | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 18  | 2     | 609 | CLA  | CMB-C2B-C1B | -3.58 | 122.96      | 128.46   |
| 18  | B     | 827 | CLA  | CMB-C2B-C3B | 3.58  | 131.37      | 124.68   |
| 18  | A     | 826 | CLA  | CMB-C2B-C3B | 3.58  | 131.37      | 124.68   |
| 27  | 5     | 620 | XAT  | C35-C15-C14 | -3.58 | 116.14      | 123.47   |
| 25  | 3     | 608 | CHL  | CHD-C4C-C3C | -3.58 | 119.58      | 124.84   |
| 18  | 5     | 614 | CLA  | CMB-C2B-C1B | -3.58 | 122.97      | 128.46   |
| 25  | 6     | 601 | CHL  | CHD-C4C-C3C | -3.58 | 119.58      | 124.84   |
| 18  | A     | 833 | CLA  | CMB-C2B-C3B | 3.57  | 131.35      | 124.68   |
| 18  | F     | 301 | CLA  | CMB-C2B-C1B | -3.56 | 122.99      | 128.46   |
| 18  | F     | 304 | CLA  | CMB-C2B-C1B | -3.56 | 123.00      | 128.46   |
| 18  | A     | 823 | CLA  | CMB-C2B-C3B | 3.55  | 131.32      | 124.68   |
| 25  | 2     | 601 | CHL  | C1B-CHB-C4A | -3.55 | 123.09      | 130.12   |
| 18  | 5     | 613 | CLA  | CMB-C2B-C1B | -3.54 | 123.02      | 128.46   |
| 27  | 5     | 620 | XAT  | C38-C25-C26 | -3.54 | 116.32      | 122.26   |
| 27  | 2     | 620 | XAT  | C4-C3-C2    | -3.54 | 103.93      | 110.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 5     | 604 | CLA  | CMB-C2B-C3B | 3.54  | 131.30      | 124.68   |
| 18  | A     | 806 | CLA  | CMB-C2B-C3B | 3.54  | 131.30      | 124.68   |
| 18  | B     | 836 | CLA  | CMB-C2B-C3B | 3.54  | 131.29      | 124.68   |
| 25  | 5     | 608 | CHL  | C1-C2-C3    | -3.53 | 121.03      | 126.75   |
| 18  | B     | 813 | CLA  | CMB-C2B-C3B | 3.53  | 131.28      | 124.68   |
| 18  | 6     | 611 | CLA  | CAB-C3B-C4B | -3.53 | 123.04      | 128.46   |
| 25  | 6     | 607 | CHL  | CAC-C3C-C4C | 3.53  | 129.38      | 124.81   |
| 18  | A     | 829 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 18  | A     | 808 | CLA  | CMB-C2B-C3B | 3.52  | 131.26      | 124.68   |
| 25  | 2     | 616 | CHL  | CHD-C4C-C3C | -3.51 | 119.68      | 124.84   |
| 25  | 2     | 608 | CHL  | C1B-CHB-C4A | -3.51 | 123.17      | 130.12   |
| 25  | 2     | 608 | CHL  | CAC-C3C-C4C | 3.51  | 129.36      | 124.81   |
| 18  | A     | 827 | CLA  | CMB-C2B-C3B | 3.51  | 131.24      | 124.68   |
| 18  | A     | 835 | CLA  | CMB-C2B-C1B | -3.50 | 123.08      | 128.46   |
| 18  | A     | 811 | CLA  | CMB-C2B-C3B | 3.50  | 131.23      | 124.68   |
| 25  | 5     | 615 | CHL  | C2D-C1D-ND  | 3.50  | 112.68      | 110.10   |
| 18  | B     | 811 | CLA  | CAB-C3B-C4B | -3.50 | 123.09      | 128.46   |
| 18  | B     | 816 | CLA  | CMB-C2B-C1B | -3.49 | 123.10      | 128.46   |
| 25  | 2     | 608 | CHL  | CHD-C4C-C3C | -3.48 | 119.72      | 124.84   |
| 18  | B     | 824 | CLA  | CMB-C2B-C1B | -3.48 | 123.11      | 128.46   |
| 18  | B     | 840 | CLA  | O2D-CGD-O1D | -3.48 | 117.03      | 123.84   |
| 18  | A     | 815 | CLA  | CMB-C2B-C1B | -3.48 | 123.12      | 128.46   |
| 18  | G     | 204 | CLA  | CMB-C2B-C1B | -3.48 | 123.12      | 128.46   |
| 18  | B     | 805 | CLA  | CMB-C2B-C1B | -3.47 | 123.12      | 128.46   |
| 18  | 3     | 604 | CLA  | CAB-C3B-C4B | -3.47 | 123.12      | 128.46   |
| 18  | 5     | 612 | CLA  | CMB-C2B-C1B | -3.47 | 123.13      | 128.46   |
| 18  | 6     | 613 | CLA  | CMB-C2B-C1B | -3.46 | 123.15      | 128.46   |
| 18  | A     | 822 | CLA  | CAB-C3B-C4B | -3.46 | 123.15      | 128.46   |
| 26  | 2     | 619 | LUT  | C4-C5-C6    | -3.45 | 113.15      | 120.85   |
| 25  | 5     | 615 | CHL  | C3B-C4B-NB  | 3.45  | 113.67      | 109.21   |
| 27  | 2     | 620 | XAT  | C30-C31-C32 | -3.44 | 112.47      | 123.22   |
| 25  | 3     | 608 | CHL  | C3B-C4B-NB  | 3.44  | 113.66      | 109.21   |
| 25  | 3     | 608 | CHL  | C2D-C1D-ND  | 3.44  | 112.64      | 110.10   |
| 25  | 2     | 606 | CHL  | CAC-C3C-C4C | 3.44  | 129.27      | 124.81   |
| 27  | 6     | 619 | XAT  | C38-C25-C24 | 3.43  | 118.14      | 114.28   |
| 18  | 2     | 612 | CLA  | CMB-C2B-C1B | -3.43 | 123.19      | 128.46   |
| 25  | 2     | 606 | CHL  | C3D-C4D-ND  | 3.43  | 115.78      | 110.24   |
| 18  | 3     | 611 | CLA  | CMB-C2B-C1B | -3.43 | 123.20      | 128.46   |
| 18  | 5     | 610 | CLA  | CMB-C2B-C1B | -3.43 | 123.20      | 128.46   |
| 25  | 5     | 608 | CHL  | C3B-C4B-NB  | 3.42  | 113.64      | 109.21   |
| 18  | A     | 801 | CLA  | CMB-C2B-C1B | -3.42 | 123.20      | 128.46   |
| 18  | 6     | 614 | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 824 | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |
| 18  | B     | 818 | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |
| 18  | 5     | 603 | CLA  | CMB-C2B-C1B | -3.42 | 123.21      | 128.46   |
| 18  | 5     | 613 | CLA  | O2D-CGD-O1D | -3.42 | 117.16      | 123.84   |
| 26  | 2     | 619 | LUT  | C15-C35-C34 | -3.42 | 116.48      | 123.47   |
| 18  | B     | 833 | CLA  | CMB-C2B-C3B | 3.41  | 131.07      | 124.68   |
| 18  | A     | 840 | CLA  | CMB-C2B-C1B | -3.41 | 123.22      | 128.46   |
| 18  | L     | 304 | CLA  | CMB-C2B-C3B | 3.41  | 131.06      | 124.68   |
| 18  | A     | 818 | CLA  | CMB-C2B-C3B | 3.41  | 131.06      | 124.68   |
| 18  | A     | 819 | CLA  | CMB-C2B-C3B | 3.41  | 131.06      | 124.68   |
| 27  | 6     | 619 | XAT  | C10-C11-C12 | -3.41 | 112.58      | 123.22   |
| 18  | 6     | 606 | CLA  | O2D-CGD-O1D | -3.40 | 117.19      | 123.84   |
| 27  | 2     | 620 | XAT  | C11-C10-C9  | -3.40 | 122.46      | 127.31   |
| 18  | B     | 837 | CLA  | CMB-C2B-C1B | -3.40 | 123.24      | 128.46   |
| 26  | 2     | 619 | LUT  | C10-C11-C12 | -3.40 | 112.62      | 123.22   |
| 18  | 2     | 614 | CLA  | CMB-C2B-C1B | -3.39 | 123.25      | 128.46   |
| 25  | 6     | 601 | CHL  | C1B-CHB-C4A | -3.39 | 123.40      | 130.12   |
| 18  | G     | 203 | CLA  | CMB-C2B-C1B | -3.39 | 123.25      | 128.46   |
| 25  | 3     | 608 | CHL  | C3D-C4D-ND  | 3.39  | 115.72      | 110.24   |
| 18  | 3     | 607 | CLA  | CMB-C2B-C1B | -3.39 | 123.26      | 128.46   |
| 25  | 5     | 615 | CHL  | C3D-C4D-ND  | 3.39  | 115.71      | 110.24   |
| 18  | A     | 843 | CLA  | CMB-C2B-C1B | -3.38 | 123.26      | 128.46   |
| 25  | 5     | 606 | CHL  | C3D-C4D-ND  | 3.38  | 115.71      | 110.24   |
| 18  | A     | 802 | CLA  | CMB-C2B-C3B | 3.38  | 131.00      | 124.68   |
| 18  | B     | 808 | CLA  | CMB-C2B-C1B | -3.38 | 123.27      | 128.46   |
| 18  | B     | 821 | CLA  | CMB-C2B-C1B | -3.38 | 123.27      | 128.46   |
| 18  | A     | 839 | CLA  | CMB-C2B-C3B | 3.38  | 130.99      | 124.68   |
| 18  | B     | 823 | CLA  | CMB-C2B-C3B | 3.38  | 130.99      | 124.68   |
| 18  | A     | 831 | CLA  | O2D-CGD-O1D | -3.37 | 117.24      | 123.84   |
| 18  | 3     | 617 | CLA  | CMB-C2B-C3B | 3.37  | 130.99      | 124.68   |
| 18  | 6     | 609 | CLA  | CMB-C2B-C1B | -3.37 | 123.29      | 128.46   |
| 18  | F     | 303 | CLA  | CMB-C2B-C1B | -3.37 | 123.29      | 128.46   |
| 18  | A     | 841 | CLA  | CMB-C2B-C1B | -3.36 | 123.30      | 128.46   |
| 18  | A     | 821 | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 18  | 5     | 611 | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 18  | B     | 840 | CLA  | CMB-C2B-C1B | -3.35 | 123.31      | 128.46   |
| 18  | L     | 303 | CLA  | CMB-C2B-C1B | -3.35 | 123.32      | 128.46   |
| 18  | 6     | 604 | CLA  | CMB-C2B-C1B | -3.35 | 123.32      | 128.46   |
| 18  | 3     | 613 | CLA  | CMB-C2B-C1B | -3.34 | 123.32      | 128.46   |
| 25  | 6     | 601 | CHL  | C3D-C4D-ND  | 3.34  | 115.65      | 110.24   |
| 18  | A     | 824 | CLA  | O2D-CGD-O1D | -3.34 | 117.30      | 123.84   |
| 25  | 5     | 606 | CHL  | C1D-ND-C4D  | -3.34 | 103.96      | 106.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 2     | 613 | CLA  | CMB-C2B-C1B | -3.34 | 123.33      | 128.46   |
| 18  | B     | 828 | CLA  | CMB-C2B-C1B | -3.34 | 123.33      | 128.46   |
| 25  | 2     | 616 | CHL  | C2D-C1D-ND  | 3.34  | 112.56      | 110.10   |
| 18  | A     | 810 | CLA  | CMB-C2B-C1B | -3.34 | 123.34      | 128.46   |
| 25  | 2     | 608 | CHL  | C3D-C4D-ND  | 3.34  | 115.63      | 110.24   |
| 18  | A     | 825 | CLA  | CMB-C2B-C1B | -3.33 | 123.34      | 128.46   |
| 18  | B     | 834 | CLA  | CMB-C2B-C1B | -3.33 | 123.34      | 128.46   |
| 18  | 6     | 608 | CLA  | CMB-C2B-C1B | -3.33 | 123.35      | 128.46   |
| 18  | A     | 830 | CLA  | CMB-C2B-C3B | 3.33  | 130.90      | 124.68   |
| 18  | A     | 854 | CLA  | CMB-C2B-C3B | 3.33  | 130.90      | 124.68   |
| 18  | 5     | 601 | CLA  | CMB-C2B-C1B | -3.33 | 123.35      | 128.46   |
| 25  | 2     | 616 | CHL  | C3B-C4B-NB  | 3.32  | 113.50      | 109.21   |
| 18  | B     | 838 | CLA  | CMB-C2B-C3B | 3.32  | 130.88      | 124.68   |
| 18  | 6     | 611 | CLA  | CMB-C2B-C1B | -3.31 | 123.37      | 128.46   |
| 18  | 2     | 603 | CLA  | CMB-C2B-C1B | -3.31 | 123.37      | 128.46   |
| 18  | A     | 835 | CLA  | O2D-CGD-O1D | -3.31 | 117.36      | 123.84   |
| 18  | A     | 822 | CLA  | CMB-C2B-C1B | -3.31 | 123.38      | 128.46   |
| 18  | A     | 804 | CLA  | CMB-C2B-C3B | 3.31  | 130.87      | 124.68   |
| 18  | 6     | 612 | CLA  | CMB-C2B-C1B | -3.31 | 123.38      | 128.46   |
| 18  | 3     | 604 | CLA  | CMB-C2B-C1B | -3.31 | 123.38      | 128.46   |
| 18  | 3     | 612 | CLA  | CMB-C2B-C1B | -3.31 | 123.38      | 128.46   |
| 25  | 2     | 607 | CHL  | C3D-C4D-ND  | 3.31  | 115.58      | 110.24   |
| 18  | B     | 841 | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 18  | 6     | 616 | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 18  | 6     | 602 | CLA  | O2D-CGD-O1D | -3.30 | 117.39      | 123.84   |
| 18  | 6     | 606 | CLA  | CMB-C2B-C1B | -3.30 | 123.39      | 128.46   |
| 18  | B     | 802 | CLA  | CMB-C2B-C1B | -3.29 | 123.40      | 128.46   |
| 18  | J     | 101 | CLA  | CMB-C2B-C1B | -3.29 | 123.40      | 128.46   |
| 18  | A     | 812 | CLA  | CMB-C2B-C1B | -3.29 | 123.41      | 128.46   |
| 18  | B     | 832 | CLA  | CMB-C2B-C3B | 3.29  | 130.83      | 124.68   |
| 25  | 5     | 608 | CHL  | C1D-ND-C4D  | -3.29 | 104.00      | 106.33   |
| 25  | 6     | 601 | CHL  | C3B-C4B-NB  | 3.29  | 113.46      | 109.21   |
| 18  | A     | 805 | CLA  | O2D-CGD-O1D | -3.29 | 117.41      | 123.84   |
| 18  | B     | 820 | CLA  | CMB-C2B-C3B | 3.29  | 130.82      | 124.68   |
| 24  | 2     | 618 | LMG  | O6-C1-O1    | -3.28 | 103.36      | 110.97   |
| 18  | K     | 203 | CLA  | CMB-C2B-C1B | -3.28 | 123.42      | 128.46   |
| 18  | B     | 811 | CLA  | CMB-C2B-C1B | -3.28 | 123.42      | 128.46   |
| 18  | A     | 838 | CLA  | CMB-C2B-C1B | -3.28 | 123.43      | 128.46   |
| 18  | B     | 817 | CLA  | CMB-C2B-C1B | -3.28 | 123.43      | 128.46   |
| 18  | 6     | 610 | CLA  | CMB-C2B-C3B | 3.28  | 130.81      | 124.68   |
| 25  | 2     | 601 | CHL  | C3D-C4D-ND  | 3.27  | 115.53      | 110.24   |
| 18  | A     | 842 | CLA  | CMB-C2B-C1B | -3.27 | 123.43      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 3     | 615 | CLA  | CMB-C2B-C1B | -3.27 | 123.44      | 128.46   |
| 18  | B     | 825 | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 18  | L     | 302 | CLA  | CMB-C2B-C3B | 3.27  | 130.79      | 124.68   |
| 24  | 2     | 617 | LMG  | O6-C1-O1    | -3.26 | 103.41      | 110.97   |
| 18  | 6     | 616 | CLA  | O2D-CGD-O1D | -3.26 | 117.47      | 123.84   |
| 18  | B     | 837 | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 18  | B     | 824 | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 18  | B     | 832 | CLA  | O2D-CGD-O1D | -3.25 | 117.48      | 123.84   |
| 26  | 3     | 618 | LUT  | C18-C5-C4   | -3.25 | 108.34      | 114.36   |
| 18  | B     | 830 | CLA  | CMB-C2B-C3B | 3.24  | 130.75      | 124.68   |
| 18  | K     | 204 | CLA  | CMB-C2B-C1B | -3.24 | 123.49      | 128.46   |
| 18  | A     | 831 | CLA  | CMB-C2B-C3B | 3.23  | 130.73      | 124.68   |
| 18  | 3     | 610 | CLA  | CMB-C2B-C3B | 3.23  | 130.73      | 124.68   |
| 18  | 3     | 609 | CLA  | O2D-CGD-O1D | -3.23 | 117.53      | 123.84   |
| 18  | A     | 820 | CLA  | O2D-CGD-O1D | -3.23 | 117.53      | 123.84   |
| 18  | B     | 812 | CLA  | CMB-C2B-C3B | 3.22  | 130.71      | 124.68   |
| 18  | 5     | 602 | CLA  | CMB-C2B-C1B | -3.22 | 123.52      | 128.46   |
| 18  | B     | 806 | CLA  | CMB-C2B-C3B | 3.21  | 130.69      | 124.68   |
| 18  | G     | 201 | CLA  | CMB-C2B-C1B | -3.21 | 123.53      | 128.46   |
| 18  | 3     | 609 | CLA  | CMB-C2B-C3B | 3.21  | 130.69      | 124.68   |
| 25  | 2     | 601 | CHL  | CHD-C4C-C3C | -3.21 | 120.12      | 124.84   |
| 18  | 2     | 610 | CLA  | CMB-C2B-C3B | 3.21  | 130.68      | 124.68   |
| 20  | A     | 847 | LHG  | O8-C23-C24  | 3.21  | 119.79      | 111.38   |
| 18  | A     | 834 | CLA  | CMB-C2B-C1B | -3.21 | 123.54      | 128.46   |
| 18  | B     | 804 | CLA  | CMB-C2B-C3B | 3.20  | 130.67      | 124.68   |
| 18  | B     | 826 | CLA  | CMB-C2B-C3B | 3.20  | 130.67      | 124.68   |
| 18  | A     | 845 | CLA  | CMB-C2B-C1B | -3.20 | 123.55      | 128.46   |
| 26  | 5     | 619 | LUT  | C18-C5-C4   | -3.20 | 108.43      | 114.36   |
| 18  | B     | 803 | CLA  | CMB-C2B-C3B | 3.20  | 130.66      | 124.68   |
| 18  | 3     | 603 | CLA  | CMB-C2B-C1B | -3.20 | 123.55      | 128.46   |
| 25  | 3     | 608 | CHL  | C1D-ND-C4D  | -3.20 | 104.06      | 106.33   |
| 27  | 6     | 619 | XAT  | C35-C15-C14 | -3.19 | 116.93      | 123.47   |
| 18  | A     | 821 | CLA  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 18  | 2     | 604 | CLA  | O2D-CGD-O1D | -3.19 | 117.60      | 123.84   |
| 25  | 6     | 607 | CHL  | C4A-NA-C1A  | 3.19  | 108.14      | 106.71   |
| 26  | 5     | 619 | LUT  | C2-C3-C4    | 3.19  | 114.67      | 110.30   |
| 18  | A     | 807 | CLA  | CMB-C2B-C3B | 3.19  | 130.64      | 124.68   |
| 25  | 6     | 607 | CHL  | C3D-C4D-ND  | 3.19  | 115.39      | 110.24   |
| 18  | 2     | 611 | CLA  | CMB-C2B-C3B | 3.19  | 130.64      | 124.68   |
| 18  | B     | 838 | CLA  | O2D-CGD-O1D | -3.18 | 117.61      | 123.84   |
| 25  | 5     | 615 | CHL  | C1D-ND-C4D  | -3.18 | 104.08      | 106.33   |
| 18  | B     | 810 | CLA  | CMB-C2B-C1B | -3.18 | 123.58      | 128.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 5     | 608 | CHL  | C3D-C4D-ND  | 3.18  | 115.38      | 110.24   |
| 18  | B     | 825 | CLA  | O2D-CGD-O1D | -3.17 | 117.63      | 123.84   |
| 18  | A     | 818 | CLA  | O2D-CGD-O1D | -3.17 | 117.63      | 123.84   |
| 25  | 2     | 616 | CHL  | C3D-C4D-ND  | 3.17  | 115.37      | 110.24   |
| 25  | 2     | 608 | CHL  | C2D-C1D-ND  | 3.17  | 112.44      | 110.10   |
| 27  | 6     | 619 | XAT  | C4-C3-C2    | -3.17 | 104.65      | 110.77   |
| 18  | 6     | 602 | CLA  | CMB-C2B-C3B | 3.17  | 130.61      | 124.68   |
| 18  | 3     | 614 | CLA  | CMB-C2B-C1B | -3.16 | 123.60      | 128.46   |
| 18  | A     | 832 | CLA  | CMB-C2B-C3B | 3.16  | 130.58      | 124.68   |
| 18  | B     | 822 | CLA  | O2D-CGD-O1D | -3.16 | 117.67      | 123.84   |
| 18  | B     | 815 | CLA  | CMB-C2B-C1B | -3.15 | 123.62      | 128.46   |
| 18  | B     | 814 | CLA  | CMB-C2B-C3B | 3.15  | 130.58      | 124.68   |
| 26  | 6     | 617 | LUT  | C18-C5-C4   | -3.15 | 108.52      | 114.36   |
| 18  | B     | 822 | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 21  | B     | 847 | BCR  | C15-C16-C17 | -3.15 | 117.03      | 123.47   |
| 18  | A     | 820 | CLA  | CMB-C2B-C3B | 3.15  | 130.57      | 124.68   |
| 18  | B     | 817 | CLA  | O2D-CGD-O1D | -3.14 | 117.69      | 123.84   |
| 23  | B     | 850 | DGD  | O5D-C6D-C5D | -3.14 | 103.23      | 109.05   |
| 25  | 6     | 601 | CHL  | C2D-C1D-ND  | 3.14  | 112.42      | 110.10   |
| 18  | K     | 206 | CLA  | CMB-C2B-C1B | -3.14 | 123.64      | 128.46   |
| 18  | B     | 820 | CLA  | O2D-CGD-O1D | -3.14 | 117.70      | 123.84   |
| 18  | B     | 826 | CLA  | O2D-CGD-O1D | -3.14 | 117.71      | 123.84   |
| 18  | B     | 808 | CLA  | O2D-CGD-O1D | -3.13 | 117.71      | 123.84   |
| 18  | B     | 807 | CLA  | CMB-C2B-C3B | 3.13  | 130.54      | 124.68   |
| 18  | 6     | 604 | CLA  | O2D-CGD-O1D | -3.13 | 117.73      | 123.84   |
| 18  | A     | 840 | CLA  | O2D-CGD-O1D | -3.12 | 117.73      | 123.84   |
| 18  | B     | 807 | CLA  | O2D-CGD-O1D | -3.12 | 117.74      | 123.84   |
| 18  | A     | 804 | CLA  | O2D-CGD-O1D | -3.11 | 117.75      | 123.84   |
| 26  | 6     | 617 | LUT  | C21-C26-C27 | -3.11 | 108.77      | 112.70   |
| 18  | A     | 836 | CLA  | CMB-C2B-C3B | 3.10  | 130.48      | 124.68   |
| 18  | A     | 837 | CLA  | O2D-CGD-O1D | -3.10 | 117.78      | 123.84   |
| 18  | A     | 828 | CLA  | CMB-C2B-C3B | 3.09  | 130.47      | 124.68   |
| 25  | 2     | 607 | CHL  | CHD-C4C-C3C | -3.09 | 120.30      | 124.84   |
| 23  | B     | 850 | DGD  | O6D-C1D-O3G | -3.09 | 102.66      | 109.97   |
| 18  | B     | 805 | CLA  | O2D-CGD-O1D | -3.09 | 117.80      | 123.84   |
| 26  | 2     | 619 | LUT  | C35-C34-C33 | -3.09 | 122.91      | 127.31   |
| 25  | 2     | 608 | CHL  | C3B-C4B-NB  | 3.09  | 113.20      | 109.21   |
| 18  | A     | 817 | CLA  | CMB-C2B-C3B | 3.09  | 130.45      | 124.68   |
| 18  | B     | 819 | CLA  | CMB-C2B-C3B | 3.09  | 130.45      | 124.68   |
| 27  | 3     | 619 | XAT  | C4-C3-C2    | -3.08 | 104.82      | 110.77   |
| 18  | 2     | 610 | CLA  | O2D-CGD-O1D | -3.08 | 117.82      | 123.84   |
| 18  | 5     | 601 | CLA  | O2D-CGD-O1D | -3.08 | 117.82      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 813 | CLA  | CMB-C2B-C3B | 3.07  | 130.43      | 124.68   |
| 18  | B     | 811 | CLA  | O2D-CGD-O1D | -3.07 | 117.83      | 123.84   |
| 18  | A     | 809 | CLA  | O2D-CGD-O1D | -3.07 | 117.84      | 123.84   |
| 25  | 5     | 607 | CHL  | CAC-C3C-C4C | 3.06  | 128.78      | 124.81   |
| 18  | B     | 804 | CLA  | O2D-CGD-O1D | -3.06 | 117.85      | 123.84   |
| 18  | 2     | 602 | CLA  | CMB-C2B-C3B | 3.06  | 130.40      | 124.68   |
| 18  | F     | 305 | CLA  | CMB-C2B-C3B | 3.05  | 130.39      | 124.68   |
| 21  | K     | 202 | BCR  | C24-C23-C22 | -3.05 | 121.62      | 126.23   |
| 18  | 2     | 609 | CLA  | CMB-C2B-C3B | 3.05  | 130.38      | 124.68   |
| 26  | 3     | 618 | LUT  | C4-C5-C6    | -3.05 | 114.06      | 120.85   |
| 27  | 3     | 619 | XAT  | O4-C5-C4    | 3.04  | 115.67      | 113.38   |
| 25  | 6     | 601 | CHL  | CAC-C3C-C4C | 3.04  | 128.76      | 124.81   |
| 21  | J     | 103 | BCR  | C7-C8-C9    | -3.04 | 121.64      | 126.23   |
| 18  | B     | 809 | CLA  | CMB-C2B-C3B | 3.04  | 130.36      | 124.68   |
| 26  | 5     | 619 | LUT  | C4-C5-C6    | -3.04 | 114.08      | 120.85   |
| 18  | A     | 823 | CLA  | O2D-CGD-O1D | -3.03 | 117.91      | 123.84   |
| 27  | 5     | 620 | XAT  | O24-C25-C38 | 3.03  | 118.69      | 115.06   |
| 18  | 3     | 606 | CLA  | CMB-C2B-C3B | 3.03  | 130.35      | 124.68   |
| 18  | A     | 832 | CLA  | O2D-CGD-O1D | -3.03 | 117.91      | 123.84   |
| 21  | J     | 102 | BCR  | C15-C16-C17 | -3.03 | 117.27      | 123.47   |
| 18  | 3     | 602 | CLA  | O2D-CGD-O1D | -3.03 | 117.92      | 123.84   |
| 18  | A     | 802 | CLA  | O2D-CGD-O1D | -3.02 | 117.93      | 123.84   |
| 18  | A     | 811 | CLA  | O2D-CGD-O1D | -3.02 | 117.93      | 123.84   |
| 18  | B     | 829 | CLA  | CMB-C2B-C3B | 3.02  | 130.33      | 124.68   |
| 18  | 3     | 602 | CLA  | CMB-C2B-C3B | 3.02  | 130.32      | 124.68   |
| 18  | B     | 810 | CLA  | O2D-CGD-O1D | -3.02 | 117.94      | 123.84   |
| 25  | 2     | 607 | CHL  | C3B-C4B-NB  | 3.02  | 113.11      | 109.21   |
| 18  | A     | 803 | CLA  | C1B-CHB-C4A | -3.01 | 124.15      | 130.12   |
| 18  | A     | 854 | CLA  | O2D-CGD-O1D | -3.01 | 117.95      | 123.84   |
| 25  | 5     | 607 | CHL  | C3D-C4D-ND  | 3.01  | 115.11      | 110.24   |
| 18  | 5     | 602 | CLA  | O2D-CGD-O1D | -3.01 | 117.96      | 123.84   |
| 25  | 2     | 606 | CHL  | CHB-C4A-NA  | 3.01  | 128.67      | 124.51   |
| 18  | B     | 829 | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 27  | 2     | 620 | XAT  | C15-C14-C13 | -3.00 | 123.03      | 127.31   |
| 21  | K     | 207 | BCR  | C15-C16-C17 | -3.00 | 117.33      | 123.47   |
| 18  | B     | 827 | CLA  | O2D-CGD-O1D | -3.00 | 117.97      | 123.84   |
| 27  | 6     | 619 | XAT  | C30-C31-C32 | -3.00 | 113.86      | 123.22   |
| 18  | 6     | 603 | CLA  | CMB-C2B-C3B | 3.00  | 130.29      | 124.68   |
| 18  | B     | 830 | CLA  | O2D-CGD-O1D | -3.00 | 117.98      | 123.84   |
| 18  | A     | 803 | CLA  | O2D-CGD-O1D | -3.00 | 117.98      | 123.84   |
| 18  | A     | 827 | CLA  | O2D-CGD-O1D | -2.99 | 117.99      | 123.84   |
| 25  | 3     | 608 | CHL  | C1B-CHB-C4A | -2.99 | 124.20      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 835 | CLA  | CMB-C2B-C3B | 2.99  | 130.27      | 124.68   |
| 18  | L     | 304 | CLA  | O2D-CGD-O1D | -2.99 | 118.00      | 123.84   |
| 18  | A     | 828 | CLA  | O2D-CGD-O1D | -2.99 | 118.00      | 123.84   |
| 18  | B     | 841 | CLA  | O2D-CGD-O1D | -2.99 | 118.00      | 123.84   |
| 26  | 3     | 618 | LUT  | C2-C3-C4    | 2.99  | 114.39      | 110.30   |
| 25  | 6     | 607 | CHL  | CMD-C2D-C3D | -2.99 | 120.74      | 127.61   |
| 18  | A     | 835 | CLA  | CMB-C2B-C3B | 2.98  | 130.26      | 124.68   |
| 18  | 5     | 614 | CLA  | CMB-C2B-C3B | 2.98  | 130.25      | 124.68   |
| 18  | B     | 818 | CLA  | O2D-CGD-O1D | -2.98 | 118.02      | 123.84   |
| 18  | B     | 831 | CLA  | CMB-C2B-C3B | 2.98  | 130.25      | 124.68   |
| 18  | B     | 839 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 18  | A     | 839 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 18  | J     | 101 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 18  | F     | 304 | CLA  | CMB-C2B-C3B | 2.97  | 130.24      | 124.68   |
| 18  | A     | 838 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 18  | 2     | 602 | CLA  | O2D-CGD-O1D | -2.97 | 118.03      | 123.84   |
| 18  | 5     | 614 | CLA  | O2D-CGD-O1D | -2.97 | 118.04      | 123.84   |
| 18  | 2     | 609 | CLA  | O2D-CGD-O1D | -2.97 | 118.04      | 123.84   |
| 18  | B     | 813 | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 18  | B     | 828 | CLA  | O2D-CGD-O1D | -2.96 | 118.04      | 123.84   |
| 18  | K     | 203 | CLA  | O2D-CGD-O1D | -2.96 | 118.05      | 123.84   |
| 18  | B     | 833 | CLA  | O2D-CGD-O1D | -2.96 | 118.06      | 123.84   |
| 26  | 2     | 619 | LUT  | C18-C5-C4   | -2.96 | 108.88      | 114.36   |
| 18  | A     | 819 | CLA  | O2D-CGD-O1D | -2.95 | 118.06      | 123.84   |
| 18  | B     | 815 | CLA  | O2D-CGD-O1D | -2.95 | 118.06      | 123.84   |
| 26  | 3     | 618 | LUT  | C20-C13-C14 | -2.95 | 118.79      | 122.92   |
| 18  | A     | 813 | CLA  | O2D-CGD-O1D | -2.95 | 118.07      | 123.84   |
| 18  | F     | 301 | CLA  | CMB-C2B-C3B | 2.95  | 130.20      | 124.68   |
| 26  | 5     | 619 | LUT  | C7-C8-C9    | -2.95 | 121.78      | 126.23   |
| 18  | A     | 816 | CLA  | O2D-CGD-O1D | -2.95 | 118.08      | 123.84   |
| 18  | A     | 814 | CLA  | O2D-CGD-O1D | -2.95 | 118.08      | 123.84   |
| 18  | B     | 835 | CLA  | O2D-CGD-O1D | -2.94 | 118.08      | 123.84   |
| 25  | 5     | 608 | CHL  | CAC-C3C-C4C | 2.94  | 128.63      | 124.81   |
| 18  | B     | 823 | CLA  | O2D-CGD-O1D | -2.94 | 118.09      | 123.84   |
| 18  | A     | 837 | CLA  | CMB-C2B-C3B | 2.94  | 130.18      | 124.68   |
| 21  | J     | 102 | BCR  | C7-C8-C9    | -2.94 | 121.80      | 126.23   |
| 18  | B     | 812 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 18  | L     | 302 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 18  | A     | 825 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 18  | B     | 834 | CLA  | O2D-CGD-O1D | -2.93 | 118.11      | 123.84   |
| 18  | A     | 836 | CLA  | O2D-CGD-O1D | -2.93 | 118.12      | 123.84   |
| 18  | B     | 821 | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 834 | CLA  | O2D-CGD-O1D | -2.92 | 118.13      | 123.84   |
| 18  | A     | 812 | CLA  | O2D-CGD-O1D | -2.92 | 118.14      | 123.84   |
| 18  | A     | 833 | CLA  | O2D-CGD-O1D | -2.91 | 118.14      | 123.84   |
| 18  | A     | 805 | CLA  | CHB-C4A-NA  | 2.91  | 128.54      | 124.51   |
| 18  | K     | 201 | CLA  | O2D-CGD-O1D | -2.91 | 118.14      | 123.84   |
| 18  | 2     | 612 | CLA  | O2D-CGD-O1D | -2.91 | 118.15      | 123.84   |
| 18  | B     | 824 | CLA  | CMB-C2B-C3B | 2.91  | 130.12      | 124.68   |
| 27  | 5     | 620 | XAT  | C4-C3-C2    | -2.91 | 105.16      | 110.77   |
| 18  | L     | 303 | CLA  | O2D-CGD-O1D | -2.91 | 118.16      | 123.84   |
| 25  | 3     | 608 | CHL  | CAC-C3C-C4C | 2.90  | 128.57      | 124.81   |
| 18  | 2     | 603 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 18  | A     | 815 | CLA  | CMB-C2B-C3B | 2.90  | 130.10      | 124.68   |
| 25  | 2     | 601 | CHL  | C4A-NA-C1A  | 2.90  | 108.01      | 106.71   |
| 18  | A     | 826 | CLA  | O2D-CGD-O1D | -2.90 | 118.17      | 123.84   |
| 25  | 2     | 601 | CHL  | CAC-C3C-C4C | 2.89  | 128.56      | 124.81   |
| 18  | 6     | 613 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 18  | A     | 801 | CLA  | CMB-C2B-C3B | 2.89  | 130.08      | 124.68   |
| 18  | B     | 831 | CLA  | O2D-CGD-O1D | -2.89 | 118.19      | 123.84   |
| 18  | A     | 808 | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 18  | A     | 806 | CLA  | O2D-CGD-O1D | -2.88 | 118.20      | 123.84   |
| 25  | 2     | 606 | CHL  | CMD-C2D-C3D | -2.88 | 120.99      | 127.61   |
| 18  | 5     | 613 | CLA  | CMB-C2B-C3B | 2.88  | 130.07      | 124.68   |
| 18  | 3     | 611 | CLA  | CMB-C2B-C3B | 2.88  | 130.06      | 124.68   |
| 27  | 2     | 620 | XAT  | C6-C7-C8    | -2.88 | 119.91      | 125.99   |
| 25  | 2     | 608 | CHL  | CMD-C2D-C3D | -2.87 | 121.00      | 127.61   |
| 25  | 5     | 606 | CHL  | CMD-C2D-C3D | -2.87 | 121.00      | 127.61   |
| 18  | B     | 816 | CLA  | CMB-C2B-C3B | 2.87  | 130.04      | 124.68   |
| 25  | 2     | 608 | CHL  | C1D-ND-C4D  | -2.86 | 104.30      | 106.33   |
| 21  | 5     | 621 | BCR  | C33-C5-C6   | -2.86 | 121.32      | 124.53   |
| 25  | 3     | 608 | CHL  | CMD-C2D-C3D | -2.86 | 121.04      | 127.61   |
| 25  | 2     | 607 | CHL  | CMD-C2D-C3D | -2.86 | 121.04      | 127.61   |
| 18  | K     | 206 | CLA  | O2D-CGD-O1D | -2.86 | 118.26      | 123.84   |
| 21  | 5     | 621 | BCR  | C15-C16-C17 | -2.85 | 117.64      | 123.47   |
| 18  | A     | 822 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 27  | 2     | 620 | XAT  | C35-C15-C14 | -2.85 | 117.64      | 123.47   |
| 21  | A     | 851 | BCR  | C24-C23-C22 | -2.85 | 121.93      | 126.23   |
| 18  | 3     | 610 | CLA  | O2D-CGD-O1D | -2.85 | 118.27      | 123.84   |
| 25  | 2     | 601 | CHL  | C2D-C1D-ND  | 2.84  | 112.20      | 110.10   |
| 18  | G     | 204 | CLA  | CMB-C2B-C3B | 2.84  | 130.00      | 124.68   |
| 18  | 2     | 611 | CLA  | CBD-CHA-C1A | 2.84  | 131.98      | 127.43   |
| 18  | G     | 201 | CLA  | O2D-CGD-O1D | -2.84 | 118.29      | 123.84   |
| 25  | 5     | 615 | CHL  | CMD-C2D-C3D | -2.84 | 121.08      | 127.61   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 5     | 612 | CLA  | CMB-C2B-C3B | 2.84  | 129.98      | 124.68   |
| 18  | B     | 809 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 18  | F     | 303 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 18  | B     | 836 | CLA  | O2D-CGD-O1D | -2.83 | 118.30      | 123.84   |
| 18  | 5     | 610 | CLA  | CMB-C2B-C3B | 2.83  | 129.98      | 124.68   |
| 18  | F     | 304 | CLA  | O2D-CGD-O1D | -2.83 | 118.31      | 123.84   |
| 25  | 2     | 616 | CHL  | CMD-C2D-C3D | -2.83 | 121.11      | 127.61   |
| 25  | 5     | 608 | CHL  | O2A-CGA-CBA | 2.83  | 120.77      | 111.91   |
| 18  | B     | 819 | CLA  | O2D-CGD-O1D | -2.82 | 118.32      | 123.84   |
| 18  | A     | 854 | CLA  | C1B-CHB-C4A | -2.82 | 124.53      | 130.12   |
| 18  | 5     | 603 | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 18  | A     | 824 | CLA  | CMB-C2B-C3B | 2.82  | 129.95      | 124.68   |
| 18  | 5     | 610 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 18  | F     | 305 | CLA  | O2D-CGD-O1D | -2.82 | 118.33      | 123.84   |
| 18  | A     | 840 | CLA  | CMB-C2B-C3B | 2.82  | 129.94      | 124.68   |
| 18  | 2     | 614 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 18  | 5     | 612 | CLA  | O2D-CGD-O1D | -2.81 | 118.34      | 123.84   |
| 18  | B     | 802 | CLA  | CMB-C2B-C3B | 2.81  | 129.93      | 124.68   |
| 18  | F     | 301 | CLA  | O2D-CGD-O1D | -2.81 | 118.35      | 123.84   |
| 18  | A     | 801 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 18  | 6     | 612 | CLA  | O2D-CGD-O1D | -2.80 | 118.36      | 123.84   |
| 23  | B     | 850 | DGD  | CDB-CCB-CBB | -2.80 | 100.21      | 114.42   |
| 18  | 6     | 613 | CLA  | CMB-C2B-C3B | 2.80  | 129.91      | 124.68   |
| 18  | 5     | 613 | CLA  | O2D-CGD-CBD | 2.80  | 116.24      | 111.27   |
| 21  | K     | 202 | BCR  | C15-C14-C13 | -2.80 | 123.32      | 127.31   |
| 18  | A     | 829 | CLA  | O2D-CGD-O1D | -2.80 | 118.37      | 123.84   |
| 18  | A     | 830 | CLA  | O2D-CGD-O1D | -2.79 | 118.39      | 123.84   |
| 18  | 6     | 609 | CLA  | CAB-C3B-C2B | 2.79  | 130.15      | 124.69   |
| 18  | 2     | 614 | CLA  | CMB-C2B-C3B | 2.79  | 129.89      | 124.68   |
| 18  | 6     | 614 | CLA  | O2D-CGD-O1D | -2.79 | 117.77      | 124.09   |
| 18  | A     | 841 | CLA  | CMB-C2B-C3B | 2.78  | 129.89      | 124.68   |
| 21  | K     | 202 | BCR  | C15-C16-C17 | -2.78 | 117.77      | 123.47   |
| 18  | 5     | 604 | CLA  | O2D-CGD-O1D | -2.78 | 118.39      | 123.84   |
| 27  | 6     | 619 | XAT  | C15-C14-C13 | -2.78 | 123.34      | 127.31   |
| 25  | 2     | 616 | CHL  | C1D-ND-C4D  | -2.78 | 104.36      | 106.33   |
| 18  | B     | 805 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 18  | B     | 813 | CLA  | CAC-C3C-C4C | 2.78  | 128.42      | 124.81   |
| 18  | 6     | 609 | CLA  | O2D-CGD-O1D | -2.78 | 118.40      | 123.84   |
| 25  | 6     | 601 | CHL  | CMD-C2D-C3D | -2.78 | 121.22      | 127.61   |
| 18  | 6     | 604 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |
| 18  | 6     | 603 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 18  | L     | 303 | CLA  | CMB-C2B-C3B | 2.78  | 129.88      | 124.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | K     | 204 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 18  | A     | 843 | CLA  | O2D-CGD-O1D | -2.78 | 118.41      | 123.84   |
| 18  | 2     | 613 | CLA  | O2D-CGD-O1D | -2.77 | 118.41      | 123.84   |
| 18  | 6     | 614 | CLA  | CAB-C3B-C2B | 2.77  | 130.12      | 124.69   |
| 18  | K     | 201 | CLA  | C1B-CHB-C4A | -2.77 | 124.63      | 130.12   |
| 18  | F     | 303 | CLA  | CMB-C2B-C3B | 2.77  | 129.86      | 124.68   |
| 25  | 2     | 607 | CHL  | C2D-C1D-ND  | 2.77  | 112.15      | 110.10   |
| 25  | 2     | 601 | CHL  | CMD-C2D-C3D | -2.77 | 121.24      | 127.61   |
| 18  | A     | 842 | CLA  | O2D-CGD-O1D | -2.77 | 117.80      | 124.09   |
| 18  | 5     | 611 | CLA  | O2D-CGD-O1D | -2.77 | 118.43      | 123.84   |
| 18  | 2     | 612 | CLA  | CMB-C2B-C3B | 2.76  | 129.85      | 124.68   |
| 18  | B     | 808 | CLA  | CMB-C2B-C3B | 2.76  | 129.84      | 124.68   |
| 18  | B     | 821 | CLA  | CMB-C2B-C3B | 2.76  | 129.84      | 124.68   |
| 18  | G     | 203 | CLA  | CMB-C2B-C3B | 2.76  | 129.83      | 124.68   |
| 18  | 2     | 603 | CLA  | CMB-C2B-C3B | 2.75  | 129.83      | 124.68   |
| 25  | 6     | 601 | CHL  | CMB-C2B-C3B | 2.75  | 129.83      | 124.68   |
| 18  | 2     | 613 | CLA  | CMB-C2B-C3B | 2.75  | 129.82      | 124.68   |
| 18  | B     | 840 | CLA  | CMB-C2B-C3B | 2.75  | 129.81      | 124.68   |
| 18  | A     | 815 | CLA  | O2D-CGD-O1D | -2.74 | 118.47      | 123.84   |
| 18  | A     | 810 | CLA  | O2D-CGD-O1D | -2.74 | 118.47      | 123.84   |
| 18  | A     | 825 | CLA  | CMB-C2B-C3B | 2.74  | 129.81      | 124.68   |
| 18  | 3     | 612 | CLA  | O2D-CGD-O1D | -2.74 | 118.48      | 123.84   |
| 21  | B     | 847 | BCR  | C15-C14-C13 | -2.74 | 123.40      | 127.31   |
| 18  | A     | 841 | CLA  | O2D-CGD-O1D | -2.74 | 118.49      | 123.84   |
| 18  | 3     | 617 | CLA  | O2D-CGD-O1D | -2.73 | 117.88      | 124.09   |
| 25  | 6     | 601 | CHL  | C1D-ND-C4D  | -2.73 | 104.39      | 106.33   |
| 18  | B     | 803 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 18  | 2     | 604 | CLA  | CHB-C4A-NA  | 2.73  | 128.29      | 124.51   |
| 18  | 6     | 614 | CLA  | CMB-C2B-C3B | 2.73  | 130.03      | 124.69   |
| 18  | A     | 845 | CLA  | O2D-CGD-O1D | -2.73 | 118.50      | 123.84   |
| 18  | J     | 101 | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 18  | B     | 837 | CLA  | CMB-C2B-C3B | 2.73  | 129.78      | 124.68   |
| 18  | G     | 203 | CLA  | O2D-CGD-O1D | -2.73 | 118.51      | 123.84   |
| 18  | 3     | 611 | CLA  | CHB-C4A-NA  | 2.73  | 128.28      | 124.51   |
| 18  | 3     | 613 | CLA  | CMB-C2B-C3B | 2.72  | 129.77      | 124.68   |
| 25  | 5     | 607 | CHL  | C3B-C4B-NB  | 2.72  | 112.73      | 109.21   |
| 18  | A     | 810 | CLA  | CMB-C2B-C3B | 2.72  | 129.77      | 124.68   |
| 18  | A     | 821 | CLA  | CMB-C2B-C3B | 2.72  | 129.77      | 124.68   |
| 18  | B     | 806 | CLA  | O2D-CGD-O1D | -2.72 | 118.52      | 123.84   |
| 21  | A     | 852 | BCR  | C33-C5-C6   | -2.72 | 121.48      | 124.53   |
| 18  | 6     | 616 | CLA  | CAB-C3B-C2B | 2.72  | 130.01      | 124.69   |
| 24  | J     | 104 | LMG  | O6-C1-O1    | -2.71 | 103.55      | 109.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | G     | 203 | CLA  | C1-C2-C3    | -2.71 | 122.36      | 126.75   |
| 18  | K     | 204 | CLA  | CAB-C3B-C2B | 2.71  | 129.99      | 124.69   |
| 21  | B     | 843 | BCR  | C27-C26-C25 | 2.71  | 126.66      | 122.73   |
| 25  | 5     | 607 | CHL  | CMD-C2D-C3D | -2.71 | 121.39      | 127.61   |
| 18  | K     | 203 | CLA  | CMB-C2B-C3B | 2.71  | 129.74      | 124.68   |
| 21  | J     | 102 | BCR  | C15-C14-C13 | -2.71 | 123.45      | 127.31   |
| 21  | A     | 852 | BCR  | C15-C16-C17 | -2.71 | 117.93      | 123.47   |
| 27  | 3     | 619 | XAT  | C30-C31-C32 | -2.70 | 114.78      | 123.22   |
| 25  | 2     | 606 | CHL  | C2A-C1A-CHA | -2.70 | 119.13      | 123.86   |
| 18  | 3     | 615 | CLA  | CMB-C2B-C3B | 2.70  | 129.74      | 124.68   |
| 21  | L     | 305 | BCR  | C15-C16-C17 | -2.70 | 117.94      | 123.47   |
| 18  | B     | 841 | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 18  | A     | 838 | CLA  | CMB-C2B-C3B | 2.70  | 129.73      | 124.68   |
| 18  | B     | 828 | CLA  | CMB-C2B-C3B | 2.70  | 129.72      | 124.68   |
| 21  | 2     | 621 | BCR  | C24-C23-C22 | -2.70 | 122.16      | 126.23   |
| 18  | A     | 843 | CLA  | CMB-C2B-C3B | 2.69  | 129.72      | 124.68   |
| 18  | 3     | 607 | CLA  | CAB-C3B-C2B | 2.69  | 129.96      | 124.69   |
| 25  | 6     | 607 | CHL  | C3B-C4B-NB  | 2.69  | 112.69      | 109.21   |
| 18  | 5     | 601 | CLA  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 20  | 5     | 622 | LHG  | O8-C23-C24  | 2.69  | 120.35      | 111.91   |
| 18  | 6     | 606 | CLA  | CMB-C2B-C3B | 2.69  | 129.71      | 124.68   |
| 18  | 6     | 612 | CLA  | CMB-C2B-C3B | 2.68  | 129.70      | 124.68   |
| 21  | 2     | 621 | BCR  | C15-C16-C17 | -2.68 | 117.98      | 123.47   |
| 18  | B     | 818 | CLA  | CMB-C2B-C3B | 2.68  | 129.70      | 124.68   |
| 20  | 6     | 620 | LHG  | O8-C23-C24  | 2.68  | 120.32      | 111.91   |
| 27  | 3     | 619 | XAT  | C19-C9-C8   | 2.68  | 122.30      | 118.08   |
| 18  | A     | 842 | CLA  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 18  | B     | 834 | CLA  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 18  | 3     | 607 | CLA  | CMB-C2B-C3B | 2.68  | 129.93      | 124.69   |
| 18  | B     | 804 | CLA  | CHB-C4A-NA  | 2.68  | 128.22      | 124.51   |
| 18  | B     | 817 | CLA  | CMB-C2B-C3B | 2.68  | 129.69      | 124.68   |
| 21  | 5     | 621 | BCR  | C15-C14-C13 | -2.68 | 123.49      | 127.31   |
| 18  | 6     | 608 | CLA  | O2D-CGD-O1D | -2.68 | 118.01      | 124.09   |
| 18  | A     | 835 | CLA  | O2D-CGD-CBD | 2.68  | 116.03      | 111.27   |
| 18  | 5     | 611 | CLA  | C1A-CHA-C4D | -2.68 | 121.97      | 125.72   |
| 25  | 5     | 608 | CHL  | C1B-CHB-C4A | -2.68 | 124.82      | 130.12   |
| 18  | 5     | 611 | CLA  | CAB-C3B-C2B | 2.67  | 129.92      | 124.69   |
| 18  | 3     | 603 | CLA  | O2D-CGD-O1D | -2.67 | 118.62      | 123.84   |
| 25  | 5     | 607 | CHL  | CHD-C4C-C3C | -2.67 | 120.92      | 124.84   |
| 25  | 5     | 606 | CHL  | CAC-C3C-C4C | 2.67  | 129.10      | 125.04   |
| 25  | 5     | 608 | CHL  | CMD-C2D-C3D | -2.66 | 121.48      | 127.61   |
| 25  | 6     | 607 | CHL  | CHD-C4C-C3C | -2.66 | 120.93      | 124.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | 5     | 620 | XAT  | C15-C14-C13 | -2.66 | 123.51      | 127.31   |
| 25  | 5     | 606 | CHL  | C1B-CHB-C4A | -2.66 | 124.85      | 130.12   |
| 18  | 6     | 608 | CLA  | CMB-C2B-C3B | 2.66  | 129.66      | 124.68   |
| 21  | B     | 845 | BCR  | C27-C26-C25 | 2.66  | 126.59      | 122.73   |
| 18  | 3     | 614 | CLA  | CAA-C2A-C3A | -2.66 | 109.90      | 116.10   |
| 21  | L     | 301 | BCR  | C15-C16-C17 | -2.65 | 118.04      | 123.47   |
| 25  | 5     | 608 | CHL  | C1C-C2C-C3C | -2.65 | 105.01      | 107.11   |
| 21  | 3     | 620 | BCR  | C3-C4-C5    | -2.65 | 109.34      | 114.08   |
| 18  | A     | 812 | CLA  | CMB-C2B-C3B | 2.65  | 129.63      | 124.68   |
| 21  | A     | 851 | BCR  | C27-C26-C25 | 2.65  | 126.57      | 122.73   |
| 18  | 3     | 603 | CLA  | CMB-C2B-C3B | 2.65  | 129.63      | 124.68   |
| 18  | B     | 812 | CLA  | CHB-C4A-NA  | 2.65  | 128.17      | 124.51   |
| 25  | 6     | 607 | CHL  | CMB-C2B-C3B | 2.64  | 129.63      | 124.68   |
| 21  | J     | 102 | BCR  | C27-C26-C25 | 2.64  | 126.57      | 122.73   |
| 18  | A     | 841 | CLA  | C1-C2-C3    | -2.64 | 121.47      | 126.04   |
| 18  | F     | 304 | CLA  | CAA-C2A-C3A | -2.64 | 109.93      | 116.10   |
| 18  | A     | 832 | CLA  | CAA-C2A-C3A | -2.64 | 109.93      | 116.10   |
| 21  | B     | 846 | BCR  | C24-C23-C22 | -2.64 | 122.24      | 126.23   |
| 18  | 5     | 611 | CLA  | CMB-C2B-C3B | 2.64  | 129.86      | 124.69   |
| 18  | A     | 845 | CLA  | CHB-C4A-NA  | 2.64  | 128.16      | 124.51   |
| 25  | 5     | 607 | CHL  | O2D-CGD-O1D | -2.64 | 118.68      | 123.84   |
| 18  | B     | 824 | CLA  | O2D-CGD-CBD | 2.64  | 115.96      | 111.27   |
| 18  | 6     | 611 | CLA  | CMB-C2B-C3B | 2.64  | 129.85      | 124.69   |
| 21  | K     | 207 | BCR  | C15-C14-C13 | -2.63 | 123.55      | 127.31   |
| 26  | 3     | 618 | LUT  | C10-C11-C12 | -2.63 | 115.00      | 123.22   |
| 18  | 3     | 607 | CLA  | O2D-CGD-O1D | -2.63 | 118.11      | 124.09   |
| 18  | 5     | 612 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 18  | A     | 835 | CLA  | CHB-C4A-NA  | 2.63  | 128.15      | 124.51   |
| 18  | L     | 304 | CLA  | CHB-C4A-NA  | 2.63  | 128.14      | 124.51   |
| 18  | B     | 816 | CLA  | O2D-CGD-O1D | -2.63 | 118.13      | 124.09   |
| 21  | A     | 849 | BCR  | C15-C16-C17 | -2.62 | 118.10      | 123.47   |
| 25  | 2     | 606 | CHL  | C1C-C2C-C3C | -2.62 | 105.03      | 107.11   |
| 18  | A     | 834 | CLA  | CMB-C2B-C3B | 2.62  | 129.58      | 124.68   |
| 18  | A     | 822 | CLA  | CAB-C3B-C2B | 2.62  | 129.81      | 124.69   |
| 18  | 5     | 602 | CLA  | CMB-C2B-C3B | 2.62  | 129.57      | 124.68   |
| 21  | J     | 103 | BCR  | C33-C5-C6   | -2.62 | 121.59      | 124.53   |
| 25  | 5     | 615 | CHL  | CMB-C2B-C3B | 2.62  | 129.57      | 124.68   |
| 21  | F     | 302 | BCR  | C15-C16-C17 | -2.62 | 118.12      | 123.47   |
| 21  | L     | 301 | BCR  | C33-C5-C6   | -2.61 | 121.59      | 124.53   |
| 18  | 6     | 609 | CLA  | CMB-C2B-C3B | 2.61  | 129.81      | 124.69   |
| 18  | 3     | 614 | CLA  | CMB-C2B-C3B | 2.61  | 129.56      | 124.68   |
| 18  | 3     | 613 | CLA  | O2D-CGD-O1D | -2.61 | 118.16      | 124.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 5     | 613 | CLA  | CHB-C4A-NA  | 2.61  | 128.12      | 124.51   |
| 18  | 6     | 611 | CLA  | CAA-C2A-C3A | -2.61 | 110.01      | 116.10   |
| 26  | 2     | 619 | LUT  | C11-C12-C13 | -2.61 | 119.09      | 126.42   |
| 21  | L     | 305 | BCR  | C33-C5-C6   | -2.61 | 121.60      | 124.53   |
| 18  | B     | 815 | CLA  | CMB-C2B-C3B | 2.61  | 129.56      | 124.68   |
| 18  | 2     | 609 | CLA  | C1B-CHB-C4A | -2.61 | 124.95      | 130.12   |
| 21  | 3     | 620 | BCR  | C2-C1-C6    | 2.61  | 114.50      | 110.48   |
| 26  | 6     | 617 | LUT  | C1-C6-C7    | -2.61 | 108.40      | 115.78   |
| 18  | B     | 802 | CLA  | C1B-CHB-C4A | -2.61 | 124.95      | 130.12   |
| 18  | 3     | 612 | CLA  | CMB-C2B-C3B | 2.60  | 129.55      | 124.68   |
| 20  | 2     | 622 | LHG  | O8-C23-C24  | 2.60  | 120.08      | 111.91   |
| 18  | 6     | 616 | CLA  | CMB-C2B-C3B | 2.60  | 129.78      | 124.69   |
| 27  | 2     | 620 | XAT  | O24-C25-C38 | 2.60  | 118.17      | 115.06   |
| 21  | L     | 305 | BCR  | C28-C27-C26 | -2.60 | 109.44      | 114.08   |
| 21  | B     | 846 | BCR  | C27-C26-C25 | 2.59  | 126.50      | 122.73   |
| 26  | 5     | 619 | LUT  | C21-C26-C27 | -2.59 | 109.42      | 112.70   |
| 18  | B     | 802 | CLA  | O2D-CGD-O1D | -2.59 | 118.77      | 123.84   |
| 18  | B     | 805 | CLA  | CHB-C4A-NA  | 2.59  | 128.10      | 124.51   |
| 18  | B     | 811 | CLA  | CAB-C3B-C2B | 2.59  | 129.76      | 124.69   |
| 18  | 3     | 604 | CLA  | CAB-C3B-C2B | 2.59  | 129.76      | 124.69   |
| 18  | B     | 810 | CLA  | CMB-C2B-C3B | 2.59  | 129.52      | 124.68   |
| 18  | B     | 824 | CLA  | CHB-C4A-NA  | 2.59  | 128.09      | 124.51   |
| 21  | A     | 856 | BCR  | C15-C16-C17 | -2.59 | 118.18      | 123.47   |
| 21  | 3     | 622 | BCR  | C24-C23-C22 | -2.58 | 122.33      | 126.23   |
| 21  | B     | 848 | BCR  | C33-C5-C6   | -2.58 | 121.63      | 124.53   |
| 18  | K     | 206 | CLA  | CMB-C2B-C3B | 2.58  | 129.51      | 124.68   |
| 21  | J     | 102 | BCR  | C24-C23-C22 | -2.58 | 122.33      | 126.23   |
| 27  | 3     | 619 | XAT  | C31-C30-C29 | -2.58 | 123.62      | 127.31   |
| 18  | 3     | 604 | CLA  | O2D-CGD-O1D | -2.58 | 118.23      | 124.09   |
| 25  | 2     | 606 | CHL  | CMB-C2B-C3B | 2.58  | 129.51      | 124.68   |
| 18  | A     | 817 | CLA  | CAA-C2A-C3A | -2.58 | 110.08      | 116.10   |
| 18  | A     | 823 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 18  | 6     | 611 | CLA  | O2D-CGD-O1D | -2.58 | 118.23      | 124.09   |
| 18  | A     | 802 | CLA  | CHB-C4A-NA  | 2.58  | 128.08      | 124.51   |
| 18  | B     | 814 | CLA  | O2D-CGD-O1D | -2.58 | 118.24      | 124.09   |
| 21  | K     | 207 | BCR  | C24-C23-C22 | -2.58 | 122.34      | 126.23   |
| 27  | 2     | 620 | XAT  | C20-C13-C12 | 2.58  | 122.14      | 118.08   |
| 18  | B     | 827 | CLA  | C1B-CHB-C4A | -2.58 | 125.02      | 130.12   |
| 18  | 6     | 612 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |
| 18  | 6     | 611 | CLA  | CAB-C3B-C2B | 2.57  | 129.73      | 124.69   |
| 18  | A     | 829 | CLA  | C1-C2-C3    | -2.57 | 121.59      | 126.04   |
| 18  | A     | 822 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 813 | CLA  | CHB-C4A-NA  | 2.57  | 128.07      | 124.51   |
| 18  | A     | 805 | CLA  | O2D-CGD-CBD | 2.57  | 115.84      | 111.27   |
| 18  | A     | 835 | CLA  | C1B-CHB-C4A | -2.57 | 125.03      | 130.12   |
| 18  | A     | 845 | CLA  | CMB-C2B-C3B | 2.57  | 129.48      | 124.68   |
| 18  | B     | 839 | CLA  | CHB-C4A-NA  | 2.57  | 128.06      | 124.51   |
| 18  | 5     | 604 | CLA  | CHB-C4A-NA  | 2.57  | 128.06      | 124.51   |
| 25  | 5     | 607 | CHL  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 20  | A     | 846 | LHG  | C11-C10-C9  | -2.56 | 101.41      | 114.42   |
| 18  | 3     | 603 | CLA  | C1B-CHB-C4A | -2.56 | 125.04      | 130.12   |
| 23  | B     | 850 | DGD  | C3G-C2G-C1G | -2.56 | 105.73      | 111.79   |
| 18  | A     | 804 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 20  | A     | 846 | LHG  | O8-C23-C24  | 2.56  | 119.94      | 111.91   |
| 18  | 6     | 606 | CLA  | O2D-CGD-CBD | 2.56  | 115.82      | 111.27   |
| 25  | 2     | 607 | CHL  | CMB-C2B-C3B | 2.56  | 129.47      | 124.68   |
| 18  | K     | 204 | CLA  | CMB-C2B-C3B | 2.56  | 129.70      | 124.69   |
| 18  | 2     | 609 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 18  | B     | 828 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 18  | 6     | 614 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 27  | 2     | 620 | XAT  | C39-C29-C28 | 2.56  | 122.11      | 118.08   |
| 18  | K     | 204 | CLA  | CHB-C4A-NA  | 2.56  | 128.05      | 124.51   |
| 18  | 6     | 610 | CLA  | C1B-CHB-C4A | -2.56 | 125.05      | 130.12   |
| 21  | K     | 207 | BCR  | C3-C4-C5    | -2.56 | 109.51      | 114.08   |
| 21  | A     | 851 | BCR  | C33-C5-C6   | -2.55 | 121.66      | 124.53   |
| 18  | 3     | 609 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 18  | B     | 803 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 18  | 3     | 612 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 18  | G     | 201 | CLA  | CMB-C2B-C3B | 2.55  | 129.45      | 124.68   |
| 18  | A     | 814 | CLA  | CHB-C4A-NA  | 2.55  | 128.04      | 124.51   |
| 18  | A     | 831 | CLA  | O2D-CGD-CBD | 2.55  | 115.80      | 111.27   |
| 21  | B     | 848 | BCR  | C7-C8-C9    | -2.55 | 122.39      | 126.23   |
| 21  | G     | 205 | BCR  | C24-C23-C22 | -2.55 | 122.39      | 126.23   |
| 18  | 3     | 604 | CLA  | CMB-C2B-C3B | 2.54  | 129.67      | 124.69   |
| 18  | B     | 811 | CLA  | CMB-C2B-C3B | 2.54  | 129.66      | 124.69   |
| 18  | A     | 854 | CLA  | C1-C2-C3    | -2.54 | 121.65      | 126.04   |
| 18  | B     | 806 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 21  | A     | 851 | BCR  | C15-C16-C17 | -2.54 | 118.27      | 123.47   |
| 18  | B     | 808 | CLA  | O2A-CGA-O1A | -2.54 | 117.18      | 123.59   |
| 18  | A     | 833 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 18  | B     | 820 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 18  | B     | 826 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 18  | B     | 834 | CLA  | CHB-C4A-NA  | 2.54  | 128.02      | 124.51   |
| 27  | 5     | 620 | XAT  | C10-C11-C12 | -2.54 | 115.31      | 123.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 820 | CLA  | C1B-CHB-C4A | -2.54 | 125.10      | 130.12   |
| 25  | 5     | 606 | CHL  | CMB-C2B-C3B | 2.53  | 129.65      | 124.69   |
| 25  | 5     | 615 | CHL  | C2A-C1A-CHA | -2.53 | 119.43      | 123.86   |
| 18  | A     | 817 | CLA  | O2D-CGD-O1D | -2.53 | 118.34      | 124.09   |
| 21  | B     | 801 | BCR  | C33-C5-C6   | -2.53 | 121.68      | 124.53   |
| 18  | A     | 817 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 18  | 3     | 602 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 21  | I     | 101 | BCR  | C15-C16-C17 | -2.53 | 118.29      | 123.47   |
| 18  | A     | 818 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 18  | A     | 826 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 18  | A     | 829 | CLA  | C1B-CHB-C4A | -2.53 | 125.11      | 130.12   |
| 21  | G     | 205 | BCR  | C33-C5-C6   | -2.53 | 121.69      | 124.53   |
| 18  | A     | 836 | CLA  | CHB-C4A-NA  | 2.53  | 128.01      | 124.51   |
| 18  | B     | 835 | CLA  | C1B-CHB-C4A | -2.53 | 125.11      | 130.12   |
| 18  | B     | 833 | CLA  | C1B-CHB-C4A | -2.52 | 125.12      | 130.12   |
| 21  | 3     | 622 | BCR  | C15-C14-C13 | -2.52 | 123.71      | 127.31   |
| 21  | B     | 843 | BCR  | C33-C5-C6   | -2.52 | 121.70      | 124.53   |
| 18  | G     | 201 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 21  | B     | 848 | BCR  | C28-C27-C26 | -2.52 | 109.58      | 114.08   |
| 18  | B     | 817 | CLA  | CHB-C4A-NA  | 2.52  | 128.00      | 124.51   |
| 18  | A     | 801 | CLA  | C1B-CHB-C4A | -2.52 | 125.13      | 130.12   |
| 18  | A     | 822 | CLA  | CMB-C2B-C3B | 2.52  | 129.62      | 124.69   |
| 21  | B     | 843 | BCR  | C24-C23-C22 | -2.52 | 122.43      | 126.23   |
| 18  | G     | 204 | CLA  | O2D-CGD-O1D | -2.52 | 118.38      | 124.09   |
| 18  | B     | 837 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 18  | 3     | 613 | CLA  | CHB-C4A-NA  | 2.51  | 127.99      | 124.51   |
| 18  | 2     | 612 | CLA  | CAA-C2A-C3A | -2.51 | 110.24      | 116.10   |
| 18  | A     | 806 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 18  | A     | 809 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 18  | 3     | 606 | CLA  | O2D-CGD-O1D | -2.51 | 118.39      | 124.09   |
| 18  | B     | 840 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 18  | G     | 203 | CLA  | C1B-CHB-C4A | -2.51 | 125.15      | 130.12   |
| 18  | 5     | 609 | CLA  | CHB-C4A-NA  | 2.51  | 127.98      | 124.51   |
| 18  | L     | 303 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 18  | A     | 807 | CLA  | O2D-CGD-O1D | -2.50 | 118.40      | 124.09   |
| 25  | 2     | 616 | CHL  | CMB-C2B-C3B | 2.50  | 129.36      | 124.68   |
| 18  | 3     | 607 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 18  | B     | 815 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 18  | B     | 825 | CLA  | C1B-CHB-C4A | -2.50 | 125.17      | 130.12   |
| 18  | B     | 808 | CLA  | CHB-C4A-NA  | 2.50  | 127.97      | 124.51   |
| 18  | A     | 825 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 18  | A     | 810 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | L     | 301 | BCR  | C15-C14-C13 | -2.49 | 123.75      | 127.31   |
| 21  | A     | 850 | BCR  | C33-C5-C6   | -2.49 | 121.73      | 124.53   |
| 21  | K     | 202 | BCR  | C33-C5-C6   | -2.49 | 121.73      | 124.53   |
| 18  | 2     | 611 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 18  | 2     | 603 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 21  | 2     | 621 | BCR  | C27-C26-C25 | 2.49  | 126.35      | 122.73   |
| 18  | K     | 206 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 18  | 6     | 606 | CLA  | CHB-C4A-NA  | 2.49  | 127.96      | 124.51   |
| 18  | A     | 815 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 18  | B     | 830 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 26  | 3     | 618 | LUT  | C15-C35-C34 | -2.49 | 118.38      | 123.47   |
| 18  | A     | 832 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 18  | 6     | 616 | CLA  | CHB-C4A-NA  | 2.49  | 127.95      | 124.51   |
| 25  | 2     | 601 | CHL  | CMB-C2B-C3B | 2.49  | 129.56      | 124.69   |
| 18  | A     | 841 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 18  | A     | 843 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 18  | K     | 203 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 18  | G     | 203 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 18  | F     | 304 | CLA  | CHB-C4A-NA  | 2.48  | 127.95      | 124.51   |
| 18  | 2     | 602 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 27  | 2     | 620 | XAT  | C24-C23-C22 | -2.48 | 105.98      | 110.77   |
| 18  | A     | 831 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | B     | 841 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | 6     | 608 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | 3     | 606 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | A     | 821 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | 6     | 610 | CLA  | O2D-CGD-O1D | -2.48 | 118.46      | 124.09   |
| 18  | B     | 822 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | B     | 807 | CLA  | C1-C2-C3    | -2.48 | 121.76      | 126.04   |
| 18  | 5     | 603 | CLA  | O2D-CGD-O1D | -2.48 | 118.46      | 124.09   |
| 18  | 5     | 610 | CLA  | C1-C2-C3    | -2.48 | 121.76      | 126.04   |
| 18  | A     | 824 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 21  | B     | 843 | BCR  | C15-C16-C17 | -2.48 | 118.40      | 123.47   |
| 18  | B     | 829 | CLA  | CHB-C4A-NA  | 2.48  | 127.94      | 124.51   |
| 18  | 6     | 602 | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 18  | 5     | 614 | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 18  | 5     | 601 | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 18  | 6     | 604 | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 20  | A     | 847 | LHG  | C11-C10-C9  | -2.47 | 101.88      | 114.42   |
| 18  | 5     | 603 | CLA  | CHB-C4A-NA  | 2.47  | 127.93      | 124.51   |
| 25  | 2     | 616 | CHL  | C1C-C2C-C3C | -2.47 | 105.16      | 107.11   |
| 18  | 3     | 614 | CLA  | O2D-CGD-O1D | -2.47 | 118.49      | 124.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | G     | 204 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 18  | K     | 201 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 18  | 6     | 603 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 25  | 2     | 608 | CHL  | CMB-C2B-C3B | 2.46  | 129.29      | 124.68   |
| 18  | B     | 810 | CLA  | CHB-C4A-NA  | 2.46  | 127.92      | 124.51   |
| 27  | 3     | 619 | XAT  | C35-C34-C33 | -2.46 | 123.80      | 127.31   |
| 18  | A     | 812 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 18  | A     | 816 | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 18  | F     | 301 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 18  | J     | 101 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 18  | 2     | 614 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 18  | A     | 828 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 18  | 5     | 602 | CLA  | C1B-CHB-C4A | -2.46 | 125.25      | 130.12   |
| 18  | B     | 839 | CLA  | O2D-CGD-O1D | -2.46 | 118.51      | 124.09   |
| 18  | 5     | 610 | CLA  | CHB-C4A-NA  | 2.46  | 127.91      | 124.51   |
| 21  | A     | 848 | BCR  | C3-C4-C5    | -2.45 | 109.70      | 114.08   |
| 18  | B     | 808 | CLA  | C1B-CHB-C4A | -2.45 | 125.26      | 130.12   |
| 18  | 6     | 609 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 18  | A     | 839 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 18  | 6     | 610 | CLA  | CHB-C4A-NA  | 2.45  | 127.90      | 124.51   |
| 25  | 5     | 608 | CHL  | CMB-C2B-C3B | 2.45  | 129.25      | 124.68   |
| 18  | A     | 822 | CLA  | C1B-CHB-C4A | -2.45 | 125.27      | 130.12   |
| 21  | A     | 856 | BCR  | C15-C14-C13 | -2.45 | 123.82      | 127.31   |
| 21  | 3     | 622 | BCR  | C11-C10-C9  | -2.44 | 123.82      | 127.31   |
| 25  | 2     | 616 | CHL  | O2D-CGD-O1D | -2.44 | 119.06      | 123.84   |
| 25  | 5     | 606 | CHL  | O2D-CGD-O1D | -2.44 | 119.06      | 123.84   |
| 21  | A     | 856 | BCR  | C24-C23-C22 | -2.44 | 122.54      | 126.23   |
| 18  | B     | 834 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 18  | L     | 302 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 18  | 2     | 604 | CLA  | O2D-CGD-CBD | 2.44  | 115.61      | 111.27   |
| 18  | A     | 805 | CLA  | C1B-CHB-C4A | -2.44 | 125.28      | 130.12   |
| 18  | 3     | 610 | CLA  | CAA-C2A-C3A | -2.44 | 110.41      | 116.10   |
| 18  | A     | 816 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 18  | A     | 827 | CLA  | CHB-C4A-NA  | 2.44  | 127.89      | 124.51   |
| 18  | 3     | 604 | CLA  | CHB-C4A-NA  | 2.44  | 127.88      | 124.51   |
| 25  | 5     | 615 | CHL  | C1C-C2C-C3C | -2.44 | 105.18      | 107.11   |
| 25  | 5     | 607 | CHL  | C2D-C1D-ND  | 2.44  | 111.90      | 110.10   |
| 18  | B     | 830 | CLA  | C1B-CHB-C4A | -2.44 | 125.29      | 130.12   |
| 21  | F     | 302 | BCR  | C27-C26-C25 | 2.43  | 126.26      | 122.73   |
| 18  | 5     | 604 | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 18  | A     | 843 | CLA  | C1B-CHB-C4A | -2.43 | 125.30      | 130.12   |
| 18  | 3     | 610 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | F     | 303 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 18  | 5     | 609 | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 18  | 6     | 611 | CLA  | CHB-C4A-NA  | 2.43  | 127.87      | 124.51   |
| 18  | A     | 802 | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 18  | A     | 840 | CLA  | C1B-CHB-C4A | -2.43 | 125.31      | 130.12   |
| 18  | B     | 811 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 18  | B     | 814 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 21  | B     | 847 | BCR  | C27-C26-C25 | 2.42  | 126.25      | 122.73   |
| 18  | B     | 818 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 25  | 5     | 606 | CHL  | OMC-CMC-C2C | -2.42 | 120.21      | 125.69   |
| 18  | 3     | 617 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 18  | B     | 819 | CLA  | CHB-C4A-NA  | 2.42  | 127.86      | 124.51   |
| 18  | 6     | 602 | CLA  | C1B-CHB-C4A | -2.42 | 125.32      | 130.12   |
| 18  | B     | 803 | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 25  | 5     | 608 | CHL  | C5-C3-C4    | 2.42  | 119.94      | 114.60   |
| 20  | 5     | 622 | LHG  | C11-C10-C9  | -2.42 | 102.15      | 114.42   |
| 18  | B     | 838 | CLA  | C1B-CHB-C4A | -2.42 | 125.33      | 130.12   |
| 21  | L     | 301 | BCR  | C27-C26-C25 | 2.42  | 126.24      | 122.73   |
| 25  | 6     | 607 | CHL  | CHD-C1D-C2D | 2.42  | 130.55      | 125.48   |
| 20  | 2     | 622 | LHG  | C11-C10-C9  | -2.42 | 102.16      | 114.42   |
| 21  | B     | 843 | BCR  | C15-C14-C13 | -2.41 | 123.86      | 127.31   |
| 18  | B     | 813 | CLA  | C1B-CHB-C4A | -2.41 | 125.33      | 130.12   |
| 18  | A     | 807 | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 21  | B     | 801 | BCR  | C27-C26-C25 | 2.41  | 126.23      | 122.73   |
| 18  | B     | 816 | CLA  | CHB-C4A-NA  | 2.41  | 127.85      | 124.51   |
| 18  | A     | 831 | CLA  | C1B-CHB-C4A | -2.41 | 125.34      | 130.12   |
| 18  | A     | 842 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 18  | 2     | 613 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 21  | B     | 844 | BCR  | C15-C16-C17 | -2.41 | 118.54      | 123.47   |
| 18  | A     | 834 | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 18  | B     | 809 | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 18  | A     | 808 | CLA  | CHB-C4A-NA  | 2.41  | 127.84      | 124.51   |
| 18  | B     | 807 | CLA  | C1B-CHB-C4A | -2.41 | 125.35      | 130.12   |
| 18  | 3     | 610 | CLA  | C1B-CHB-C4A | -2.40 | 125.35      | 130.12   |
| 21  | B     | 846 | BCR  | C33-C5-C6   | -2.40 | 121.83      | 124.53   |
| 18  | A     | 830 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 27  | 6     | 619 | XAT  | C39-C29-C28 | 2.40  | 121.86      | 118.08   |
| 21  | A     | 856 | BCR  | C11-C10-C9  | -2.40 | 123.88      | 127.31   |
| 18  | F     | 305 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 18  | B     | 836 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 18  | A     | 834 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 18  | A     | 825 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 2     | 607 | CHL  | C1D-ND-C4D  | -2.40 | 104.63      | 106.33   |
| 18  | B     | 819 | CLA  | C1B-CHB-C4A | -2.40 | 125.36      | 130.12   |
| 18  | 6     | 613 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 18  | B     | 825 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 18  | 3     | 614 | CLA  | CHB-C4A-NA  | 2.40  | 127.83      | 124.51   |
| 21  | B     | 848 | BCR  | C35-C13-C14 | -2.40 | 119.56      | 122.92   |
| 18  | B     | 831 | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 18  | B     | 840 | CLA  | C1B-CHB-C4A | -2.39 | 125.38      | 130.12   |
| 21  | A     | 856 | BCR  | C3-C4-C5    | -2.39 | 109.80      | 114.08   |
| 18  | A     | 806 | CLA  | C1B-CHB-C4A | -2.39 | 125.38      | 130.12   |
| 18  | A     | 813 | CLA  | CHB-C4A-NA  | 2.39  | 127.82      | 124.51   |
| 18  | A     | 827 | CLA  | C1B-CHB-C4A | -2.39 | 125.38      | 130.12   |
| 21  | K     | 207 | BCR  | C27-C26-C25 | 2.39  | 126.20      | 122.73   |
| 21  | G     | 205 | BCR  | C15-C16-C17 | -2.39 | 118.58      | 123.47   |
| 18  | 3     | 609 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 21  | B     | 845 | BCR  | C24-C23-C22 | -2.39 | 122.63      | 126.23   |
| 18  | B     | 808 | CLA  | C1-C2-C3    | -2.39 | 122.89      | 126.75   |
| 18  | A     | 828 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 21  | A     | 852 | BCR  | C27-C26-C25 | 2.39  | 126.19      | 122.73   |
| 26  | 2     | 619 | LUT  | C20-C13-C14 | -2.39 | 119.58      | 122.92   |
| 18  | 3     | 602 | CLA  | C1B-CHB-C4A | -2.39 | 125.39      | 130.12   |
| 18  | A     | 838 | CLA  | CHB-C4A-NA  | 2.38  | 127.81      | 124.51   |
| 18  | F     | 305 | CLA  | CHB-C4A-NA  | 2.38  | 127.81      | 124.51   |
| 18  | A     | 830 | CLA  | CHB-C4A-NA  | 2.38  | 127.81      | 124.51   |
| 18  | A     | 823 | CLA  | C1B-CHB-C4A | -2.38 | 125.40      | 130.12   |
| 21  | B     | 847 | BCR  | C11-C10-C9  | -2.38 | 123.91      | 127.31   |
| 21  | 5     | 621 | BCR  | C27-C26-C25 | 2.38  | 126.19      | 122.73   |
| 18  | 3     | 615 | CLA  | C1B-CHB-C4A | -2.38 | 125.40      | 130.12   |
| 21  | A     | 856 | BCR  | C27-C26-C25 | 2.38  | 126.19      | 122.73   |
| 18  | 6     | 609 | CLA  | CAA-C2A-C3A | -2.38 | 110.55      | 116.10   |
| 25  | 5     | 606 | CHL  | C1C-C2C-C3C | -2.38 | 105.23      | 107.11   |
| 18  | B     | 821 | CLA  | CHB-C4A-NA  | 2.38  | 127.80      | 124.51   |
| 18  | B     | 823 | CLA  | CHB-C4A-NA  | 2.37  | 127.80      | 124.51   |
| 27  | 5     | 620 | XAT  | C18-C5-C4   | 2.37  | 116.95      | 114.28   |
| 18  | A     | 809 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 18  | 2     | 610 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 18  | 6     | 612 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 18  | 5     | 610 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 21  | F     | 302 | BCR  | C33-C5-C6   | -2.37 | 121.86      | 124.53   |
| 18  | A     | 812 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 18  | A     | 837 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 18  | B     | 829 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 838 | CLA  | CHB-C4A-NA  | 2.37  | 127.79      | 124.51   |
| 18  | 3     | 611 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 21  | A     | 849 | BCR  | C33-C5-C6   | -2.37 | 121.87      | 124.53   |
| 18  | 6     | 603 | CLA  | C1B-CHB-C4A | -2.37 | 125.42      | 130.12   |
| 18  | A     | 819 | CLA  | C1B-CHB-C4A | -2.37 | 125.43      | 130.12   |
| 18  | 3     | 603 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 18  | A     | 819 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 18  | B     | 833 | CLA  | CHB-C4A-NA  | 2.37  | 127.78      | 124.51   |
| 21  | L     | 305 | BCR  | C15-C14-C13 | -2.36 | 123.94      | 127.31   |
| 18  | A     | 826 | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 18  | A     | 833 | CLA  | C1B-CHB-C4A | -2.36 | 125.44      | 130.12   |
| 18  | B     | 841 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 18  | A     | 836 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 18  | B     | 812 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 18  | 2     | 611 | CLA  | C1B-CHB-C4A | -2.36 | 125.45      | 130.12   |
| 18  | B     | 807 | CLA  | CHB-C4A-NA  | 2.35  | 127.77      | 124.51   |
| 18  | A     | 804 | CLA  | C1B-CHB-C4A | -2.35 | 125.45      | 130.12   |
| 18  | 3     | 613 | CLA  | C1B-CHB-C4A | -2.35 | 125.46      | 130.12   |
| 27  | 5     | 620 | XAT  | C30-C31-C32 | -2.35 | 115.88      | 123.22   |
| 21  | A     | 849 | BCR  | C15-C14-C13 | -2.35 | 123.95      | 127.31   |
| 18  | A     | 837 | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 18  | B     | 832 | CLA  | CHB-C4A-NA  | 2.35  | 127.76      | 124.51   |
| 18  | 3     | 606 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 18  | A     | 814 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 25  | 5     | 607 | CHL  | CHD-C1D-C2D | 2.35  | 130.41      | 125.48   |
| 18  | 2     | 604 | CLA  | C1-C2-C3    | -2.35 | 122.95      | 126.75   |
| 23  | B     | 850 | DGD  | CFB-CEB-CDB | -2.35 | 102.51      | 114.42   |
| 18  | B     | 818 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 18  | B     | 839 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 18  | 5     | 610 | CLA  | O2A-CGA-O1A | -2.35 | 117.67      | 123.59   |
| 27  | 2     | 620 | XAT  | C28-C29-C30 | -2.35 | 115.34      | 118.94   |
| 18  | A     | 839 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 18  | 3     | 617 | CLA  | C1B-CHB-C4A | -2.35 | 125.47      | 130.12   |
| 25  | 2     | 601 | CHL  | C1C-C2C-C3C | -2.34 | 105.25      | 107.11   |
| 18  | B     | 811 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 21  | A     | 850 | BCR  | C27-C26-C25 | 2.34  | 126.13      | 122.73   |
| 25  | 2     | 601 | CHL  | O2D-CGD-O1D | -2.34 | 119.26      | 123.84   |
| 21  | B     | 845 | BCR  | C33-C5-C6   | -2.34 | 121.90      | 124.53   |
| 18  | B     | 837 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 18  | 3     | 615 | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 18  | B     | 823 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 20  | A     | 846 | LHG  | C20-C19-C18 | -2.34 | 102.55      | 114.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 841 | CLA  | C1B-CHB-C4A | -2.34 | 125.48      | 130.12   |
| 18  | 3     | 617 | CLA  | CAA-C2A-C3A | -2.34 | 110.64      | 116.10   |
| 18  | 2     | 612 | CLA  | CHB-C4A-NA  | 2.34  | 127.75      | 124.51   |
| 18  | 5     | 603 | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 18  | A     | 811 | CLA  | CHB-C4A-NA  | 2.34  | 127.74      | 124.51   |
| 18  | B     | 806 | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 18  | A     | 807 | CLA  | C1B-CHB-C4A | -2.34 | 125.49      | 130.12   |
| 21  | A     | 848 | BCR  | C27-C26-C25 | 2.33  | 126.12      | 122.73   |
| 18  | F     | 303 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 18  | 6     | 613 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 25  | 2     | 607 | CHL  | O2D-CGD-O1D | -2.33 | 119.29      | 123.84   |
| 18  | L     | 304 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 18  | 5     | 614 | CLA  | C1B-CHB-C4A | -2.33 | 125.51      | 130.12   |
| 18  | 3     | 610 | CLA  | CMA-C3A-C2A | -2.32 | 110.67      | 116.10   |
| 24  | 2     | 617 | LMG  | O1-C1-C2    | -2.32 | 105.42      | 108.15   |
| 18  | G     | 201 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 21  | G     | 205 | BCR  | C27-C26-C25 | 2.32  | 126.10      | 122.73   |
| 18  | A     | 811 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 18  | B     | 821 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 21  | A     | 851 | BCR  | C15-C14-C13 | -2.32 | 124.00      | 127.31   |
| 18  | A     | 832 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 18  | F     | 301 | CLA  | C1B-CHB-C4A | -2.32 | 125.52      | 130.12   |
| 25  | 5     | 607 | CHL  | OMC-CMC-C2C | -2.32 | 120.44      | 125.69   |
| 25  | 6     | 601 | CHL  | C1C-C2C-C3C | -2.32 | 105.27      | 107.11   |
| 18  | 2     | 604 | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 24  | 2     | 618 | LMG  | O3-C3-C2    | -2.32 | 104.99      | 110.35   |
| 18  | 5     | 612 | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 18  | B     | 805 | CLA  | O2A-CGA-O1A | -2.32 | 117.74      | 123.59   |
| 23  | B     | 850 | DGD  | C3D-C4D-C5D | -2.32 | 106.11      | 110.24   |
| 18  | 2     | 603 | CLA  | C1B-CHB-C4A | -2.32 | 125.53      | 130.12   |
| 21  | B     | 844 | BCR  | C33-C5-C6   | -2.32 | 121.93      | 124.53   |
| 21  | 2     | 621 | BCR  | C15-C14-C13 | -2.31 | 124.01      | 127.31   |
| 21  | K     | 202 | BCR  | C27-C26-C25 | 2.31  | 126.09      | 122.73   |
| 27  | 3     | 619 | XAT  | C25-C24-C23 | -2.31 | 108.18      | 112.75   |
| 18  | B     | 804 | CLA  | C1B-CHB-C4A | -2.31 | 125.54      | 130.12   |
| 18  | A     | 841 | CLA  | O2A-CGA-O1A | -2.31 | 117.77      | 123.59   |
| 18  | 2     | 602 | CLA  | C1B-CHB-C4A | -2.31 | 125.55      | 130.12   |
| 18  | B     | 809 | CLA  | CHB-C4A-NA  | 2.31  | 127.70      | 124.51   |
| 18  | B     | 826 | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 20  | A     | 846 | LHG  | C18-C17-C16 | -2.30 | 102.74      | 114.42   |
| 21  | B     | 845 | BCR  | C15-C16-C17 | -2.30 | 118.76      | 123.47   |
| 18  | A     | 840 | CLA  | CHB-C4A-NA  | 2.30  | 127.69      | 124.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 3     | 615 | CLA  | CAA-C2A-C3A | -2.30 | 110.73      | 116.10   |
| 18  | B     | 836 | CLA  | C1B-CHB-C4A | -2.30 | 125.56      | 130.12   |
| 21  | 2     | 621 | BCR  | C33-C5-C6   | -2.30 | 121.95      | 124.53   |
| 21  | B     | 801 | BCR  | C24-C23-C22 | -2.30 | 122.77      | 126.23   |
| 18  | B     | 814 | CLA  | C1B-CHB-C4A | -2.30 | 125.57      | 130.12   |
| 18  | B     | 836 | CLA  | CHD-C1D-ND  | -2.29 | 122.34      | 124.45   |
| 18  | A     | 838 | CLA  | C1B-CHB-C4A | -2.29 | 125.57      | 130.12   |
| 18  | L     | 303 | CLA  | C1B-CHB-C4A | -2.29 | 125.57      | 130.12   |
| 18  | A     | 815 | CLA  | C1B-CHB-C4A | -2.29 | 125.57      | 130.12   |
| 25  | 3     | 608 | CHL  | CBC-CAC-C3C | -2.29 | 106.11      | 112.43   |
| 18  | B     | 825 | CLA  | O2A-CGA-O1A | -2.29 | 117.81      | 123.59   |
| 18  | A     | 820 | CLA  | CHB-C4A-NA  | 2.29  | 127.68      | 124.51   |
| 26  | 6     | 617 | LUT  | C11-C12-C13 | -2.29 | 119.98      | 126.42   |
| 18  | K     | 204 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 18  | 6     | 609 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 26  | 3     | 618 | LUT  | C20-C13-C12 | 2.29  | 121.69      | 118.08   |
| 18  | A     | 818 | CLA  | C1B-CHB-C4A | -2.29 | 125.58      | 130.12   |
| 18  | B     | 816 | CLA  | C1B-CHB-C4A | -2.29 | 125.59      | 130.12   |
| 27  | 6     | 619 | XAT  | C24-C23-C22 | -2.29 | 106.36      | 110.77   |
| 18  | A     | 808 | CLA  | C1B-CHB-C4A | -2.29 | 125.59      | 130.12   |
| 18  | B     | 822 | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 18  | 6     | 604 | CLA  | C1B-CHB-C4A | -2.28 | 125.59      | 130.12   |
| 18  | B     | 832 | CLA  | C1B-CHB-C4A | -2.28 | 125.60      | 130.12   |
| 18  | 3     | 604 | CLA  | C1B-CHB-C4A | -2.28 | 125.60      | 130.12   |
| 18  | B     | 827 | CLA  | CHB-C4A-NA  | 2.28  | 127.66      | 124.51   |
| 18  | A     | 818 | CLA  | O2D-CGD-CBD | 2.28  | 115.32      | 111.27   |
| 25  | 2     | 601 | CHL  | C1D-ND-C4D  | -2.28 | 104.72      | 106.33   |
| 18  | L     | 303 | CLA  | CHD-C1D-ND  | -2.28 | 122.36      | 124.45   |
| 18  | 6     | 614 | CLA  | CAA-C2A-C3A | -2.28 | 110.78      | 116.10   |
| 18  | 6     | 614 | CLA  | CMA-C3A-C2A | -2.28 | 110.78      | 116.10   |
| 18  | 5     | 601 | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 21  | J     | 103 | BCR  | C15-C14-C13 | -2.28 | 124.06      | 127.31   |
| 21  | F     | 302 | BCR  | C24-C23-C22 | -2.28 | 122.79      | 126.23   |
| 18  | A     | 813 | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 18  | B     | 820 | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 18  | B     | 831 | CLA  | C1B-CHB-C4A | -2.28 | 125.61      | 130.12   |
| 18  | 3     | 613 | CLA  | C1-C2-C3    | -2.27 | 122.11      | 126.04   |
| 18  | K     | 206 | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 24  | J     | 104 | LMG  | O3-C3-C2    | -2.27 | 105.10      | 110.35   |
| 18  | G     | 204 | CLA  | C1B-CHB-C4A | -2.27 | 125.62      | 130.12   |
| 21  | J     | 103 | BCR  | C28-C27-C26 | -2.27 | 110.03      | 114.08   |
| 21  | 3     | 622 | BCR  | C15-C16-C17 | -2.27 | 118.83      | 123.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 805 | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 18  | 3     | 612 | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 21  | A     | 849 | BCR  | C27-C26-C25 | 2.27  | 126.02      | 122.73   |
| 18  | 2     | 613 | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 18  | B     | 808 | CLA  | O2D-CGD-CBD | 2.27  | 115.30      | 111.27   |
| 18  | 5     | 613 | CLA  | C1B-CHB-C4A | -2.27 | 125.63      | 130.12   |
| 18  | B     | 826 | CLA  | O2D-CGD-CBD | 2.27  | 115.29      | 111.27   |
| 21  | 2     | 621 | BCR  | C11-C10-C9  | -2.27 | 124.08      | 127.31   |
| 18  | A     | 821 | CLA  | C1B-CHB-C4A | -2.26 | 125.63      | 130.12   |
| 18  | 3     | 611 | CLA  | CAA-C2A-C3A | -2.26 | 110.82      | 116.10   |
| 18  | B     | 810 | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 18  | 6     | 606 | CLA  | C1B-CHB-C4A | -2.26 | 125.64      | 130.12   |
| 18  | J     | 101 | CLA  | C1B-CHB-C4A | -2.26 | 125.65      | 130.12   |
| 27  | 5     | 620 | XAT  | C19-C9-C8   | 2.26  | 121.63      | 118.08   |
| 21  | A     | 850 | BCR  | C24-C23-C22 | -2.26 | 122.83      | 126.23   |
| 18  | 3     | 607 | CLA  | C1B-CHB-C4A | -2.26 | 125.65      | 130.12   |
| 25  | 3     | 608 | CHL  | CMB-C2B-C3B | 2.25  | 128.89      | 124.68   |
| 25  | 6     | 607 | CHL  | O2D-CGD-O1D | -2.25 | 118.98      | 124.09   |
| 18  | A     | 817 | CLA  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 18  | L     | 302 | CLA  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 18  | B     | 835 | CLA  | CHB-C4A-NA  | 2.25  | 127.62      | 124.51   |
| 25  | 5     | 615 | CHL  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 26  | 2     | 619 | LUT  | C2-C3-C4    | 2.25  | 113.38      | 110.30   |
| 18  | 6     | 611 | CLA  | C1B-CHB-C4A | -2.25 | 125.66      | 130.12   |
| 25  | 6     | 601 | CHL  | O2D-CGD-O1D | -2.25 | 118.98      | 124.09   |
| 18  | B     | 803 | CLA  | O2A-CGA-O1A | -2.25 | 117.92      | 123.59   |
| 21  | B     | 847 | BCR  | C33-C5-C6   | -2.25 | 122.01      | 124.53   |
| 18  | A     | 843 | CLA  | CHD-C1D-ND  | -2.24 | 122.39      | 124.45   |
| 26  | 5     | 619 | LUT  | C11-C12-C13 | -2.24 | 120.12      | 126.42   |
| 27  | 5     | 620 | XAT  | O24-C25-C26 | -2.24 | 57.10       | 58.96    |
| 18  | B     | 815 | CLA  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 18  | A     | 836 | CLA  | CHD-C1D-ND  | -2.24 | 122.40      | 124.45   |
| 18  | 2     | 614 | CLA  | C1B-CHB-C4A | -2.24 | 125.68      | 130.12   |
| 25  | 2     | 601 | CHL  | CHD-C1D-C2D | 2.24  | 130.18      | 125.48   |
| 18  | 5     | 602 | CLA  | CHB-C4A-NA  | 2.24  | 127.61      | 124.51   |
| 21  | B     | 845 | BCR  | C15-C14-C13 | -2.24 | 124.12      | 127.31   |
| 18  | A     | 824 | CLA  | C1B-CHB-C4A | -2.24 | 125.69      | 130.12   |
| 21  | A     | 848 | BCR  | C24-C23-C22 | -2.24 | 122.86      | 126.23   |
| 21  | J     | 103 | BCR  | C15-C16-C17 | -2.24 | 118.89      | 123.47   |
| 25  | 2     | 607 | CHL  | C4A-NA-C1A  | 2.24  | 107.71      | 106.71   |
| 21  | 3     | 620 | BCR  | C15-C16-C17 | -2.24 | 118.89      | 123.47   |
| 18  | F     | 304 | CLA  | C1B-CHB-C4A | -2.24 | 125.69      | 130.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 817 | CLA  | C1B-CHB-C4A | -2.23 | 125.69      | 130.12   |
| 18  | 3     | 611 | CLA  | O2D-CGD-O1D | -2.23 | 119.02      | 124.09   |
| 27  | 5     | 620 | XAT  | C20-C13-C12 | 2.23  | 121.59      | 118.08   |
| 26  | 6     | 617 | LUT  | C15-C35-C34 | -2.23 | 118.90      | 123.47   |
| 18  | B     | 824 | CLA  | C1B-CHB-C4A | -2.23 | 125.70      | 130.12   |
| 18  | 5     | 611 | CLA  | C1B-CHB-C4A | -2.23 | 125.70      | 130.12   |
| 18  | B     | 828 | CLA  | O2A-CGA-O1A | -2.23 | 117.97      | 123.59   |
| 21  | B     | 844 | BCR  | C27-C26-C25 | 2.23  | 125.96      | 122.73   |
| 18  | 3     | 614 | CLA  | C1B-CHB-C4A | -2.22 | 125.71      | 130.12   |
| 18  | A     | 811 | CLA  | CHD-C1D-ND  | -2.22 | 122.41      | 124.45   |
| 18  | B     | 832 | CLA  | CHD-C1D-ND  | -2.22 | 122.41      | 124.45   |
| 25  | 5     | 606 | CHL  | C2A-C1A-CHA | -2.22 | 119.98      | 123.86   |
| 18  | A     | 829 | CLA  | CHB-C4A-NA  | 2.22  | 127.58      | 124.51   |
| 18  | B     | 804 | CLA  | O2D-CGD-CBD | 2.22  | 115.21      | 111.27   |
| 21  | 5     | 621 | BCR  | C11-C10-C9  | -2.22 | 124.15      | 127.31   |
| 18  | A     | 842 | CLA  | C1B-CHB-C4A | -2.21 | 125.73      | 130.12   |
| 18  | A     | 809 | CLA  | O2D-CGD-CBD | 2.21  | 115.20      | 111.27   |
| 18  | B     | 814 | CLA  | CHD-C1D-ND  | -2.21 | 122.42      | 124.45   |
| 18  | B     | 802 | CLA  | O2A-CGA-O1A | -2.21 | 118.01      | 123.59   |
| 21  | G     | 205 | BCR  | C7-C8-C9    | -2.21 | 122.89      | 126.23   |
| 21  | 3     | 622 | BCR  | C33-C5-C6   | -2.21 | 122.05      | 124.53   |
| 18  | A     | 816 | CLA  | CHD-C1D-ND  | -2.21 | 122.42      | 124.45   |
| 21  | B     | 844 | BCR  | C15-C14-C13 | -2.21 | 124.16      | 127.31   |
| 21  | I     | 101 | BCR  | C33-C5-C6   | -2.21 | 122.05      | 124.53   |
| 18  | 6     | 616 | CLA  | C1B-CHB-C4A | -2.21 | 125.75      | 130.12   |
| 21  | A     | 851 | BCR  | C2-C1-C6    | 2.21  | 113.88      | 110.48   |
| 21  | 3     | 620 | BCR  | C28-C27-C26 | -2.21 | 110.14      | 114.08   |
| 25  | 2     | 608 | CHL  | O2D-CGD-O1D | -2.21 | 119.08      | 124.09   |
| 25  | 5     | 615 | CHL  | O2D-CGD-O1D | -2.20 | 119.54      | 123.84   |
| 18  | 2     | 612 | CLA  | C1B-CHB-C4A | -2.20 | 125.77      | 130.12   |
| 18  | B     | 822 | CLA  | C1-C2-C3    | -2.20 | 122.24      | 126.04   |
| 20  | 2     | 622 | LHG  | C27-C26-C25 | -2.20 | 103.27      | 114.42   |
| 18  | G     | 201 | CLA  | CHD-C1D-ND  | -2.20 | 122.44      | 124.45   |
| 18  | A     | 845 | CLA  | O2A-CGA-O1A | -2.19 | 118.05      | 123.59   |
| 18  | 6     | 608 | CLA  | C1B-CHB-C4A | -2.19 | 125.77      | 130.12   |
| 18  | 6     | 606 | CLA  | C2A-C1A-CHA | 2.19  | 126.11      | 122.71   |
| 21  | B     | 843 | BCR  | C7-C8-C9    | -2.19 | 122.92      | 126.23   |
| 21  | J     | 103 | BCR  | C3-C4-C5    | -2.19 | 110.16      | 114.08   |
| 18  | B     | 813 | CLA  | O2A-CGA-O1A | -2.19 | 118.06      | 123.59   |
| 24  | 2     | 618 | LMG  | O1-C1-C2    | -2.19 | 105.58      | 108.15   |
| 18  | A     | 833 | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 21  | L     | 301 | BCR  | C2-C1-C6    | 2.19  | 113.85      | 110.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | 6     | 607 | CHL  | C1C-C2C-C3C | -2.19 | 105.38      | 107.11   |
| 21  | A     | 852 | BCR  | C7-C8-C9    | -2.19 | 122.93      | 126.23   |
| 18  | A     | 812 | CLA  | CHD-C1D-ND  | -2.19 | 122.44      | 124.45   |
| 18  | A     | 829 | CLA  | O2A-CGA-O1A | -2.18 | 118.08      | 123.59   |
| 21  | I     | 101 | BCR  | C15-C14-C13 | -2.18 | 124.19      | 127.31   |
| 18  | B     | 828 | CLA  | CHB-C4A-NA  | 2.18  | 127.53      | 124.51   |
| 18  | A     | 845 | CLA  | C1B-CHB-C4A | -2.18 | 125.80      | 130.12   |
| 18  | 2     | 609 | CLA  | CHD-C1D-ND  | -2.18 | 122.45      | 124.45   |
| 24  | 2     | 617 | LMG  | O3-C3-C2    | -2.18 | 105.31      | 110.35   |
| 18  | A     | 810 | CLA  | C1B-CHB-C4A | -2.18 | 125.81      | 130.12   |
| 23  | B     | 850 | DGD  | CBB-CAB-C9B | -2.18 | 103.38      | 114.42   |
| 18  | B     | 802 | CLA  | CHB-C4A-NA  | 2.17  | 127.52      | 124.51   |
| 18  | B     | 834 | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 18  | B     | 838 | CLA  | O2A-CGA-O1A | -2.17 | 118.11      | 123.59   |
| 18  | B     | 841 | CLA  | O2A-CGA-O1A | -2.17 | 118.11      | 123.59   |
| 21  | 3     | 620 | BCR  | C24-C23-C22 | -2.17 | 122.95      | 126.23   |
| 18  | B     | 809 | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 18  | 6     | 614 | CLA  | CHB-C4A-NA  | 2.17  | 127.52      | 124.51   |
| 18  | B     | 819 | CLA  | CHD-C1D-ND  | -2.17 | 122.46      | 124.45   |
| 21  | F     | 302 | BCR  | C15-C14-C13 | -2.17 | 124.22      | 127.31   |
| 25  | 5     | 607 | CHL  | C1C-C2C-C3C | -2.17 | 105.39      | 107.11   |
| 18  | A     | 837 | CLA  | O2D-CGD-CBD | 2.17  | 115.12      | 111.27   |
| 20  | 5     | 622 | LHG  | C27-C26-C25 | -2.16 | 103.44      | 114.42   |
| 25  | 2     | 607 | CHL  | OMC-CMC-C2C | -2.16 | 120.80      | 125.69   |
| 25  | 6     | 607 | CHL  | OMC-CMC-C2C | -2.16 | 120.80      | 125.69   |
| 18  | 5     | 614 | CLA  | CHD-C1D-ND  | -2.16 | 122.47      | 124.45   |
| 21  | B     | 846 | BCR  | C15-C14-C13 | -2.16 | 124.22      | 127.31   |
| 27  | 5     | 620 | XAT  | O4-C5-C6    | -2.16 | 57.17       | 58.96    |
| 18  | B     | 841 | CLA  | CHD-C1D-ND  | -2.16 | 122.47      | 124.45   |
| 18  | K     | 203 | CLA  | C1B-CHB-C4A | -2.16 | 125.84      | 130.12   |
| 21  | A     | 849 | BCR  | C24-C23-C22 | -2.16 | 122.97      | 126.23   |
| 25  | 3     | 608 | CHL  | O2D-CGD-O1D | -2.16 | 119.19      | 124.09   |
| 21  | 3     | 622 | BCR  | C27-C26-C25 | 2.16  | 125.86      | 122.73   |
| 20  | A     | 846 | LHG  | C27-C26-C25 | -2.16 | 103.47      | 114.42   |
| 18  | B     | 806 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 18  | A     | 801 | CLA  | O2A-CGA-O1A | -2.15 | 118.16      | 123.59   |
| 18  | A     | 804 | CLA  | O2D-CGD-CBD | 2.15  | 115.09      | 111.27   |
| 18  | B     | 807 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 18  | B     | 837 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 21  | L     | 305 | BCR  | C2-C1-C6    | 2.15  | 113.79      | 110.48   |
| 18  | B     | 825 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 21  | A     | 850 | BCR  | C11-C10-C9  | -2.15 | 124.24      | 127.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | B     | 821 | CLA  | CHD-C1D-ND  | -2.15 | 122.48      | 124.45   |
| 27  | 3     | 619 | XAT  | C10-C11-C12 | -2.14 | 116.53      | 123.22   |
| 18  | 6     | 613 | CLA  | O2A-CGA-O1A | -2.14 | 117.96      | 123.30   |
| 21  | 3     | 620 | BCR  | C8-C7-C6    | -2.14 | 121.19      | 127.20   |
| 18  | B     | 813 | CLA  | CHD-C1D-ND  | -2.14 | 122.49      | 124.45   |
| 18  | A     | 838 | CLA  | O2A-CGA-O1A | -2.14 | 118.19      | 123.59   |
| 18  | 3     | 602 | CLA  | O2A-CGA-O1A | -2.14 | 118.19      | 123.59   |
| 21  | J     | 102 | BCR  | C2-C1-C6    | 2.14  | 113.78      | 110.48   |
| 26  | 2     | 619 | LUT  | C40-C33-C32 | 2.14  | 121.45      | 118.08   |
| 18  | A     | 832 | CLA  | CMA-C3A-C2A | -2.14 | 111.10      | 116.10   |
| 18  | B     | 826 | CLA  | O2A-CGA-O1A | -2.14 | 118.19      | 123.59   |
| 18  | A     | 803 | CLA  | CHD-C1D-ND  | -2.14 | 122.49      | 124.45   |
| 18  | 5     | 609 | CLA  | CHD-C1D-ND  | -2.14 | 122.49      | 124.45   |
| 18  | A     | 820 | CLA  | CHD-C1D-ND  | -2.13 | 122.49      | 124.45   |
| 18  | A     | 832 | CLA  | CHD-C1D-ND  | -2.13 | 122.49      | 124.45   |
| 18  | 2     | 602 | CLA  | CHD-C1D-ND  | -2.13 | 122.49      | 124.45   |
| 18  | A     | 854 | CLA  | CHB-C4A-NA  | 2.13  | 127.46      | 124.51   |
| 18  | A     | 815 | CLA  | CHD-C1D-ND  | -2.13 | 122.50      | 124.45   |
| 18  | 3     | 604 | CLA  | CHD-C1D-ND  | -2.13 | 122.50      | 124.45   |
| 18  | B     | 832 | CLA  | O2D-CGD-CBD | 2.12  | 115.04      | 111.27   |
| 25  | 2     | 607 | CHL  | C1C-C2C-C3C | -2.12 | 105.43      | 107.11   |
| 26  | 2     | 619 | LUT  | C39-C29-C28 | 2.12  | 121.42      | 118.08   |
| 18  | 6     | 604 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 18  | 3     | 607 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 18  | A     | 838 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 18  | B     | 818 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 25  | 5     | 615 | CHL  | CHB-C4A-NA  | 2.12  | 127.44      | 124.51   |
| 21  | L     | 305 | BCR  | C24-C23-C22 | -2.12 | 123.04      | 126.23   |
| 18  | B     | 812 | CLA  | CHD-C1D-ND  | -2.12 | 122.51      | 124.45   |
| 21  | A     | 851 | BCR  | C38-C26-C25 | -2.12 | 122.15      | 124.53   |
| 21  | L     | 305 | BCR  | C29-C30-C25 | 2.11  | 113.74      | 110.48   |
| 18  | A     | 826 | CLA  | O2A-CGA-O1A | -2.11 | 118.26      | 123.59   |
| 18  | 5     | 602 | CLA  | CHD-C1D-ND  | -2.11 | 122.51      | 124.45   |
| 18  | A     | 842 | CLA  | O2A-CGA-O1A | -2.11 | 118.04      | 123.30   |
| 18  | B     | 807 | CLA  | O2A-CGA-O1A | -2.11 | 118.28      | 123.59   |
| 18  | A     | 827 | CLA  | O2A-CGA-O1A | -2.11 | 118.28      | 123.59   |
| 18  | A     | 801 | CLA  | CHB-C4A-NA  | 2.10  | 127.42      | 124.51   |
| 26  | 6     | 617 | LUT  | C31-C32-C33 | -2.10 | 120.50      | 126.42   |
| 18  | B     | 802 | CLA  | C1-C2-C3    | -2.10 | 122.41      | 126.04   |
| 18  | A     | 806 | CLA  | O2A-CGA-O1A | -2.10 | 118.29      | 123.59   |
| 18  | B     | 809 | CLA  | O2A-CGA-O1A | -2.10 | 118.29      | 123.59   |
| 18  | F     | 303 | CLA  | O2A-CGA-O1A | -2.10 | 118.07      | 123.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | 2     | 610 | CLA  | CHB-C4A-NA  | 2.10  | 127.41      | 124.51   |
| 18  | F     | 303 | CLA  | CHD-C1D-ND  | -2.10 | 122.53      | 124.45   |
| 21  | F     | 302 | BCR  | C11-C10-C9  | -2.10 | 124.32      | 127.31   |
| 18  | B     | 832 | CLA  | O2A-CGA-O1A | -2.10 | 118.07      | 123.30   |
| 18  | A     | 805 | CLA  | O2A-CGA-O1A | -2.10 | 118.30      | 123.59   |
| 18  | B     | 811 | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 21  | L     | 305 | BCR  | C7-C8-C9    | -2.09 | 123.07      | 126.23   |
| 18  | B     | 806 | CLA  | O2A-CGA-O1A | -2.09 | 118.31      | 123.59   |
| 18  | A     | 839 | CLA  | CHD-C1D-ND  | -2.09 | 122.53      | 124.45   |
| 18  | B     | 841 | CLA  | C1-C2-C3    | -2.09 | 122.43      | 126.04   |
| 24  | J     | 104 | LMG  | O2-C2-C1    | -2.09 | 104.97      | 110.05   |
| 25  | 2     | 606 | CHL  | O2D-CGD-O1D | -2.09 | 119.75      | 123.84   |
| 25  | 2     | 607 | CHL  | CHD-C1D-C2D | 2.09  | 129.86      | 125.48   |
| 21  | B     | 848 | BCR  | C29-C30-C25 | 2.09  | 113.69      | 110.48   |
| 18  | A     | 808 | CLA  | O2A-CGA-O1A | -2.09 | 118.10      | 123.30   |
| 21  | B     | 848 | BCR  | C15-C14-C13 | -2.09 | 124.33      | 127.31   |
| 25  | 2     | 616 | CHL  | OMC-CMC-C2C | -2.09 | 120.97      | 125.69   |
| 18  | 6     | 614 | CLA  | CHD-C1D-ND  | -2.08 | 122.54      | 124.45   |
| 18  | 5     | 604 | CLA  | CHD-C1D-ND  | -2.08 | 122.54      | 124.45   |
| 26  | 3     | 618 | LUT  | C1-C6-C7    | -2.08 | 109.89      | 115.78   |
| 18  | A     | 810 | CLA  | O2A-CGA-O1A | -2.08 | 118.11      | 123.30   |
| 21  | G     | 205 | BCR  | C15-C14-C13 | -2.08 | 124.34      | 127.31   |
| 18  | 6     | 603 | CLA  | CHD-C1D-ND  | -2.08 | 122.54      | 124.45   |
| 18  | B     | 824 | CLA  | O2A-CGA-O1A | -2.08 | 118.11      | 123.30   |
| 25  | 5     | 615 | CHL  | C4D-CHA-C1A | -2.08 | 118.72      | 121.25   |
| 18  | A     | 839 | CLA  | O2A-CGA-O1A | -2.08 | 118.34      | 123.59   |
| 18  | 6     | 604 | CLA  | O2A-CGA-O1A | -2.08 | 118.34      | 123.59   |
| 18  | A     | 835 | CLA  | O2A-CGA-O1A | -2.08 | 118.35      | 123.59   |
| 25  | 2     | 608 | CHL  | C1C-C2C-C3C | -2.08 | 105.47      | 107.11   |
| 18  | B     | 835 | CLA  | CHD-C1D-ND  | -2.08 | 122.55      | 124.45   |
| 18  | 6     | 602 | CLA  | CHD-C1D-ND  | -2.07 | 122.55      | 124.45   |
| 25  | 6     | 607 | CHL  | C2D-C1D-ND  | 2.07  | 111.63      | 110.10   |
| 18  | B     | 833 | CLA  | O2A-CGA-O1A | -2.07 | 118.14      | 123.30   |
| 18  | B     | 828 | CLA  | CHD-C1D-ND  | -2.07 | 122.55      | 124.45   |
| 18  | B     | 833 | CLA  | CHD-C1D-ND  | -2.07 | 122.55      | 124.45   |
| 24  | 2     | 617 | LMG  | O2-C2-C1    | -2.07 | 105.02      | 110.05   |
| 18  | A     | 808 | CLA  | CHD-C1D-ND  | -2.07 | 122.56      | 124.45   |
| 18  | A     | 825 | CLA  | CHD-C1D-ND  | -2.07 | 122.56      | 124.45   |
| 18  | A     | 812 | CLA  | O2A-CGA-O1A | -2.07 | 118.38      | 123.59   |
| 18  | B     | 815 | CLA  | O2A-CGA-O1A | -2.07 | 118.38      | 123.59   |
| 18  | B     | 830 | CLA  | CHD-C1D-ND  | -2.07 | 122.56      | 124.45   |
| 18  | B     | 833 | CLA  | CAA-C2A-C3A | -2.06 | 107.12      | 112.78   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 814 | CLA  | O2A-CGA-O1A | -2.06 | 118.38      | 123.59   |
| 18  | 6     | 610 | CLA  | O2A-CGA-O1A | -2.06 | 118.16      | 123.30   |
| 21  | B     | 843 | BCR  | C38-C26-C25 | -2.06 | 122.21      | 124.53   |
| 18  | A     | 854 | CLA  | O2A-CGA-O1A | -2.06 | 118.39      | 123.59   |
| 21  | B     | 847 | BCR  | C7-C8-C9    | -2.06 | 123.12      | 126.23   |
| 18  | 3     | 611 | CLA  | C2A-C1A-CHA | 2.06  | 127.45      | 123.85   |
| 21  | J     | 103 | BCR  | C24-C23-C22 | -2.06 | 123.12      | 126.23   |
| 25  | 5     | 608 | CHL  | OMC-CMC-C2C | -2.06 | 121.04      | 125.69   |
| 18  | A     | 803 | CLA  | O2A-CGA-O1A | -2.06 | 118.40      | 123.59   |
| 18  | 3     | 613 | CLA  | O2A-CGA-O1A | -2.05 | 118.41      | 123.59   |
| 18  | A     | 843 | CLA  | C1-C2-C3    | -2.05 | 122.49      | 126.04   |
| 21  | B     | 846 | BCR  | C15-C16-C17 | -2.05 | 119.27      | 123.47   |
| 18  | B     | 829 | CLA  | C2D-C1D-ND  | -2.05 | 108.59      | 110.10   |
| 18  | A     | 814 | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 18  | A     | 815 | CLA  | O2A-CGA-O1A | -2.05 | 118.19      | 123.30   |
| 25  | 6     | 601 | CHL  | OMC-CMC-C2C | -2.05 | 121.05      | 125.69   |
| 18  | 2     | 614 | CLA  | CHD-C1D-ND  | -2.05 | 122.57      | 124.45   |
| 21  | A     | 850 | BCR  | C7-C8-C9    | -2.05 | 123.14      | 126.23   |
| 25  | 3     | 608 | CHL  | C1C-C2C-C3C | -2.05 | 104.81      | 106.96   |
| 25  | 5     | 607 | CHL  | C4D-CHA-C1A | -2.05 | 118.76      | 121.25   |
| 21  | B     | 801 | BCR  | C15-C16-C17 | -2.04 | 119.29      | 123.47   |
| 21  | A     | 850 | BCR  | C15-C16-C17 | -2.04 | 119.29      | 123.47   |
| 18  | B     | 838 | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 18  | L     | 304 | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 18  | 5     | 612 | CLA  | O2A-CGA-O1A | -2.04 | 118.21      | 123.30   |
| 21  | L     | 305 | BCR  | C11-C10-C9  | -2.04 | 124.40      | 127.31   |
| 25  | 2     | 608 | CHL  | OMC-CMC-C2C | -2.04 | 121.07      | 125.69   |
| 26  | 5     | 619 | LUT  | C17-C1-C6   | -2.04 | 106.99      | 110.30   |
| 26  | 3     | 618 | LUT  | C21-C26-C27 | -2.04 | 110.12      | 112.70   |
| 25  | 3     | 608 | CHL  | CAA-C2A-C3A | -2.04 | 111.34      | 116.10   |
| 18  | A     | 827 | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 18  | B     | 813 | CLA  | C1-C2-C3    | -2.04 | 122.52      | 126.04   |
| 18  | G     | 204 | CLA  | CHD-C1D-ND  | -2.04 | 122.58      | 124.45   |
| 21  | A     | 851 | BCR  | C37-C22-C21 | -2.04 | 120.07      | 122.92   |
| 21  | K     | 202 | BCR  | C35-C13-C14 | -2.04 | 120.07      | 122.92   |
| 18  | A     | 804 | CLA  | C1-C2-C3    | -2.04 | 122.52      | 126.04   |
| 18  | B     | 837 | CLA  | O2D-CGD-CBD | 2.03  | 114.88      | 111.27   |
| 18  | A     | 804 | CLA  | O2A-CGA-O1A | -2.03 | 118.46      | 123.59   |
| 23  | B     | 850 | DGD  | C5B-C4B-C3B | -2.03 | 104.10      | 114.42   |
| 18  | 3     | 617 | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 25  | 2     | 601 | CHL  | O1D-CGD-CBD | -2.03 | 120.33      | 124.48   |
| 25  | 6     | 607 | CHL  | C4D-CHA-C1A | -2.03 | 118.78      | 121.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | 2     | 618 | LMG  | C1-C2-C3    | -2.03 | 105.77      | 110.00   |
| 18  | A     | 854 | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 18  | 5     | 602 | CLA  | O2A-CGA-O1A | -2.03 | 118.24      | 123.30   |
| 18  | A     | 845 | CLA  | CHD-C1D-ND  | -2.03 | 122.59      | 124.45   |
| 18  | A     | 835 | CLA  | C1-C2-C3    | -2.03 | 122.54      | 126.04   |
| 27  | 2     | 620 | XAT  | C10-C11-C12 | -2.03 | 116.89      | 123.22   |
| 18  | B     | 819 | CLA  | O2A-CGA-O1A | -2.02 | 118.25      | 123.30   |
| 18  | A     | 818 | CLA  | O2A-CGA-O1A | -2.02 | 118.48      | 123.59   |
| 18  | A     | 837 | CLA  | O2A-CGA-O1A | -2.02 | 118.26      | 123.30   |
| 21  | A     | 851 | BCR  | C8-C7-C6    | -2.02 | 121.52      | 127.20   |
| 18  | 6     | 603 | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 24  | J     | 104 | LMG  | O1-C7-C8    | -2.02 | 106.02      | 110.90   |
| 18  | K     | 203 | CLA  | O2A-CGA-O1A | -2.02 | 118.26      | 123.30   |
| 18  | G     | 203 | CLA  | O2A-CGA-O1A | -2.02 | 118.49      | 123.59   |
| 18  | A     | 819 | CLA  | O2A-CGA-O1A | -2.02 | 118.26      | 123.30   |
| 21  | A     | 852 | BCR  | C24-C23-C22 | -2.02 | 123.18      | 126.23   |
| 18  | 6     | 609 | CLA  | CHD-C1D-ND  | -2.02 | 122.60      | 124.45   |
| 18  | 5     | 611 | CLA  | CHD-C1D-ND  | -2.02 | 122.60      | 124.45   |
| 18  | A     | 837 | CLA  | CHD-C1D-ND  | -2.02 | 122.60      | 124.45   |
| 18  | A     | 841 | CLA  | CHD-C1D-ND  | -2.02 | 122.60      | 124.45   |
| 18  | L     | 302 | CLA  | CHD-C1D-ND  | -2.02 | 122.60      | 124.45   |
| 23  | B     | 850 | DGD  | O3E-C3E-C2E | -2.02 | 105.69      | 110.35   |
| 24  | J     | 104 | LMG  | C1-C2-C3    | -2.02 | 105.80      | 110.00   |
| 27  | 6     | 619 | XAT  | O24-C25-C26 | -2.02 | 57.29       | 58.96    |
| 18  | 2     | 609 | CLA  | O2A-CGA-O1A | -2.02 | 118.50      | 123.59   |
| 25  | 2     | 601 | CHL  | OMC-CMC-C2C | -2.02 | 121.13      | 125.69   |
| 21  | B     | 848 | BCR  | C15-C16-C17 | -2.02 | 119.35      | 123.47   |
| 21  | I     | 101 | BCR  | C28-C27-C26 | -2.02 | 110.48      | 114.08   |
| 18  | B     | 805 | CLA  | O2D-CGD-CBD | 2.01  | 114.85      | 111.27   |
| 18  | 5     | 601 | CLA  | CHD-C1D-ND  | -2.01 | 122.60      | 124.45   |
| 18  | 3     | 602 | CLA  | O2D-CGD-CBD | 2.01  | 114.84      | 111.27   |
| 18  | K     | 206 | CLA  | O2A-CGA-O1A | -2.01 | 118.28      | 123.30   |
| 18  | A     | 834 | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 18  | A     | 843 | CLA  | C2D-C1D-ND  | -2.01 | 108.62      | 110.10   |
| 21  | L     | 301 | BCR  | C24-C23-C22 | -2.01 | 123.20      | 126.23   |
| 18  | B     | 822 | CLA  | O2A-CGA-O1A | -2.01 | 118.52      | 123.59   |
| 21  | A     | 852 | BCR  | C15-C14-C13 | -2.01 | 124.44      | 127.31   |
| 21  | B     | 846 | BCR  | C38-C26-C25 | -2.01 | 122.27      | 124.53   |
| 27  | 2     | 620 | XAT  | C20-C13-C14 | -2.01 | 120.11      | 122.92   |
| 18  | 2     | 613 | CLA  | O2A-CGA-O1A | -2.01 | 118.30      | 123.30   |
| 18  | A     | 829 | CLA  | CHD-C1D-ND  | -2.01 | 122.61      | 124.45   |
| 27  | 6     | 619 | XAT  | C19-C9-C8   | 2.01  | 121.24      | 118.08   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 18  | A     | 825 | CLA  | O2A-CGA-O1A | -2.01 | 118.53      | 123.59   |
| 18  | A     | 821 | CLA  | O2A-CGA-O1A | -2.01 | 118.30      | 123.30   |
| 18  | 6     | 612 | CLA  | O2A-CGA-O1A | -2.00 | 118.30      | 123.30   |
| 25  | 2     | 608 | CHL  | CAA-C2A-C3A | -2.00 | 111.42      | 116.10   |
| 18  | B     | 827 | CLA  | CHD-C1D-ND  | -2.00 | 122.61      | 124.45   |
| 23  | B     | 850 | DGD  | CAB-C9B-C8B | -2.00 | 104.25      | 114.42   |
| 18  | A     | 809 | CLA  | O2A-CGA-O1A | -2.00 | 118.31      | 123.30   |
| 18  | B     | 827 | CLA  | O2A-CGA-O1A | -2.00 | 118.31      | 123.30   |
| 26  | 3     | 618 | LUT  | C17-C1-C6   | -2.00 | 107.05      | 110.30   |
| 21  | A     | 849 | BCR  | C11-C10-C9  | -2.00 | 124.45      | 127.31   |
| 18  | A     | 817 | CLA  | CHD-C1D-ND  | -2.00 | 122.61      | 124.45   |

All (180) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 18  | A     | 801 | CLA  | ND   |
| 18  | A     | 802 | CLA  | ND   |
| 18  | A     | 803 | CLA  | ND   |
| 18  | A     | 804 | CLA  | ND   |
| 18  | A     | 805 | CLA  | ND   |
| 18  | A     | 806 | CLA  | ND   |
| 18  | A     | 807 | CLA  | ND   |
| 18  | A     | 808 | CLA  | ND   |
| 18  | A     | 809 | CLA  | ND   |
| 18  | A     | 810 | CLA  | ND   |
| 18  | A     | 811 | CLA  | ND   |
| 18  | A     | 812 | CLA  | ND   |
| 18  | A     | 813 | CLA  | ND   |
| 18  | A     | 814 | CLA  | ND   |
| 18  | A     | 815 | CLA  | ND   |
| 18  | A     | 816 | CLA  | ND   |
| 18  | A     | 817 | CLA  | ND   |
| 18  | A     | 818 | CLA  | ND   |
| 18  | A     | 819 | CLA  | ND   |
| 18  | A     | 820 | CLA  | ND   |
| 18  | A     | 821 | CLA  | ND   |
| 18  | A     | 822 | CLA  | ND   |
| 18  | A     | 823 | CLA  | ND   |
| 18  | A     | 824 | CLA  | ND   |
| 18  | A     | 825 | CLA  | ND   |
| 18  | A     | 826 | CLA  | ND   |
| 18  | A     | 827 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 18  | A     | 828 | CLA  | ND   |
| 18  | A     | 829 | CLA  | ND   |
| 18  | A     | 830 | CLA  | ND   |
| 18  | A     | 831 | CLA  | ND   |
| 18  | A     | 832 | CLA  | ND   |
| 18  | A     | 833 | CLA  | ND   |
| 18  | A     | 834 | CLA  | ND   |
| 18  | A     | 835 | CLA  | ND   |
| 18  | A     | 836 | CLA  | ND   |
| 18  | A     | 837 | CLA  | ND   |
| 18  | A     | 838 | CLA  | ND   |
| 18  | A     | 839 | CLA  | ND   |
| 18  | A     | 840 | CLA  | ND   |
| 18  | A     | 841 | CLA  | ND   |
| 18  | A     | 842 | CLA  | ND   |
| 18  | A     | 843 | CLA  | ND   |
| 18  | A     | 845 | CLA  | ND   |
| 18  | A     | 854 | CLA  | ND   |
| 18  | B     | 802 | CLA  | ND   |
| 18  | B     | 803 | CLA  | ND   |
| 18  | B     | 804 | CLA  | ND   |
| 18  | B     | 805 | CLA  | ND   |
| 18  | B     | 806 | CLA  | ND   |
| 18  | B     | 807 | CLA  | ND   |
| 18  | B     | 808 | CLA  | ND   |
| 18  | B     | 809 | CLA  | ND   |
| 18  | B     | 810 | CLA  | ND   |
| 18  | B     | 811 | CLA  | ND   |
| 18  | B     | 812 | CLA  | ND   |
| 18  | B     | 813 | CLA  | ND   |
| 18  | B     | 814 | CLA  | ND   |
| 18  | B     | 815 | CLA  | ND   |
| 18  | B     | 816 | CLA  | ND   |
| 18  | B     | 817 | CLA  | ND   |
| 18  | B     | 818 | CLA  | ND   |
| 18  | B     | 819 | CLA  | ND   |
| 18  | B     | 820 | CLA  | ND   |
| 18  | B     | 821 | CLA  | ND   |
| 18  | B     | 822 | CLA  | ND   |
| 18  | B     | 823 | CLA  | ND   |
| 18  | B     | 824 | CLA  | ND   |
| 18  | B     | 825 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 18  | B     | 826 | CLA  | ND   |
| 18  | B     | 827 | CLA  | ND   |
| 18  | B     | 828 | CLA  | ND   |
| 18  | B     | 829 | CLA  | ND   |
| 18  | B     | 830 | CLA  | ND   |
| 18  | B     | 831 | CLA  | ND   |
| 18  | B     | 832 | CLA  | ND   |
| 18  | B     | 833 | CLA  | ND   |
| 18  | B     | 834 | CLA  | ND   |
| 18  | B     | 835 | CLA  | ND   |
| 18  | B     | 836 | CLA  | ND   |
| 18  | B     | 837 | CLA  | ND   |
| 18  | B     | 838 | CLA  | ND   |
| 18  | B     | 839 | CLA  | ND   |
| 18  | B     | 840 | CLA  | ND   |
| 18  | B     | 841 | CLA  | ND   |
| 18  | F     | 301 | CLA  | ND   |
| 18  | F     | 303 | CLA  | ND   |
| 18  | F     | 304 | CLA  | ND   |
| 18  | F     | 305 | CLA  | ND   |
| 18  | G     | 201 | CLA  | ND   |
| 18  | G     | 203 | CLA  | ND   |
| 18  | G     | 204 | CLA  | ND   |
| 18  | J     | 101 | CLA  | ND   |
| 18  | K     | 201 | CLA  | ND   |
| 18  | K     | 203 | CLA  | ND   |
| 18  | K     | 204 | CLA  | ND   |
| 18  | K     | 206 | CLA  | ND   |
| 18  | L     | 302 | CLA  | ND   |
| 18  | L     | 303 | CLA  | ND   |
| 18  | L     | 304 | CLA  | ND   |
| 18  | 2     | 602 | CLA  | ND   |
| 18  | 2     | 603 | CLA  | ND   |
| 18  | 2     | 604 | CLA  | ND   |
| 18  | 2     | 609 | CLA  | ND   |
| 18  | 2     | 610 | CLA  | ND   |
| 18  | 2     | 611 | CLA  | ND   |
| 18  | 2     | 612 | CLA  | ND   |
| 18  | 2     | 613 | CLA  | ND   |
| 18  | 2     | 614 | CLA  | ND   |
| 18  | 6     | 602 | CLA  | ND   |
| 18  | 6     | 603 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 18  | 6     | 604 | CLA  | ND   |
| 18  | 6     | 606 | CLA  | ND   |
| 18  | 6     | 608 | CLA  | ND   |
| 18  | 6     | 609 | CLA  | ND   |
| 18  | 6     | 610 | CLA  | ND   |
| 18  | 6     | 611 | CLA  | ND   |
| 18  | 6     | 612 | CLA  | ND   |
| 18  | 6     | 613 | CLA  | ND   |
| 18  | 6     | 614 | CLA  | ND   |
| 18  | 6     | 616 | CLA  | ND   |
| 18  | 3     | 602 | CLA  | ND   |
| 18  | 3     | 603 | CLA  | ND   |
| 18  | 3     | 604 | CLA  | ND   |
| 18  | 3     | 606 | CLA  | ND   |
| 18  | 3     | 607 | CLA  | ND   |
| 18  | 3     | 609 | CLA  | ND   |
| 18  | 3     | 610 | CLA  | ND   |
| 18  | 3     | 611 | CLA  | ND   |
| 18  | 3     | 612 | CLA  | ND   |
| 18  | 3     | 613 | CLA  | ND   |
| 18  | 3     | 614 | CLA  | ND   |
| 18  | 3     | 615 | CLA  | ND   |
| 18  | 3     | 617 | CLA  | ND   |
| 18  | 5     | 601 | CLA  | ND   |
| 18  | 5     | 602 | CLA  | ND   |
| 18  | 5     | 603 | CLA  | ND   |
| 18  | 5     | 604 | CLA  | ND   |
| 18  | 5     | 609 | CLA  | ND   |
| 18  | 5     | 610 | CLA  | ND   |
| 18  | 5     | 611 | CLA  | ND   |
| 18  | 5     | 612 | CLA  | ND   |
| 18  | 5     | 613 | CLA  | ND   |
| 18  | 5     | 614 | CLA  | ND   |
| 25  | 2     | 601 | CHL  | ND   |
| 25  | 2     | 601 | CHL  | NC   |
| 25  | 2     | 601 | CHL  | NA   |
| 25  | 2     | 606 | CHL  | ND   |
| 25  | 2     | 606 | CHL  | NC   |
| 25  | 2     | 606 | CHL  | NA   |
| 25  | 2     | 607 | CHL  | ND   |
| 25  | 2     | 607 | CHL  | NC   |
| 25  | 2     | 607 | CHL  | NA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 25  | 2     | 608 | CHL  | ND   |
| 25  | 2     | 608 | CHL  | NC   |
| 25  | 2     | 608 | CHL  | NA   |
| 25  | 2     | 616 | CHL  | ND   |
| 25  | 2     | 616 | CHL  | NC   |
| 25  | 2     | 616 | CHL  | NA   |
| 25  | 6     | 601 | CHL  | ND   |
| 25  | 6     | 601 | CHL  | NC   |
| 25  | 6     | 601 | CHL  | NA   |
| 25  | 6     | 607 | CHL  | ND   |
| 25  | 6     | 607 | CHL  | NC   |
| 25  | 6     | 607 | CHL  | NA   |
| 25  | 3     | 608 | CHL  | ND   |
| 25  | 3     | 608 | CHL  | NC   |
| 25  | 3     | 608 | CHL  | NA   |
| 25  | 5     | 606 | CHL  | ND   |
| 25  | 5     | 606 | CHL  | NC   |
| 25  | 5     | 606 | CHL  | NA   |
| 25  | 5     | 607 | CHL  | ND   |
| 25  | 5     | 607 | CHL  | NC   |
| 25  | 5     | 607 | CHL  | NA   |
| 25  | 5     | 608 | CHL  | ND   |
| 25  | 5     | 608 | CHL  | NC   |
| 25  | 5     | 608 | CHL  | NA   |
| 25  | 5     | 615 | CHL  | ND   |
| 25  | 5     | 615 | CHL  | NC   |
| 25  | 5     | 615 | CHL  | NA   |

All (1358) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 801 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 802 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 802 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 805 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 805 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 806 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 806 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 809 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 809 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 811 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 818 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 818 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 818 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 821 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 821 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 821 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 823 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 824 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 824 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 825 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 826 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 828 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 828 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 828 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 831 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 832 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 832 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 832 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 834 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 837 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 841 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 845 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 845 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 845 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 854 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 854 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 854 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 854 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 854 | CLA  | C2-C3-C5-C6     |
| 18  | A     | 854 | CLA  | C4-C3-C5-C6     |
| 18  | B     | 802 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 802 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 806 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 810 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 811 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 813 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 813 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 813 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 815 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 815 | CLA  | C4-C3-C5-C6     |
| 18  | B     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 822 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 822 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 822 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 822 | CLA  | C4-C3-C5-C6     |
| 18  | B     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 826 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 826 | CLA  | C4-C3-C5-C6     |
| 18  | B     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 831 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 834 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 835 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 837 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 837 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 841 | CLA  | C14-C13-C15-C16 |
| 18  | F     | 301 | CLA  | CBD-CGD-O2D-CED |
| 18  | J     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 18  | K     | 206 | CLA  | CBD-CGD-O2D-CED |
| 18  | 2     | 602 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 2     | 602 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 2     | 603 | CLA  | CBD-CGD-O2D-CED |
| 18  | 2     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 2     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 2     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 2     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 2     | 610 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 2     | 610 | CLA  | CBD-CGD-O2D-CED |
| 18  | 2     | 614 | CLA  | CBD-CGD-O2D-CED |
| 18  | 6     | 603 | CLA  | C2-C3-C5-C6     |
| 18  | 6     | 603 | CLA  | C4-C3-C5-C6     |
| 18  | 6     | 604 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 6     | 609 | CLA  | CBD-CGD-O2D-CED |
| 18  | 6     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 6     | 613 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 6     | 613 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 6     | 616 | CLA  | CBD-CGD-O2D-CED |
| 18  | 3     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 3     | 602 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 3     | 607 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 3     | 610 | CLA  | CBD-CGD-O2D-CED |
| 18  | 3     | 612 | CLA  | CBD-CGD-O2D-CED |
| 18  | 5     | 604 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 5     | 604 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 5     | 604 | CLA  | CBD-CGD-O2D-CED |
| 18  | 5     | 609 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 5     | 609 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 5     | 609 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 5     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 5     | 611 | CLA  | CMA-C3A-C4A-NA  |
| 18  | 5     | 611 | CLA  | CBD-CGD-O2D-CED |
| 18  | 5     | 614 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 5     | 614 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 5     | 614 | CLA  | CBD-CGD-O2D-CED |
| 19  | A     | 844 | PQN  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 844 | PQN  | C14-C13-C15-C16 |
| 19  | A     | 844 | PQN  | C24-C23-C25-C26 |
| 20  | A     | 846 | LHG  | C4-O6-P-O5      |
| 20  | A     | 846 | LHG  | O7-C5-C6-O8     |
| 20  | A     | 847 | LHG  | C3-O3-P-O4      |
| 20  | A     | 847 | LHG  | C3-O3-P-O5      |
| 20  | A     | 847 | LHG  | C4-O6-P-O5      |
| 20  | A     | 847 | LHG  | O7-C5-C6-O8     |
| 20  | B     | 851 | LHG  | C1-C2-C3-O3     |
| 20  | B     | 851 | LHG  | C4-O6-P-O5      |
| 20  | B     | 851 | LHG  | O9-C7-O7-C5     |
| 20  | B     | 851 | LHG  | C8-C7-O7-C5     |
| 20  | 2     | 622 | LHG  | C1-C2-C3-O3     |
| 20  | 2     | 622 | LHG  | C3-O3-P-O5      |
| 20  | 2     | 622 | LHG  | C4-O6-P-O3      |
| 20  | 2     | 622 | LHG  | C4-O6-P-O4      |
| 20  | 2     | 622 | LHG  | C4-O6-P-O5      |
| 20  | 6     | 620 | LHG  | O1-C1-C2-O2     |
| 20  | 6     | 620 | LHG  | O1-C1-C2-C3     |
| 20  | 6     | 620 | LHG  | C3-O3-P-O4      |
| 20  | 6     | 620 | LHG  | C3-O3-P-O6      |
| 20  | 6     | 620 | LHG  | C4-O6-P-O3      |
| 20  | 6     | 620 | LHG  | C4-O6-P-O4      |
| 20  | 5     | 622 | LHG  | C1-C2-C3-O3     |
| 20  | 5     | 622 | LHG  | C4-O6-P-O4      |
| 21  | A     | 849 | BCR  | C7-C8-C9-C34    |
| 21  | A     | 851 | BCR  | C7-C8-C9-C34    |
| 21  | A     | 851 | BCR  | C37-C22-C23-C24 |
| 21  | A     | 851 | BCR  | C22-C23-C24-C25 |
| 21  | A     | 851 | BCR  | C23-C24-C25-C30 |
| 21  | A     | 852 | BCR  | C1-C6-C7-C8     |
| 21  | A     | 852 | BCR  | C7-C8-C9-C10    |
| 21  | A     | 852 | BCR  | C7-C8-C9-C34    |
| 21  | A     | 852 | BCR  | C21-C22-C23-C24 |
| 21  | A     | 852 | BCR  | C37-C22-C23-C24 |
| 21  | A     | 856 | BCR  | C23-C24-C25-C30 |
| 21  | B     | 801 | BCR  | C7-C8-C9-C10    |
| 21  | B     | 801 | BCR  | C7-C8-C9-C34    |
| 21  | B     | 843 | BCR  | C7-C8-C9-C34    |
| 21  | B     | 843 | BCR  | C37-C22-C23-C24 |
| 21  | B     | 844 | BCR  | C7-C8-C9-C34    |
| 21  | B     | 844 | BCR  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | B     | 845 | BCR  | C14-C15-C16-C17 |
| 21  | B     | 845 | BCR  | C16-C17-C18-C36 |
| 21  | B     | 845 | BCR  | C17-C18-C19-C20 |
| 21  | B     | 845 | BCR  | C18-C19-C20-C21 |
| 21  | B     | 845 | BCR  | C21-C22-C23-C24 |
| 21  | B     | 845 | BCR  | C37-C22-C23-C24 |
| 21  | B     | 846 | BCR  | C7-C8-C9-C34    |
| 21  | B     | 846 | BCR  | C13-C14-C15-C16 |
| 21  | B     | 846 | BCR  | C14-C15-C16-C17 |
| 21  | B     | 846 | BCR  | C16-C17-C18-C19 |
| 21  | B     | 846 | BCR  | C16-C17-C18-C36 |
| 21  | B     | 846 | BCR  | C36-C18-C19-C20 |
| 21  | B     | 846 | BCR  | C18-C19-C20-C21 |
| 21  | B     | 846 | BCR  | C20-C21-C22-C37 |
| 21  | B     | 846 | BCR  | C22-C23-C24-C25 |
| 21  | B     | 847 | BCR  | C23-C24-C25-C30 |
| 21  | B     | 848 | BCR  | C1-C6-C7-C8     |
| 21  | B     | 848 | BCR  | C7-C8-C9-C10    |
| 21  | B     | 848 | BCR  | C11-C10-C9-C8   |
| 21  | B     | 848 | BCR  | C11-C10-C9-C34  |
| 21  | B     | 848 | BCR  | C10-C11-C12-C13 |
| 21  | B     | 848 | BCR  | C11-C12-C13-C35 |
| 21  | F     | 302 | BCR  | C10-C11-C12-C13 |
| 21  | F     | 302 | BCR  | C11-C12-C13-C35 |
| 21  | F     | 302 | BCR  | C14-C15-C16-C17 |
| 21  | F     | 302 | BCR  | C16-C17-C18-C36 |
| 21  | G     | 205 | BCR  | C23-C24-C25-C30 |
| 21  | I     | 101 | BCR  | C14-C15-C16-C17 |
| 21  | J     | 102 | BCR  | C6-C7-C8-C9     |
| 21  | J     | 103 | BCR  | C1-C6-C7-C8     |
| 21  | J     | 103 | BCR  | C6-C7-C8-C9     |
| 21  | J     | 103 | BCR  | C11-C10-C9-C8   |
| 21  | J     | 103 | BCR  | C11-C12-C13-C14 |
| 21  | J     | 103 | BCR  | C11-C12-C13-C35 |
| 21  | J     | 103 | BCR  | C14-C15-C16-C17 |
| 21  | J     | 103 | BCR  | C18-C19-C20-C21 |
| 21  | J     | 103 | BCR  | C20-C21-C22-C23 |
| 21  | J     | 103 | BCR  | C20-C21-C22-C37 |
| 21  | J     | 103 | BCR  | C22-C23-C24-C25 |
| 21  | K     | 202 | BCR  | C7-C8-C9-C34    |
| 21  | K     | 207 | BCR  | C6-C7-C8-C9     |
| 21  | K     | 207 | BCR  | C18-C19-C20-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | K     | 207 | BCR  | C21-C22-C23-C24 |
| 21  | K     | 207 | BCR  | C22-C23-C24-C25 |
| 21  | L     | 301 | BCR  | C1-C6-C7-C8     |
| 21  | L     | 305 | BCR  | C7-C8-C9-C34    |
| 21  | L     | 305 | BCR  | C21-C22-C23-C24 |
| 21  | L     | 305 | BCR  | C37-C22-C23-C24 |
| 21  | L     | 305 | BCR  | C22-C23-C24-C25 |
| 21  | L     | 305 | BCR  | C23-C24-C25-C26 |
| 21  | L     | 305 | BCR  | C23-C24-C25-C30 |
| 21  | 3     | 620 | BCR  | C6-C7-C8-C9     |
| 21  | 3     | 620 | BCR  | C7-C8-C9-C10    |
| 21  | 3     | 620 | BCR  | C7-C8-C9-C34    |
| 21  | 3     | 620 | BCR  | C20-C21-C22-C23 |
| 21  | 3     | 620 | BCR  | C20-C21-C22-C37 |
| 21  | 3     | 620 | BCR  | C23-C24-C25-C30 |
| 21  | 3     | 622 | BCR  | C6-C7-C8-C9     |
| 21  | 3     | 622 | BCR  | C7-C8-C9-C10    |
| 21  | 3     | 622 | BCR  | C7-C8-C9-C34    |
| 21  | 3     | 622 | BCR  | C22-C23-C24-C25 |
| 21  | 5     | 621 | BCR  | C20-C21-C22-C37 |
| 21  | 5     | 621 | BCR  | C23-C24-C25-C30 |
| 23  | B     | 850 | DGD  | O1B-C1B-O2G-C2G |
| 24  | J     | 104 | LMG  | O6-C1-O1-C7     |
| 24  | 2     | 617 | LMG  | C2-C1-O1-C7     |
| 24  | 2     | 617 | LMG  | O6-C1-O1-C7     |
| 25  | 2     | 616 | CHL  | CHA-CBD-CGD-O1D |
| 25  | 2     | 616 | CHL  | CHA-CBD-CGD-O2D |
| 25  | 5     | 606 | CHL  | C1C-C2C-CMC-OMC |
| 25  | 5     | 608 | CHL  | C2A-CAA-CBA-CGA |
| 26  | 2     | 619 | LUT  | C5-C6-C7-C8     |
| 26  | 2     | 619 | LUT  | C7-C8-C9-C10    |
| 26  | 2     | 619 | LUT  | C7-C8-C9-C19    |
| 26  | 6     | 617 | LUT  | C6-C7-C8-C9     |
| 26  | 6     | 617 | LUT  | C11-C10-C9-C8   |
| 26  | 6     | 617 | LUT  | C11-C10-C9-C19  |
| 26  | 6     | 617 | LUT  | C10-C11-C12-C13 |
| 26  | 6     | 617 | LUT  | C30-C31-C32-C33 |
| 26  | 3     | 618 | LUT  | C5-C6-C7-C8     |
| 26  | 3     | 618 | LUT  | C11-C10-C9-C8   |
| 26  | 3     | 618 | LUT  | C11-C10-C9-C19  |
| 26  | 3     | 618 | LUT  | C10-C11-C12-C13 |
| 26  | 3     | 618 | LUT  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | 3     | 618 | LUT  | C20-C13-C14-C15 |
| 26  | 3     | 618 | LUT  | C26-C27-C28-C29 |
| 26  | 5     | 619 | LUT  | C5-C6-C7-C8     |
| 26  | 5     | 619 | LUT  | C12-C13-C14-C15 |
| 26  | 5     | 619 | LUT  | C20-C13-C14-C15 |
| 26  | 5     | 619 | LUT  | C14-C15-C35-C34 |
| 27  | 2     | 620 | XAT  | O4-C6-C7-C8     |
| 18  | F     | 303 | CLA  | O1D-CGD-O2D-CED |
| 18  | 2     | 603 | CLA  | O1D-CGD-O2D-CED |
| 18  | 6     | 606 | CLA  | O1D-CGD-O2D-CED |
| 18  | 6     | 609 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 801 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 811 | CLA  | O1D-CGD-O2D-CED |
| 18  | 5     | 604 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 802 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 812 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 822 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 809 | CLA  | CBD-CGD-O2D-CED |
| 18  | F     | 303 | CLA  | CBD-CGD-O2D-CED |
| 18  | K     | 201 | CLA  | CBD-CGD-O2D-CED |
| 18  | K     | 204 | CLA  | CBD-CGD-O2D-CED |
| 18  | 2     | 613 | CLA  | CBD-CGD-O2D-CED |
| 18  | 6     | 603 | CLA  | CBD-CGD-O2D-CED |
| 18  | 6     | 606 | CLA  | CBD-CGD-O2D-CED |
| 18  | 6     | 613 | CLA  | CBD-CGD-O2D-CED |
| 18  | 3     | 603 | CLA  | CBD-CGD-O2D-CED |
| 18  | 5     | 613 | CLA  | CBD-CGD-O2D-CED |
| 25  | 5     | 608 | CHL  | CBD-CGD-O2D-CED |
| 20  | 6     | 620 | LHG  | O10-C23-O8-C6   |
| 24  | J     | 104 | LMG  | O10-C28-O8-C9   |
| 18  | B     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 811 | CLA  | O1D-CGD-O2D-CED |
| 18  | K     | 206 | CLA  | O1D-CGD-O2D-CED |
| 18  | 6     | 616 | CLA  | O1D-CGD-O2D-CED |
| 18  | 3     | 603 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 834 | CLA  | O1D-CGD-O2D-CED |
| 18  | 3     | 610 | CLA  | O1D-CGD-O2D-CED |
| 18  | 5     | 611 | CLA  | O1D-CGD-O2D-CED |
| 20  | 6     | 620 | LHG  | C24-C23-O8-C6   |
| 18  | A     | 814 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 841 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 854 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 810 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 813 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 819 | CLA  | CBD-CGD-O2D-CED |
| 18  | G     | 201 | CLA  | CBD-CGD-O2D-CED |
| 18  | K     | 203 | CLA  | CBD-CGD-O2D-CED |
| 18  | 2     | 602 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 845 | CLA  | O1A-CGA-O2A-C1  |
| 18  | 3     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 20  | 5     | 622 | LHG  | O10-C23-O8-C6   |
| 18  | B     | 810 | CLA  | O1A-CGA-O2A-C1  |
| 18  | B     | 806 | CLA  | O1D-CGD-O2D-CED |
| 18  | 3     | 612 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 834 | CLA  | O1D-CGD-O2D-CED |
| 18  | 2     | 610 | CLA  | O1D-CGD-O2D-CED |
| 18  | 2     | 614 | CLA  | O1D-CGD-O2D-CED |
| 18  | 5     | 614 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 829 | CLA  | CBD-CGD-O2D-CED |
| 18  | G     | 203 | CLA  | CBD-CGD-O2D-CED |
| 25  | 2     | 601 | CHL  | CBD-CGD-O2D-CED |
| 25  | 5     | 615 | CHL  | CBD-CGD-O2D-CED |
| 18  | F     | 301 | CLA  | O1D-CGD-O2D-CED |
| 18  | 6     | 613 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 805 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 818 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 829 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 843 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 815 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 826 | CLA  | C3-C5-C6-C7     |
| 19  | A     | 844 | PQN  | C13-C15-C16-C17 |
| 18  | A     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 845 | CLA  | CBA-CGA-O2A-C1  |
| 18  | 3     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 20  | 5     | 622 | LHG  | C24-C23-O8-C6   |
| 23  | B     | 850 | DGD  | C2B-C1B-O2G-C2G |
| 18  | 2     | 613 | CLA  | O1D-CGD-O2D-CED |
| 18  | 5     | 613 | CLA  | O1D-CGD-O2D-CED |
| 18  | K     | 204 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 839 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 839 | CLA  | C2-C3-C5-C6     |
| 18  | A     | 824 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 832 | CLA  | CBD-CGD-O2D-CED |
| 25  | 2     | 606 | CHL  | CBD-CGD-O2D-CED |
| 18  | A     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 830 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 833 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 843 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 817 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 835 | CLA  | C2A-CAA-CBA-CGA |
| 18  | G     | 203 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 6     | 616 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 801 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 806 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 839 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 18  | 6     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 831 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 809 | CLA  | O1D-CGD-O2D-CED |
| 18  | K     | 201 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 18  | 6     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 5     | 608 | CHL  | O1D-CGD-O2D-CED |
| 21  | B     | 845 | BCR  | C13-C14-C15-C16 |
| 21  | B     | 845 | BCR  | C15-C16-C17-C18 |
| 21  | B     | 846 | BCR  | C19-C20-C21-C22 |
| 18  | A     | 803 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 818 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 803 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 821 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 835 | CLA  | CBD-CGD-O2D-CED |
| 25  | 2     | 616 | CHL  | CBD-CGD-O2D-CED |
| 20  | 2     | 622 | LHG  | O2-C2-C3-O3     |
| 20  | 5     | 622 | LHG  | O2-C2-C3-O3     |
| 18  | A     | 826 | CLA  | C3-C5-C6-C7     |
| 19  | B     | 842 | PQN  | C13-C15-C16-C17 |
| 18  | A     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 818 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 839 | CLA  | O1A-CGA-O2A-C1  |
| 24  | J     | 104 | LMG  | O6-C5-C6-O5     |
| 18  | A     | 802 | CLA  | O1D-CGD-O2D-CED |
| 25  | 5     | 607 | CHL  | CBD-CGD-O2D-CED |
| 18  | B     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 839 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 804 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 804 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 854 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 809 | CLA  | C3-C5-C6-C7     |
| 24  | J     | 104 | LMG  | C29-C28-O8-C9   |
| 18  | A     | 822 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 845 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 840 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 818 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 840 | CLA  | C2-C3-C5-C6     |
| 18  | F     | 305 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 6     | 603 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 18  | G     | 203 | CLA  | CBA-CGA-O2A-C1  |
| 20  | 2     | 622 | LHG  | C23-C24-C25-C26 |
| 18  | A     | 812 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 819 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 854 | CLA  | O1D-CGD-O2D-CED |
| 18  | K     | 203 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 834 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 807 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 815 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 810 | CLA  | O1D-CGD-O2D-CED |
| 18  | 2     | 602 | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 846 | BCR  | C15-C16-C17-C18 |
| 21  | B     | 848 | BCR  | C9-C10-C11-C12  |
| 21  | F     | 302 | BCR  | C9-C10-C11-C12  |
| 21  | F     | 302 | BCR  | C13-C14-C15-C16 |
| 21  | J     | 102 | BCR  | C9-C10-C11-C12  |
| 20  | A     | 846 | LHG  | C7-C8-C9-C10    |
| 18  | B     | 806 | CLA  | C15-C16-C17-C18 |
| 18  | B     | 813 | CLA  | C5-C6-C7-C8     |
| 20  | B     | 851 | LHG  | O2-C2-C3-O3     |
| 23  | B     | 850 | DGD  | C2E-C1E-O5D-C6D |
| 24  | J     | 104 | LMG  | C2-C1-O1-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 828 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 803 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 827 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 839 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 841 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 841 | CLA  | C14-C13-C15-C16 |
| 18  | B     | 825 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 813 | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 201 | CLA  | O1D-CGD-O2D-CED |
| 18  | F     | 304 | CLA  | CBD-CGD-O2D-CED |
| 21  | B     | 844 | BCR  | C37-C22-C23-C24 |
| 21  | B     | 845 | BCR  | C7-C8-C9-C34    |
| 21  | J     | 102 | BCR  | C11-C12-C13-C35 |
| 21  | J     | 103 | BCR  | C37-C22-C23-C24 |
| 21  | K     | 207 | BCR  | C11-C12-C13-C35 |
| 21  | 3     | 622 | BCR  | C37-C22-C23-C24 |
| 27  | 2     | 620 | XAT  | C7-C8-C9-C19    |
| 21  | A     | 851 | BCR  | C21-C22-C23-C24 |
| 21  | B     | 848 | BCR  | C11-C12-C13-C14 |
| 21  | 3     | 622 | BCR  | C21-C22-C23-C24 |
| 27  | 2     | 620 | XAT  | C7-C8-C9-C10    |
| 27  | 5     | 620 | XAT  | C27-C28-C29-C30 |
| 23  | B     | 850 | DGD  | C1A-C2A-C3A-C4A |
| 24  | 2     | 618 | LMG  | O6-C5-C6-O5     |
| 18  | A     | 841 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 843 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 818 | CLA  | C10-C11-C12-C13 |
| 18  | A     | 829 | CLA  | C13-C15-C16-C17 |
| 18  | A     | 835 | CLA  | C5-C6-C7-C8     |
| 18  | A     | 841 | CLA  | C5-C6-C7-C8     |
| 18  | B     | 803 | CLA  | C10-C11-C12-C13 |
| 18  | B     | 825 | CLA  | C13-C15-C16-C17 |
| 18  | B     | 840 | CLA  | C15-C16-C17-C18 |
| 20  | A     | 846 | LHG  | C28-C29-C30-C31 |
| 18  | A     | 831 | CLA  | C5-C6-C7-C8     |
| 20  | A     | 846 | LHG  | C23-C24-C25-C26 |
| 20  | A     | 847 | LHG  | C7-C8-C9-C10    |
| 20  | 6     | 620 | LHG  | C23-C24-C25-C26 |
| 18  | 6     | 602 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 830 | CLA  | C15-C16-C17-C18 |
| 18  | A     | 814 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 843 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 825 | CLA  | C10-C11-C12-C13 |
| 18  | B     | 826 | CLA  | C5-C6-C7-C8     |
| 24  | J     | 104 | LMG  | C28-C29-C30-C31 |
| 18  | A     | 808 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 828 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 813 | CLA  | C15-C16-C17-C18 |
| 18  | A     | 826 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 21  | J     | 103 | BCR  | C9-C10-C11-C12  |
| 18  | A     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 818 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 18  | G     | 201 | CLA  | C2A-CAA-CBA-CGA |
| 18  | G     | 203 | CLA  | O1D-CGD-O2D-CED |
| 25  | 5     | 615 | CHL  | O1D-CGD-O2D-CED |
| 18  | A     | 834 | CLA  | C5-C6-C7-C8     |
| 18  | B     | 815 | CLA  | C8-C10-C11-C12  |
| 18  | 2     | 609 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 849 | BCR  | C6-C7-C8-C9     |
| 18  | B     | 827 | CLA  | CBD-CGD-O2D-CED |
| 23  | B     | 850 | DGD  | O6E-C1E-O5D-C6D |
| 21  | G     | 205 | BCR  | C10-C11-C12-C13 |
| 21  | J     | 103 | BCR  | C10-C11-C12-C13 |
| 26  | 2     | 619 | LUT  | C10-C11-C12-C13 |
| 26  | 5     | 619 | LUT  | C30-C31-C32-C33 |
| 23  | B     | 850 | DGD  | O6E-C5E-C6E-O5E |
| 24  | 2     | 617 | LMG  | C4-C5-C6-O5     |
| 18  | B     | 840 | CLA  | C13-C15-C16-C17 |
| 18  | B     | 828 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 804 | CLA  | C8-C10-C11-C12  |
| 18  | B     | 807 | CLA  | C10-C11-C12-C13 |
| 18  | A     | 829 | CLA  | O1D-CGD-O2D-CED |
| 24  | J     | 104 | LMG  | C4-C5-C6-O5     |
| 18  | A     | 843 | CLA  | O1A-CGA-O2A-C1  |
| 18  | G     | 203 | CLA  | O1A-CGA-O2A-C1  |
| 25  | 2     | 606 | CHL  | O1D-CGD-O2D-CED |
| 18  | B     | 807 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 844 | PQN  | C18-C20-C21-C22 |
| 20  | A     | 847 | LHG  | C3-O3-P-O6      |
| 20  | A     | 847 | LHG  | C4-O6-P-O3      |
| 20  | 5     | 622 | LHG  | C4-O6-P-O3      |
| 20  | 2     | 622 | LHG  | C7-C8-C9-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | 6     | 603 | CLA  | CBA-CGA-O2A-C1  |
| 25  | 2     | 601 | CHL  | O1D-CGD-O2D-CED |
| 18  | B     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 3     | 613 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 839 | CLA  | C13-C15-C16-C17 |
| 18  | A     | 854 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 804 | CLA  | C2A-CAA-CBA-CGA |
| 18  | K     | 201 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 6     | 603 | CLA  | C6-C7-C8-C10    |
| 21  | J     | 103 | BCR  | C15-C16-C17-C18 |
| 26  | 2     | 619 | LUT  | C9-C10-C11-C12  |
| 18  | B     | 811 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 852 | BCR  | C16-C17-C18-C36 |
| 21  | A     | 852 | BCR  | C20-C21-C22-C37 |
| 21  | B     | 845 | BCR  | C20-C21-C22-C37 |
| 21  | I     | 101 | BCR  | C20-C21-C22-C37 |
| 21  | J     | 103 | BCR  | C16-C17-C18-C36 |
| 21  | K     | 207 | BCR  | C16-C17-C18-C36 |
| 21  | L     | 301 | BCR  | C16-C17-C18-C36 |
| 21  | L     | 301 | BCR  | C20-C21-C22-C37 |
| 21  | 2     | 621 | BCR  | C20-C21-C22-C37 |
| 21  | 5     | 621 | BCR  | C16-C17-C18-C36 |
| 26  | 2     | 619 | LUT  | C11-C10-C9-C19  |
| 26  | 6     | 617 | LUT  | C39-C29-C30-C31 |
| 26  | 6     | 617 | LUT  | C40-C33-C34-C35 |
| 18  | 3     | 613 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 824 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 832 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 812 | CLA  | C16-C17-C18-C20 |
| 18  | A     | 825 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 831 | CLA  | O1D-CGD-O2D-CED |
| 20  | 5     | 622 | LHG  | C5-C4-O6-P      |
| 20  | 5     | 622 | LHG  | C23-C24-C25-C26 |
| 21  | A     | 852 | BCR  | C16-C17-C18-C19 |
| 21  | B     | 845 | BCR  | C16-C17-C18-C19 |
| 21  | B     | 845 | BCR  | C20-C21-C22-C23 |
| 21  | B     | 846 | BCR  | C20-C21-C22-C23 |
| 21  | F     | 302 | BCR  | C16-C17-C18-C19 |
| 21  | J     | 102 | BCR  | C11-C10-C9-C8   |
| 21  | J     | 103 | BCR  | C16-C17-C18-C19 |
| 21  | L     | 301 | BCR  | C11-C10-C9-C8   |
| 21  | 5     | 621 | BCR  | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | 2     | 619 | LUT  | C11-C10-C9-C8   |
| 26  | 6     | 617 | LUT  | C28-C29-C30-C31 |
| 26  | 6     | 617 | LUT  | C32-C33-C34-C35 |
| 23  | B     | 850 | DGD  | C9A-CAA-CBA-CCA |
| 18  | 2     | 609 | CLA  | C6-C7-C8-C10    |
| 18  | 3     | 613 | CLA  | C6-C7-C8-C9     |
| 18  | B     | 835 | CLA  | O1D-CGD-O2D-CED |
| 20  | A     | 846 | LHG  | C13-C14-C15-C16 |
| 18  | 3     | 613 | CLA  | C2-C3-C5-C6     |
| 18  | A     | 804 | CLA  | C11-C10-C8-C9   |
| 18  | A     | 841 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 806 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 809 | CLA  | C11-C10-C8-C9   |
| 18  | A     | 818 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 838 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 25  | 2     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 25  | 6     | 601 | CHL  | C2A-CAA-CBA-CGA |
| 18  | 6     | 603 | CLA  | O1A-CGA-O2A-C1  |
| 27  | 5     | 620 | XAT  | C27-C28-C29-C39 |
| 23  | B     | 850 | DGD  | C4B-C5B-C6B-C7B |
| 20  | A     | 847 | LHG  | O1-C1-C2-C3     |
| 20  | 5     | 622 | LHG  | O1-C1-C2-C3     |
| 21  | F     | 302 | BCR  | C11-C12-C13-C14 |
| 21  | J     | 103 | BCR  | C21-C22-C23-C24 |
| 21  | L     | 305 | BCR  | C7-C8-C9-C10    |
| 20  | A     | 846 | LHG  | C9-C10-C11-C12  |
| 20  | 6     | 620 | LHG  | C7-C8-C9-C10    |
| 18  | A     | 814 | CLA  | C16-C17-C18-C19 |
| 18  | K     | 201 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 823 | CLA  | CBD-CGD-O2D-CED |
| 18  | B     | 803 | CLA  | O1D-CGD-O2D-CED |
| 20  | 5     | 622 | LHG  | C11-C10-C9-C8   |
| 23  | B     | 850 | DGD  | CAB-CBB-CCB-CDB |
| 18  | A     | 803 | CLA  | O1D-CGD-O2D-CED |
| 25  | 2     | 616 | CHL  | O1D-CGD-O2D-CED |
| 18  | A     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 18  | A     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 810 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 813 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 840 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 3     | 603 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 5     | 612 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 821 | CLA  | O1D-CGD-O2D-CED |
| 18  | 3     | 613 | CLA  | C6-C7-C8-C10    |
| 18  | 2     | 609 | CLA  | C4-C3-C5-C6     |
| 25  | 5     | 607 | CHL  | O1D-CGD-O2D-CED |
| 18  | A     | 826 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 825 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 806 | CLA  | C2-C1-O2A-CGA   |
| 18  | A     | 829 | CLA  | C2-C1-O2A-CGA   |
| 18  | B     | 809 | CLA  | C10-C11-C12-C13 |
| 18  | B     | 836 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 848 | BCR  | C23-C24-C25-C26 |
| 21  | A     | 848 | BCR  | C23-C24-C25-C30 |
| 21  | A     | 851 | BCR  | C23-C24-C25-C26 |
| 21  | A     | 852 | BCR  | C5-C6-C7-C8     |
| 21  | A     | 856 | BCR  | C1-C6-C7-C8     |
| 21  | A     | 856 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 846 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 846 | BCR  | C23-C24-C25-C30 |
| 21  | B     | 847 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 848 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 848 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 848 | BCR  | C23-C24-C25-C30 |
| 21  | G     | 205 | BCR  | C23-C24-C25-C26 |
| 21  | J     | 103 | BCR  | C5-C6-C7-C8     |
| 21  | J     | 103 | BCR  | C23-C24-C25-C26 |
| 21  | J     | 103 | BCR  | C23-C24-C25-C30 |
| 21  | K     | 207 | BCR  | C23-C24-C25-C30 |
| 21  | L     | 301 | BCR  | C5-C6-C7-C8     |
| 21  | L     | 305 | BCR  | C5-C6-C7-C8     |
| 21  | 3     | 620 | BCR  | C23-C24-C25-C26 |
| 21  | 5     | 621 | BCR  | C1-C6-C7-C8     |
| 21  | 5     | 621 | BCR  | C5-C6-C7-C8     |
| 21  | 5     | 621 | BCR  | C23-C24-C25-C26 |
| 26  | 6     | 617 | LUT  | C5-C6-C7-C8     |
| 19  | A     | 844 | PQN  | C15-C16-C17-C18 |
| 24  | 2     | 617 | LMG  | O6-C5-C6-O5     |
| 23  | B     | 850 | DGD  | CBA-CCA-CDA-CEA |
| 18  | A     | 804 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 827 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 831 | CLA  | C11-C10-C8-C7   |
| 18  | A     | 831 | CLA  | C12-C13-C15-C16 |
| 18  | A     | 841 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 841 | CLA  | C12-C13-C15-C16 |
| 18  | B     | 805 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 806 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 809 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 809 | CLA  | C12-C13-C15-C16 |
| 18  | B     | 815 | CLA  | C6-C7-C8-C10    |
| 18  | B     | 825 | CLA  | C11-C10-C8-C7   |
| 18  | 2     | 609 | CLA  | C2-C3-C5-C6     |
| 19  | B     | 842 | PQN  | C22-C23-C25-C26 |
| 18  | A     | 814 | CLA  | C5-C6-C7-C8     |
| 18  | A     | 829 | CLA  | C10-C11-C12-C13 |
| 20  | A     | 847 | LHG  | C24-C23-O8-C6   |
| 18  | A     | 803 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 803 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 2     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 6     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 818 | CLA  | C5-C6-C7-C8     |
| 23  | B     | 850 | DGD  | CAA-CBA-CCA-CDA |
| 23  | B     | 850 | DGD  | O6D-C1D-O3G-C3G |
| 18  | A     | 843 | CLA  | C5-C6-C7-C8     |
| 18  | A     | 839 | CLA  | O1D-CGD-O2D-CED |
| 20  | A     | 846 | LHG  | C32-C33-C34-C35 |
| 20  | A     | 846 | LHG  | C8-C7-O7-C5     |
| 20  | 2     | 622 | LHG  | C8-C7-O7-C5     |
| 21  | L     | 301 | BCR  | C10-C11-C12-C13 |
| 18  | B     | 813 | CLA  | C13-C15-C16-C17 |
| 18  | A     | 812 | CLA  | C16-C17-C18-C19 |
| 18  | 6     | 603 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 826 | CLA  | C11-C10-C8-C9   |
| 18  | A     | 827 | CLA  | C11-C12-C13-C14 |
| 18  | A     | 831 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 805 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 815 | CLA  | C6-C7-C8-C9     |
| 18  | 3     | 602 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 804 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 18  | G     | 204 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 6     | 602 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | 2     | 621 | BCR  | C11-C12-C13-C35 |
| 21  | A     | 848 | BCR  | C21-C22-C23-C24 |
| 18  | A     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 845 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 823 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 2     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 6     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 3     | 603 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 5     | 612 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 814 | CLA  | C16-C17-C18-C20 |
| 18  | 2     | 609 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 835 | CLA  | C13-C15-C16-C17 |
| 18  | 5     | 611 | CLA  | CMA-C3A-C4A-CHB |
| 18  | B     | 841 | CLA  | C13-C15-C16-C17 |
| 18  | B     | 807 | CLA  | C4-C3-C5-C6     |
| 20  | A     | 846 | LHG  | C4-C5-C6-O8     |
| 20  | 5     | 622 | LHG  | C24-C25-C26-C27 |
| 18  | A     | 815 | CLA  | O1D-CGD-O2D-CED |
| 18  | F     | 304 | CLA  | O1D-CGD-O2D-CED |
| 18  | B     | 840 | CLA  | CAA-CBA-CGA-O2A |
| 20  | 5     | 622 | LHG  | O1-C1-C2-O2     |
| 20  | 2     | 622 | LHG  | C11-C12-C13-C14 |
| 20  | 2     | 622 | LHG  | C27-C28-C29-C30 |
| 21  | J     | 102 | BCR  | C11-C10-C9-C34  |
| 21  | J     | 103 | BCR  | C11-C10-C9-C34  |
| 21  | L     | 305 | BCR  | C16-C17-C18-C36 |
| 18  | A     | 835 | CLA  | C4-C3-C5-C6     |
| 18  | B     | 825 | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 18  | B     | 841 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 842 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 828 | CLA  | O1A-CGA-O2A-C1  |
| 19  | B     | 842 | PQN  | C20-C21-C22-C23 |
| 20  | 6     | 620 | LHG  | C24-C25-C26-C27 |
| 18  | B     | 809 | CLA  | C13-C15-C16-C17 |
| 18  | A     | 808 | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 848 | BCR  | C12-C13-C14-C15 |
| 23  | B     | 850 | DGD  | C2A-C3A-C4A-C5A |
| 18  | A     | 812 | CLA  | C11-C12-C13-C15 |
| 18  | A     | 814 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 827 | CLA  | C11-C12-C13-C15 |
| 18  | A     | 829 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 829 | CLA  | C11-C12-C13-C15 |
| 18  | A     | 839 | CLA  | C12-C13-C15-C16 |
| 18  | A     | 843 | CLA  | C6-C7-C8-C10    |
| 18  | B     | 805 | CLA  | C11-C12-C13-C15 |
| 18  | B     | 825 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 841 | CLA  | C12-C13-C15-C16 |
| 19  | A     | 844 | PQN  | C22-C23-C25-C26 |
| 18  | A     | 812 | CLA  | C11-C12-C13-C14 |
| 18  | A     | 829 | CLA  | C11-C12-C13-C14 |
| 18  | B     | 803 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 805 | CLA  | C6-C7-C8-C9     |
| 18  | B     | 806 | CLA  | C11-C12-C13-C14 |
| 18  | B     | 826 | CLA  | C11-C12-C13-C14 |
| 18  | B     | 836 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 841 | CLA  | C11-C12-C13-C14 |
| 18  | A     | 805 | CLA  | C6-C7-C8-C10    |
| 21  | B     | 846 | BCR  | C7-C8-C9-C10    |
| 21  | K     | 202 | BCR  | C7-C8-C9-C10    |
| 24  | J     | 104 | LMG  | C30-C31-C32-C33 |
| 18  | A     | 819 | CLA  | CBD-CGD-O2D-CED |
| 20  | 6     | 620 | LHG  | O6-C4-C5-C6     |
| 20  | 6     | 620 | LHG  | C11-C10-C9-C8   |
| 18  | A     | 835 | CLA  | C2-C3-C5-C6     |
| 20  | A     | 846 | LHG  | O9-C7-O7-C5     |
| 23  | B     | 850 | DGD  | C9B-CAB-CBB-CCB |
| 18  | B     | 811 | CLA  | C6-C7-C8-C9     |
| 20  | A     | 846 | LHG  | C27-C28-C29-C30 |
| 18  | B     | 841 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 18  | 6     | 604 | CLA  | C3A-C2A-CAA-CBA |
| 23  | B     | 850 | DGD  | CCA-CDA-CEA-CFA |
| 20  | B     | 851 | LHG  | C4-C5-C6-O8     |
| 20  | 2     | 622 | LHG  | C4-C5-C6-O8     |
| 23  | B     | 850 | DGD  | O1G-C1G-C2G-C3G |
| 23  | B     | 850 | DGD  | C4E-C5E-C6E-O5E |
| 18  | B     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 18  | B     | 807 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 827 | CLA  | O1D-CGD-O2D-CED |
| 18  | 6     | 602 | CLA  | O1D-CGD-O2D-CED |
| 20  | 2     | 622 | LHG  | C12-C13-C14-C15 |
| 25  | 5     | 606 | CHL  | C3C-C2C-CMC-OMC |
| 18  | B     | 823 | CLA  | O1D-CGD-O2D-CED |
| 20  | B     | 851 | LHG  | C24-C23-O8-C6   |
| 18  | 6     | 608 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 814 | CLA  | C15-C16-C17-C18 |
| 19  | A     | 844 | PQN  | C25-C26-C27-C28 |
| 23  | B     | 850 | DGD  | C6B-C7B-C8B-C9B |
| 18  | A     | 805 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 854 | CLA  | C2-C1-O2A-CGA   |
| 18  | B     | 806 | CLA  | C2-C1-O2A-CGA   |
| 18  | B     | 815 | CLA  | C2-C1-O2A-CGA   |
| 18  | A     | 826 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 806 | CLA  | C11-C10-C8-C9   |
| 18  | A     | 818 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 834 | CLA  | C6-C7-C8-C9     |
| 18  | B     | 813 | CLA  | C11-C12-C13-C14 |
| 18  | B     | 825 | CLA  | C6-C7-C8-C9     |
| 18  | B     | 826 | CLA  | C6-C7-C8-C9     |
| 19  | B     | 842 | PQN  | C16-C17-C18-C19 |
| 18  | B     | 813 | CLA  | C2C-C3C-CAC-CBC |
| 18  | A     | 829 | CLA  | C15-C16-C17-C18 |
| 18  | B     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 25  | 2     | 607 | CHL  | CBD-CGD-O2D-CED |
| 21  | A     | 848 | BCR  | C1-C6-C7-C8     |
| 21  | A     | 848 | BCR  | C5-C6-C7-C8     |
| 21  | A     | 849 | BCR  | C1-C6-C7-C8     |
| 21  | A     | 849 | BCR  | C5-C6-C7-C8     |
| 21  | A     | 850 | BCR  | C1-C6-C7-C8     |
| 21  | A     | 850 | BCR  | C5-C6-C7-C8     |
| 21  | A     | 851 | BCR  | C1-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | A     | 851 | BCR  | C5-C6-C7-C8     |
| 21  | A     | 856 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 801 | BCR  | C1-C6-C7-C8     |
| 21  | B     | 801 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 801 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 843 | BCR  | C1-C6-C7-C8     |
| 21  | B     | 843 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 843 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 843 | BCR  | C23-C24-C25-C30 |
| 21  | B     | 844 | BCR  | C1-C6-C7-C8     |
| 21  | B     | 844 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 845 | BCR  | C1-C6-C7-C8     |
| 21  | B     | 845 | BCR  | C5-C6-C7-C8     |
| 21  | B     | 845 | BCR  | C23-C24-C25-C26 |
| 21  | B     | 845 | BCR  | C23-C24-C25-C30 |
| 21  | B     | 846 | BCR  | C1-C6-C7-C8     |
| 21  | B     | 846 | BCR  | C5-C6-C7-C8     |
| 21  | G     | 205 | BCR  | C1-C6-C7-C8     |
| 21  | G     | 205 | BCR  | C5-C6-C7-C8     |
| 21  | K     | 202 | BCR  | C1-C6-C7-C8     |
| 21  | K     | 202 | BCR  | C5-C6-C7-C8     |
| 21  | K     | 202 | BCR  | C23-C24-C25-C26 |
| 21  | K     | 207 | BCR  | C1-C6-C7-C8     |
| 21  | K     | 207 | BCR  | C5-C6-C7-C8     |
| 21  | K     | 207 | BCR  | C23-C24-C25-C26 |
| 21  | L     | 301 | BCR  | C23-C24-C25-C26 |
| 21  | L     | 305 | BCR  | C1-C6-C7-C8     |
| 21  | 2     | 621 | BCR  | C1-C6-C7-C8     |
| 21  | 2     | 621 | BCR  | C5-C6-C7-C8     |
| 21  | 2     | 621 | BCR  | C23-C24-C25-C26 |
| 21  | 2     | 621 | BCR  | C23-C24-C25-C30 |
| 21  | 3     | 622 | BCR  | C23-C24-C25-C26 |
| 21  | 3     | 622 | BCR  | C23-C24-C25-C30 |
| 18  | A     | 834 | CLA  | C8-C10-C11-C12  |
| 18  | A     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 18  | J     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 21  | A     | 849 | BCR  | C7-C8-C9-C10    |
| 21  | B     | 843 | BCR  | C21-C22-C23-C24 |
| 21  | J     | 102 | BCR  | C7-C8-C9-C10    |
| 25  | 5     | 607 | CHL  | C1A-C2A-CAA-CBA |
| 18  | B     | 811 | CLA  | C6-C7-C8-C10    |
| 18  | B     | 807 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | A     | 847 | LHG  | O2-C2-C3-O3     |
| 18  | K     | 201 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 818 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 818 | CLA  | C12-C13-C15-C16 |
| 18  | A     | 826 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 827 | CLA  | C12-C13-C15-C16 |
| 18  | A     | 834 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 839 | CLA  | C6-C7-C8-C10    |
| 18  | B     | 803 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 806 | CLA  | C11-C12-C13-C15 |
| 18  | B     | 806 | CLA  | C12-C13-C15-C16 |
| 18  | B     | 807 | CLA  | C12-C13-C15-C16 |
| 18  | B     | 825 | CLA  | C6-C7-C8-C10    |
| 18  | B     | 826 | CLA  | C11-C12-C13-C15 |
| 18  | B     | 841 | CLA  | C11-C12-C13-C15 |
| 18  | 3     | 602 | CLA  | C6-C7-C8-C10    |
| 19  | B     | 842 | PQN  | C21-C22-C23-C25 |
| 21  | J     | 103 | BCR  | C13-C14-C15-C16 |
| 18  | 2     | 604 | CLA  | CBA-CGA-O2A-C1  |
| 21  | A     | 856 | BCR  | C20-C21-C22-C37 |
| 21  | B     | 843 | BCR  | C20-C21-C22-C37 |
| 21  | B     | 844 | BCR  | C20-C21-C22-C37 |
| 21  | B     | 845 | BCR  | C35-C13-C14-C15 |
| 21  | K     | 202 | BCR  | C20-C21-C22-C37 |
| 21  | 3     | 620 | BCR  | C16-C17-C18-C36 |
| 26  | 5     | 619 | LUT  | C11-C10-C9-C19  |
| 18  | A     | 806 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 822 | CLA  | C3-C5-C6-C7     |
| 18  | B     | 822 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 806 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 808 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 810 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 819 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 829 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 832 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 845 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 819 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 830 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 832 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 836 | CLA  | CAD-CBD-CGD-O2D |
| 18  | F     | 301 | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | 2     | 604 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 2     | 613 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 6     | 606 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 6     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 5     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 5     | 612 | CLA  | CAD-CBD-CGD-O2D |
| 20  | B     | 851 | LHG  | C6-C5-O7-C7     |
| 21  | A     | 849 | BCR  | C22-C23-C24-C25 |
| 21  | 2     | 621 | BCR  | C6-C7-C8-C9     |
| 18  | A     | 825 | CLA  | CBA-CGA-O2A-C1  |
| 20  | A     | 847 | LHG  | C4-C5-C6-O8     |
| 20  | 2     | 622 | LHG  | C2-C3-O3-P      |
| 18  | 2     | 604 | CLA  | O1A-CGA-O2A-C1  |
| 18  | B     | 832 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 806 | CLA  | C16-C17-C18-C19 |
| 24  | J     | 104 | LMG  | O9-C10-O7-C8    |
| 18  | A     | 814 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 840 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 841 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 805 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 805 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 810 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 810 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 821 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 821 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 18  | J     | 101 | CLA  | CHA-CBD-CGD-O1D |
| 18  | J     | 101 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 5     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 24  | J     | 104 | LMG  | C29-C30-C31-C32 |
| 21  | B     | 845 | BCR  | C11-C10-C9-C8   |
| 23  | B     | 850 | DGD  | C2D-C1D-O3G-C3G |
| 20  | 2     | 622 | LHG  | O7-C5-C6-O8     |
| 23  | B     | 850 | DGD  | O1G-C1G-C2G-O2G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 833 | CLA  | CBD-CGD-O2D-CED |
| 20  | 5     | 622 | LHG  | C28-C29-C30-C31 |
| 18  | A     | 819 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 812 | CLA  | C15-C16-C17-C18 |
| 18  | A     | 829 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 851 | BCR  | C11-C12-C13-C35 |
| 21  | K     | 207 | BCR  | C37-C22-C23-C24 |
| 20  | 2     | 622 | LHG  | O1-C1-C2-C3     |
| 20  | 2     | 622 | LHG  | C24-C25-C26-C27 |
| 18  | A     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 6     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 5     | 610 | CLA  | C1A-C2A-CAA-CBA |
| 25  | 2     | 608 | CHL  | CHA-CBD-CGD-O2D |
| 25  | 5     | 608 | CHL  | C1A-C2A-CAA-CBA |
| 25  | 2     | 607 | CHL  | O1D-CGD-O2D-CED |
| 18  | A     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 20  | A     | 847 | LHG  | C4-O6-P-O4      |
| 20  | 5     | 622 | LHG  | C3-O3-P-O4      |
| 18  | A     | 827 | CLA  | C16-C17-C18-C20 |
| 18  | A     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 20  | A     | 846 | LHG  | O6-C4-C5-C6     |
| 20  | A     | 847 | LHG  | O6-C4-C5-C6     |
| 20  | A     | 846 | LHG  | C24-C25-C26-C27 |
| 18  | B     | 802 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 3     | 613 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 806 | CLA  | C16-C17-C18-C19 |
| 18  | A     | 814 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 815 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 816 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 826 | CLA  | CAD-CBD-CGD-O1D |
| 18  | A     | 834 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 817 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 821 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 837 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 840 | CLA  | CAD-CBD-CGD-O1D |
| 18  | J     | 101 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 6     | 616 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 5     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 25  | 5     | 607 | CHL  | CAD-CBD-CGD-O1D |
| 18  | A     | 831 | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 807 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 840 | CLA  | C6-C7-C8-C10    |
| 18  | 3     | 611 | CLA  | CAD-CBD-CGD-O2D |
| 20  | A     | 846 | LHG  | O6-C4-C5-O7     |
| 20  | A     | 847 | LHG  | O6-C4-C5-O7     |
| 20  | 6     | 620 | LHG  | O6-C4-C5-O7     |
| 25  | 3     | 608 | CHL  | CAD-CBD-CGD-O2D |
| 18  | B     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 811 | CLA  | C3-C5-C6-C7     |
| 18  | 3     | 617 | CLA  | CAD-CBD-CGD-O1D |
| 20  | B     | 851 | LHG  | O7-C5-C6-O8     |
| 23  | B     | 850 | DGD  | C6A-C7A-C8A-C9A |
| 18  | A     | 831 | CLA  | C15-C16-C17-C18 |
| 21  | B     | 801 | BCR  | C14-C15-C16-C17 |
| 18  | A     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 818 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 827 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 829 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 839 | CLA  | C6-C7-C8-C9     |
| 18  | A     | 843 | CLA  | C6-C7-C8-C9     |
| 18  | B     | 806 | CLA  | C14-C13-C15-C16 |
| 18  | B     | 807 | CLA  | C14-C13-C15-C16 |
| 18  | 3     | 602 | CLA  | C6-C7-C8-C9     |
| 21  | B     | 848 | BCR  | C6-C7-C8-C9     |
| 20  | A     | 846 | LHG  | C11-C12-C13-C14 |
| 18  | B     | 841 | CLA  | C3-C5-C6-C7     |
| 21  | F     | 302 | BCR  | C15-C16-C17-C18 |
| 20  | 5     | 622 | LHG  | C12-C13-C14-C15 |
| 18  | A     | 806 | CLA  | C16-C17-C18-C20 |
| 21  | 5     | 621 | BCR  | C7-C8-C9-C10    |
| 26  | 6     | 617 | LUT  | C20-C13-C14-C15 |
| 18  | A     | 829 | CLA  | C16-C17-C18-C20 |
| 18  | B     | 831 | CLA  | C1-C2-C3-C4     |
| 18  | 6     | 604 | CLA  | C1-C2-C3-C4     |
| 18  | B     | 833 | CLA  | O1D-CGD-O2D-CED |
| 23  | B     | 850 | DGD  | C4D-C5D-C6D-O5D |
| 18  | A     | 829 | CLA  | CAA-CBA-CGA-O2A |
| 20  | 2     | 622 | LHG  | O6-C4-C5-C6     |
| 18  | A     | 802 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 841 | CLA  | C2A-CAA-CBA-CGA |
| 18  | K     | 206 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 5     | 613 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 805 | CLA  | C2-C1-O2A-CGA   |
| 18  | B     | 803 | CLA  | C2-C1-O2A-CGA   |
| 18  | B     | 826 | CLA  | C2-C1-O2A-CGA   |
| 20  | 6     | 620 | LHG  | C2-C3-O3-P      |
| 20  | 2     | 622 | LHG  | O6-C4-C5-O7     |
| 20  | 5     | 622 | LHG  | O6-C4-C5-O7     |
| 21  | B     | 801 | BCR  | C23-C24-C25-C30 |
| 21  | F     | 302 | BCR  | C23-C24-C25-C26 |
| 21  | F     | 302 | BCR  | C23-C24-C25-C30 |
| 21  | K     | 202 | BCR  | C23-C24-C25-C30 |
| 21  | L     | 301 | BCR  | C23-C24-C25-C30 |
| 18  | A     | 826 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 3     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 20  | A     | 846 | LHG  | C3-O3-P-O6      |
| 20  | B     | 851 | LHG  | C4-O6-P-O3      |
| 20  | 2     | 622 | LHG  | C3-O3-P-O6      |
| 20  | A     | 846 | LHG  | C25-C26-C27-C28 |
| 18  | B     | 822 | CLA  | C6-C7-C8-C10    |
| 23  | B     | 850 | DGD  | CCB-CDB-CEB-CFB |
| 18  | A     | 818 | CLA  | C11-C10-C8-C7   |
| 18  | A     | 830 | CLA  | C11-C12-C13-C15 |
| 18  | A     | 841 | CLA  | C11-C10-C8-C7   |
| 18  | 3     | 602 | CLA  | C11-C10-C8-C7   |
| 19  | B     | 842 | PQN  | C16-C17-C18-C20 |
| 18  | B     | 805 | CLA  | C11-C12-C13-C14 |
| 18  | B     | 809 | CLA  | C14-C13-C15-C16 |
| 18  | B     | 840 | CLA  | C6-C7-C8-C9     |
| 19  | B     | 842 | PQN  | C21-C22-C23-C24 |
| 21  | 5     | 621 | BCR  | C9-C10-C11-C12  |
| 18  | B     | 840 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 827 | CLA  | C16-C17-C18-C19 |
| 18  | A     | 831 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 21  | K     | 202 | BCR  | C13-C14-C15-C16 |
| 20  | 5     | 622 | LHG  | O6-C4-C5-C6     |
| 18  | A     | 814 | CLA  | C3-C5-C6-C7     |
| 18  | 5     | 609 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 6     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 832 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 827 | CLA  | C2-C1-O2A-CGA   |
| 18  | B     | 805 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | 5     | 602 | CLA  | C2A-CAA-CBA-CGA |
| 20  | A     | 847 | LHG  | O10-C23-C24-C25 |
| 25  | 2     | 606 | CHL  | C2A-CAA-CBA-CGA |
| 20  | 5     | 622 | LHG  | C27-C28-C29-C30 |
| 18  | A     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 18  | B     | 841 | CLA  | C3A-C2A-CAA-CBA |
| 25  | 6     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 18  | A     | 854 | CLA  | C11-C12-C13-C14 |
| 18  | B     | 807 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 828 | CLA  | C14-C13-C15-C16 |
| 19  | B     | 842 | PQN  | C26-C27-C28-C30 |
| 18  | B     | 832 | CLA  | CAA-CBA-CGA-O2A |
| 21  | A     | 848 | BCR  | C20-C21-C22-C37 |
| 21  | A     | 852 | BCR  | C11-C10-C9-C34  |
| 18  | B     | 833 | CLA  | CAA-CBA-CGA-O2A |
| 18  | K     | 203 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 829 | CLA  | C16-C17-C18-C19 |
| 20  | 6     | 620 | LHG  | O2-C2-C3-O3     |
| 18  | B     | 822 | CLA  | O1D-CGD-O2D-CED |
| 21  | A     | 856 | BCR  | C7-C8-C9-C34    |
| 25  | 2     | 616 | CHL  | CAA-CBA-CGA-O1A |
| 20  | A     | 846 | LHG  | C31-C32-C33-C34 |
| 21  | L     | 301 | BCR  | C21-C22-C23-C24 |
| 18  | A     | 840 | CLA  | CAA-CBA-CGA-O1A |
| 23  | B     | 850 | DGD  | O6D-C5D-C6D-O5D |
| 18  | A     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 5     | 614 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 854 | CLA  | C6-C7-C8-C10    |
| 18  | B     | 826 | CLA  | C11-C10-C8-C7   |
| 18  | B     | 836 | CLA  | C11-C10-C8-C7   |
| 18  | A     | 839 | CLA  | C15-C16-C17-C18 |
| 25  | 6     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 25  | 2     | 607 | CHL  | C3C-C2C-CMC-OMC |
| 25  | 5     | 615 | CHL  | C3C-C2C-CMC-OMC |
| 18  | A     | 833 | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 833 | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 834 | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 834 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | 5     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 826 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 839 | CLA  | C2A-CAA-CBA-CGA |
| 18  | L     | 302 | CLA  | C2A-CAA-CBA-CGA |
| 18  | 2     | 604 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 831 | CLA  | O2A-C1-C2-C3    |
| 25  | 5     | 608 | CHL  | CBA-CGA-O2A-C1  |
| 18  | A     | 831 | CLA  | C13-C15-C16-C17 |
| 18  | 5     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 25  | 2     | 601 | CHL  | CAA-CBA-CGA-O2A |
| 18  | 3     | 613 | CLA  | C5-C6-C7-C8     |
| 18  | B     | 841 | CLA  | CBD-CGD-O2D-CED |
| 25  | 2     | 601 | CHL  | CAA-CBA-CGA-O1A |
| 18  | B     | 806 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 852 | BCR  | C11-C10-C9-C8   |
| 18  | A     | 833 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 835 | CLA  | CAA-CBA-CGA-O1A |
| 25  | 2     | 616 | CHL  | CAA-CBA-CGA-O2A |
| 24  | J     | 104 | LMG  | O1-C7-C8-O7     |
| 18  | A     | 801 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 856 | BCR  | C19-C20-C21-C22 |
| 26  | 6     | 617 | LUT  | C9-C10-C11-C12  |
| 27  | 6     | 619 | XAT  | C29-C30-C31-C32 |
| 18  | 2     | 603 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 834 | CLA  | C10-C11-C12-C13 |
| 18  | G     | 204 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 841 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 804 | CLA  | C2-C1-O2A-CGA   |
| 18  | A     | 825 | CLA  | C2-C1-O2A-CGA   |
| 18  | 6     | 603 | CLA  | C2-C1-O2A-CGA   |
| 21  | B     | 843 | BCR  | C18-C19-C20-C21 |
| 26  | 5     | 619 | LUT  | C10-C11-C12-C13 |
| 18  | A     | 840 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 5     | 609 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 5     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 839 | CLA  | C11-C12-C13-C14 |
| 25  | 5     | 608 | CHL  | O1A-CGA-O2A-C1  |
| 20  | A     | 846 | LHG  | C17-C18-C19-C20 |
| 18  | K     | 203 | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 801 | CLA  | CAA-CBA-CGA-O2A |
| 23  | B     | 850 | DGD  | C8A-C9A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 819 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 827 | CLA  | C2A-CAA-CBA-CGA |
| 21  | A     | 849 | BCR  | C23-C24-C25-C30 |
| 21  | A     | 850 | BCR  | C23-C24-C25-C30 |
| 21  | F     | 302 | BCR  | C1-C6-C7-C8     |
| 21  | I     | 101 | BCR  | C1-C6-C7-C8     |
| 21  | J     | 102 | BCR  | C23-C24-C25-C30 |
| 21  | 3     | 620 | BCR  | C1-C6-C7-C8     |
| 21  | 3     | 622 | BCR  | C1-C6-C7-C8     |
| 21  | 3     | 622 | BCR  | C5-C6-C7-C8     |
| 18  | A     | 842 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 2     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 813 | CLA  | C8-C10-C11-C12  |
| 18  | L     | 304 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 810 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 18  | K     | 206 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 612 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 5     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 18  | K     | 206 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 841 | CLA  | C3-C5-C6-C7     |
| 18  | A     | 801 | CLA  | C6-C7-C8-C10    |
| 18  | A     | 803 | CLA  | C12-C13-C15-C16 |
| 18  | A     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 20  | A     | 847 | LHG  | O1-C1-C2-O2     |
| 20  | 2     | 622 | LHG  | O1-C1-C2-O2     |
| 21  | 2     | 621 | BCR  | C19-C20-C21-C22 |
| 24  | 2     | 618 | LMG  | C4-C5-C6-O5     |
| 23  | B     | 850 | DGD  | CEB-CFB-CGB-CHB |
| 18  | B     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 810 | CLA  | CAA-CBA-CGA-O1A |
| 18  | G     | 204 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 2     | 613 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 612 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 5     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 21  | B     | 845 | BCR  | C11-C10-C9-C34  |
| 21  | L     | 301 | BCR  | C11-C10-C9-C34  |
| 20  | 5     | 622 | LHG  | O7-C7-C8-C9     |
| 18  | A     | 818 | CLA  | C11-C10-C8-C9   |
| 18  | B     | 805 | CLA  | C14-C13-C15-C16 |
| 18  | A     | 803 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 830 | CLA  | C3A-C2A-CAA-CBA |
| 20  | A     | 847 | LHG  | O10-C23-O8-C6   |
| 18  | A     | 823 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 820 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 827 | CLA  | CAD-CBD-CGD-O2D |
| 18  | A     | 833 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 811 | CLA  | CAD-CBD-CGD-O2D |
| 18  | B     | 812 | CLA  | CAD-CBD-CGD-O2D |
| 18  | L     | 304 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 2     | 602 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 2     | 603 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 3     | 609 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 3     | 610 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 5     | 611 | CLA  | CAD-CBD-CGD-O2D |
| 18  | F     | 303 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 608 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 2     | 609 | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 842 | CLA  | CAA-CBA-CGA-O1A |
| 20  | A     | 846 | LHG  | O8-C23-C24-C25  |
| 21  | J     | 103 | BCR  | C7-C8-C9-C10    |
| 27  | 5     | 620 | XAT  | O24-C26-C27-C28 |
| 25  | 5     | 608 | CHL  | CAA-CBA-CGA-O2A |
| 18  | 6     | 608 | CLA  | CAA-CBA-CGA-O1A |
| 20  | A     | 846 | LHG  | C16-C17-C18-C19 |
| 18  | A     | 806 | CLA  | O2A-C1-C2-C3    |
| 18  | A     | 801 | CLA  | C16-C17-C18-C20 |
| 20  | 2     | 622 | LHG  | O9-C7-O7-C5     |
| 18  | A     | 809 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 809 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 840 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 803 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 807 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 808 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 808 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 824 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 824 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 828 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 833 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 836 | CLA  | CHA-CBD-CGD-O1D |
| 18  | B     | 841 | CLA  | CHA-CBD-CGD-O1D |
| 18  | F     | 305 | CLA  | CHA-CBD-CGD-O1D |
| 18  | F     | 305 | CLA  | CHA-CBD-CGD-O2D |
| 18  | G     | 203 | CLA  | CHA-CBD-CGD-O1D |
| 18  | G     | 203 | CLA  | CHA-CBD-CGD-O2D |
| 18  | K     | 201 | CLA  | CHA-CBD-CGD-O1D |
| 18  | K     | 204 | CLA  | CHA-CBD-CGD-O1D |
| 18  | K     | 204 | CLA  | CHA-CBD-CGD-O2D |
| 18  | L     | 302 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 6     | 602 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 6     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 5     | 613 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 5     | 613 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 5     | 614 | CLA  | CHA-CBD-CGD-O2D |
| 25  | 2     | 601 | CHL  | CHA-CBD-CGD-O1D |
| 25  | 2     | 601 | CHL  | CHA-CBD-CGD-O2D |
| 26  | 5     | 619 | LUT  | C29-C30-C31-C32 |
| 18  | A     | 821 | CLA  | CAA-CBA-CGA-O2A |
| 18  | F     | 303 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 23  | B     | 850 | DGD  | O2G-C2G-C3G-O3G |
| 18  | F     | 305 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 845 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 604 | CLA  | O1D-CGD-O2D-CED |
| 20  | 2     | 622 | LHG  | C28-C29-C30-C31 |
| 18  | A     | 839 | CLA  | C5-C6-C7-C8     |
| 18  | B     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 18  | 6     | 604 | CLA  | CBD-CGD-O2D-CED |
| 20  | A     | 847 | LHG  | C10-C11-C12-C13 |
| 18  | B     | 806 | CLA  | C2-C3-C5-C6     |
| 18  | B     | 828 | CLA  | C11-C10-C8-C9   |
| 18  | K     | 204 | CLA  | C4C-C3C-CAC-CBC |
| 18  | 2     | 613 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 5     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 813 | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 20  | 6     | 620 | LHG  | C8-C7-O7-C5     |
| 18  | 5     | 610 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 821 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 18  | G     | 201 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 6     | 602 | CLA  | CAA-CBA-CGA-O1A |
| 25  | 2     | 606 | CHL  | CAA-CBA-CGA-O2A |
| 18  | 2     | 609 | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 807 | CLA  | CHA-CBD-CGD-O2D |
| 18  | A     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 18  | A     | 854 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 814 | CLA  | CHA-CBD-CGD-O2D |
| 18  | B     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 18  | B     | 841 | CLA  | C1A-C2A-CAA-CBA |
| 18  | K     | 201 | CLA  | C1A-C2A-CAA-CBA |
| 18  | 3     | 611 | CLA  | CHA-CBD-CGD-O2D |
| 18  | 5     | 603 | CLA  | CHA-CBD-CGD-O2D |
| 25  | 2     | 601 | CHL  | C1A-C2A-CAA-CBA |
| 25  | 6     | 607 | CHL  | CHA-CBD-CGD-O2D |
| 18  | 3     | 602 | CLA  | C11-C12-C13-C15 |
| 18  | A     | 854 | CLA  | C13-C15-C16-C17 |
| 18  | B     | 840 | CLA  | C2-C1-O2A-CGA   |
| 18  | A     | 812 | CLA  | C5-C6-C7-C8     |
| 20  | A     | 846 | LHG  | O10-C23-C24-C25 |
| 18  | A     | 802 | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 18  | B     | 825 | CLA  | C16-C17-C18-C19 |
| 25  | 5     | 608 | CHL  | CAA-CBA-CGA-O1A |
| 18  | A     | 843 | CLA  | C10-C11-C12-C13 |
| 18  | B     | 826 | CLA  | C13-C15-C16-C17 |
| 18  | A     | 831 | CLA  | C2-C3-C5-C6     |
| 21  | F     | 302 | BCR  | C6-C7-C8-C9     |
| 21  | I     | 101 | BCR  | C6-C7-C8-C9     |
| 18  | 2     | 609 | CLA  | O1A-CGA-O2A-C1  |
| 20  | A     | 846 | LHG  | C3-O3-P-O5      |
| 23  | B     | 850 | DGD  | CEA-CFA-CGA-CHA |
| 18  | 2     | 609 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 21  | J     | 102 | BCR  | C16-C17-C18-C36 |
| 21  | A     | 849 | BCR  | C23-C24-C25-C26 |
| 21  | F     | 302 | BCR  | C5-C6-C7-C8     |
| 21  | I     | 101 | BCR  | C5-C6-C7-C8     |
| 18  | B     | 828 | CLA  | C5-C6-C7-C8     |
| 18  | A     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 18  | F     | 305 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | A     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 5     | 601 | CLA  | CAA-CBA-CGA-O2A |
| 24  | J     | 104 | LMG  | C10-C11-C12-C13 |
| 18  | A     | 831 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 803 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 835 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 838 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 841 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 2     | 602 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 2     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 6     | 602 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 6     | 603 | CLA  | CAD-CBD-CGD-O1D |
| 18  | 6     | 604 | CLA  | CAD-CBD-CGD-O1D |
| 18  | B     | 806 | CLA  | CAA-CBA-CGA-O1A |
| 18  | 6     | 603 | CLA  | CAA-CBA-CGA-O2A |
| 19  | B     | 842 | PQN  | C19-C18-C20-C21 |
| 18  | A     | 833 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 824 | CLA  | CAA-CBA-CGA-O2A |
| 18  | B     | 816 | CLA  | CAA-CBA-CGA-O2A |
| 18  | G     | 201 | CLA  | CAA-CBA-CGA-O2A |
| 25  | 2     | 606 | CHL  | CAA-CBA-CGA-O1A |
| 18  | A     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 806 | CLA  | C10-C11-C12-C13 |
| 18  | 5     | 601 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 845 | CLA  | CAA-CBA-CGA-O1A |
| 18  | B     | 806 | CLA  | C4-C3-C5-C6     |
| 18  | A     | 807 | CLA  | CHA-CBD-CGD-O1D |
| 18  | A     | 843 | CLA  | C11-C12-C13-C15 |
| 18  | B     | 828 | CLA  | C11-C10-C8-C7   |
| 18  | G     | 204 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 6     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 3     | 614 | CLA  | CHA-CBD-CGD-O1D |
| 18  | 3     | 617 | CLA  | CAD-CBD-CGD-O2D |
| 18  | 5     | 603 | CLA  | CHA-CBD-CGD-O1D |
| 25  | 6     | 607 | CHL  | CAD-CBD-CGD-O2D |
| 25  | 3     | 608 | CHL  | CHA-CBD-CGD-O1D |
| 18  | A     | 824 | CLA  | CAA-CBA-CGA-O1A |
| 23  | B     | 850 | DGD  | O1B-C1B-C2B-C3B |
| 18  | 3     | 602 | CLA  | CAA-CBA-CGA-O2A |
| 20  | A     | 847 | LHG  | O8-C23-C24-C25  |
| 21  | J     | 102 | BCR  | C11-C12-C13-C14 |
| 18  | A     | 802 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | B     | 816 | CLA  | CAA-CBA-CGA-O1A |
| 18  | A     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 18  | 6     | 603 | CLA  | CAA-CBA-CGA-O1A |

There are no ring outliers.

171 monomers are involved in 423 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | B     | 840 | CLA  | 4       | 0            |
| 18  | B     | 832 | CLA  | 1       | 0            |
| 18  | B     | 837 | CLA  | 2       | 0            |
| 18  | G     | 204 | CLA  | 2       | 0            |
| 18  | B     | 825 | CLA  | 3       | 0            |
| 18  | A     | 823 | CLA  | 1       | 0            |
| 18  | 6     | 603 | CLA  | 2       | 0            |
| 27  | 5     | 620 | XAT  | 31      | 0            |
| 18  | 5     | 611 | CLA  | 2       | 0            |
| 19  | A     | 844 | PQN  | 1       | 0            |
| 18  | A     | 819 | CLA  | 3       | 0            |
| 18  | 6     | 613 | CLA  | 1       | 0            |
| 18  | A     | 820 | CLA  | 5       | 0            |
| 18  | 3     | 602 | CLA  | 1       | 0            |
| 21  | B     | 846 | BCR  | 1       | 0            |
| 21  | I     | 101 | BCR  | 2       | 0            |
| 18  | B     | 819 | CLA  | 3       | 0            |
| 24  | J     | 104 | LMG  | 1       | 0            |
| 18  | B     | 803 | CLA  | 2       | 0            |
| 20  | A     | 847 | LHG  | 2       | 0            |
| 18  | A     | 839 | CLA  | 3       | 0            |
| 18  | B     | 802 | CLA  | 3       | 0            |
| 21  | B     | 843 | BCR  | 4       | 0            |
| 18  | A     | 830 | CLA  | 2       | 0            |
| 18  | A     | 831 | CLA  | 2       | 0            |
| 18  | A     | 845 | CLA  | 1       | 0            |
| 18  | B     | 806 | CLA  | 2       | 0            |
| 18  | A     | 801 | CLA  | 1       | 0            |
| 18  | B     | 827 | CLA  | 3       | 0            |
| 18  | 3     | 614 | CLA  | 2       | 0            |
| 25  | 6     | 607 | CHL  | 6       | 0            |
| 18  | A     | 828 | CLA  | 1       | 0            |
| 18  | 3     | 609 | CLA  | 7       | 0            |
| 18  | 5     | 602 | CLA  | 5       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | 5     | 610 | CLA  | 3       | 0            |
| 27  | 2     | 620 | XAT  | 24      | 0            |
| 18  | B     | 826 | CLA  | 3       | 0            |
| 18  | 5     | 613 | CLA  | 3       | 0            |
| 18  | A     | 826 | CLA  | 5       | 0            |
| 21  | K     | 207 | BCR  | 2       | 0            |
| 18  | B     | 814 | CLA  | 1       | 0            |
| 18  | A     | 821 | CLA  | 2       | 0            |
| 20  | 5     | 622 | LHG  | 5       | 0            |
| 18  | A     | 805 | CLA  | 3       | 0            |
| 21  | A     | 851 | BCR  | 1       | 0            |
| 21  | A     | 848 | BCR  | 3       | 0            |
| 18  | A     | 824 | CLA  | 2       | 0            |
| 18  | 3     | 613 | CLA  | 3       | 0            |
| 18  | J     | 101 | CLA  | 1       | 0            |
| 18  | B     | 821 | CLA  | 2       | 0            |
| 18  | A     | 854 | CLA  | 6       | 0            |
| 18  | 5     | 614 | CLA  | 2       | 0            |
| 18  | 2     | 613 | CLA  | 1       | 0            |
| 18  | A     | 811 | CLA  | 3       | 0            |
| 22  | C     | 101 | SF4  | 7       | 0            |
| 18  | B     | 811 | CLA  | 1       | 0            |
| 21  | A     | 850 | BCR  | 1       | 0            |
| 18  | A     | 835 | CLA  | 4       | 0            |
| 18  | 2     | 610 | CLA  | 4       | 0            |
| 25  | 5     | 607 | CHL  | 14      | 0            |
| 18  | B     | 807 | CLA  | 1       | 0            |
| 18  | L     | 304 | CLA  | 1       | 0            |
| 18  | 5     | 601 | CLA  | 2       | 0            |
| 18  | B     | 830 | CLA  | 1       | 0            |
| 18  | A     | 842 | CLA  | 2       | 0            |
| 18  | B     | 815 | CLA  | 3       | 0            |
| 18  | A     | 827 | CLA  | 5       | 0            |
| 21  | 3     | 622 | BCR  | 3       | 0            |
| 18  | 2     | 614 | CLA  | 2       | 0            |
| 19  | B     | 842 | PQN  | 5       | 0            |
| 18  | A     | 816 | CLA  | 1       | 0            |
| 18  | 3     | 606 | CLA  | 3       | 0            |
| 18  | F     | 305 | CLA  | 1       | 0            |
| 18  | B     | 836 | CLA  | 1       | 0            |
| 18  | B     | 829 | CLA  | 1       | 0            |
| 18  | 3     | 611 | CLA  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | A     | 843 | CLA  | 6       | 0            |
| 25  | 6     | 601 | CHL  | 2       | 0            |
| 18  | A     | 802 | CLA  | 2       | 0            |
| 21  | B     | 845 | BCR  | 2       | 0            |
| 21  | B     | 801 | BCR  | 2       | 0            |
| 18  | A     | 832 | CLA  | 2       | 0            |
| 18  | B     | 841 | CLA  | 2       | 0            |
| 18  | A     | 818 | CLA  | 1       | 0            |
| 18  | K     | 201 | CLA  | 1       | 0            |
| 21  | 2     | 621 | BCR  | 5       | 0            |
| 25  | 3     | 608 | CHL  | 1       | 0            |
| 20  | B     | 851 | LHG  | 1       | 0            |
| 18  | 2     | 602 | CLA  | 3       | 0            |
| 26  | 5     | 619 | LUT  | 2       | 0            |
| 18  | A     | 806 | CLA  | 5       | 0            |
| 18  | 3     | 612 | CLA  | 1       | 0            |
| 18  | B     | 833 | CLA  | 5       | 0            |
| 18  | A     | 837 | CLA  | 2       | 0            |
| 18  | B     | 805 | CLA  | 2       | 0            |
| 18  | B     | 818 | CLA  | 3       | 0            |
| 21  | J     | 103 | BCR  | 5       | 0            |
| 20  | A     | 846 | LHG  | 1       | 0            |
| 18  | B     | 823 | CLA  | 3       | 0            |
| 25  | 2     | 601 | CHL  | 1       | 0            |
| 18  | 5     | 604 | CLA  | 1       | 0            |
| 18  | A     | 814 | CLA  | 6       | 0            |
| 18  | A     | 838 | CLA  | 2       | 0            |
| 21  | B     | 848 | BCR  | 4       | 0            |
| 18  | B     | 838 | CLA  | 2       | 0            |
| 18  | A     | 813 | CLA  | 1       | 0            |
| 18  | B     | 839 | CLA  | 3       | 0            |
| 26  | 3     | 618 | LUT  | 1       | 0            |
| 18  | B     | 828 | CLA  | 5       | 0            |
| 18  | L     | 303 | CLA  | 2       | 0            |
| 18  | B     | 809 | CLA  | 4       | 0            |
| 21  | K     | 202 | BCR  | 3       | 0            |
| 25  | 2     | 616 | CHL  | 1       | 0            |
| 21  | L     | 301 | BCR  | 1       | 0            |
| 18  | 5     | 612 | CLA  | 1       | 0            |
| 18  | A     | 803 | CLA  | 2       | 0            |
| 18  | A     | 833 | CLA  | 3       | 0            |
| 21  | F     | 302 | BCR  | 4       | 0            |

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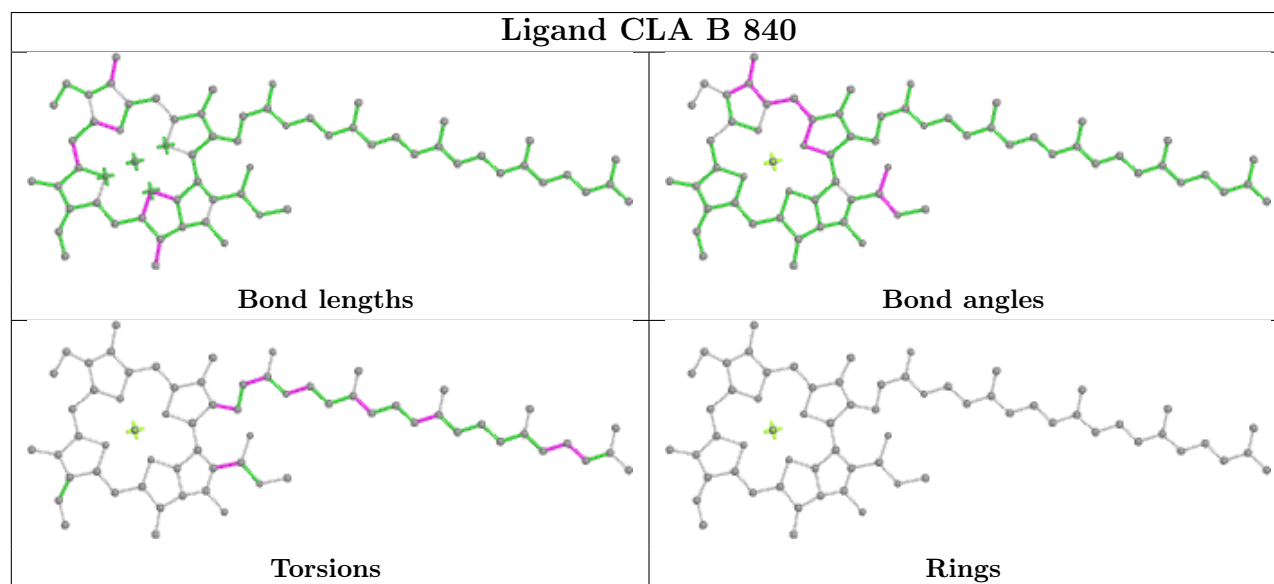
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | A     | 829 | CLA  | 9       | 0            |
| 21  | B     | 847 | BCR  | 2       | 0            |
| 21  | 3     | 620 | BCR  | 5       | 0            |
| 21  | A     | 856 | BCR  | 4       | 0            |
| 18  | B     | 831 | CLA  | 2       | 0            |
| 22  | C     | 102 | SF4  | 4       | 0            |
| 18  | B     | 834 | CLA  | 1       | 0            |
| 25  | 2     | 607 | CHL  | 5       | 0            |
| 18  | A     | 808 | CLA  | 2       | 0            |
| 25  | 5     | 608 | CHL  | 4       | 0            |
| 18  | B     | 816 | CLA  | 2       | 0            |
| 20  | 2     | 622 | LHG  | 3       | 0            |
| 18  | B     | 822 | CLA  | 1       | 0            |
| 25  | 2     | 606 | CHL  | 9       | 0            |
| 18  | A     | 840 | CLA  | 1       | 0            |
| 18  | A     | 834 | CLA  | 2       | 0            |
| 21  | J     | 102 | BCR  | 1       | 0            |
| 18  | 5     | 609 | CLA  | 1       | 0            |
| 18  | K     | 203 | CLA  | 1       | 0            |
| 18  | A     | 841 | CLA  | 2       | 0            |
| 18  | K     | 204 | CLA  | 2       | 0            |
| 18  | A     | 817 | CLA  | 1       | 0            |
| 18  | F     | 304 | CLA  | 2       | 0            |
| 18  | B     | 824 | CLA  | 3       | 0            |
| 18  | A     | 809 | CLA  | 6       | 0            |
| 21  | G     | 205 | BCR  | 3       | 0            |
| 21  | A     | 849 | BCR  | 2       | 0            |
| 18  | A     | 822 | CLA  | 1       | 0            |
| 18  | 6     | 609 | CLA  | 2       | 0            |
| 18  | B     | 817 | CLA  | 4       | 0            |
| 18  | 3     | 603 | CLA  | 2       | 0            |
| 18  | G     | 201 | CLA  | 2       | 0            |
| 18  | 3     | 617 | CLA  | 1       | 0            |
| 27  | 3     | 619 | XAT  | 17      | 0            |
| 18  | B     | 813 | CLA  | 8       | 0            |
| 18  | B     | 835 | CLA  | 3       | 0            |
| 21  | L     | 305 | BCR  | 1       | 0            |
| 27  | 6     | 619 | XAT  | 13      | 0            |
| 18  | 2     | 604 | CLA  | 3       | 0            |
| 18  | B     | 812 | CLA  | 3       | 0            |
| 18  | L     | 302 | CLA  | 4       | 0            |
| 21  | B     | 844 | BCR  | 1       | 0            |

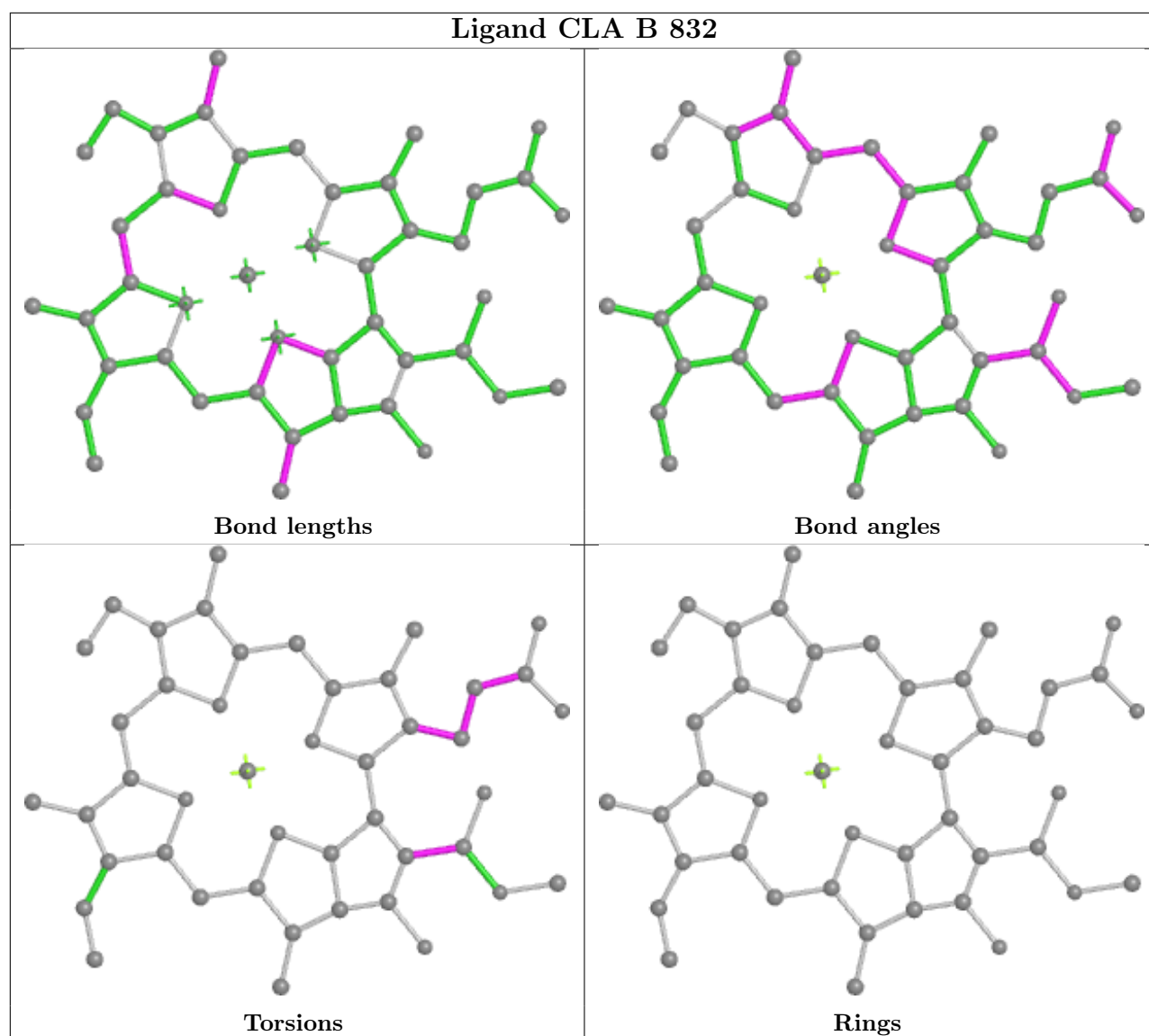
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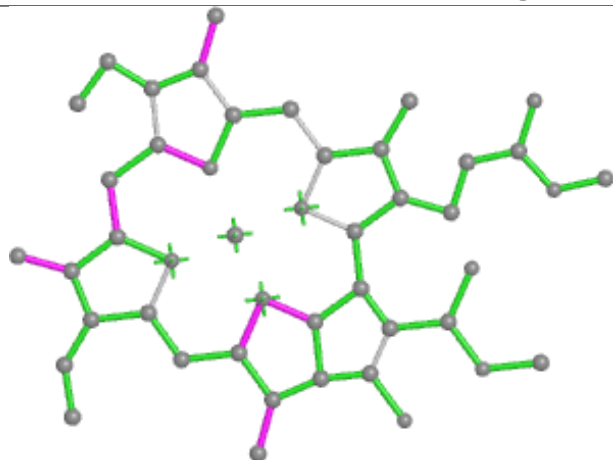
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 18  | A     | 810 | CLA  | 2       | 0            |
| 18  | 3     | 604 | CLA  | 1       | 0            |
| 21  | A     | 852 | BCR  | 4       | 0            |
| 23  | B     | 850 | DGD  | 4       | 0            |
| 18  | B     | 808 | CLA  | 1       | 0            |
| 18  | F     | 301 | CLA  | 2       | 0            |
| 20  | 6     | 620 | LHG  | 1       | 0            |
| 26  | 6     | 617 | LUT  | 3       | 0            |
| 21  | 5     | 621 | BCR  | 2       | 0            |
| 26  | 2     | 619 | LUT  | 2       | 0            |
| 18  | A     | 812 | CLA  | 7       | 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.

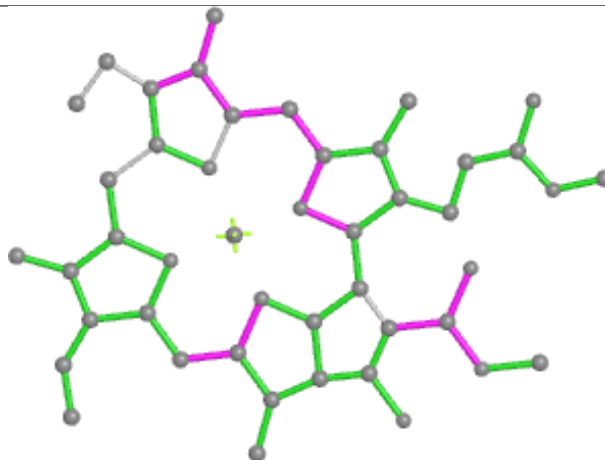




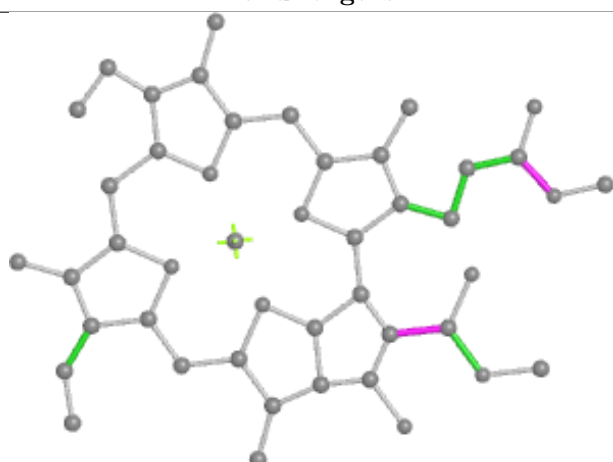
## Ligand CLA B 837



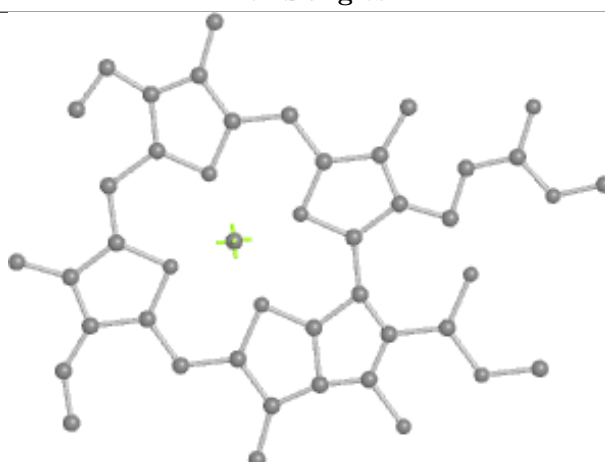
Bond lengths



Bond angles

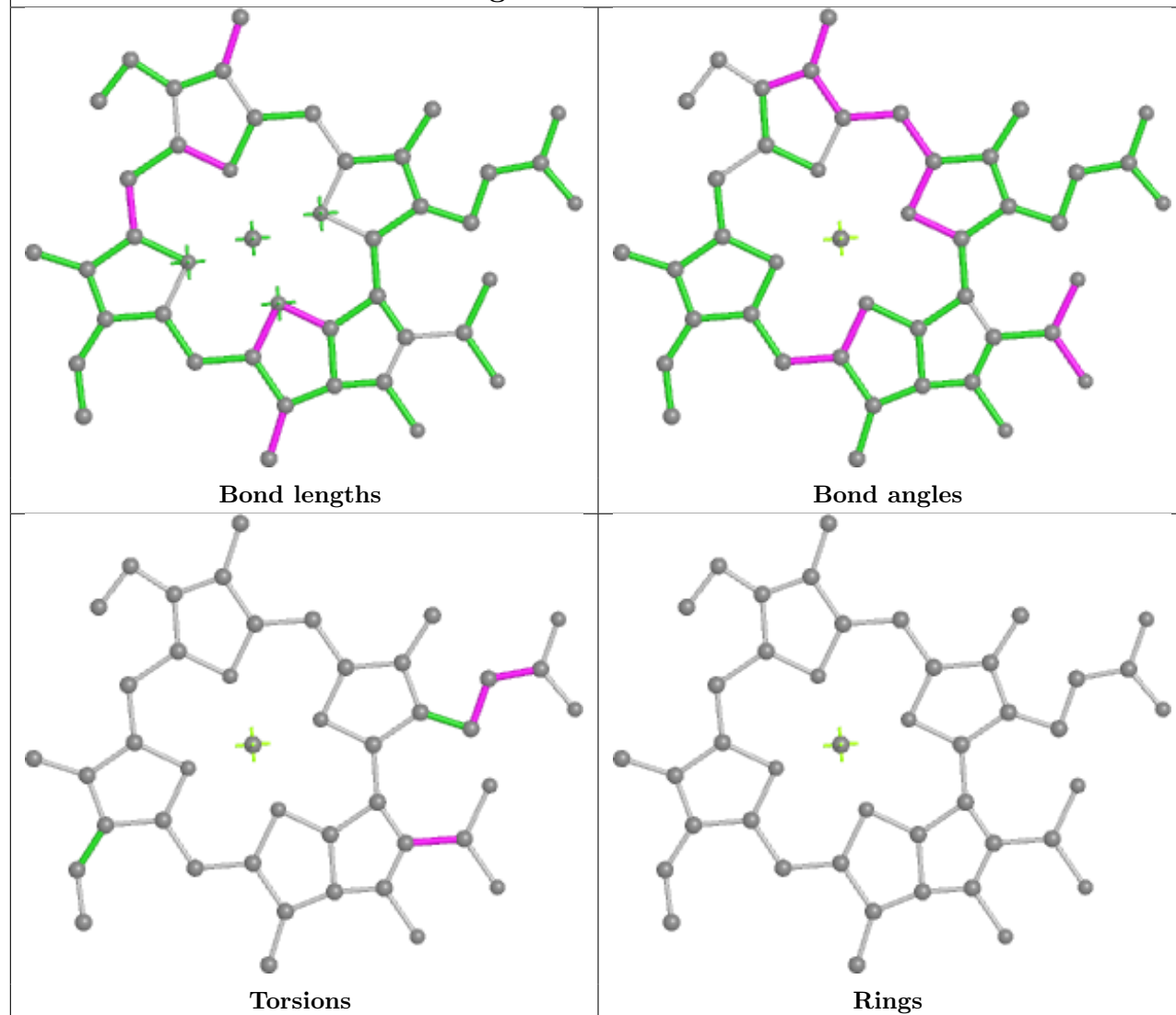


Torsions

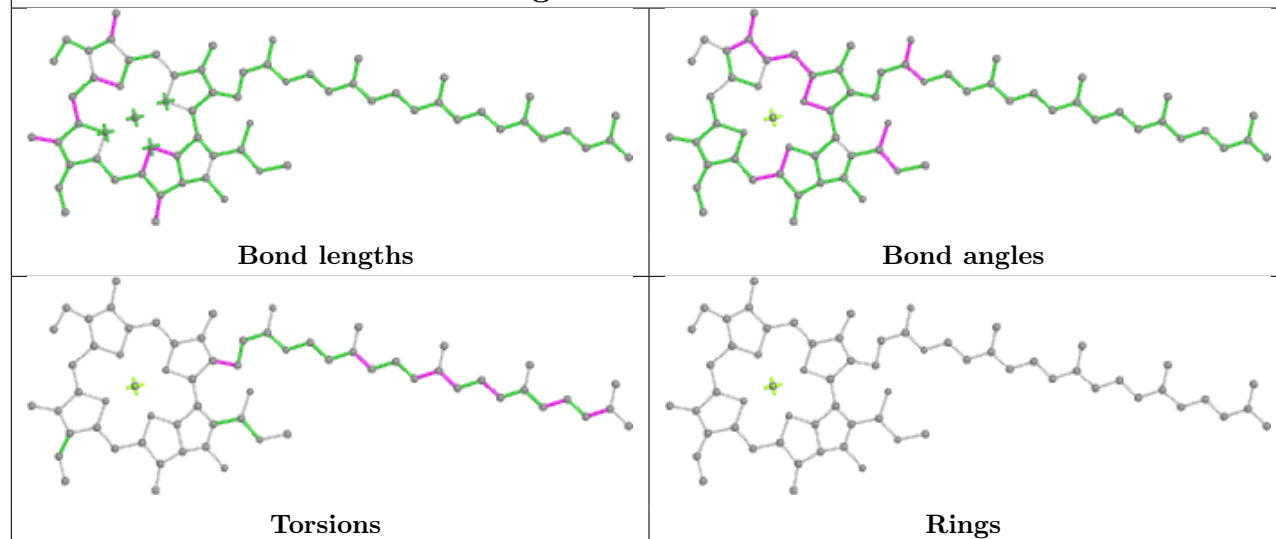


Rings

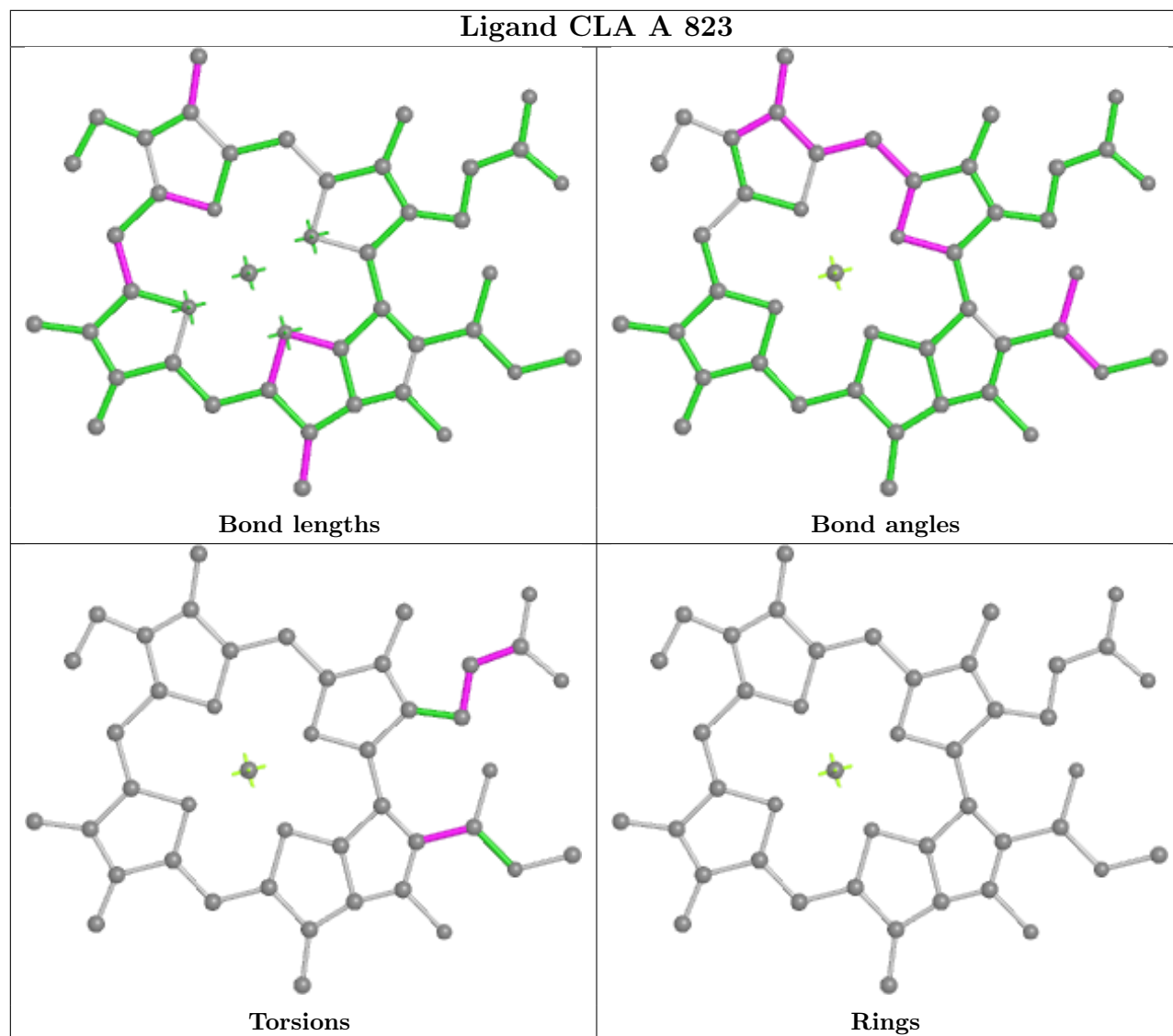
## Ligand CLA G 204

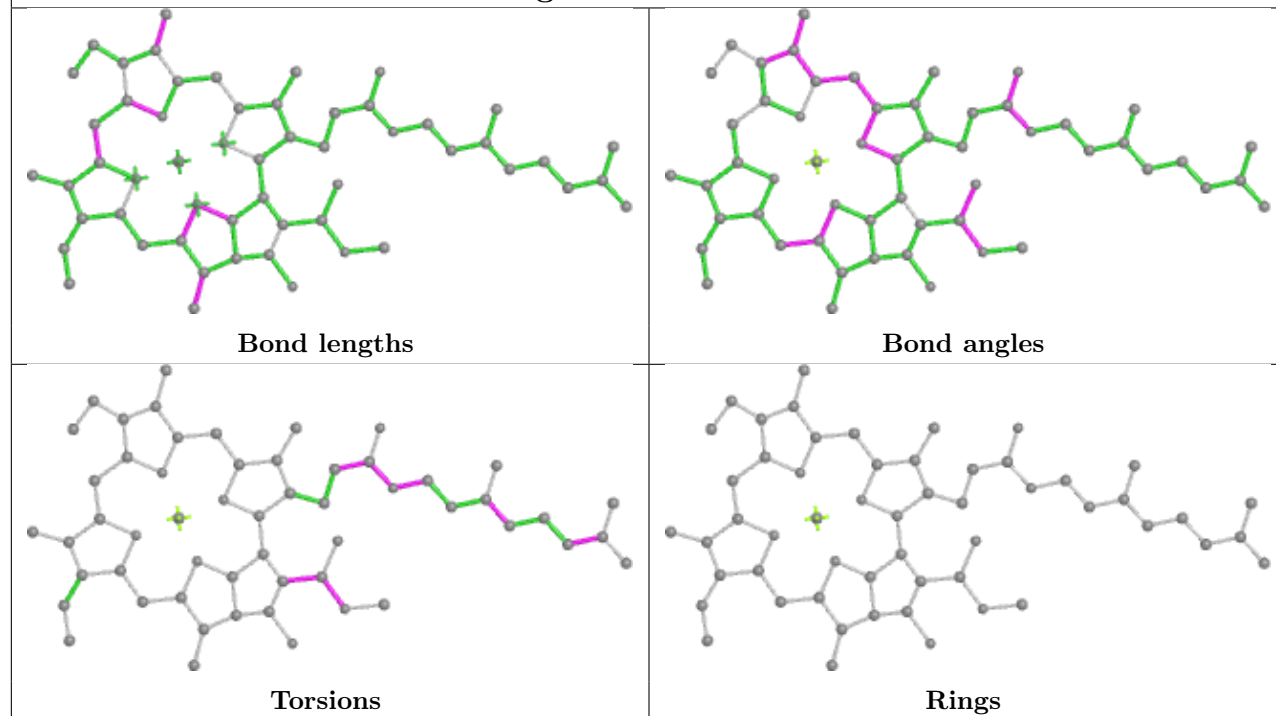
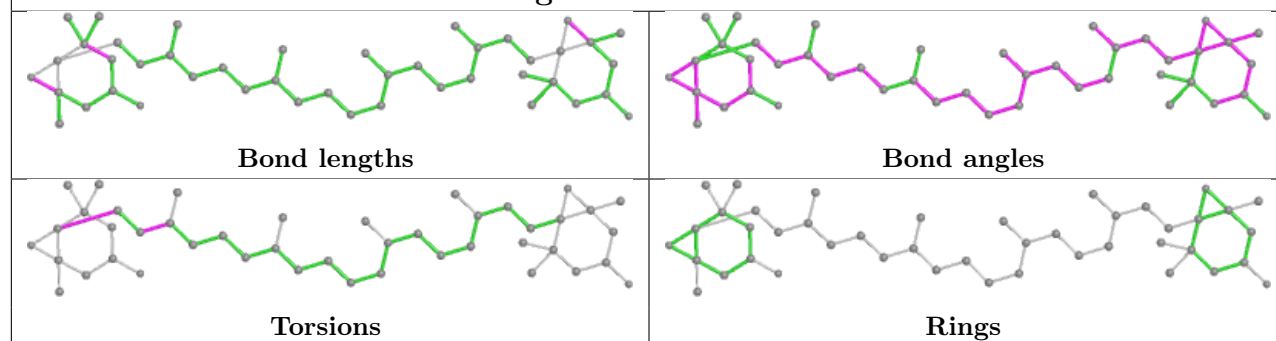


## Ligand CLA B 825

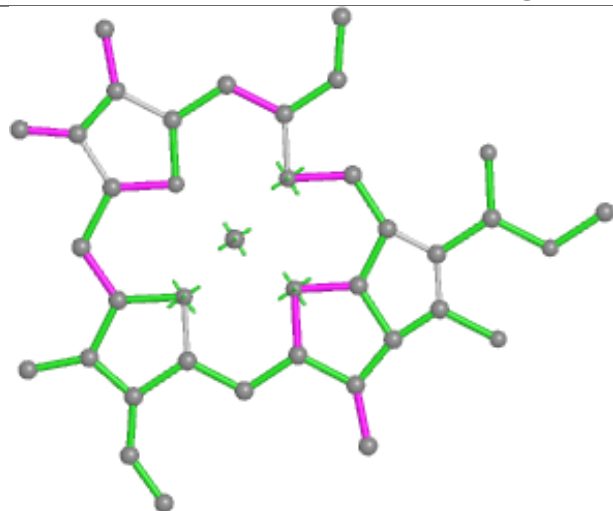


## Ligand CLA A 823

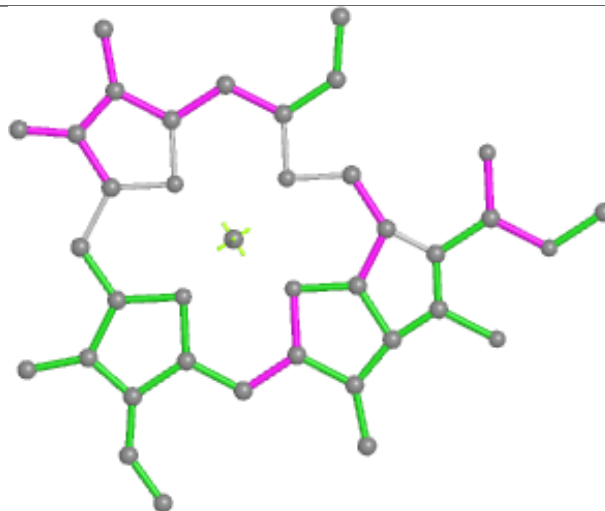


**Ligand CLA 6 603****Ligand XAT 5 620**

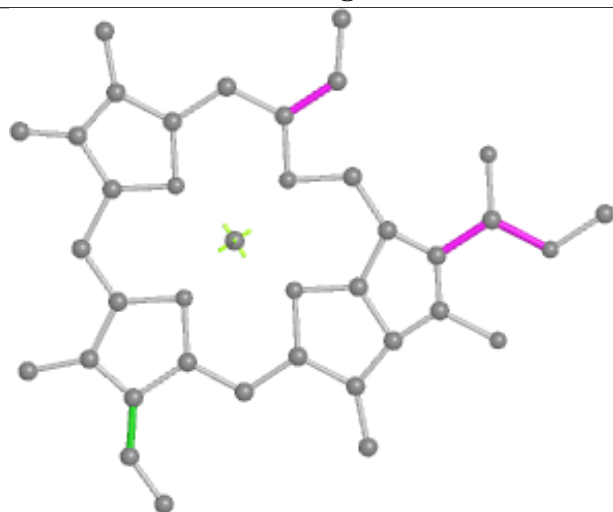
## Ligand CLA 5 611



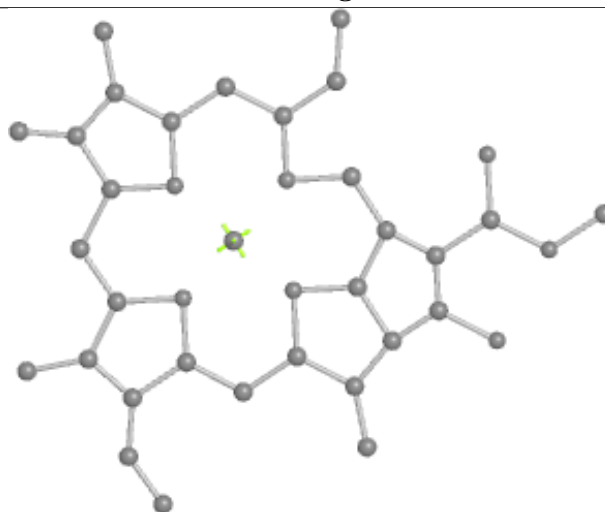
Bond lengths



Bond angles



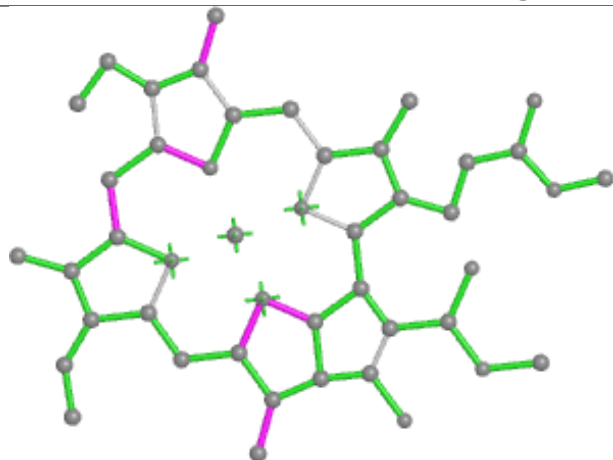
Torsions



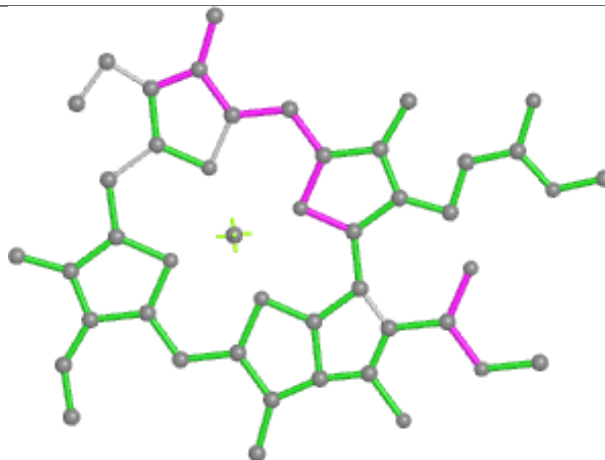
Rings



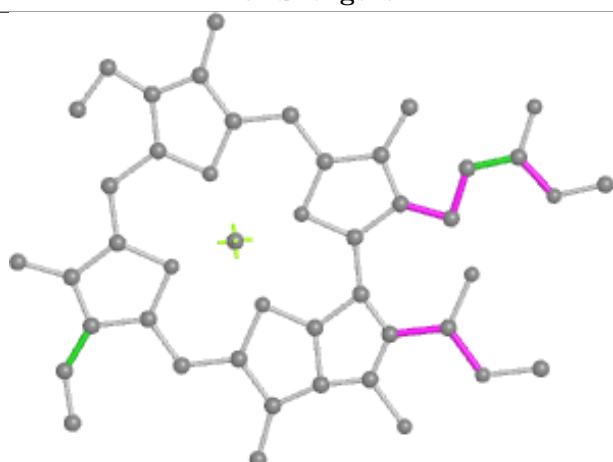
## Ligand CLA B 810



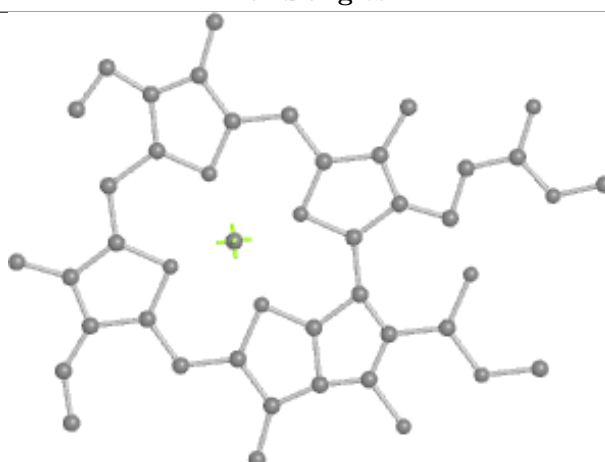
Bond lengths



Bond angles

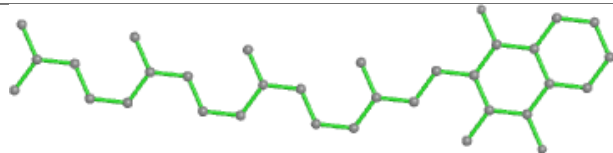


Torsions

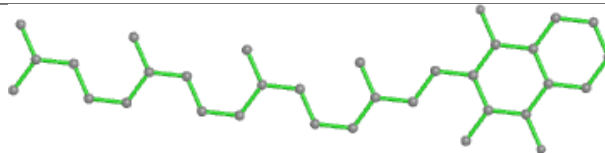


Rings

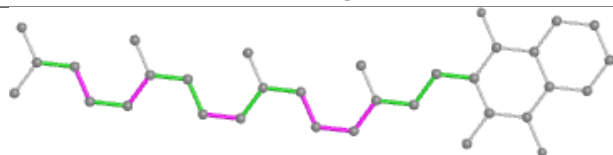
## Ligand PQN A 844



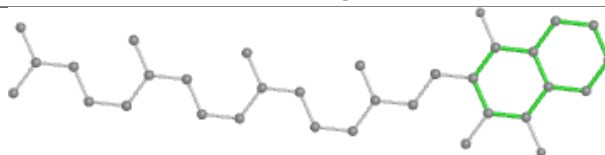
Bond lengths



Bond angles

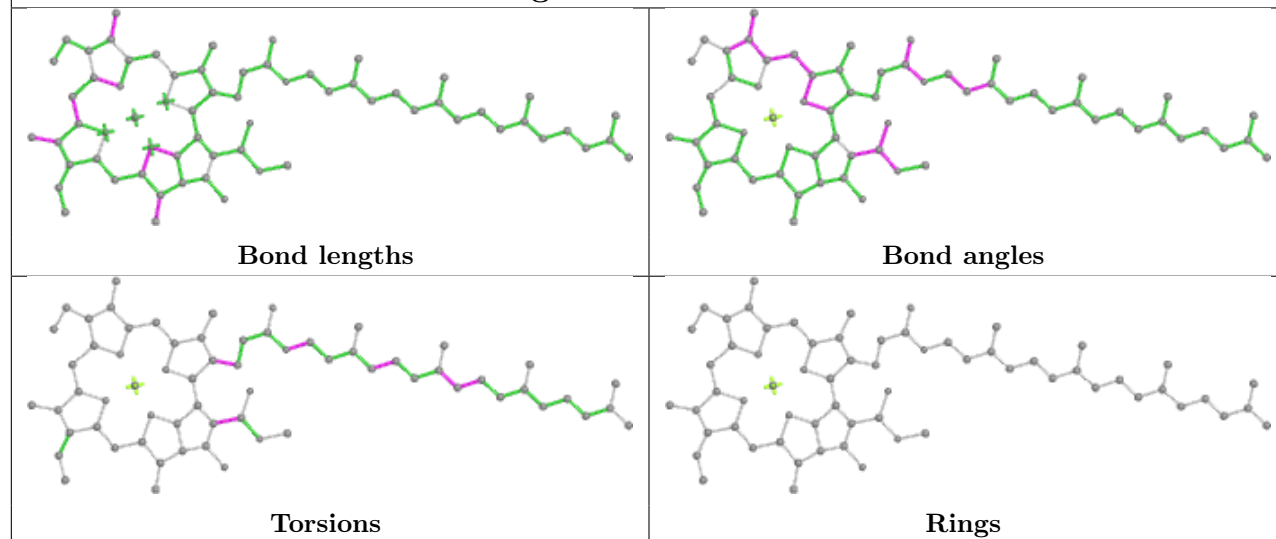


Torsions

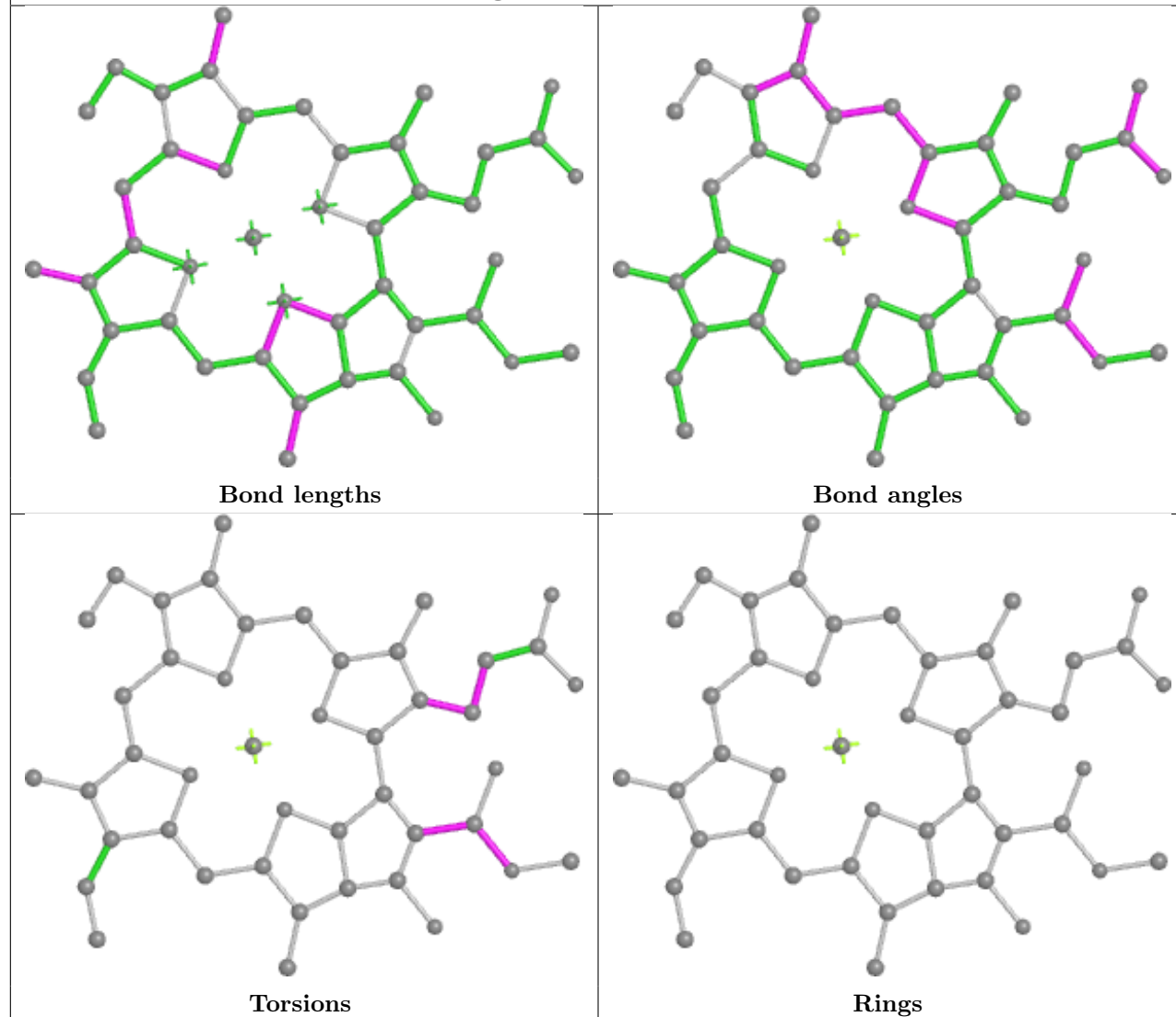


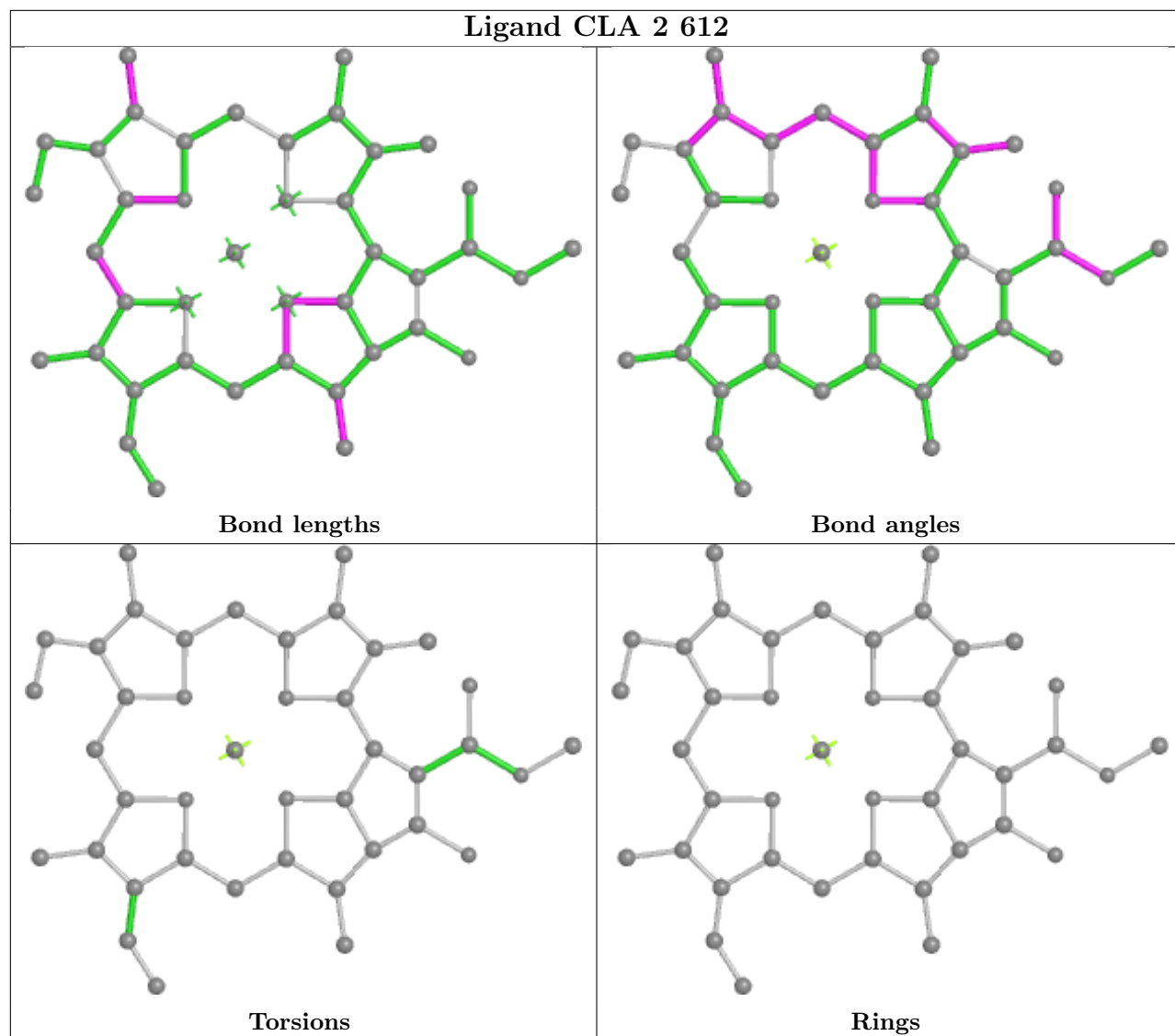
Rings

## Ligand CLA A 804

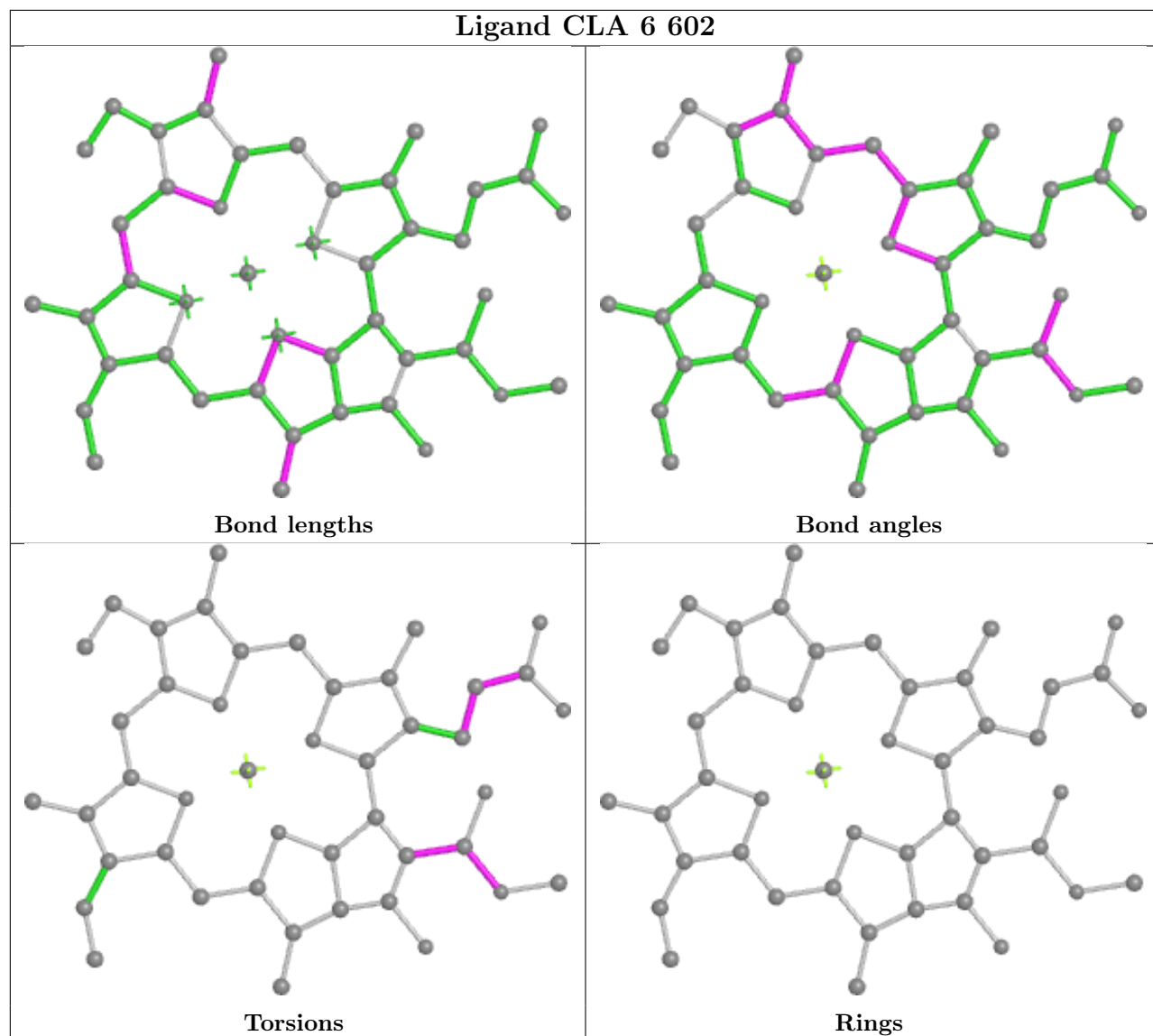


## Ligand CLA A 819

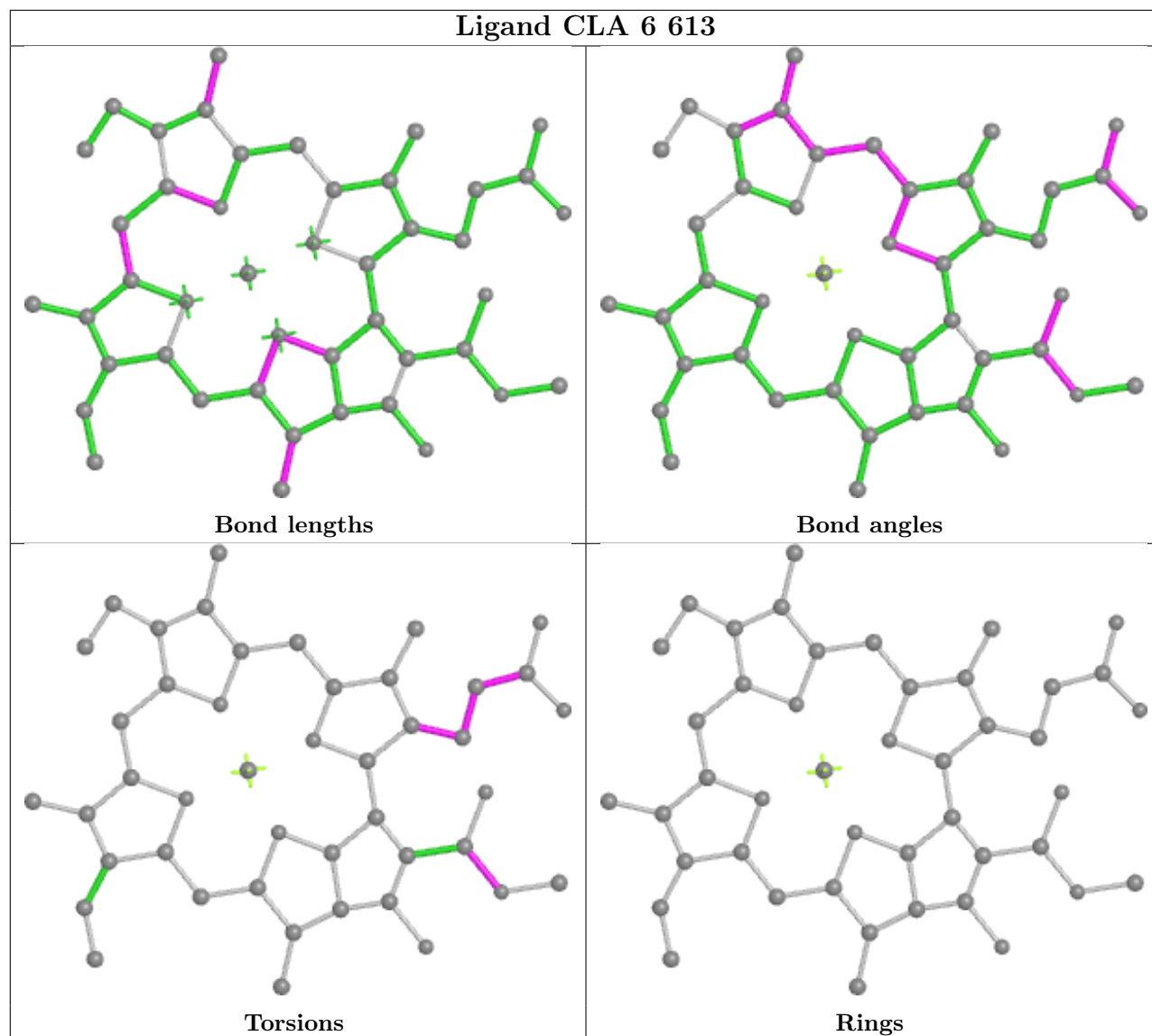




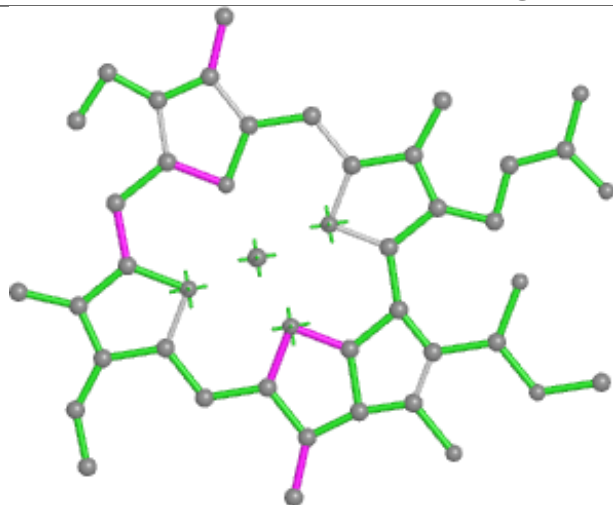
## Ligand CLA 6 602



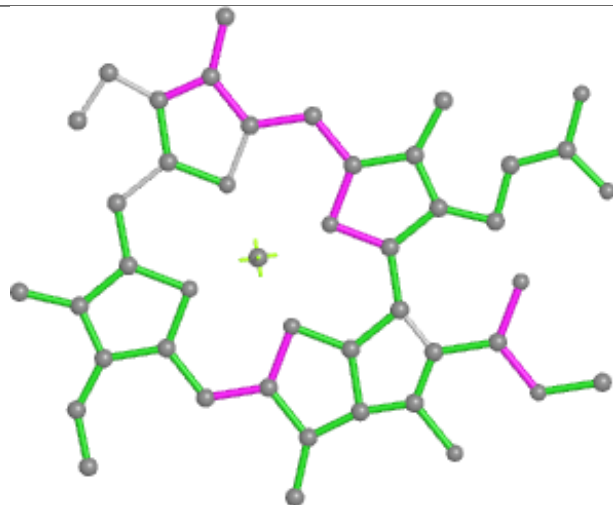
## Ligand CLA 6 613



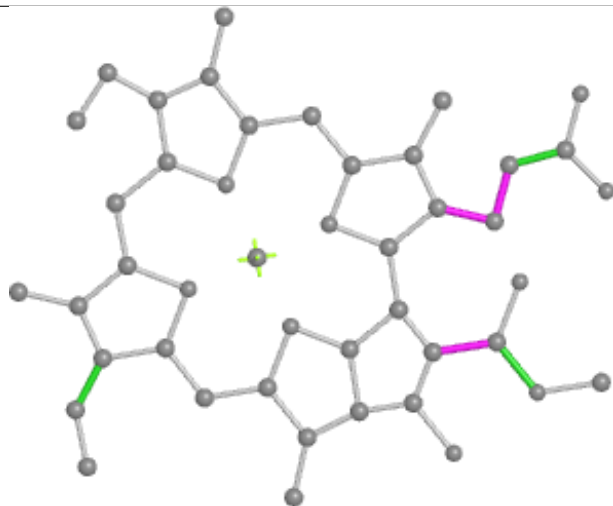
## Ligand CLA A 820



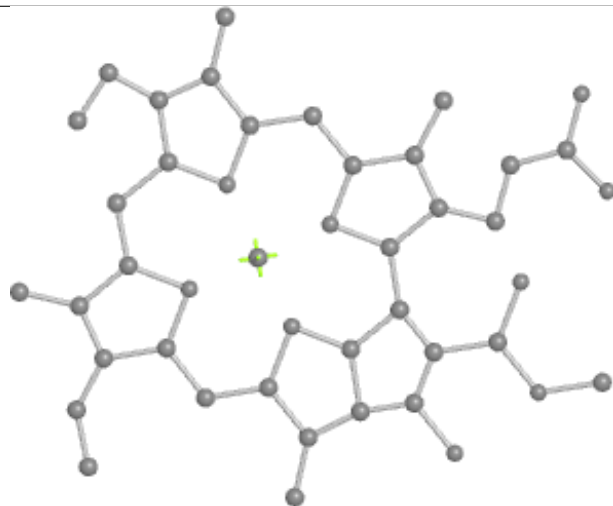
Bond lengths



Bond angles

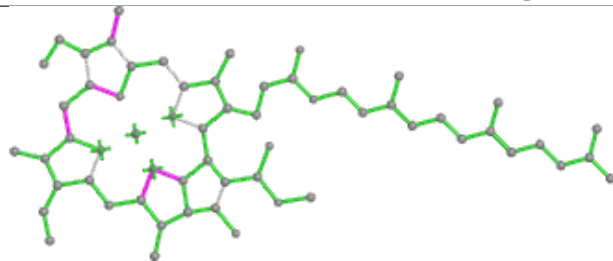


Torsions

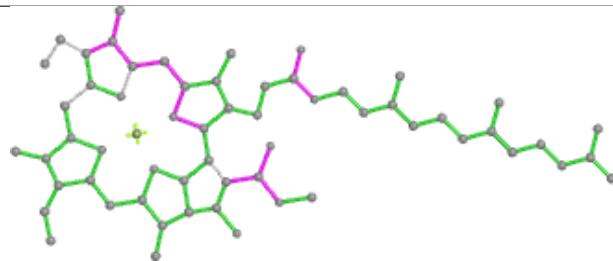


Rings

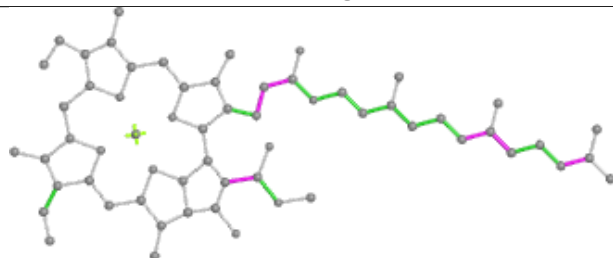
## Ligand CLA 3 602



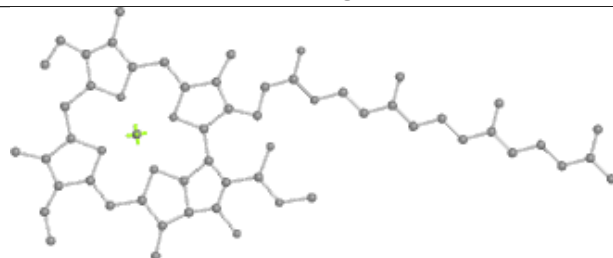
Bond lengths



Bond angles

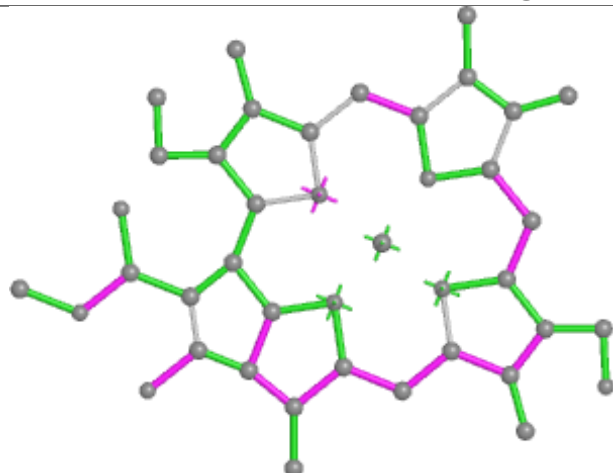


Torsions

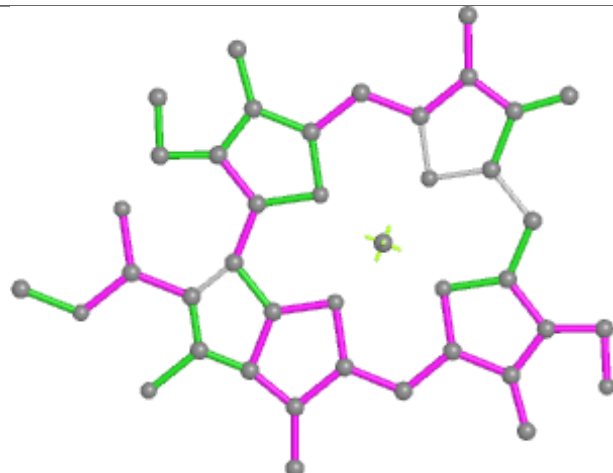


Rings

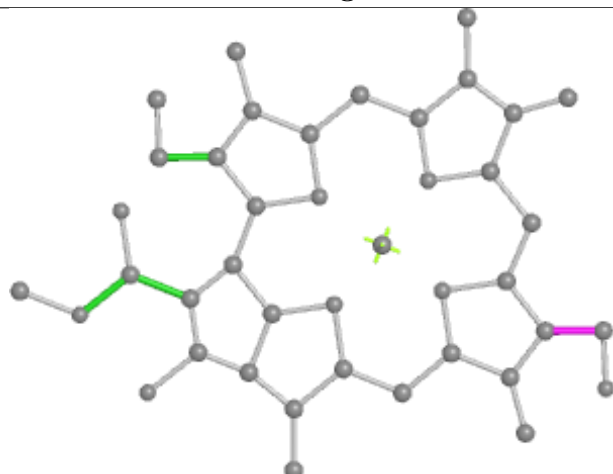
## Ligand CHL 5 606



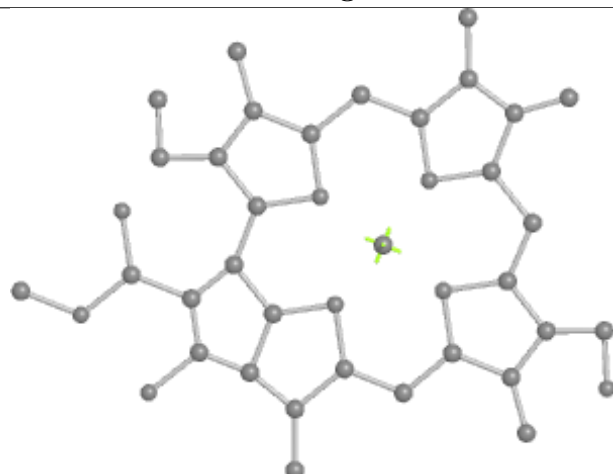
Bond lengths



Bond angles

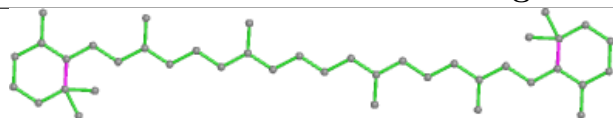


Torsions

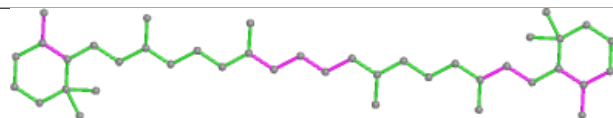


Rings

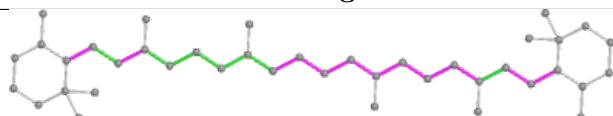
## Ligand BCR B 846



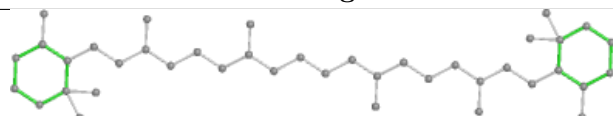
Bond lengths



Bond angles

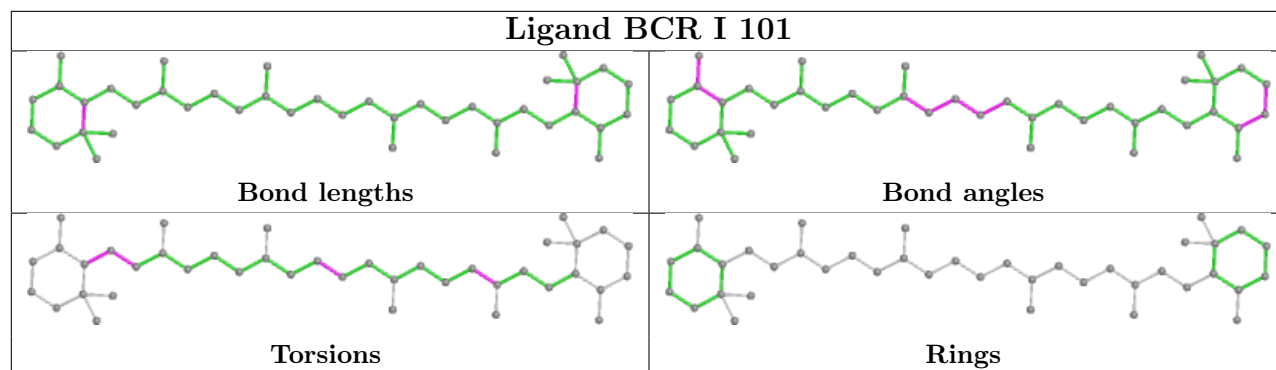


Torsions

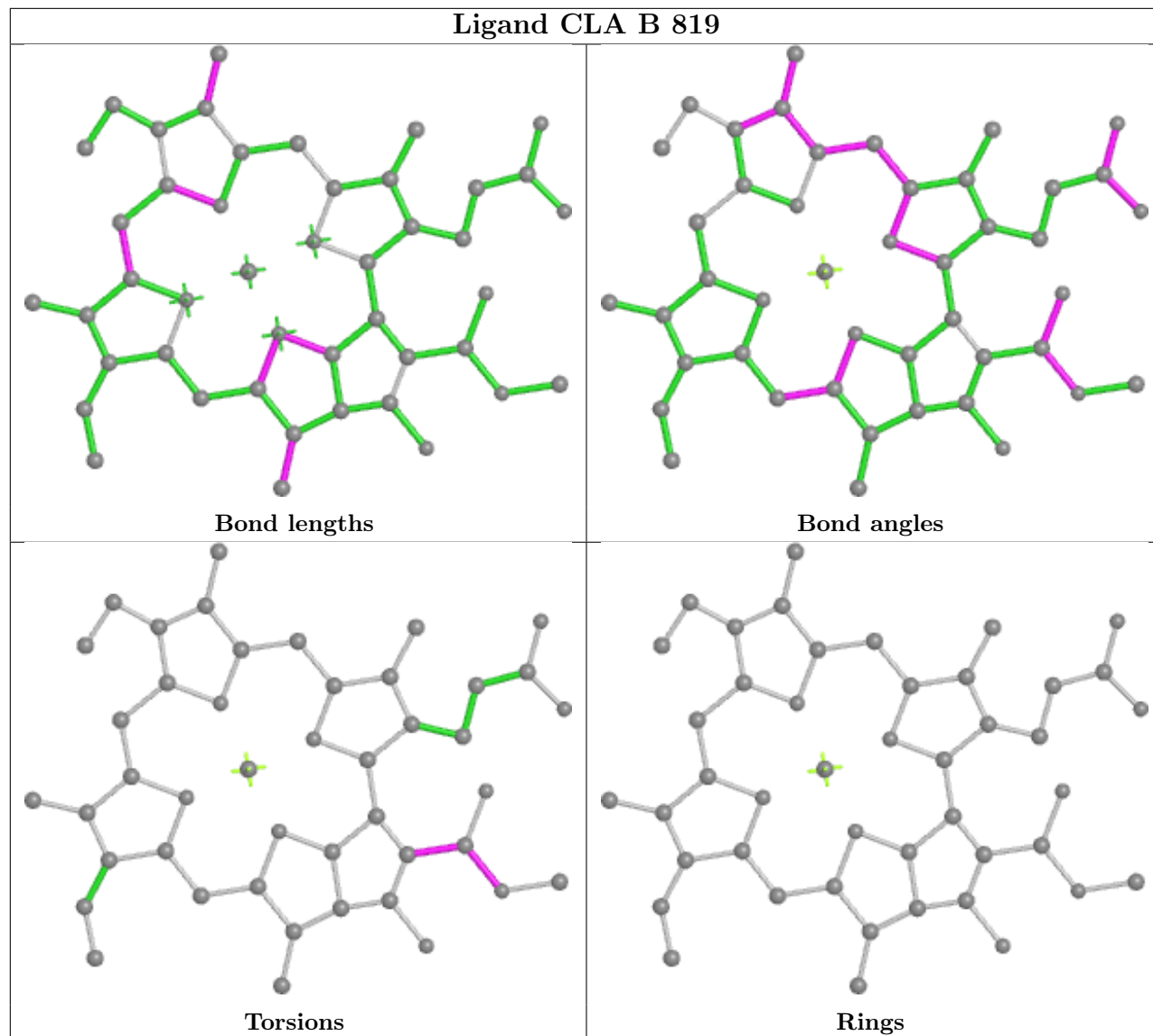


Rings

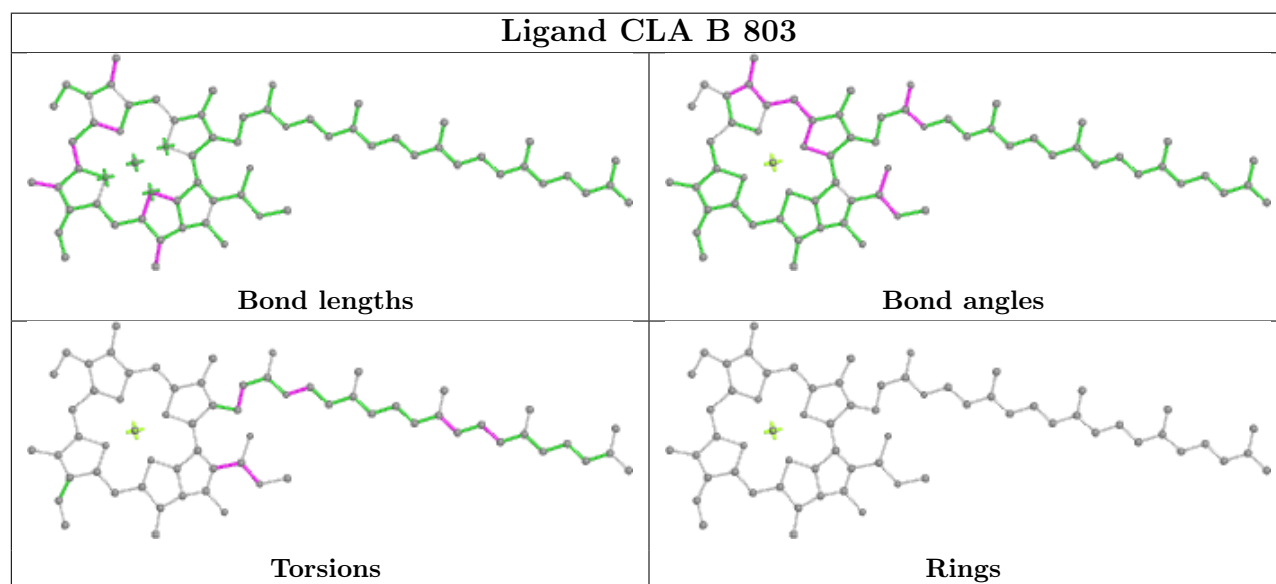
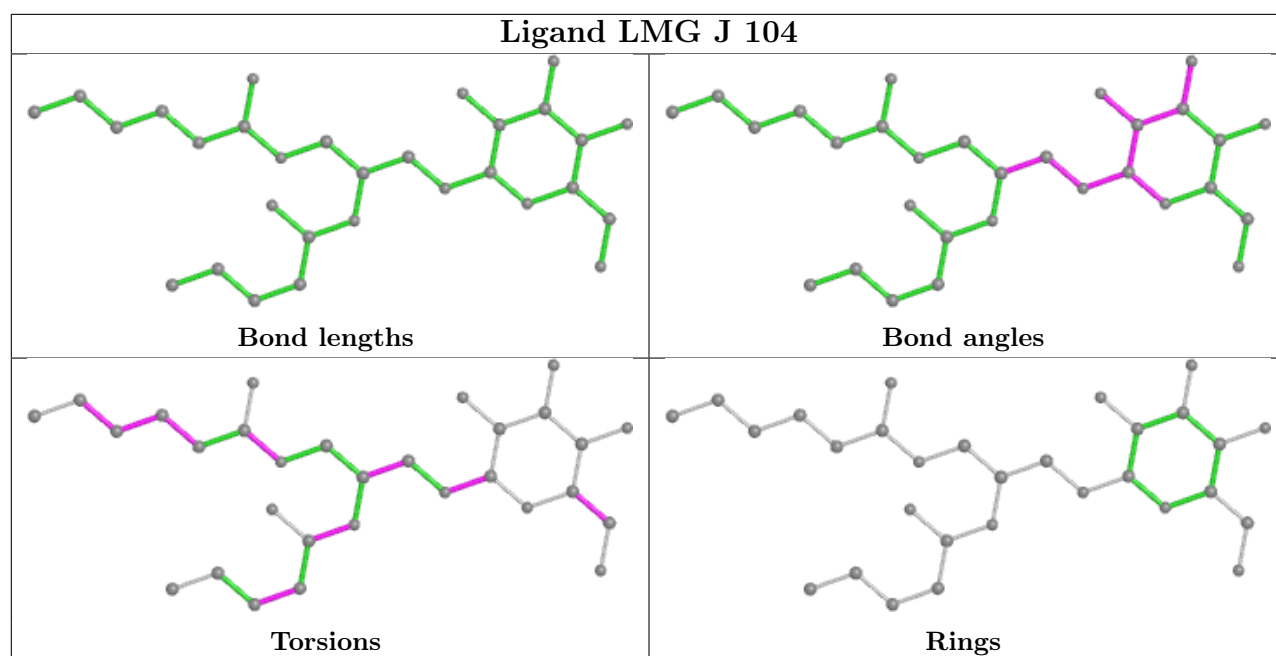
## Ligand BCR I 101

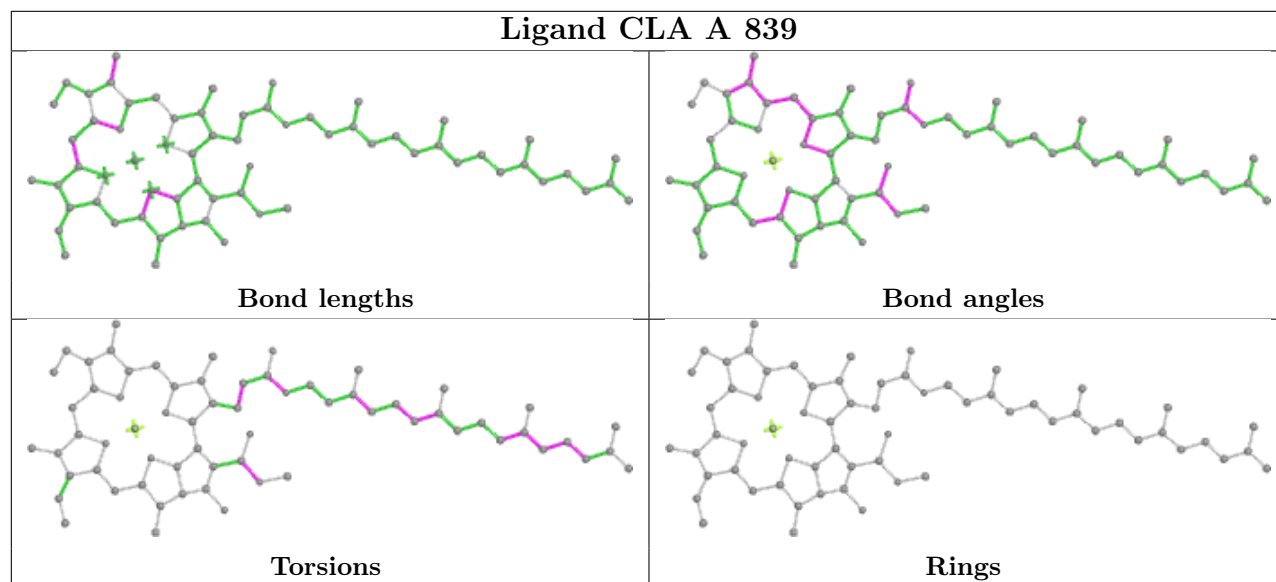
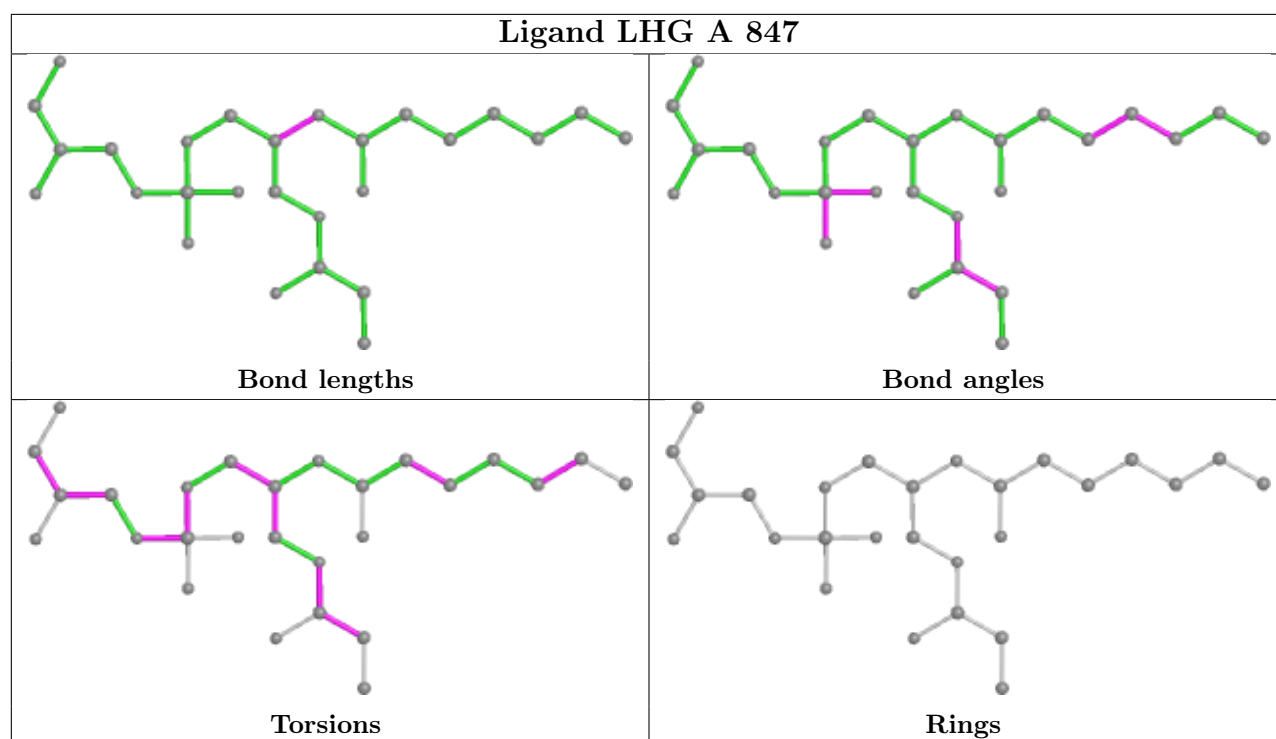


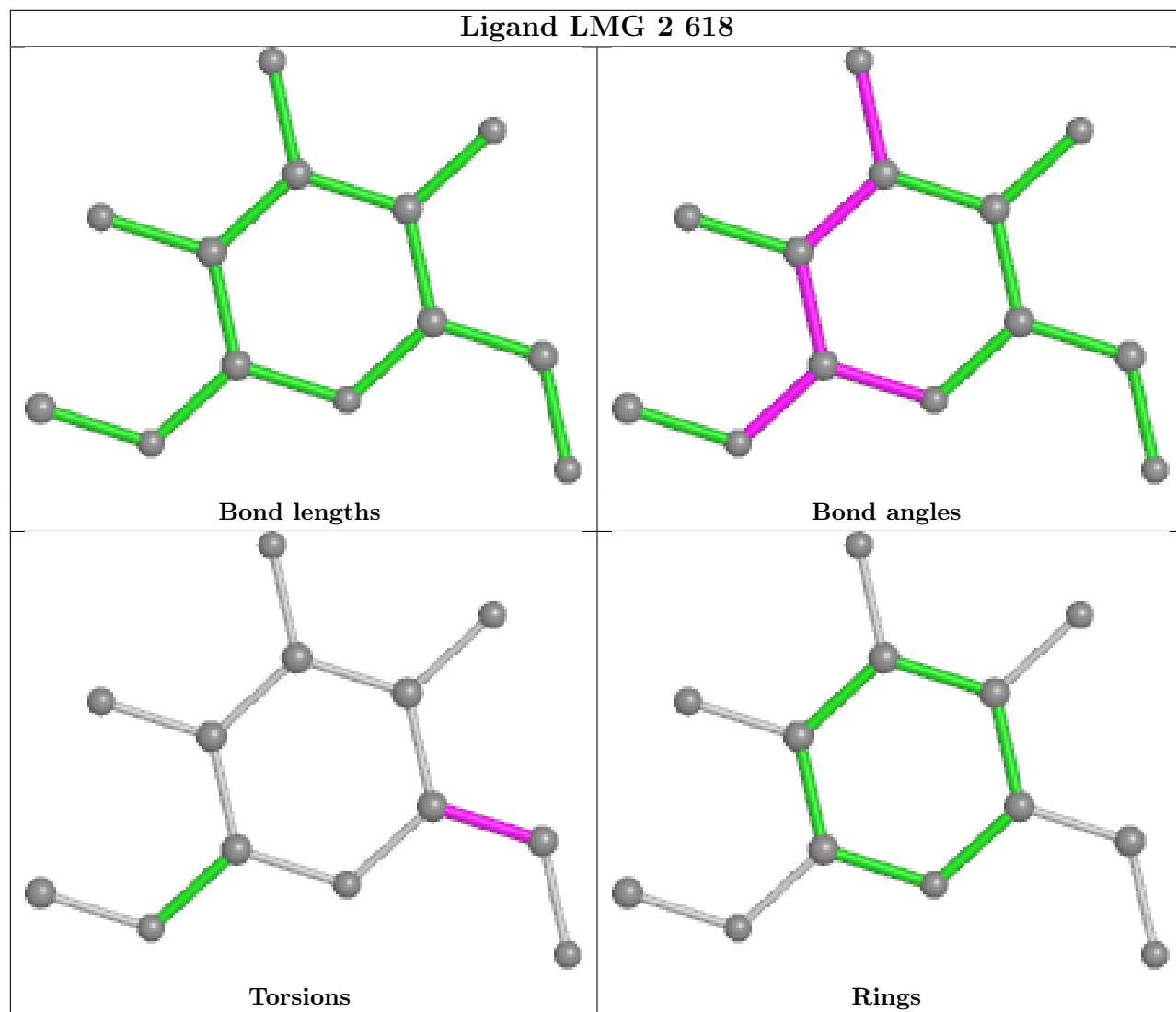
## Ligand CLA B 819

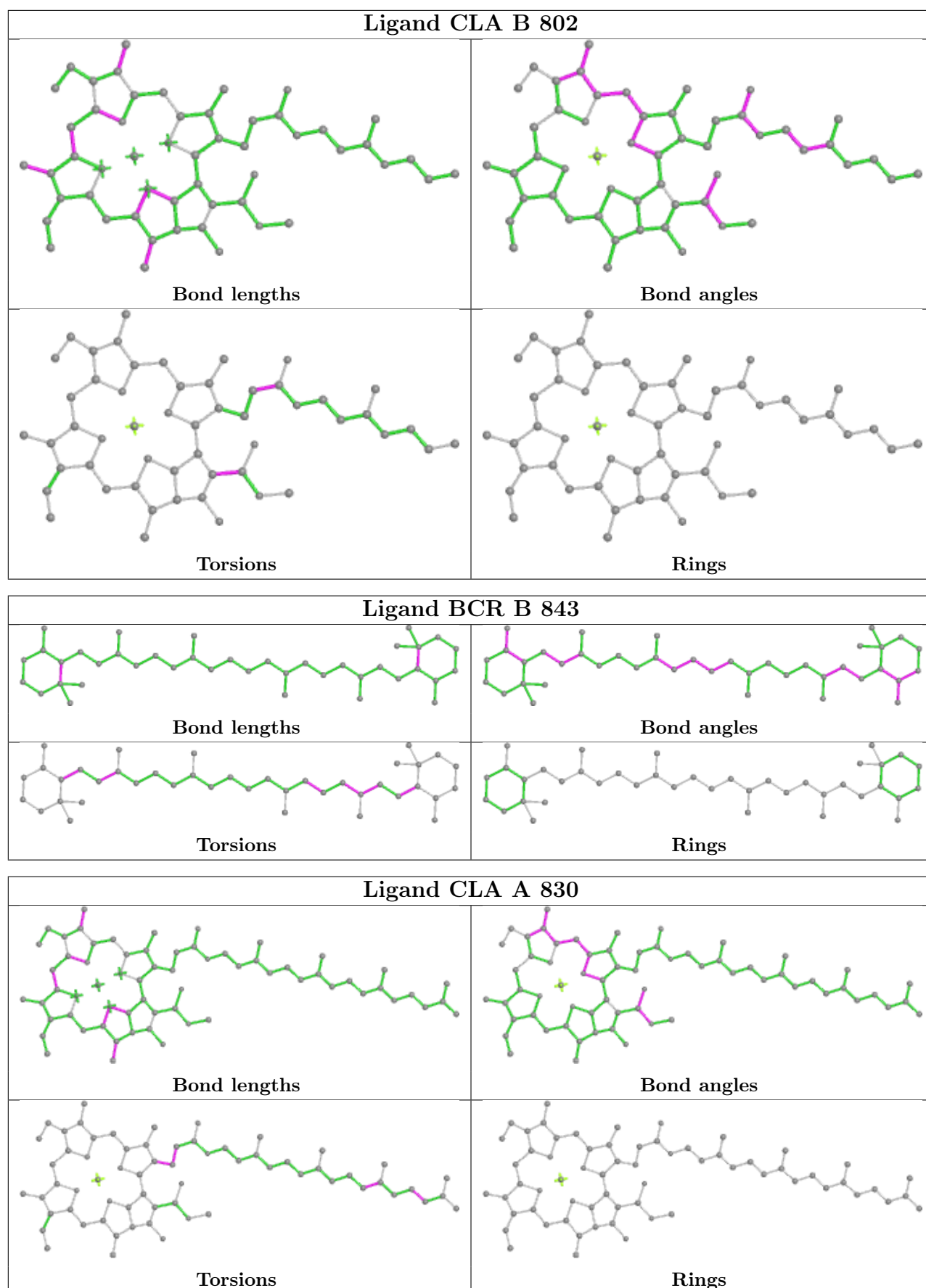




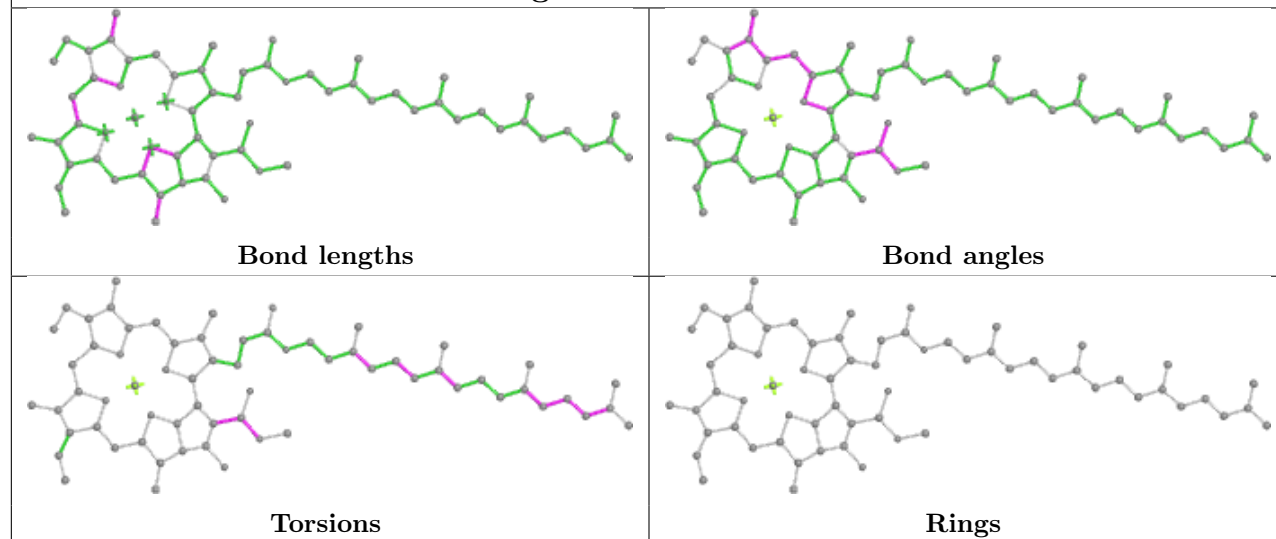




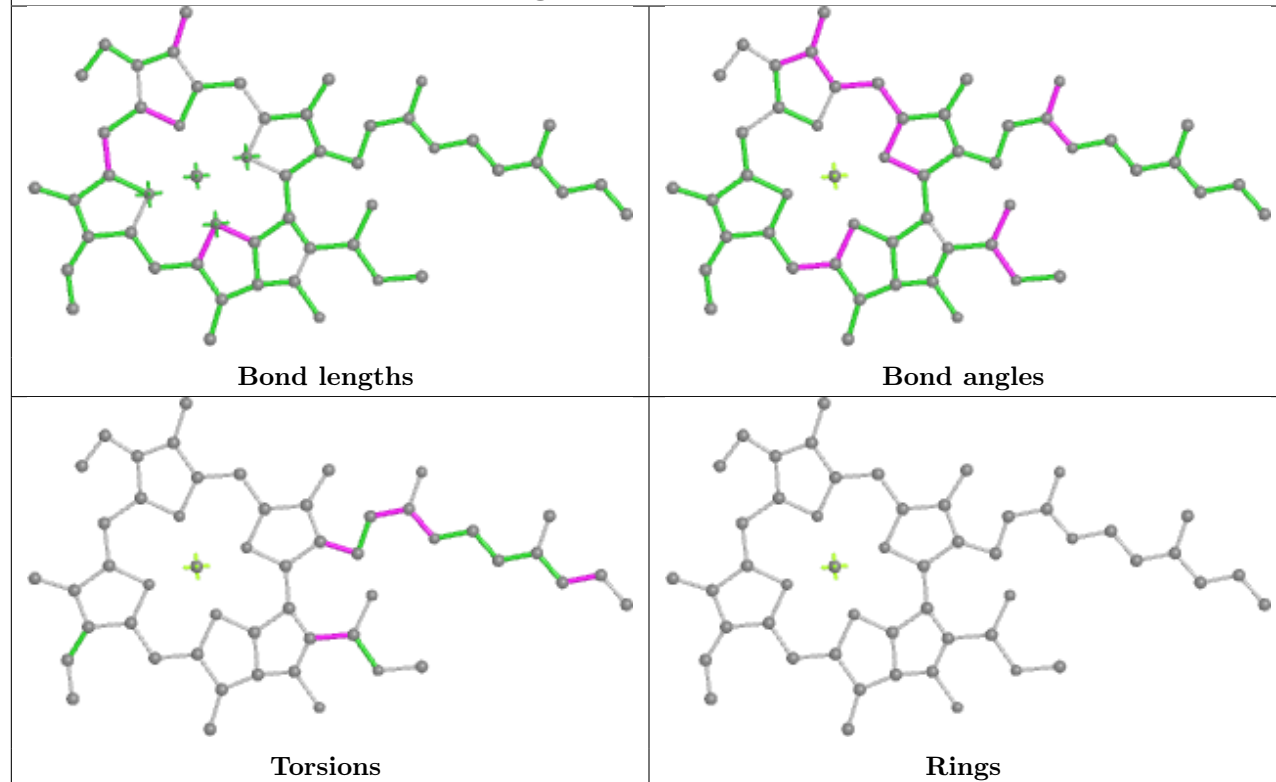


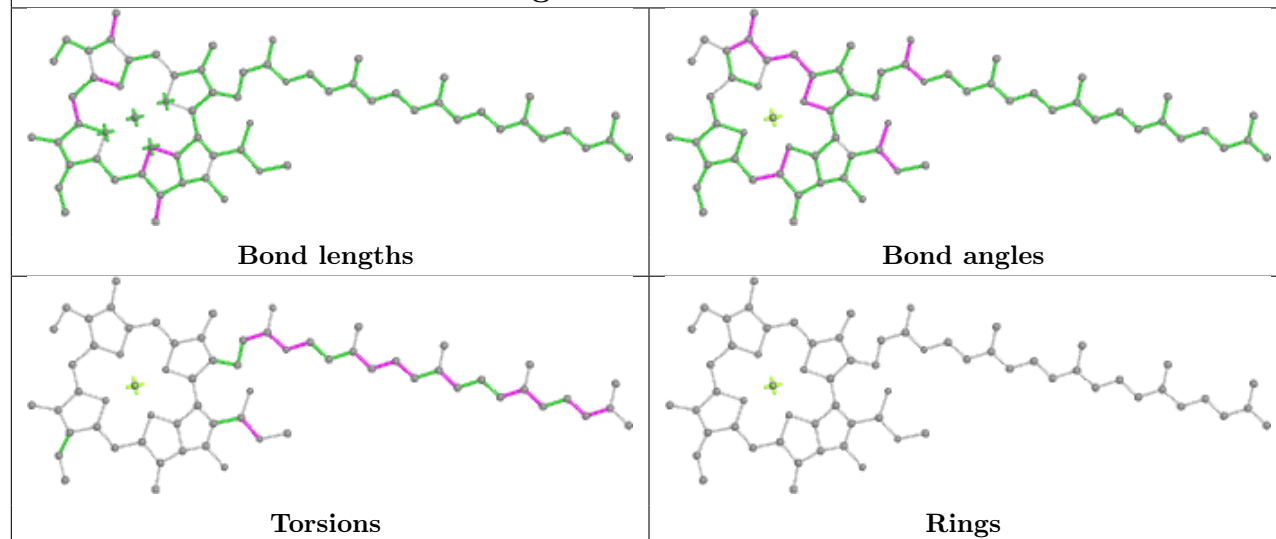
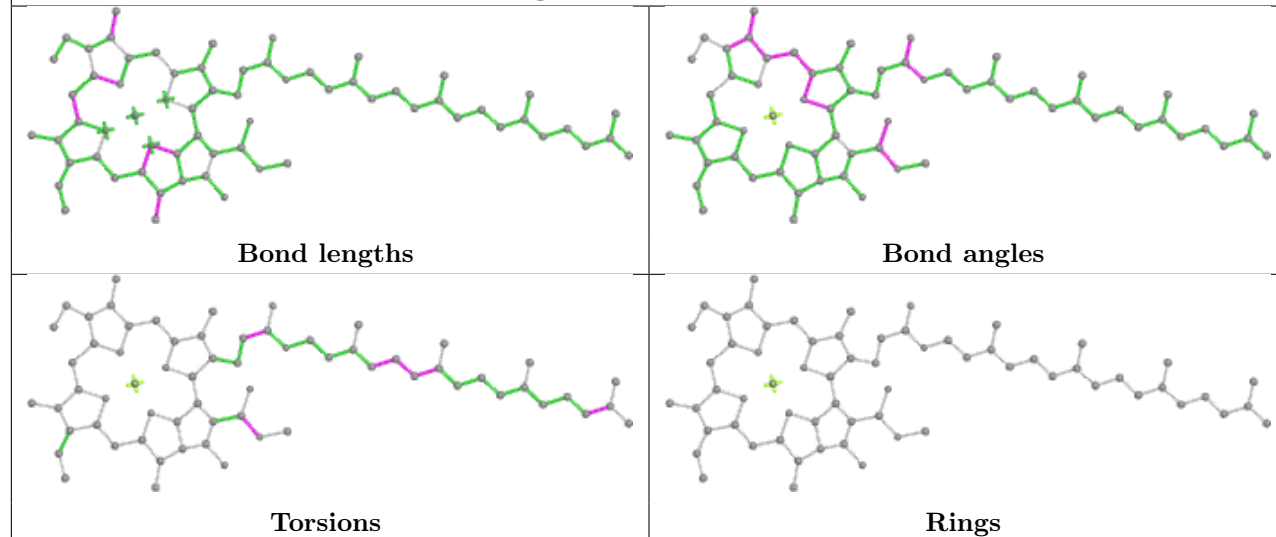


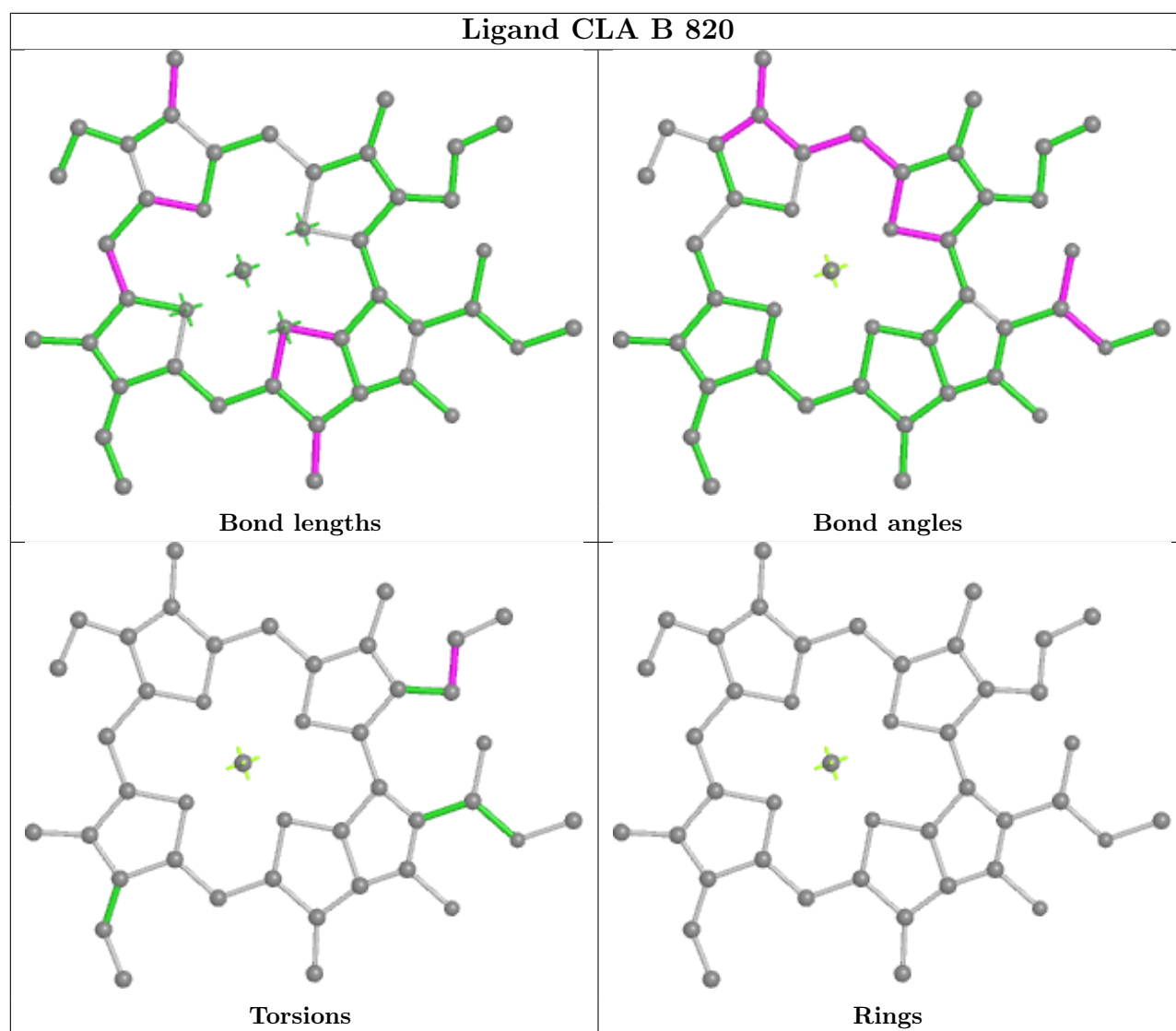
## Ligand CLA A 831

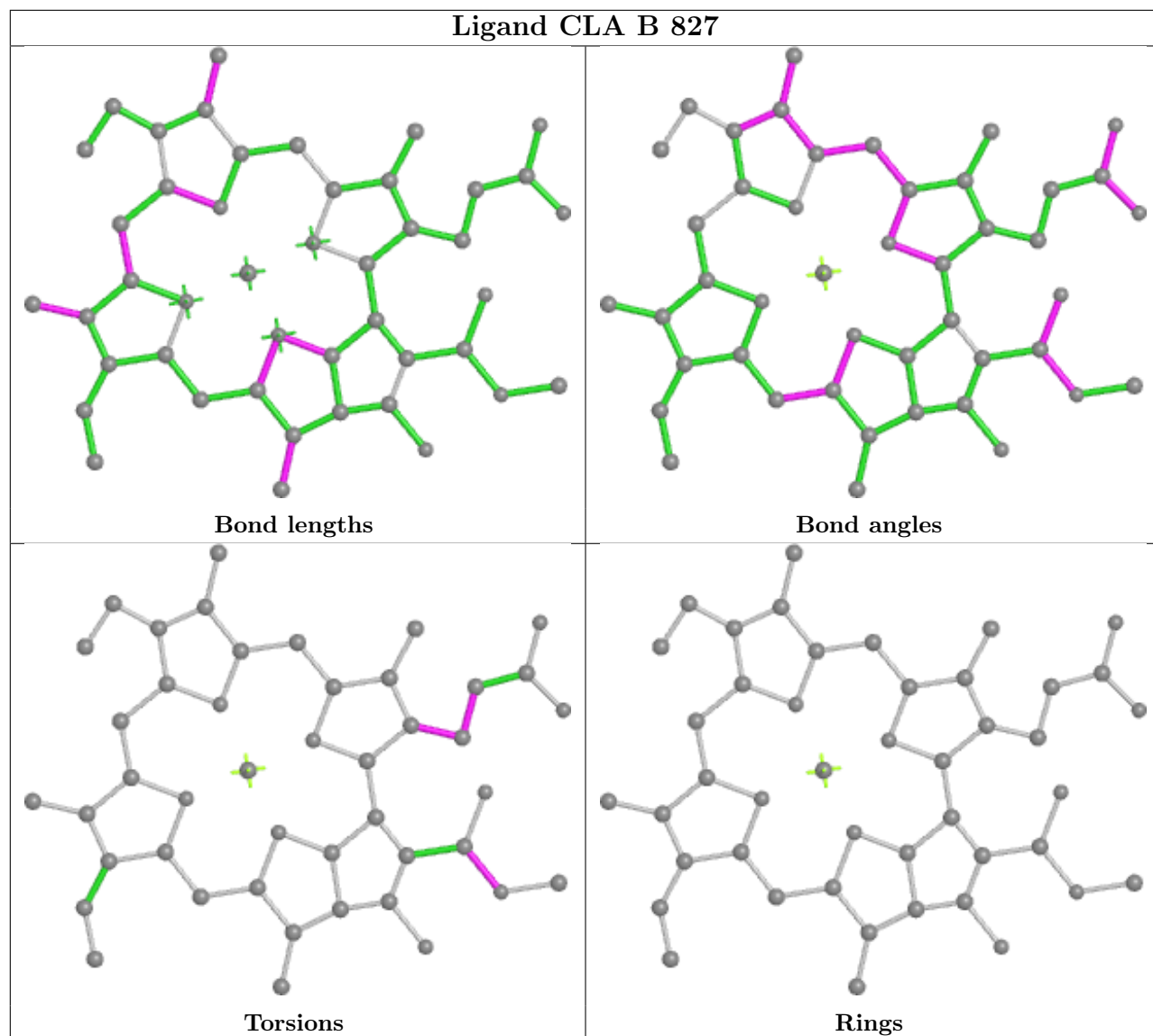


## Ligand CLA A 845

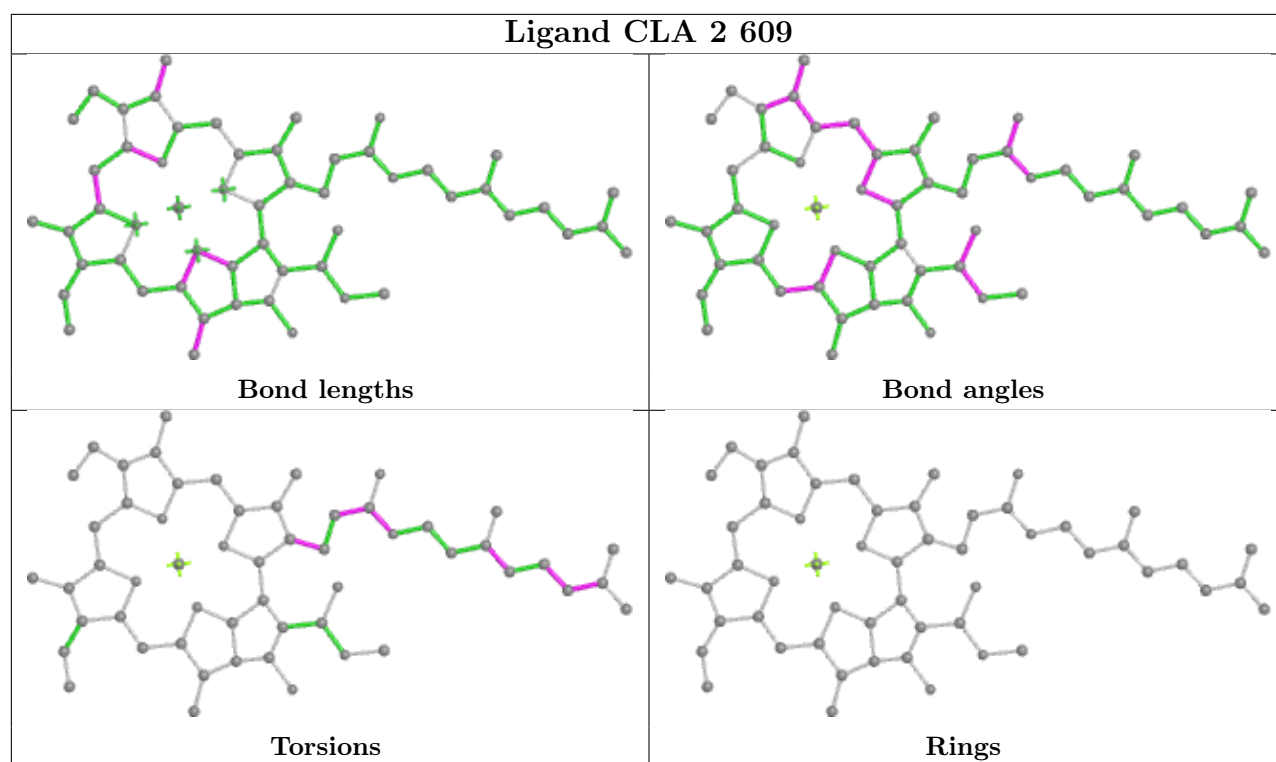


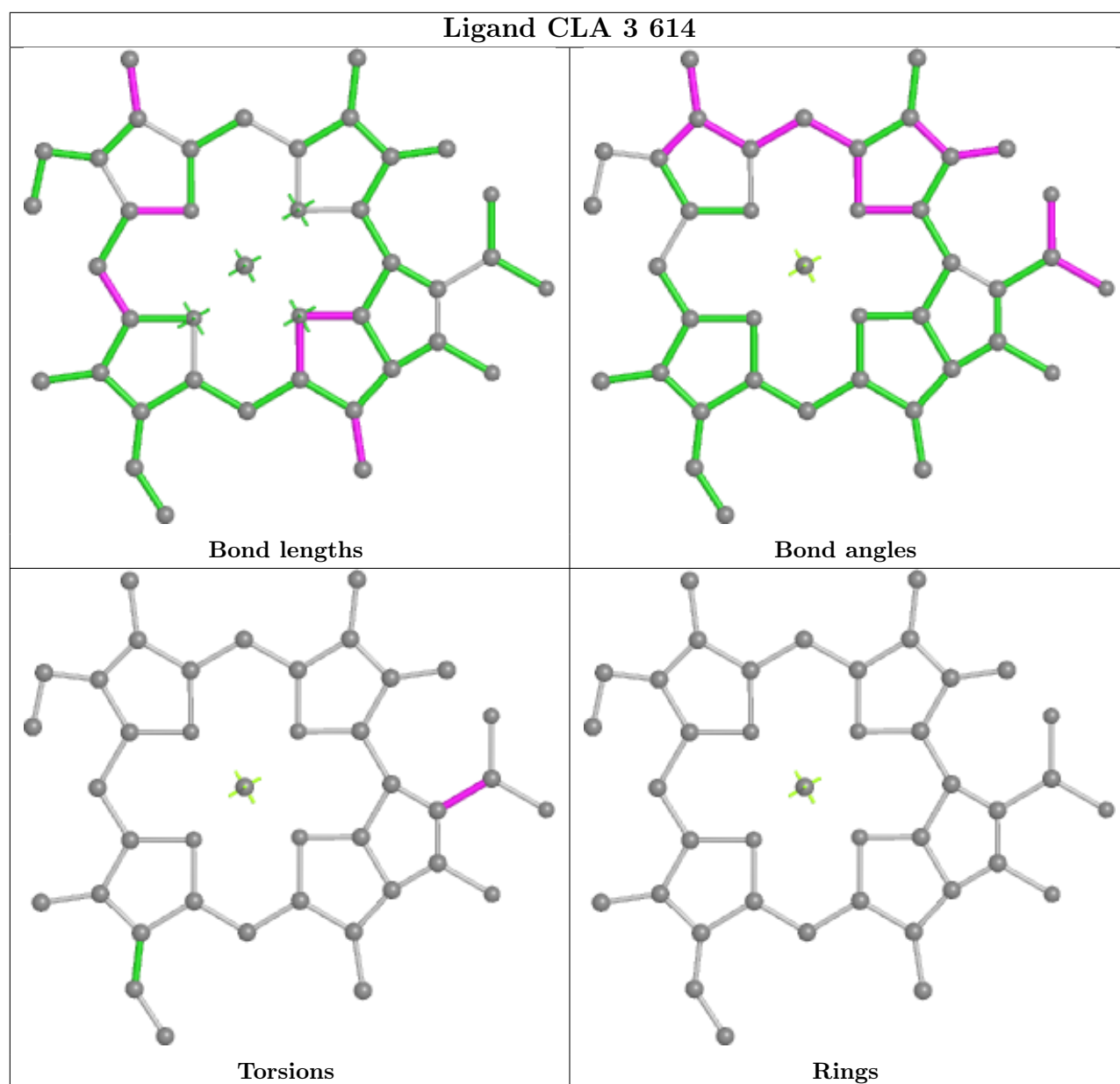
**Ligand CLA B 806****Ligand CLA A 801**



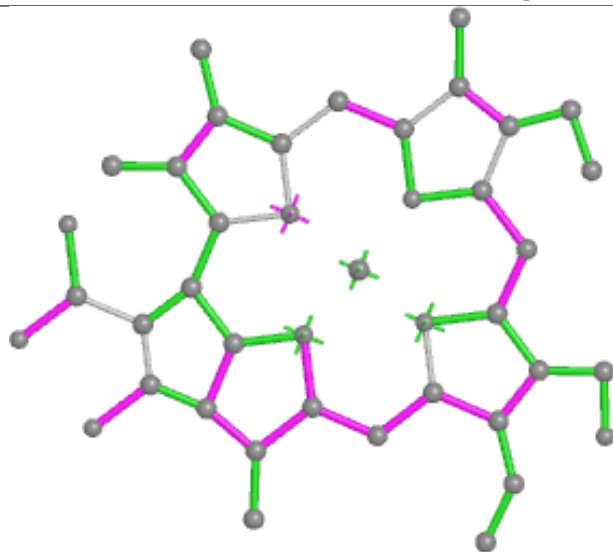




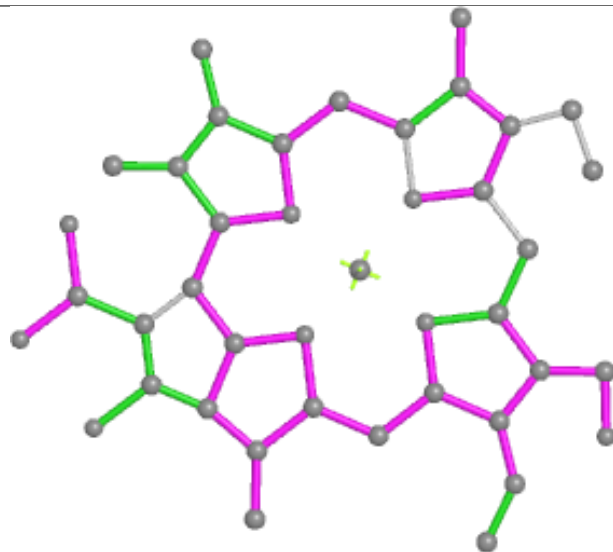




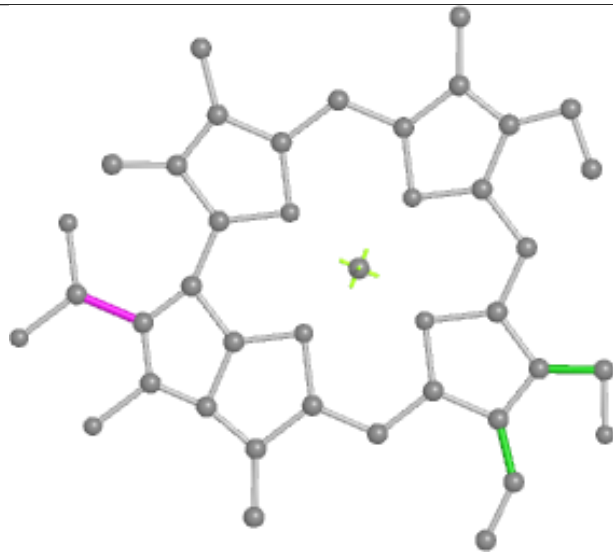
## Ligand CHL 6 607



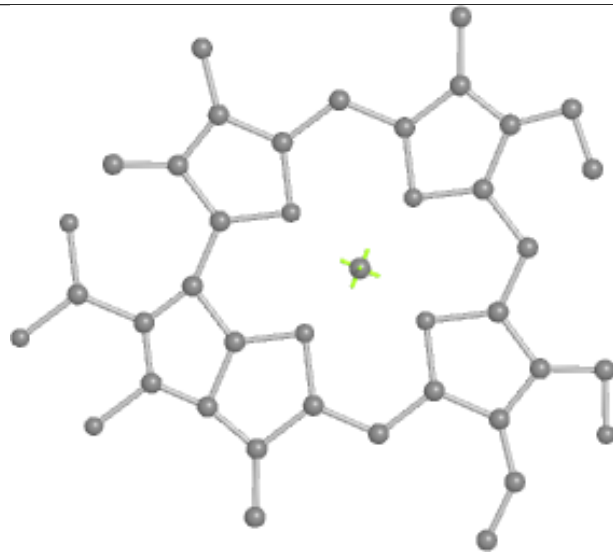
Bond lengths



Bond angles

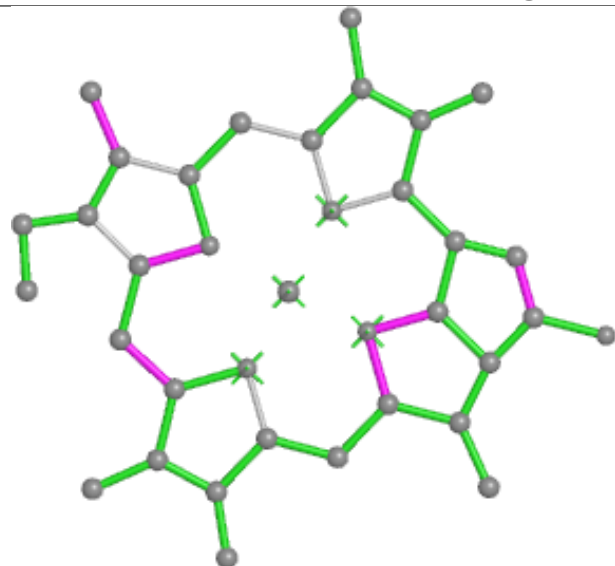


Torsions

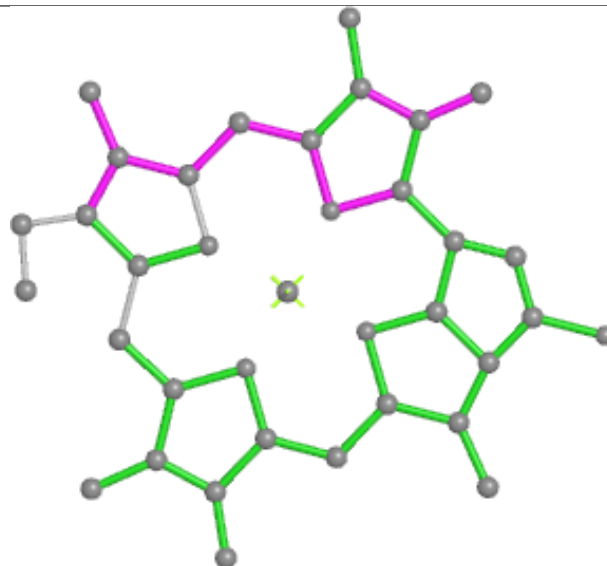


Rings

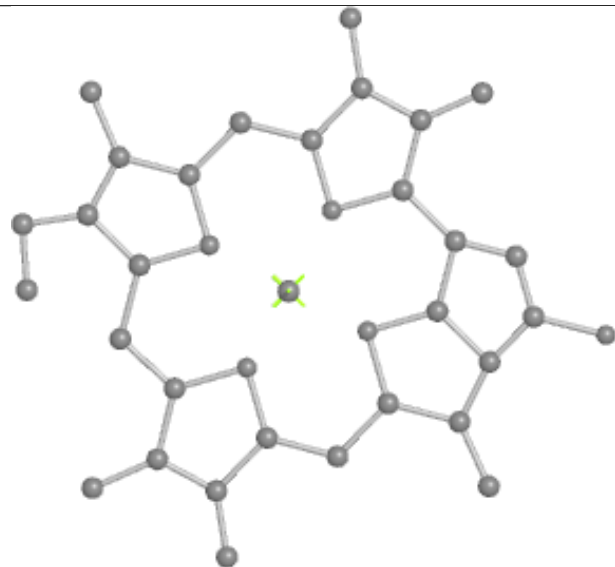
## Ligand CLA 3 615



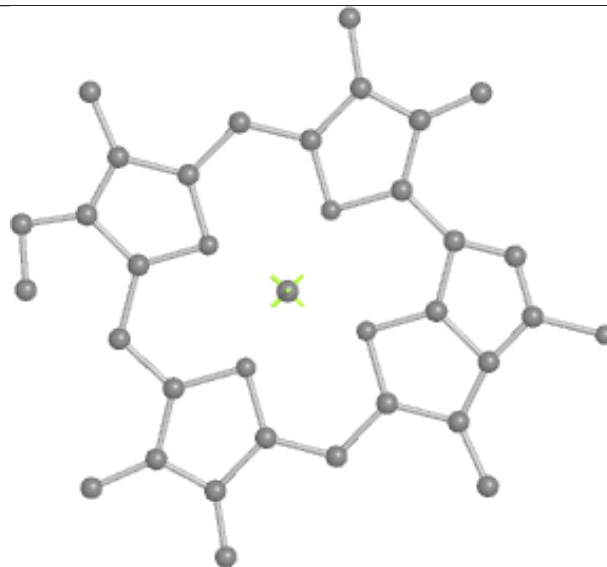
Bond lengths



Bond angles

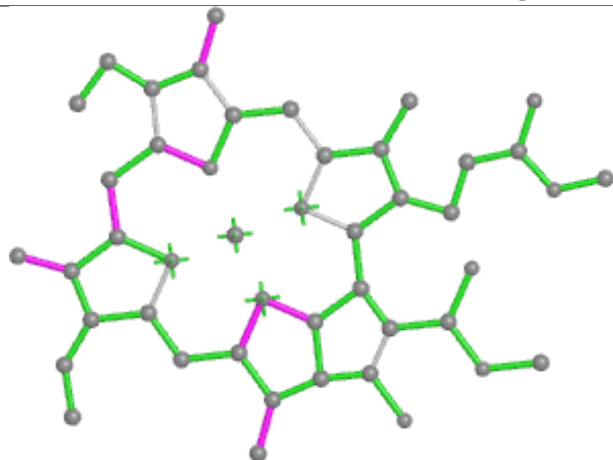


Torsions

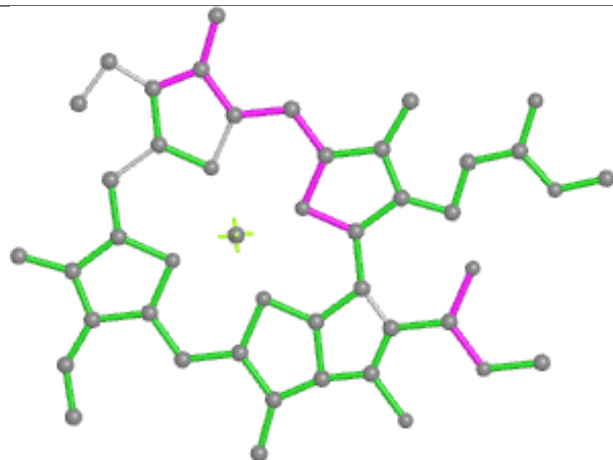


Rings

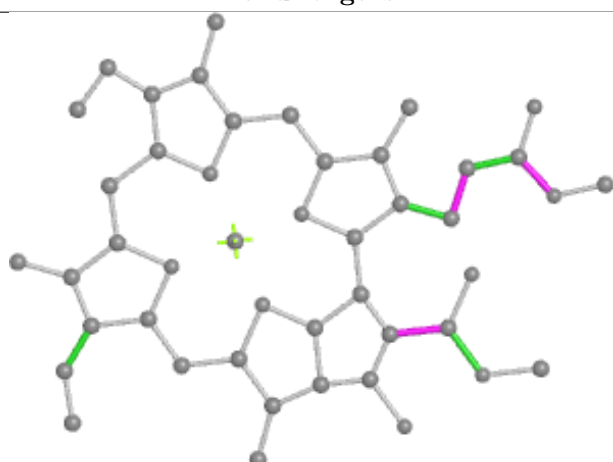
## Ligand CLA A 828



Bond lengths



Bond angles

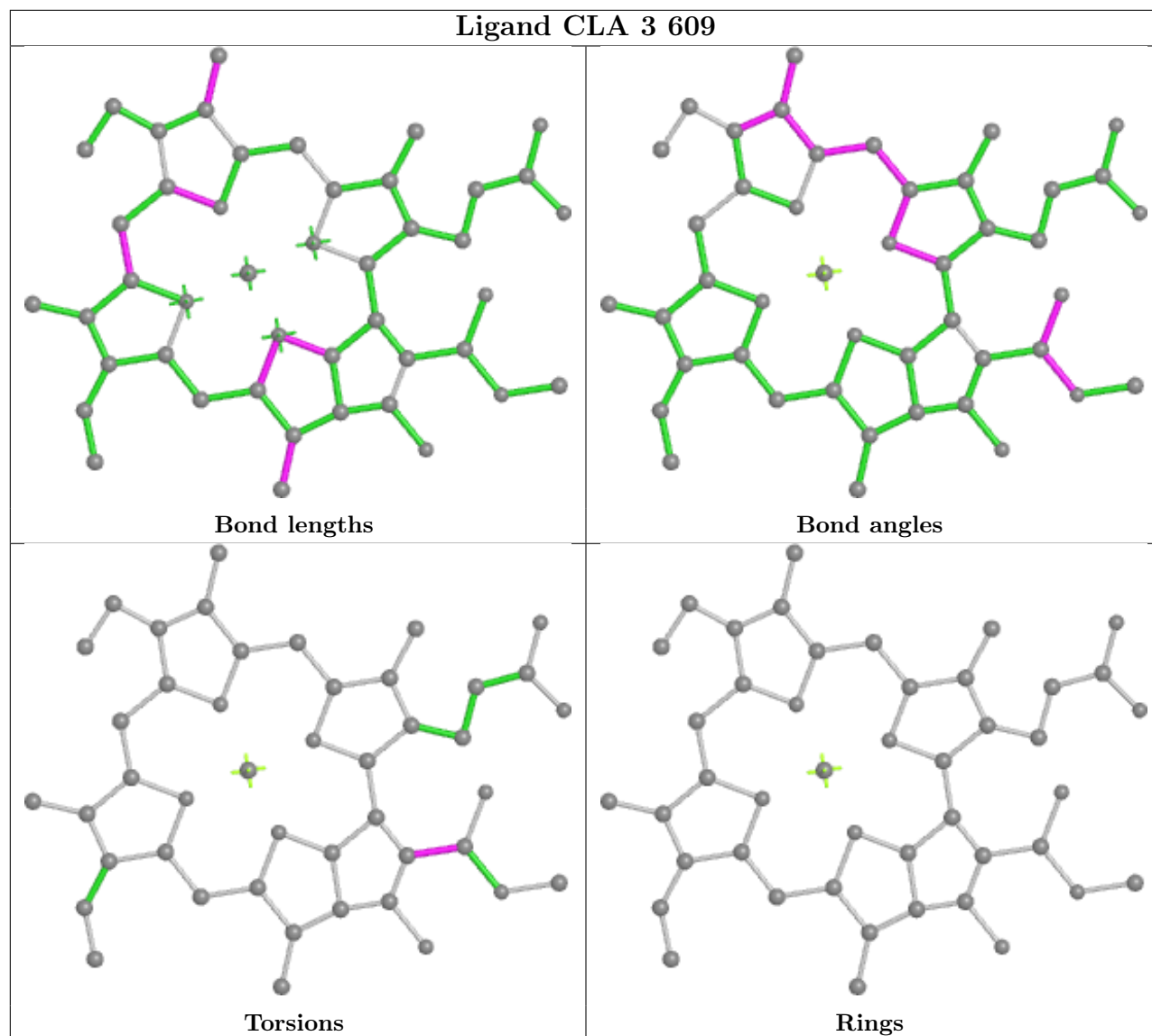


Torsions

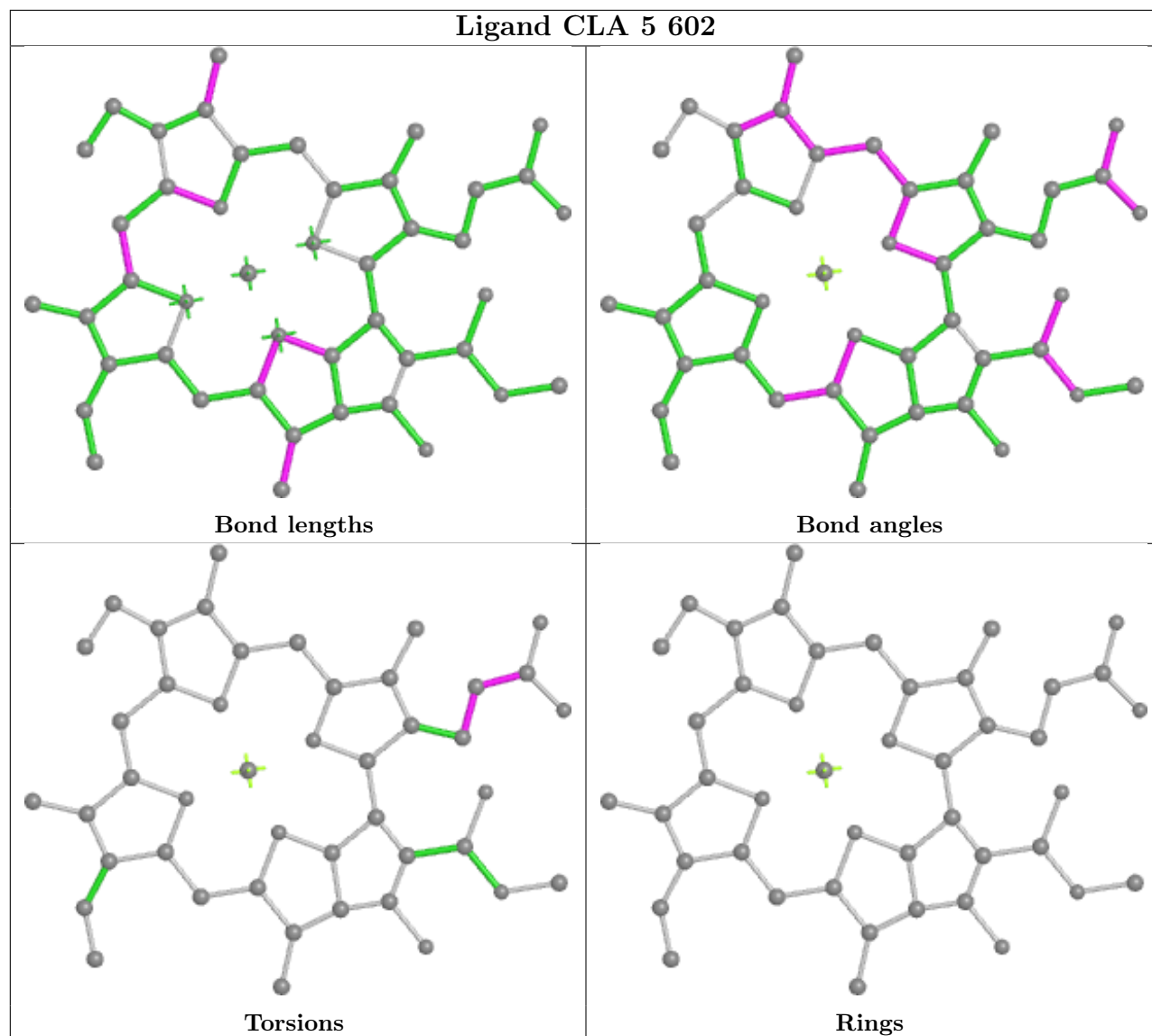


Rings

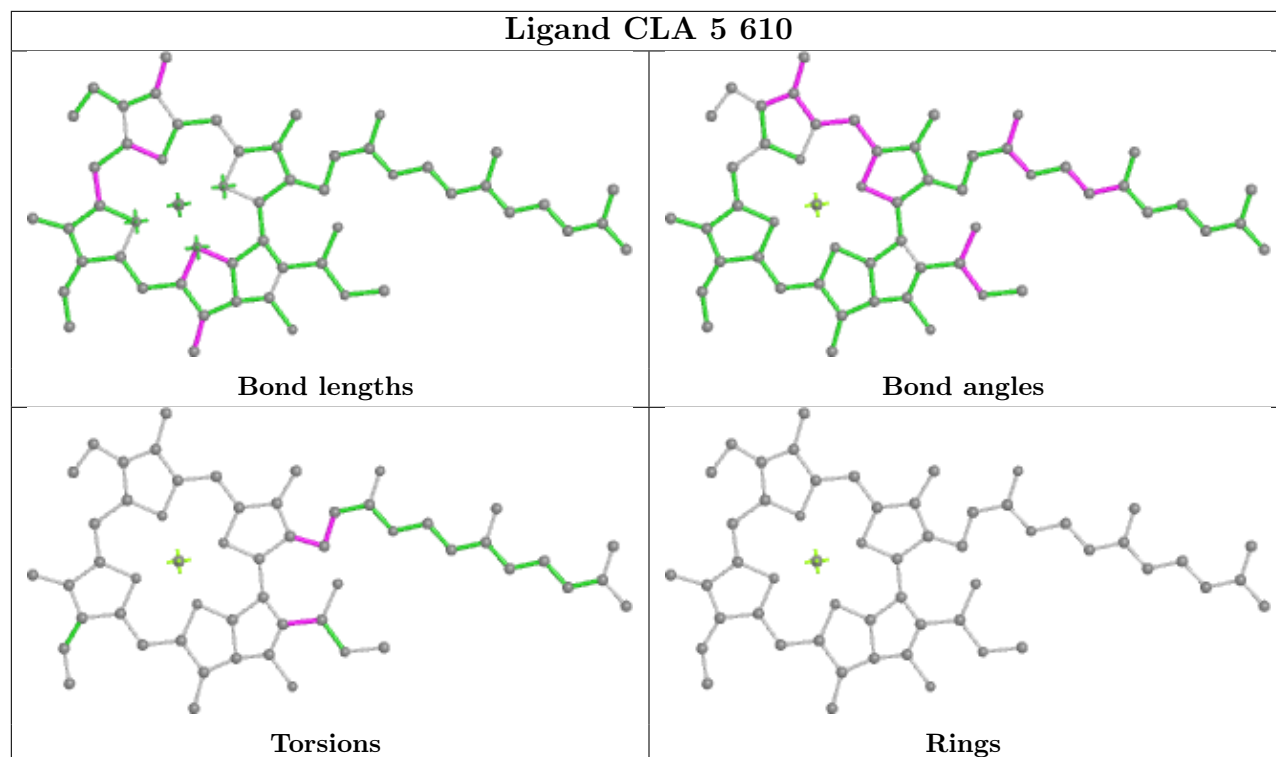
## Ligand CLA 3 609



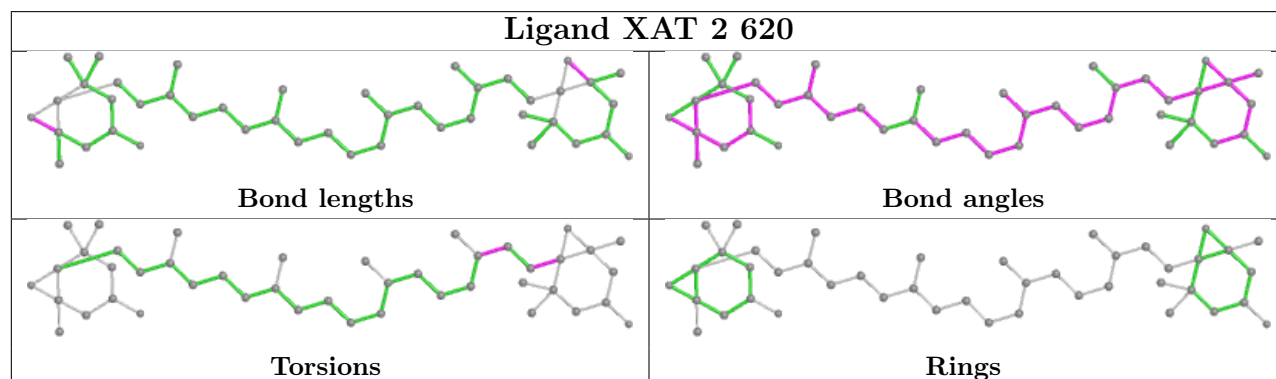
## Ligand CLA 5 602



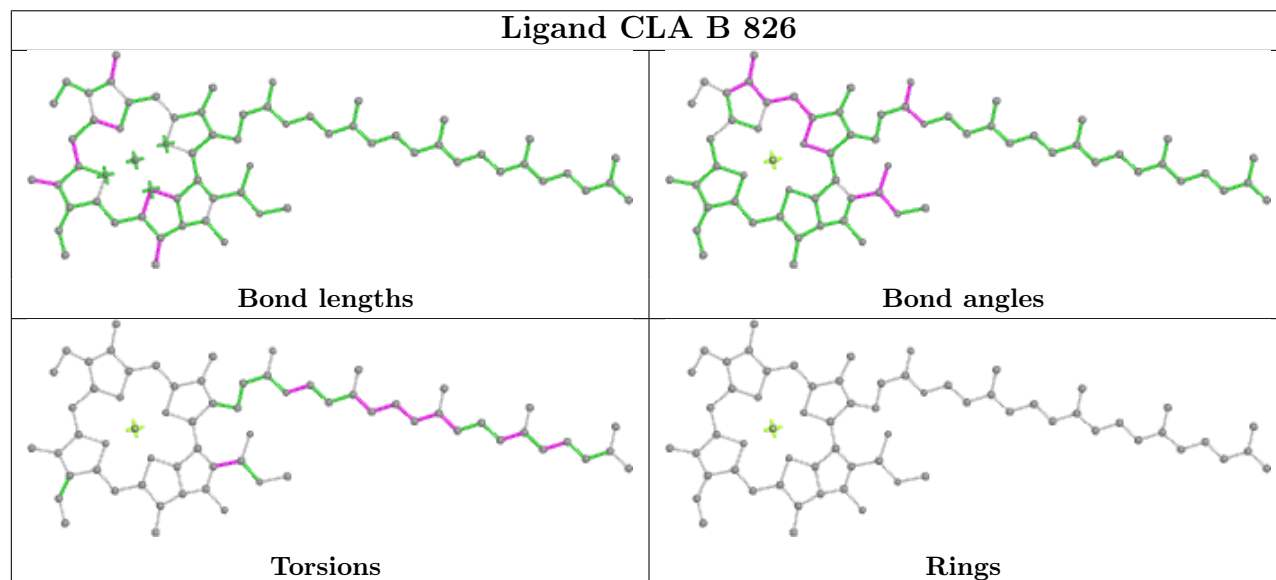
## Ligand CLA 5 610



## Ligand XAT 2 620

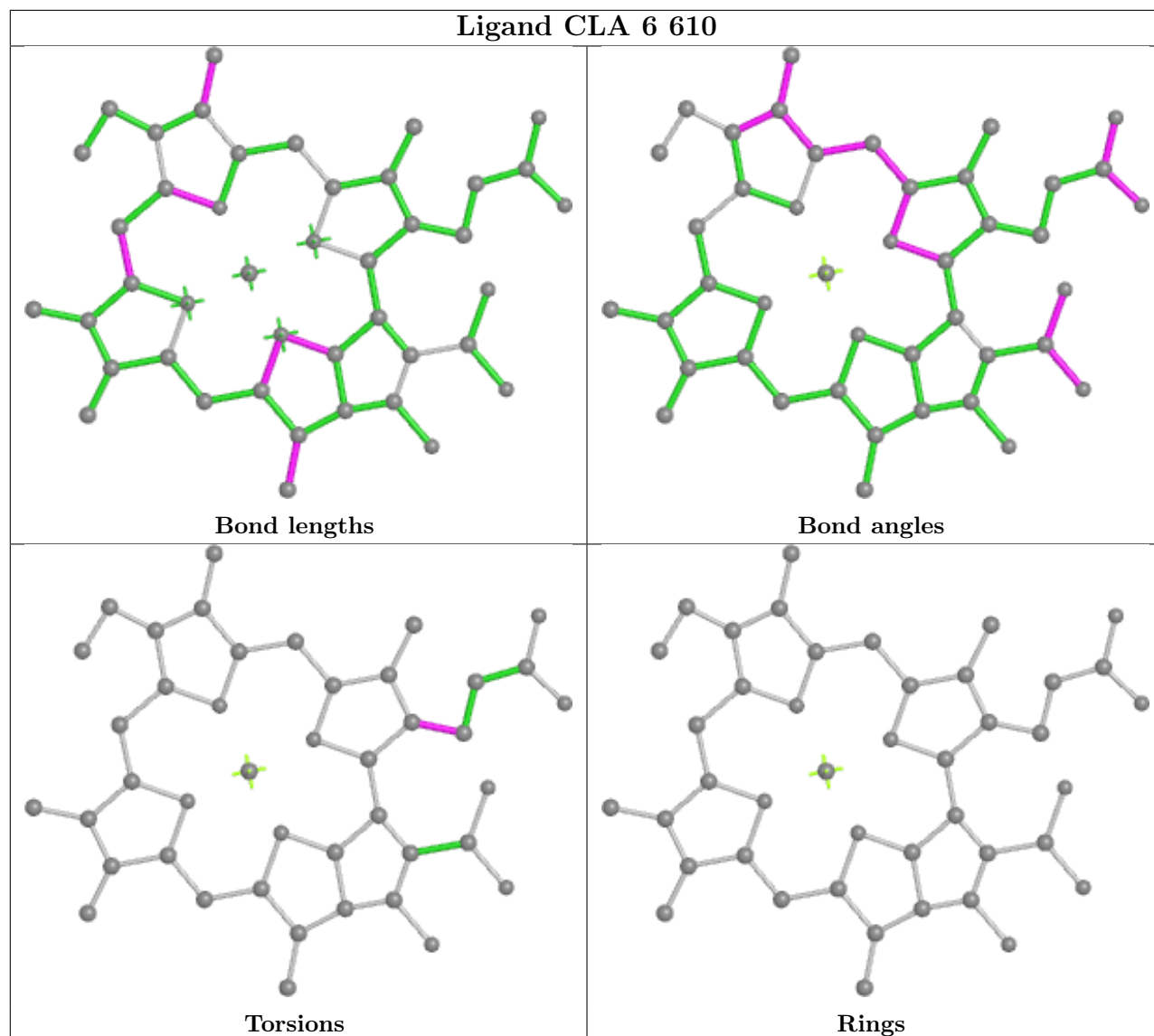


## Ligand CLA B 826

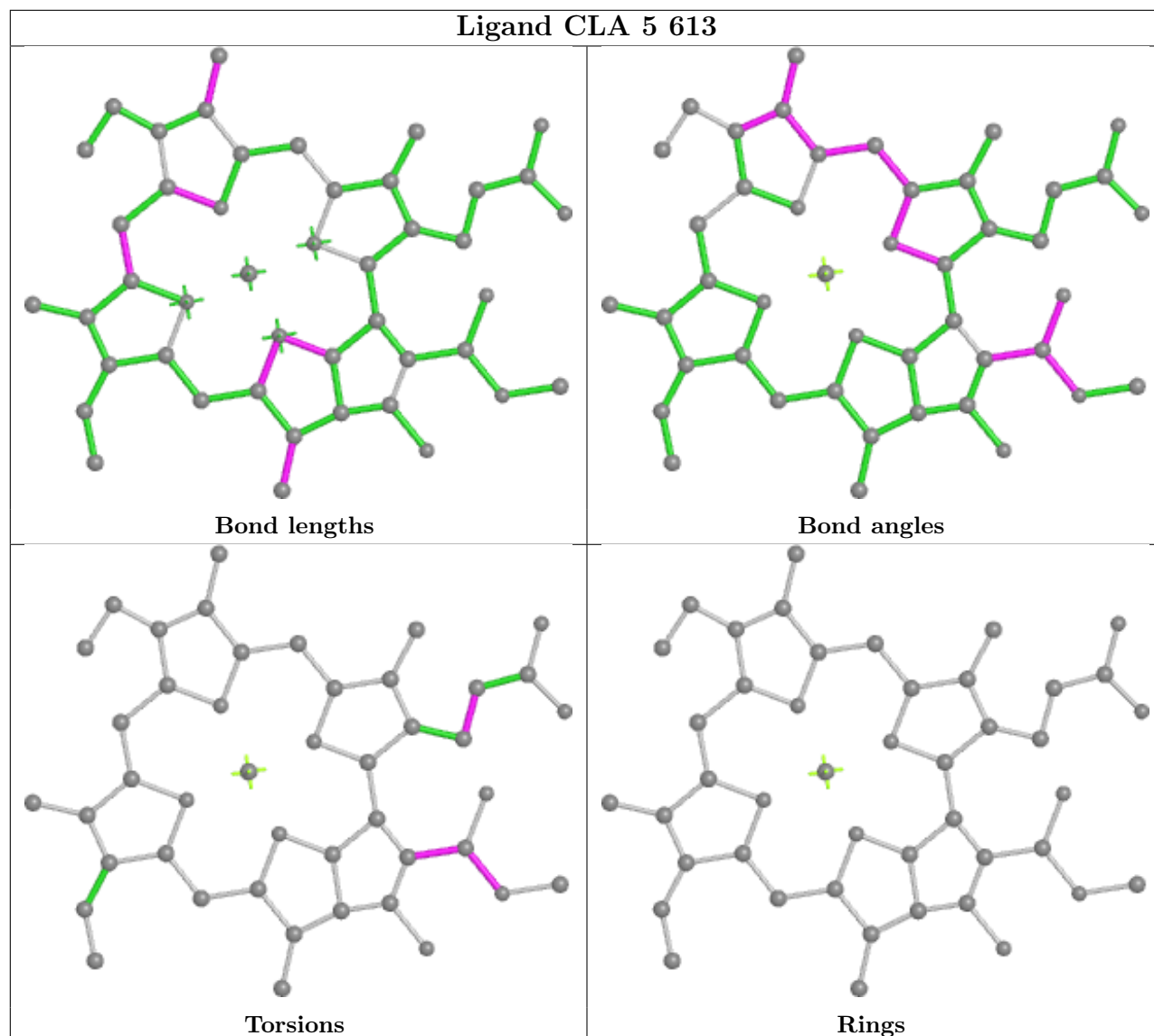




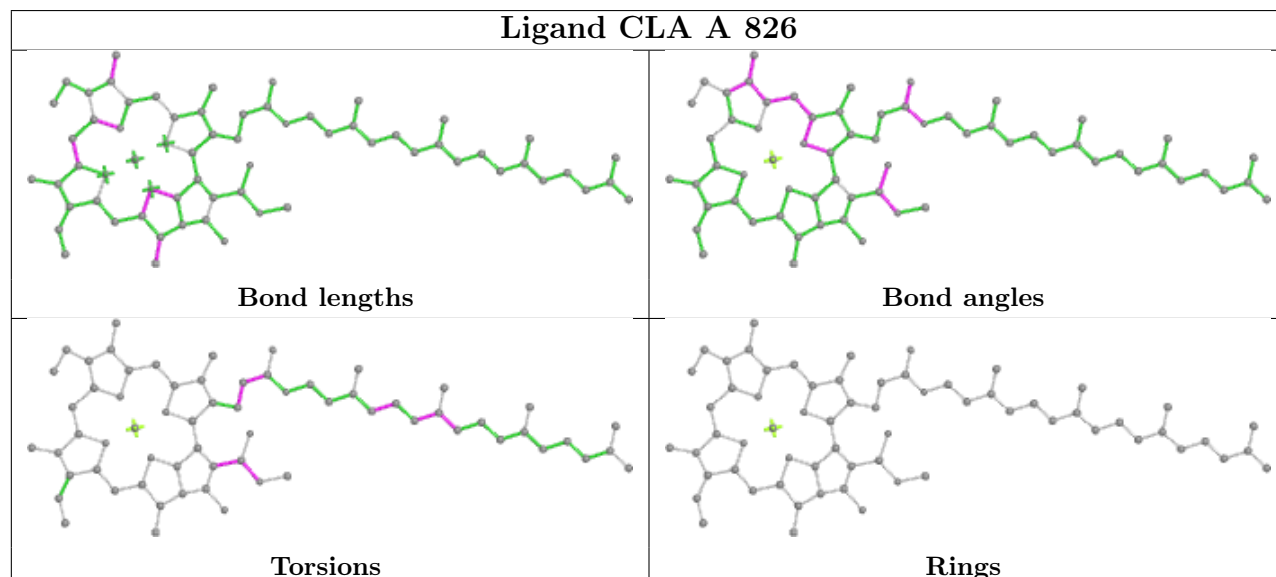
## Ligand CLA 6 610

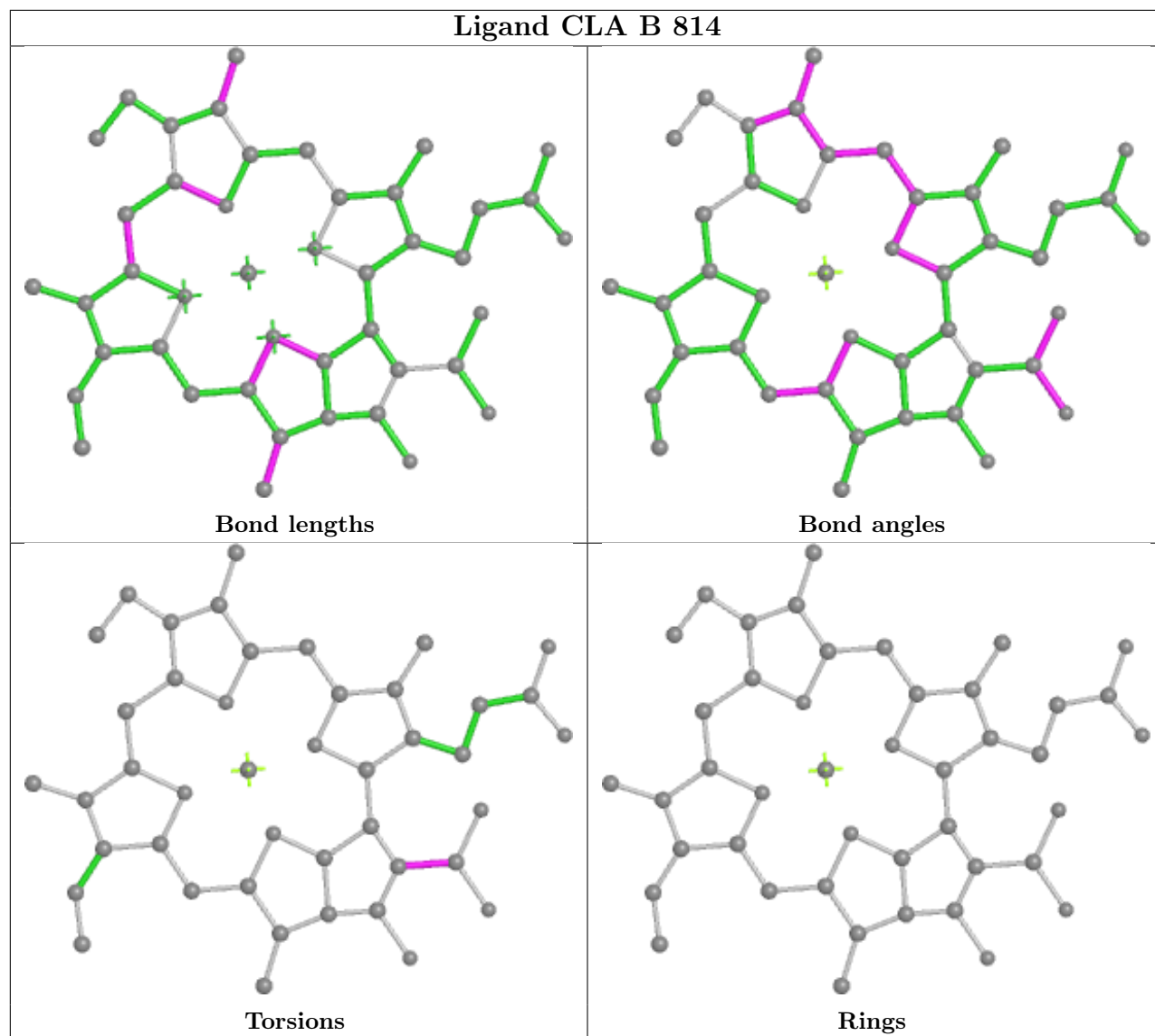
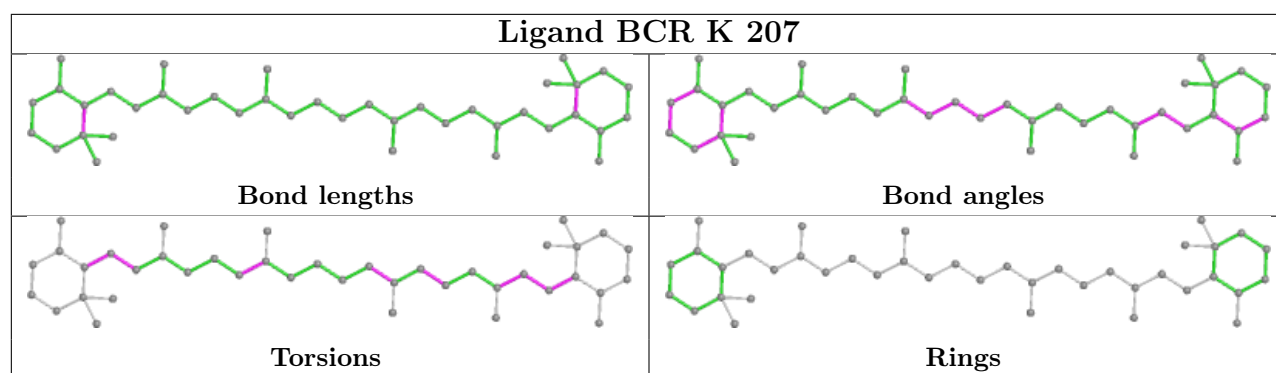


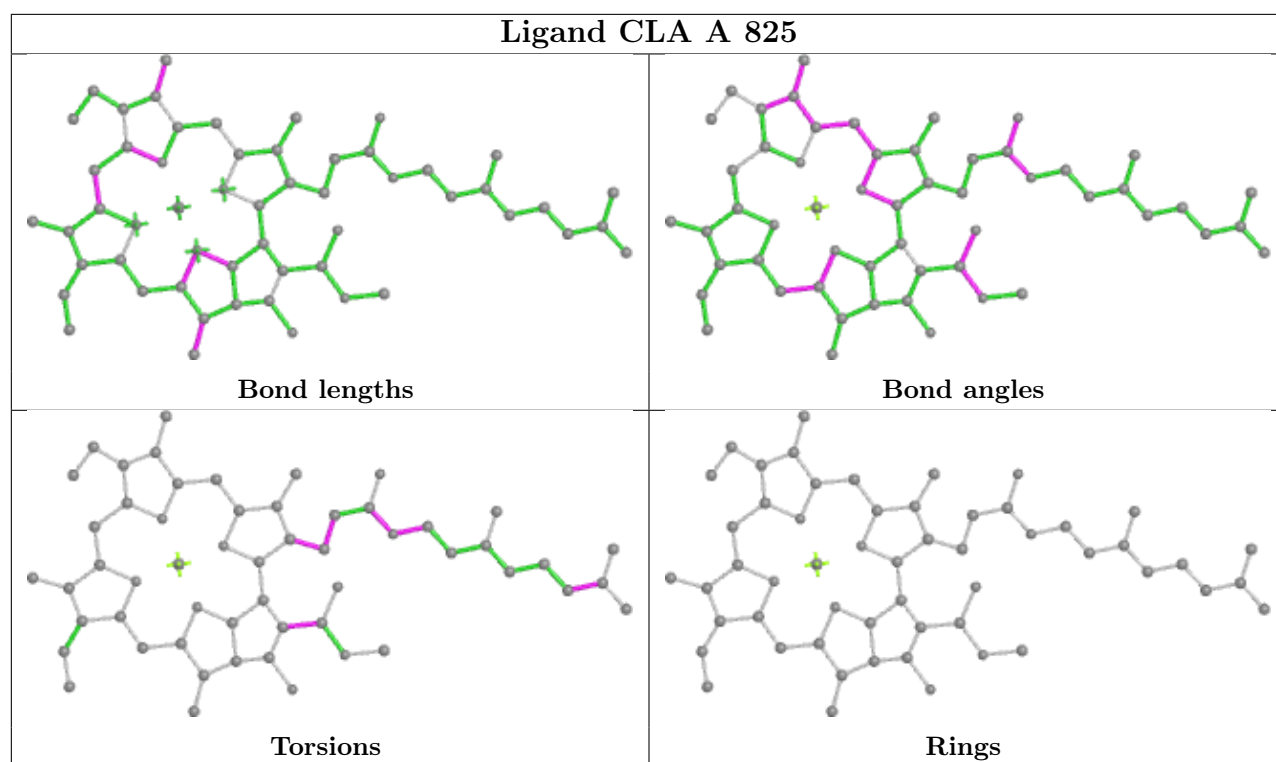
## Ligand CLA 5 613



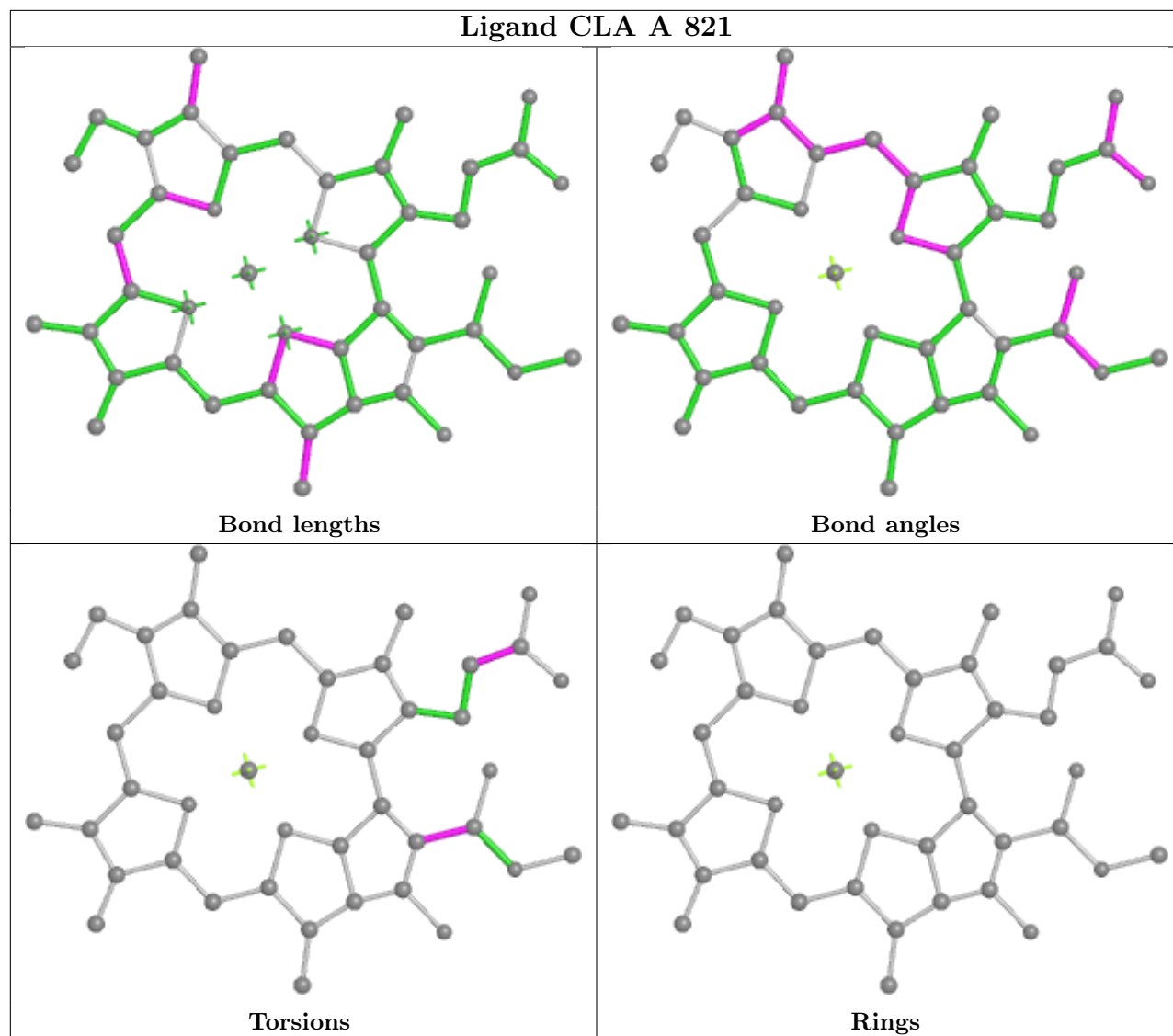
## Ligand CLA A 826



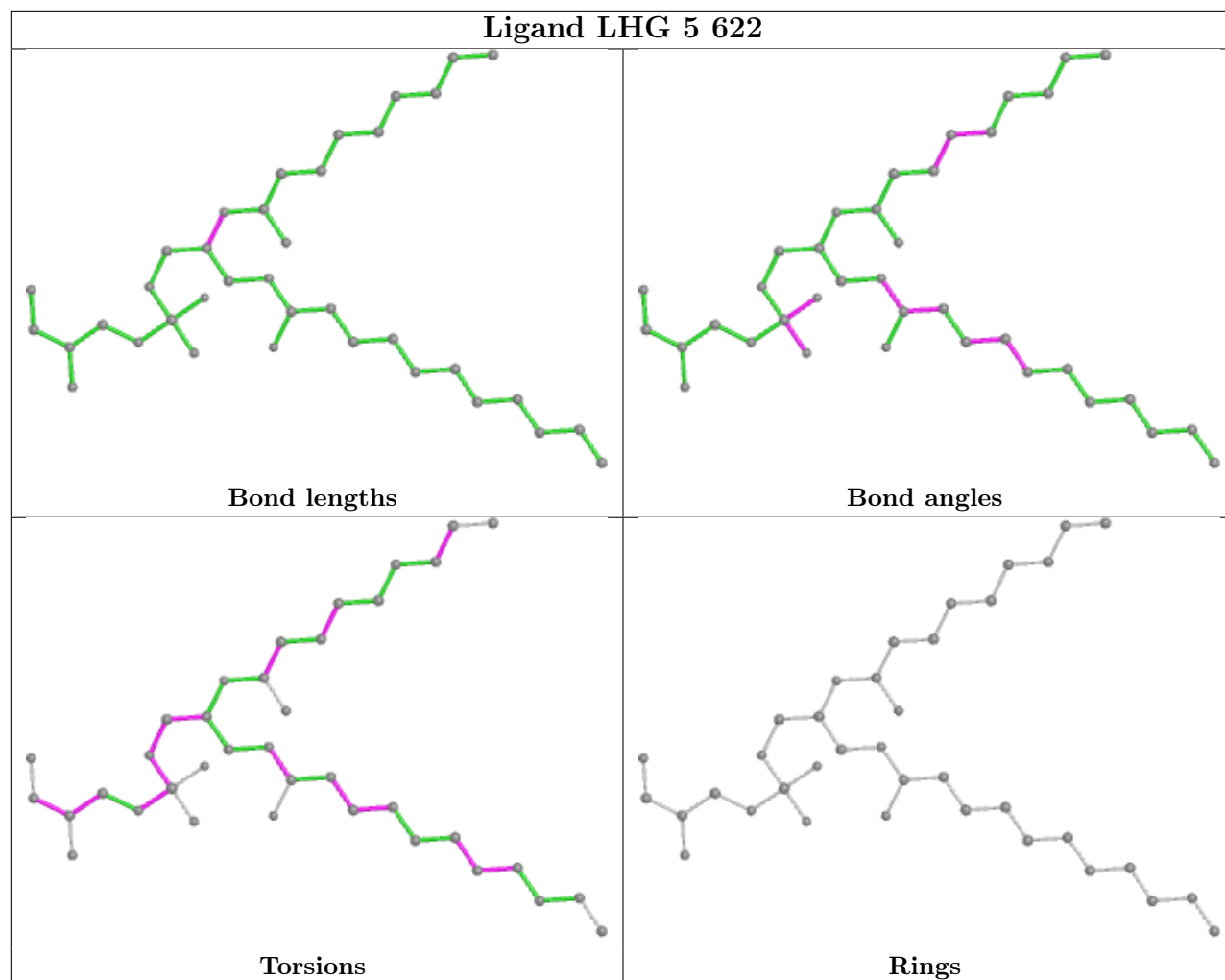




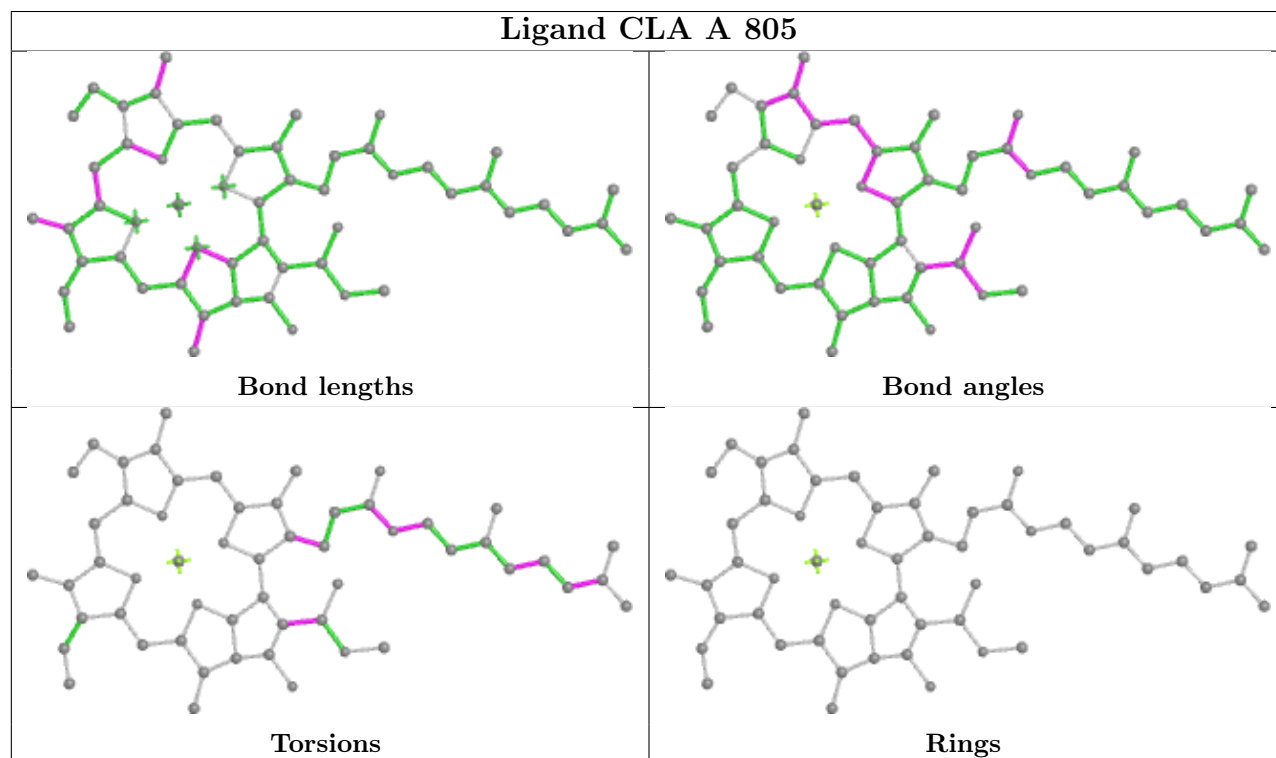
## Ligand CLA A 821

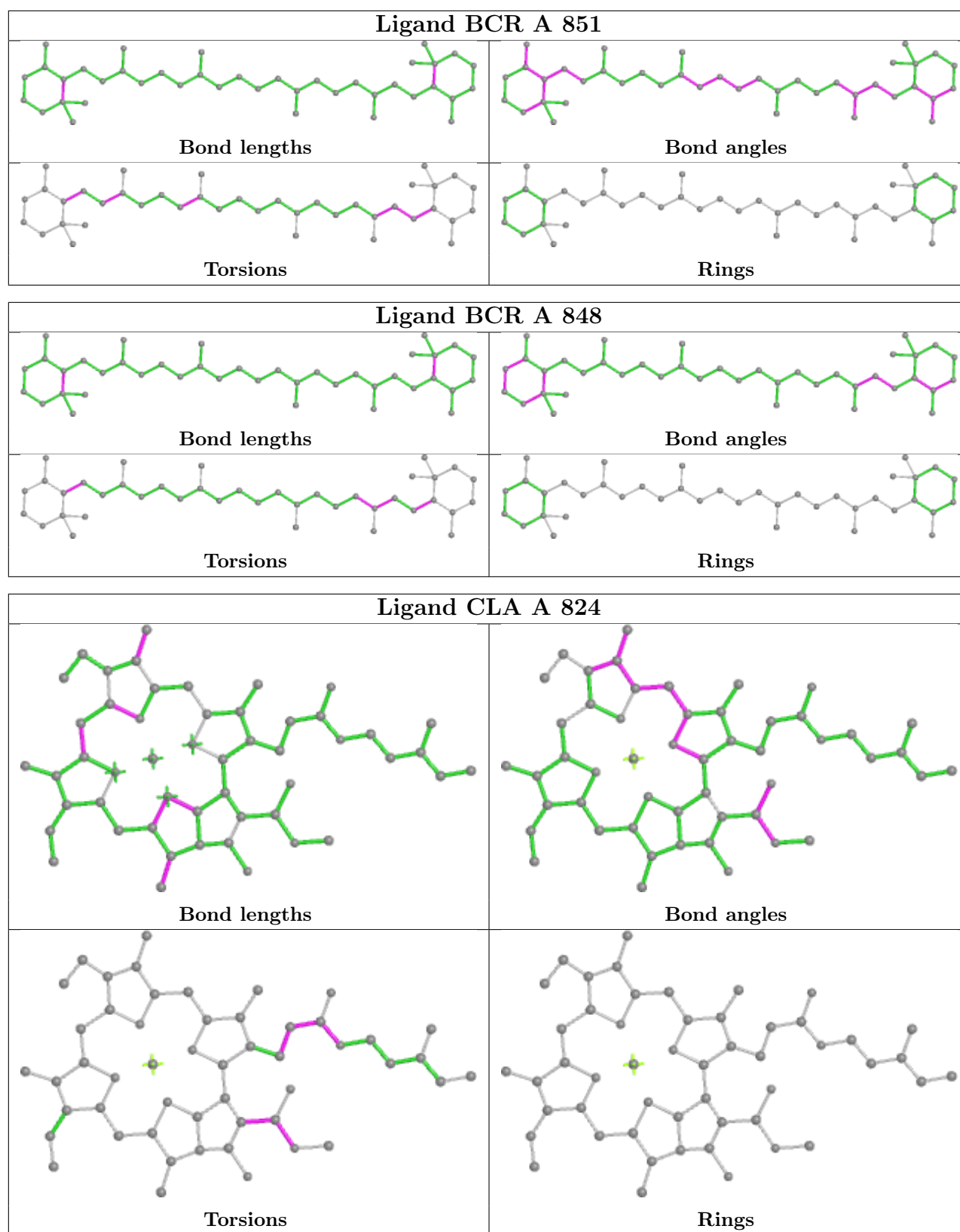


## Ligand LHG 5 622

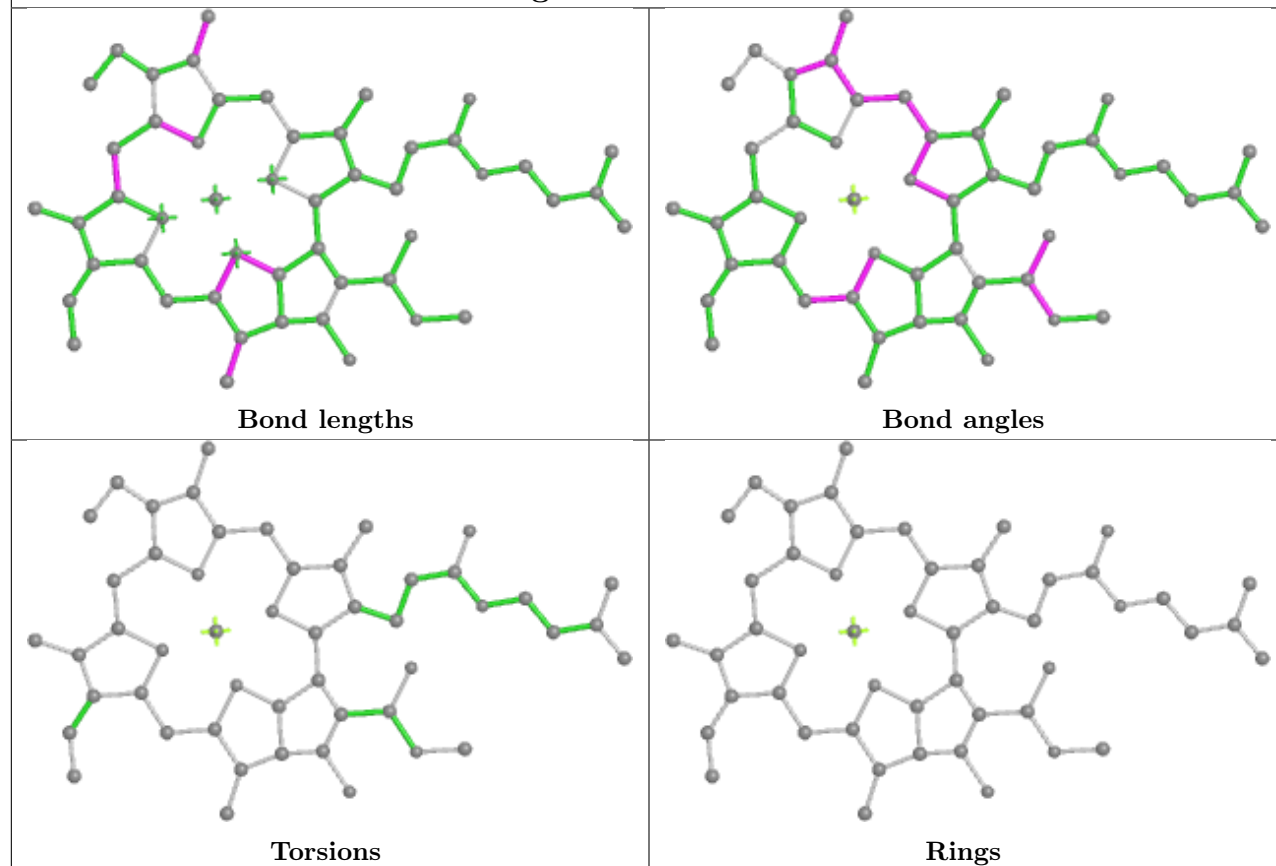


## Ligand CLA A 805

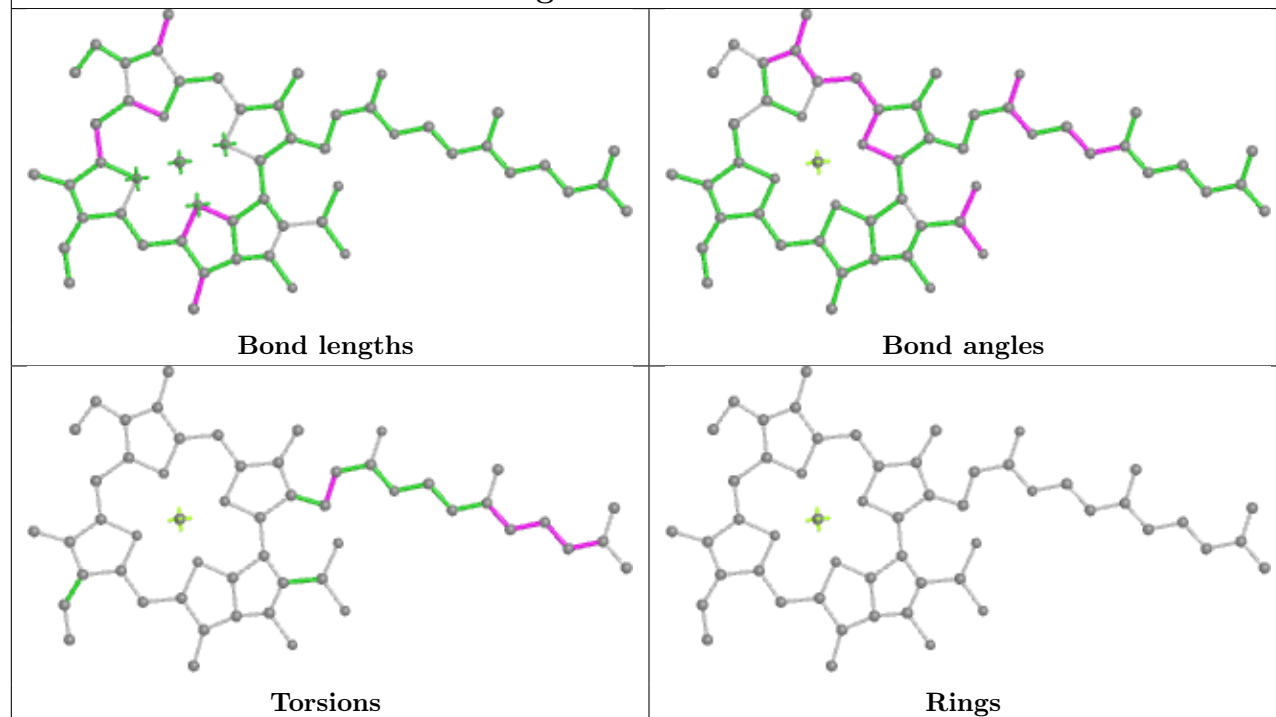




## Ligand CLA A 836

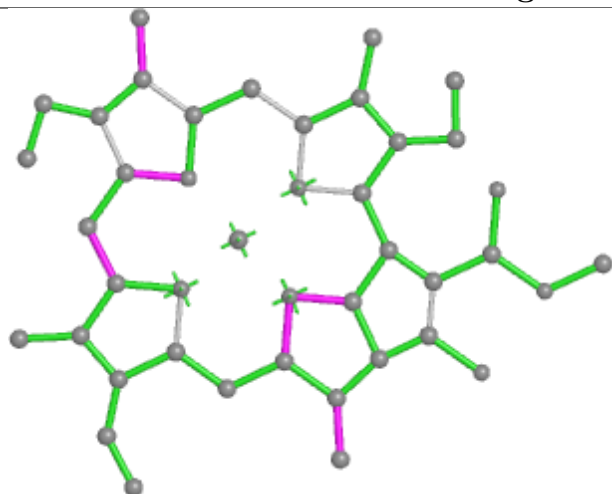


## Ligand CLA 3 613

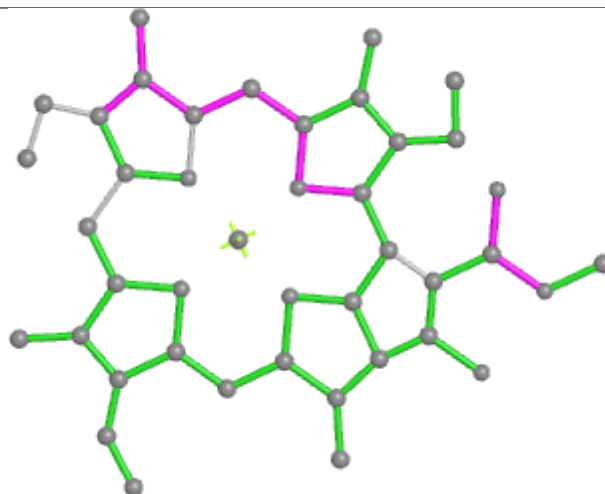




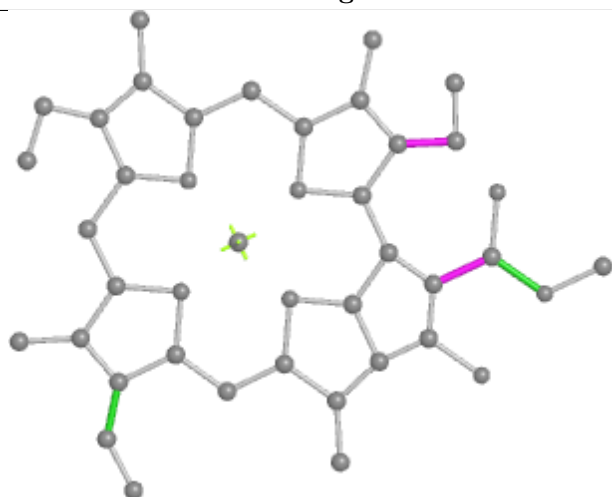
## Ligand CLA J 101



Bond lengths



Bond angles

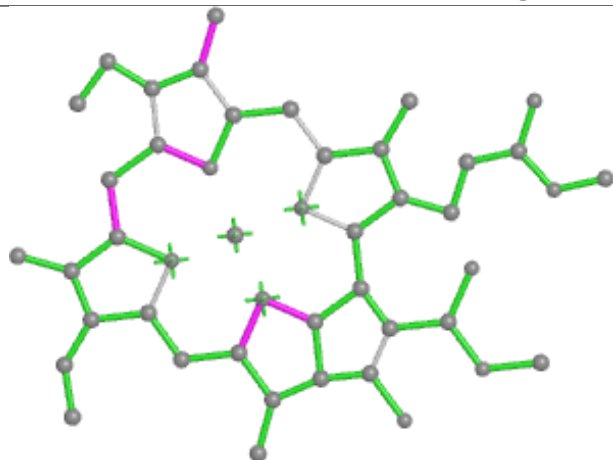


Torsions

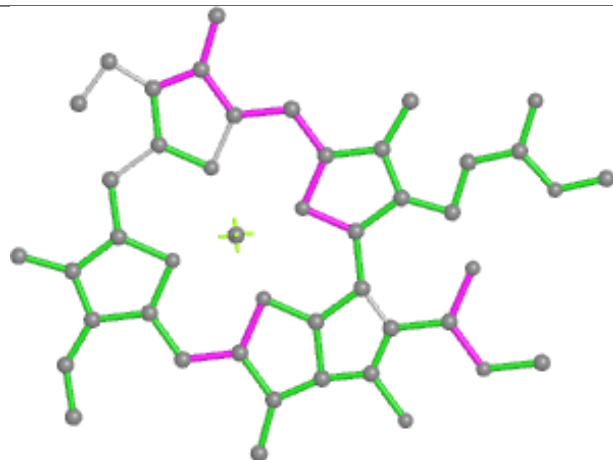


Rings

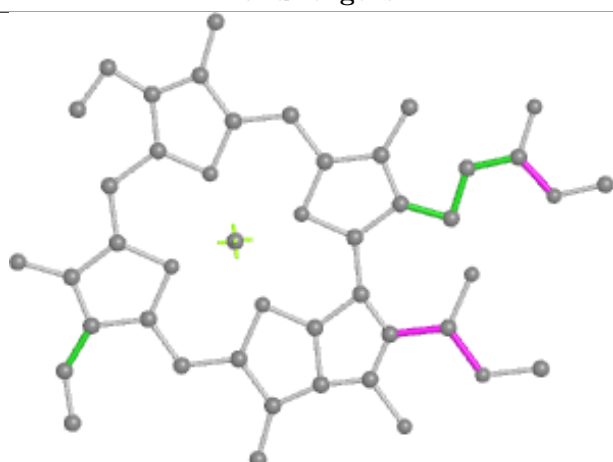
## Ligand CLA B 821



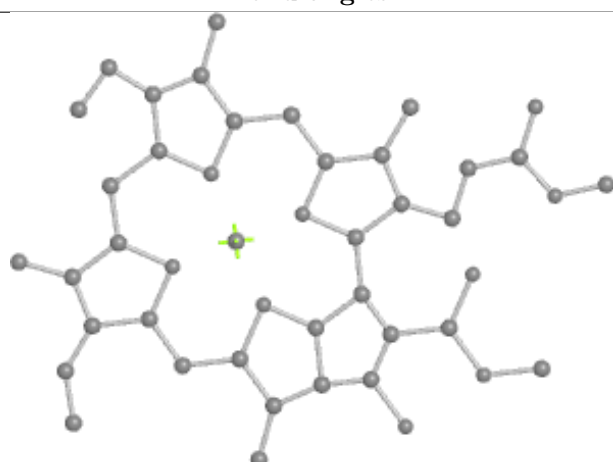
Bond lengths



Bond angles

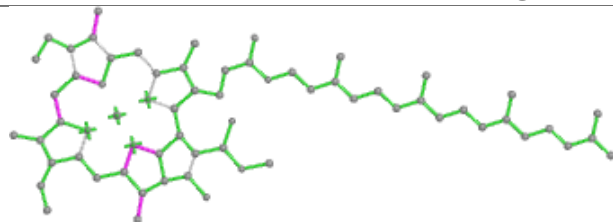


Torsions

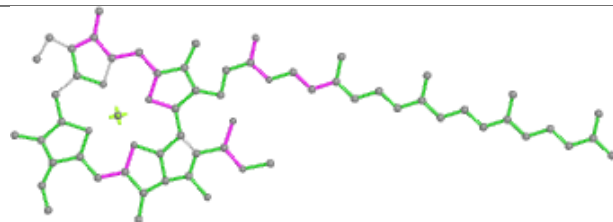


Rings

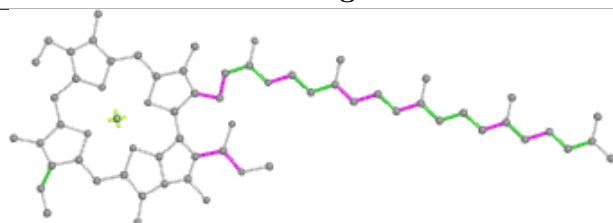
## Ligand CLA A 854



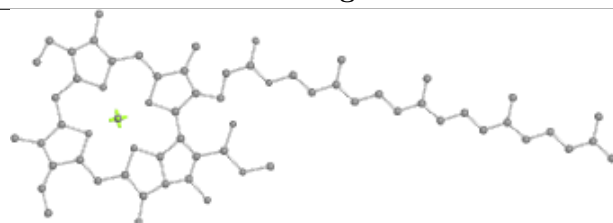
Bond lengths



Bond angles

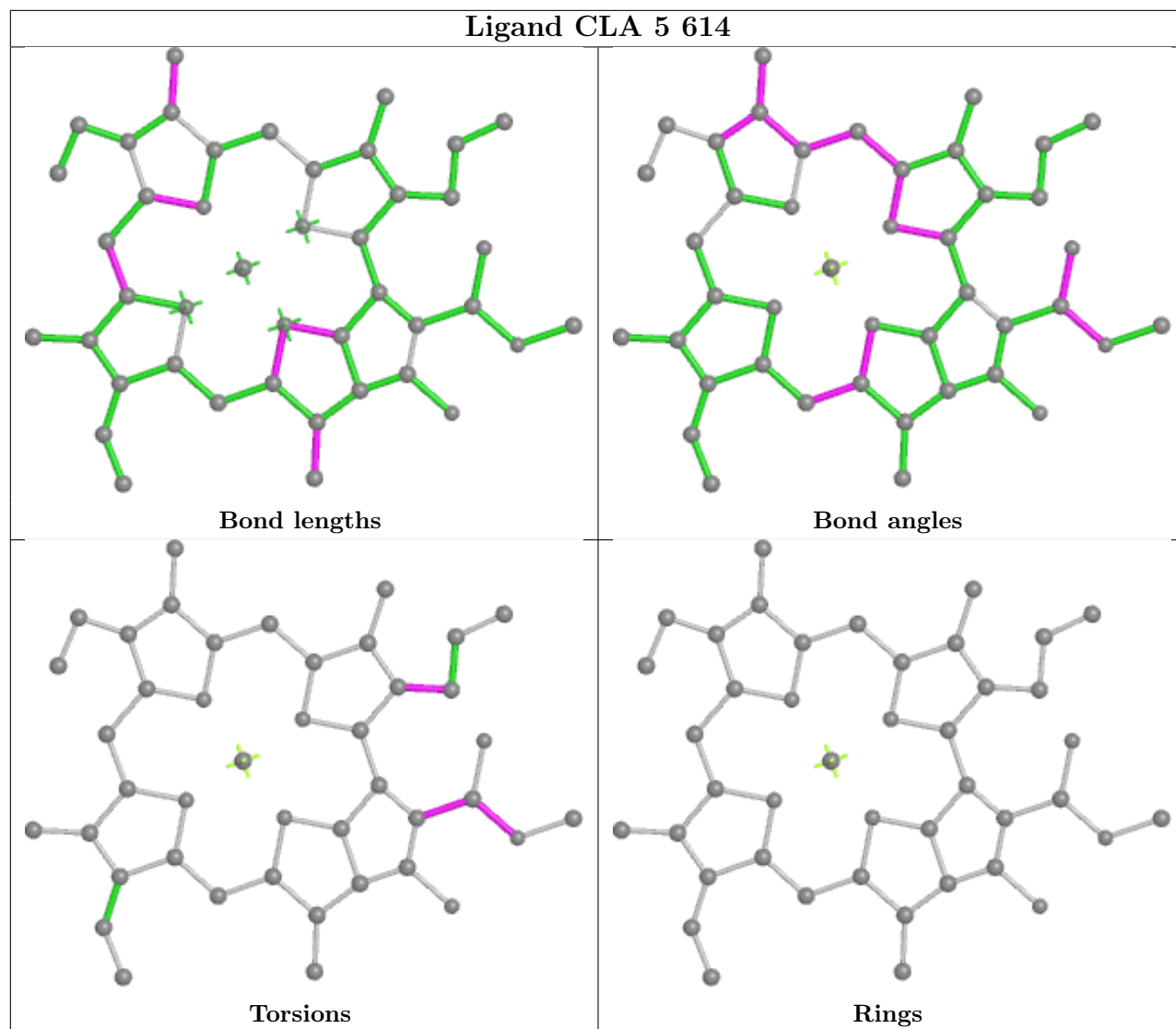


Torsions

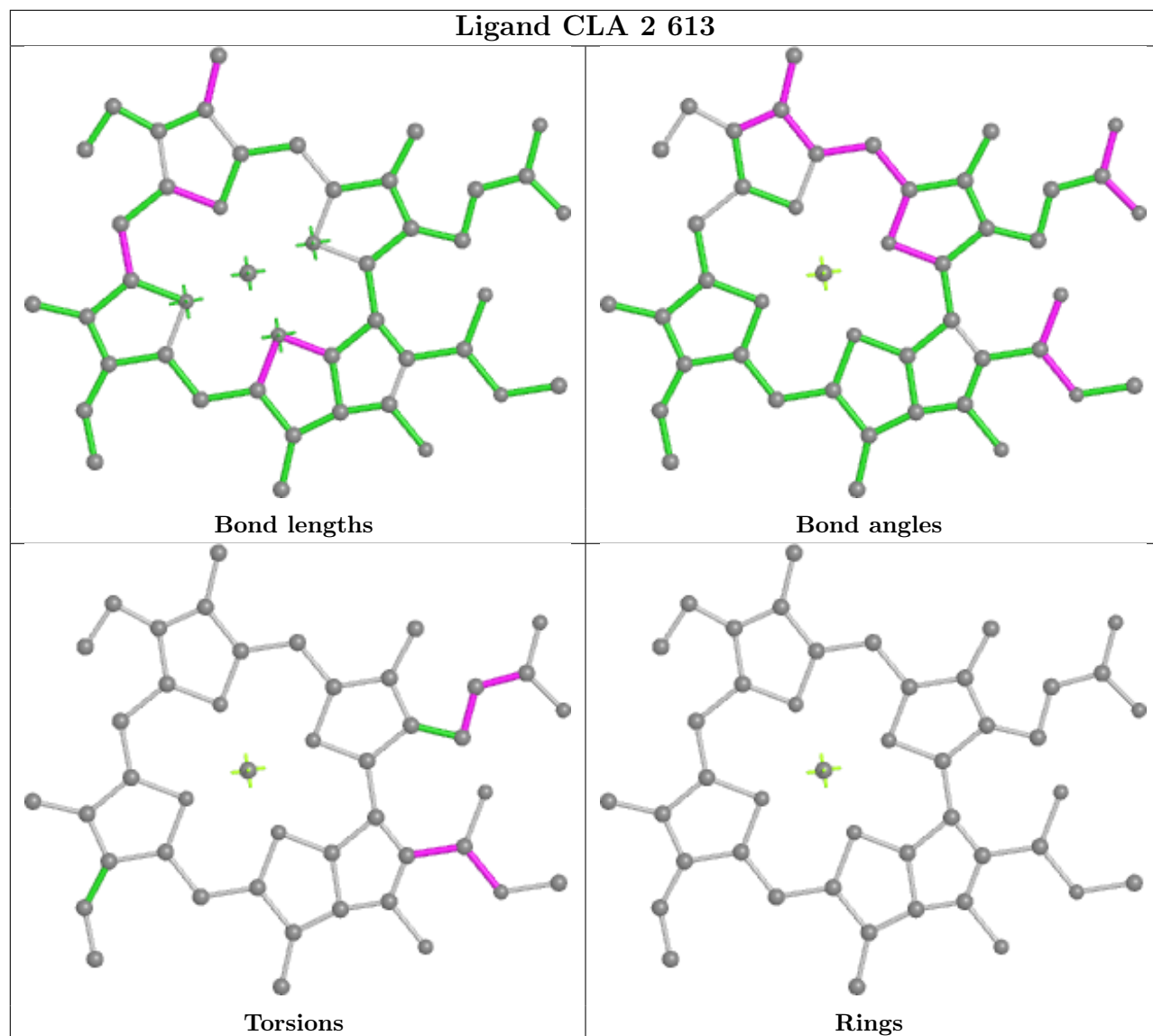


Rings

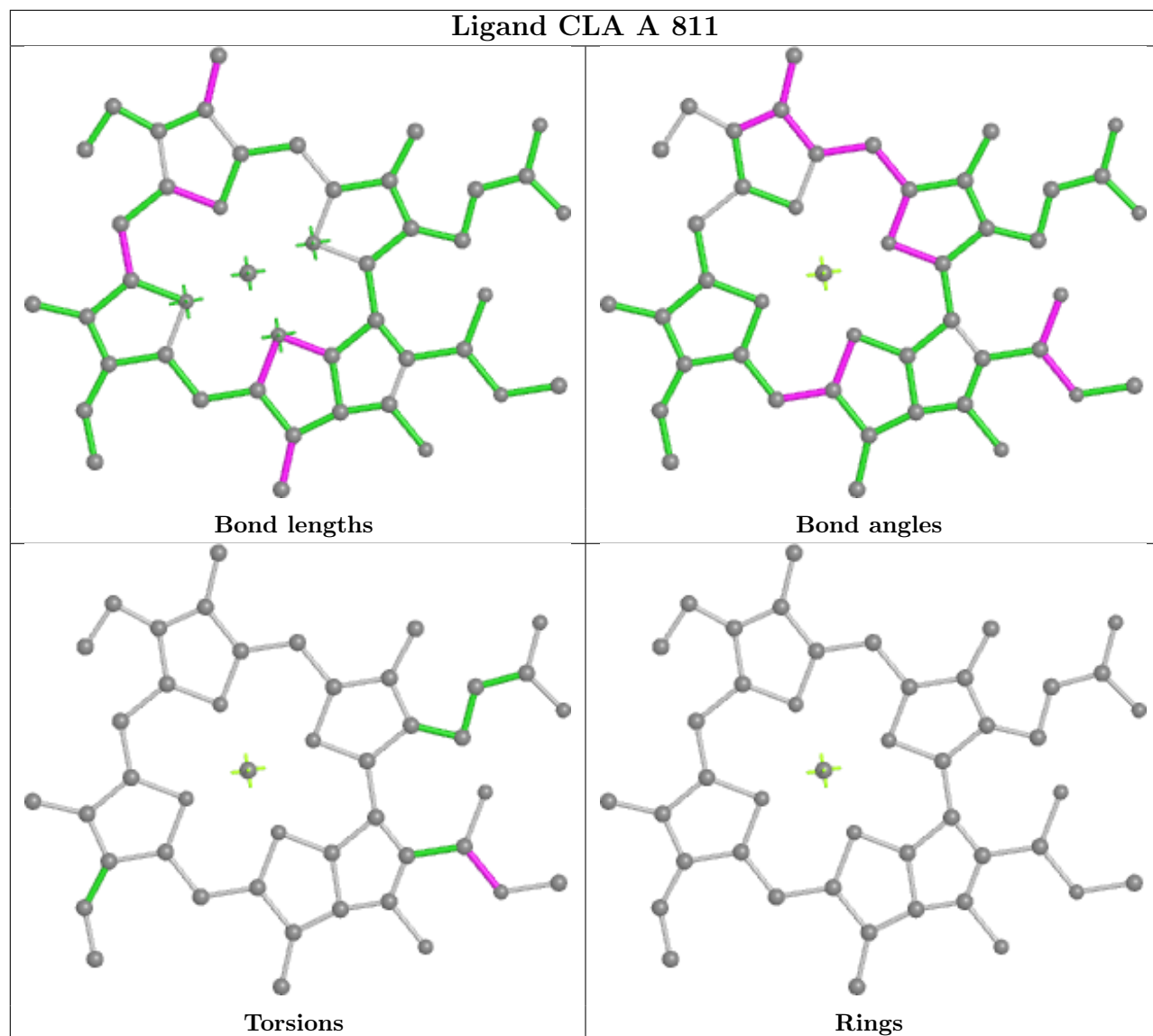
## Ligand CLA 5 614

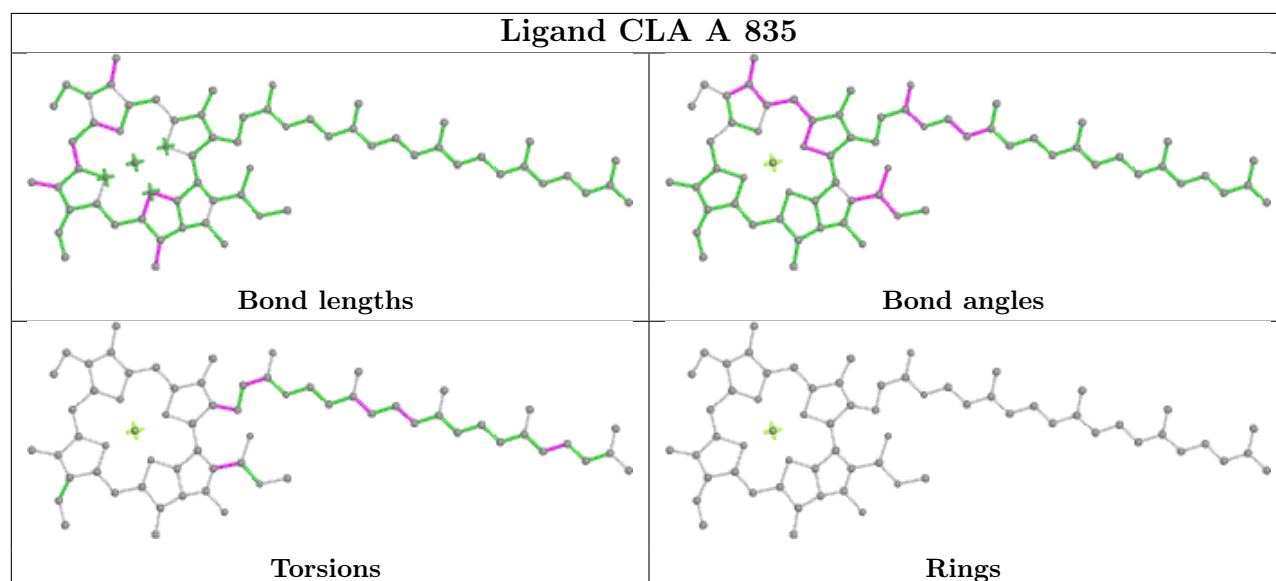
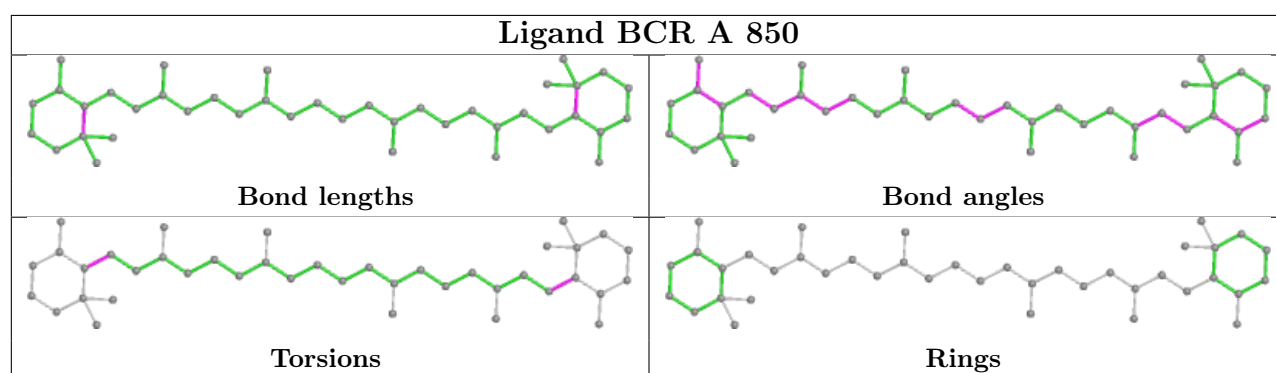
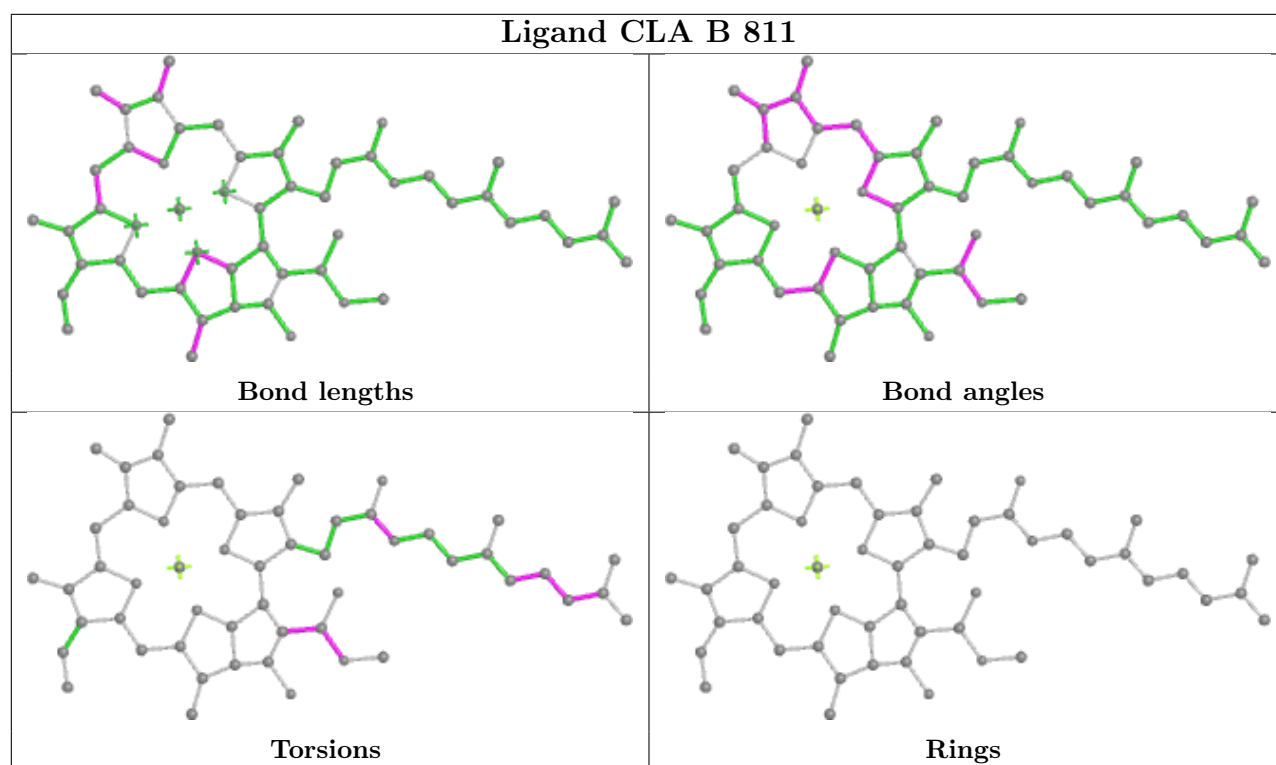


## Ligand CLA 2 613

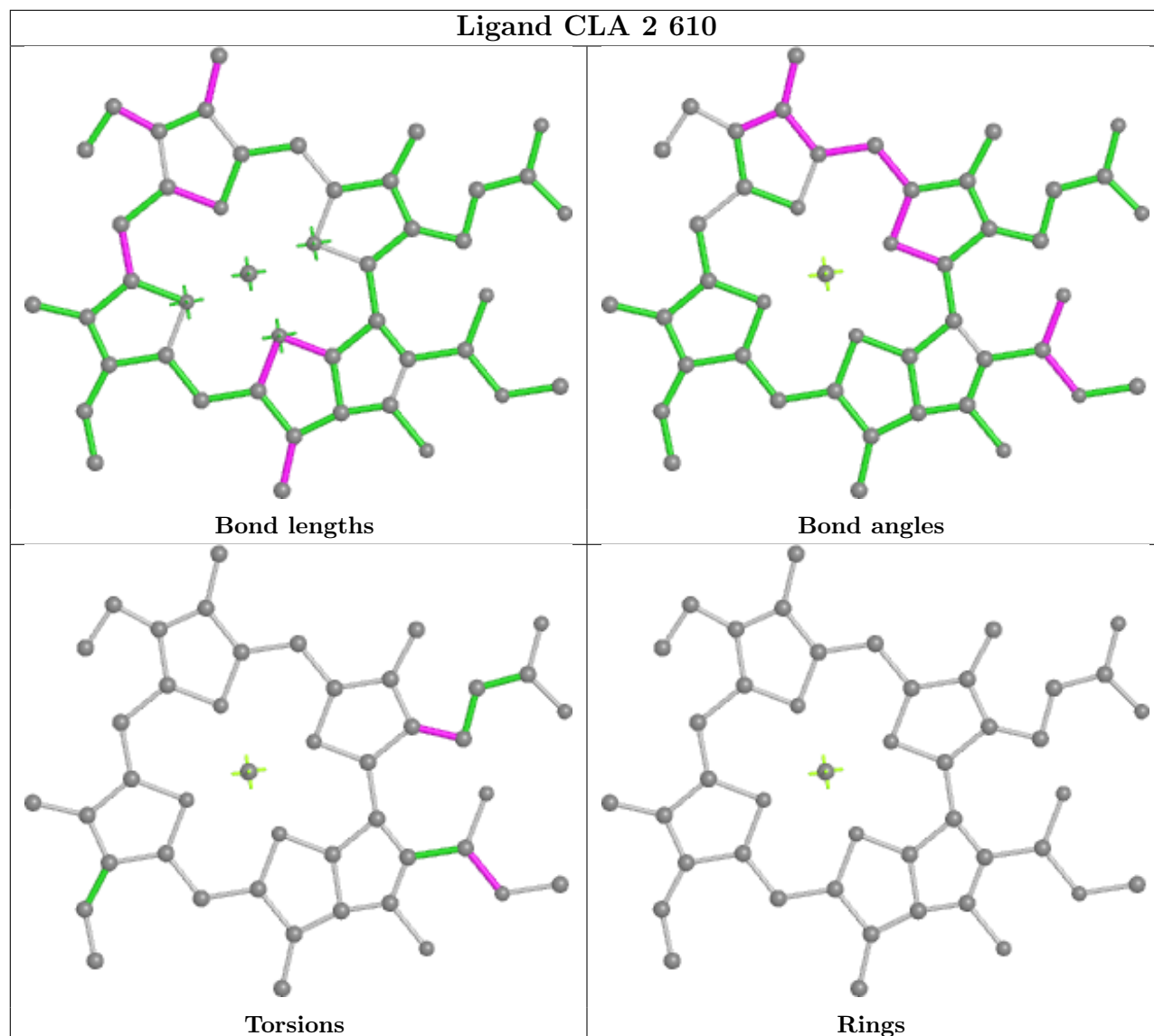


## Ligand CLA A 811

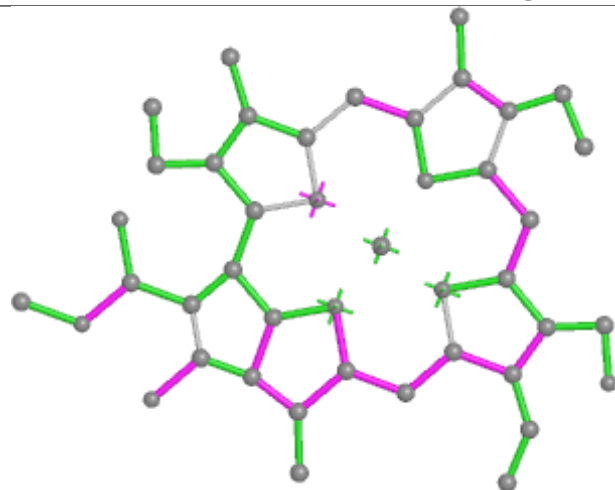




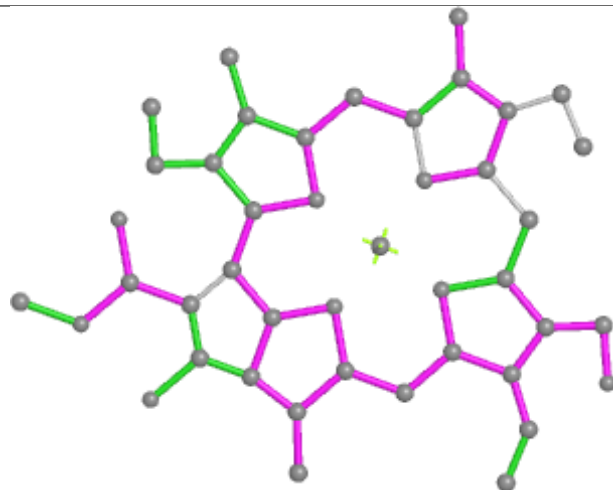
## Ligand CLA 2 610



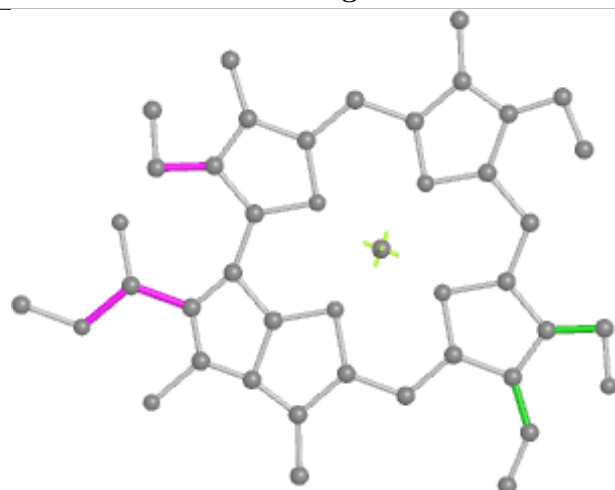
## Ligand CHL 5 607



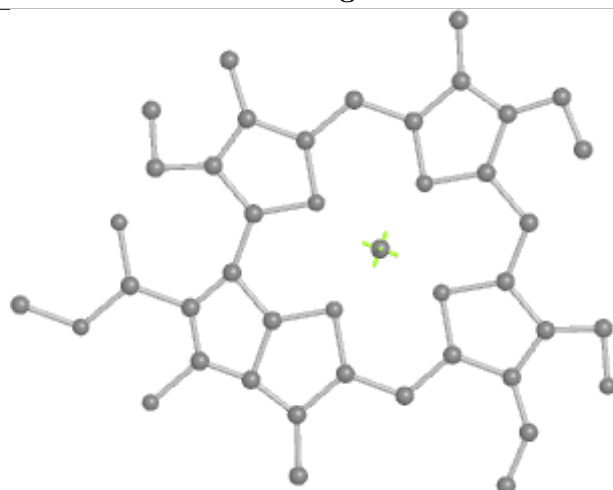
Bond lengths



Bond angles

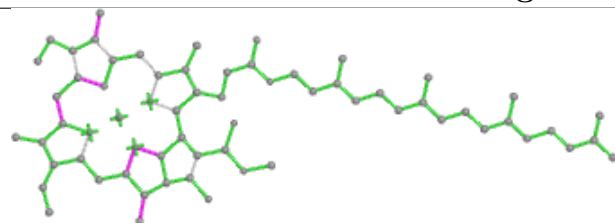


Torsions

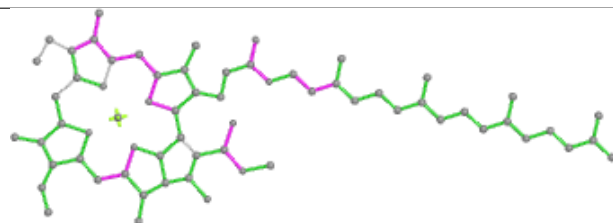


Rings

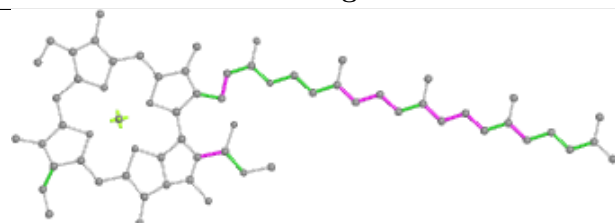
## Ligand CLA B 807



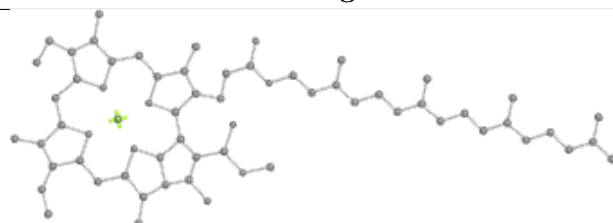
Bond lengths



Bond angles



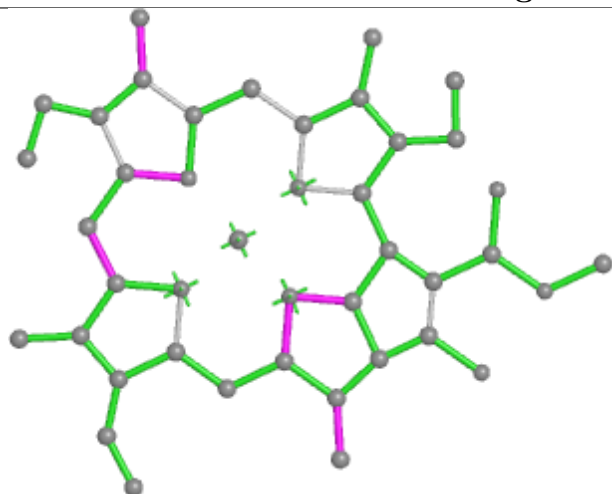
Torsions



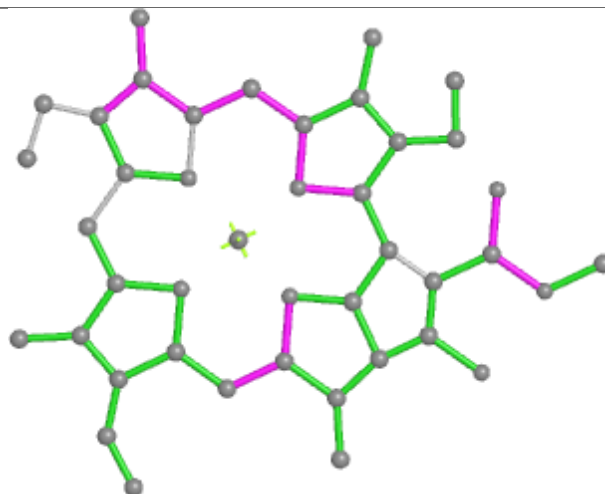
Rings



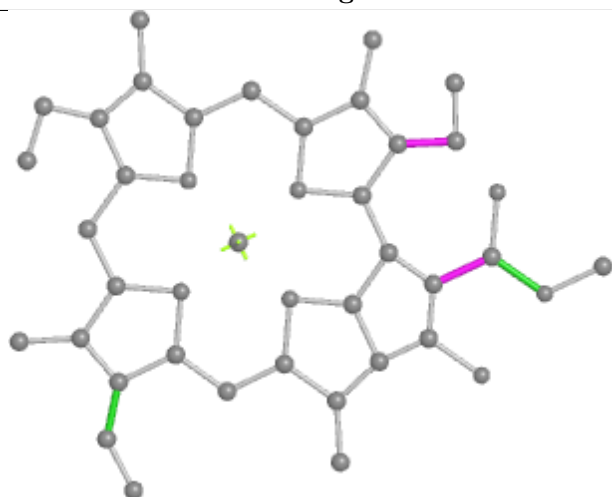
## Ligand CLA L 304



Bond lengths



Bond angles

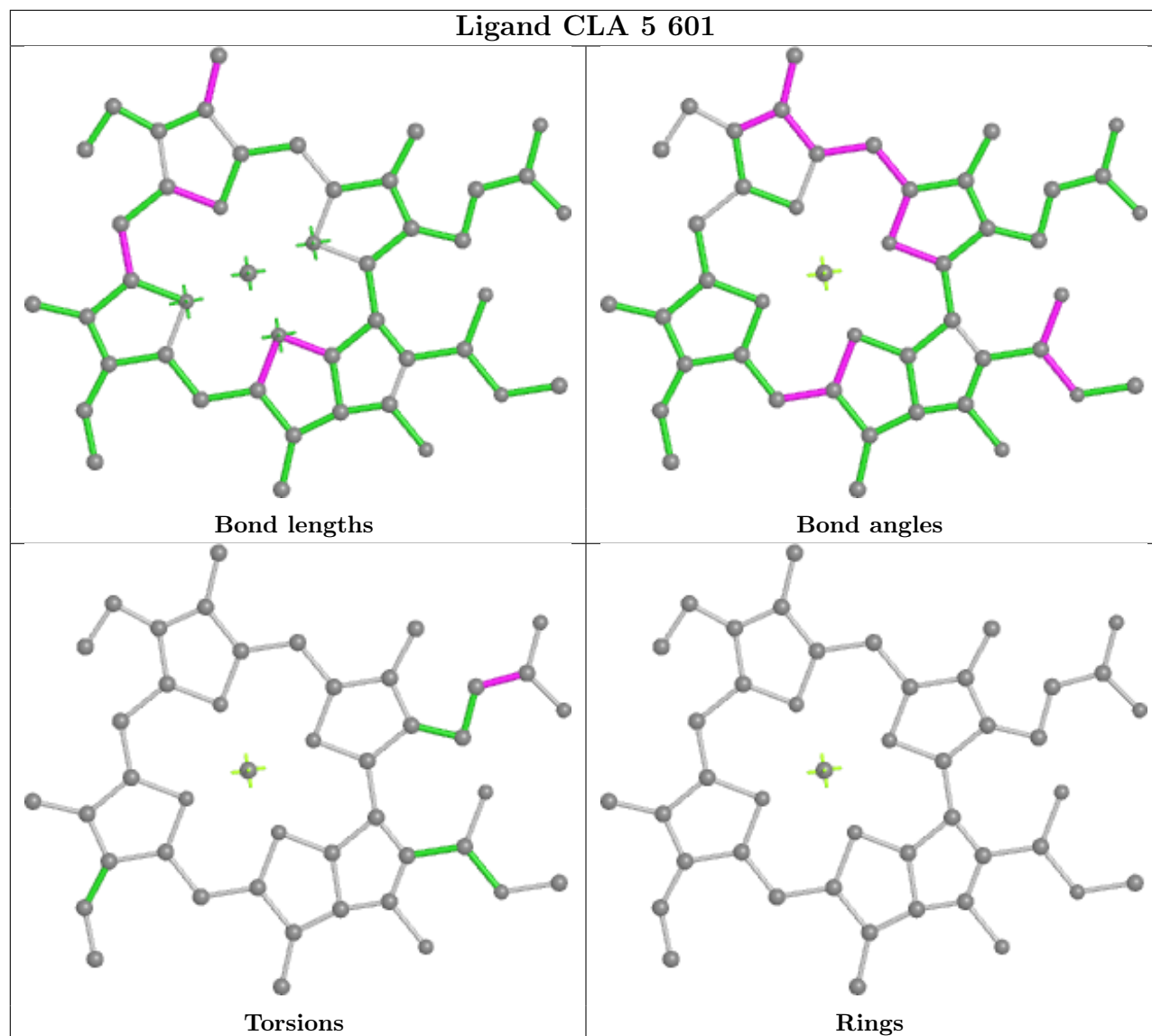


Torsions

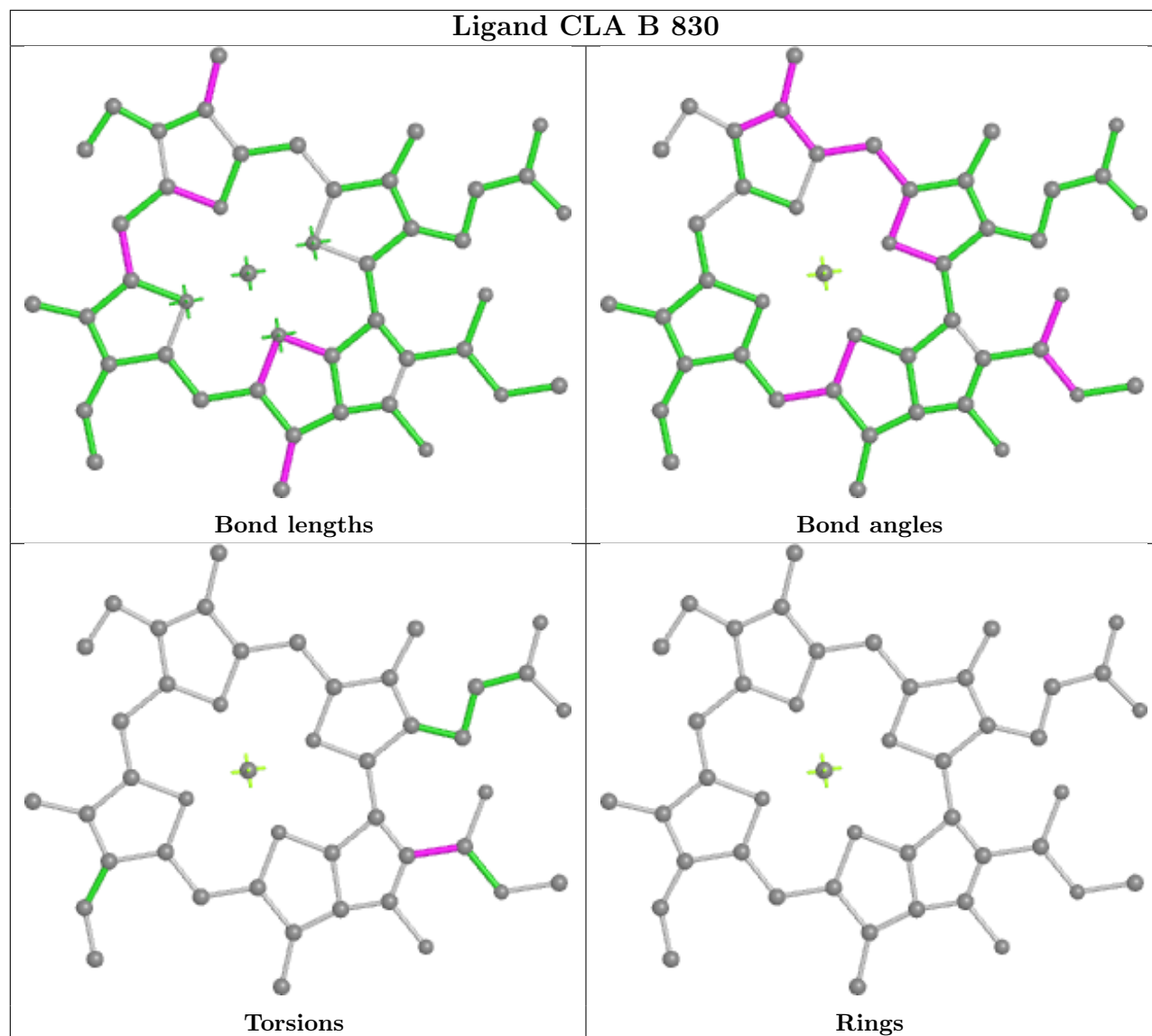


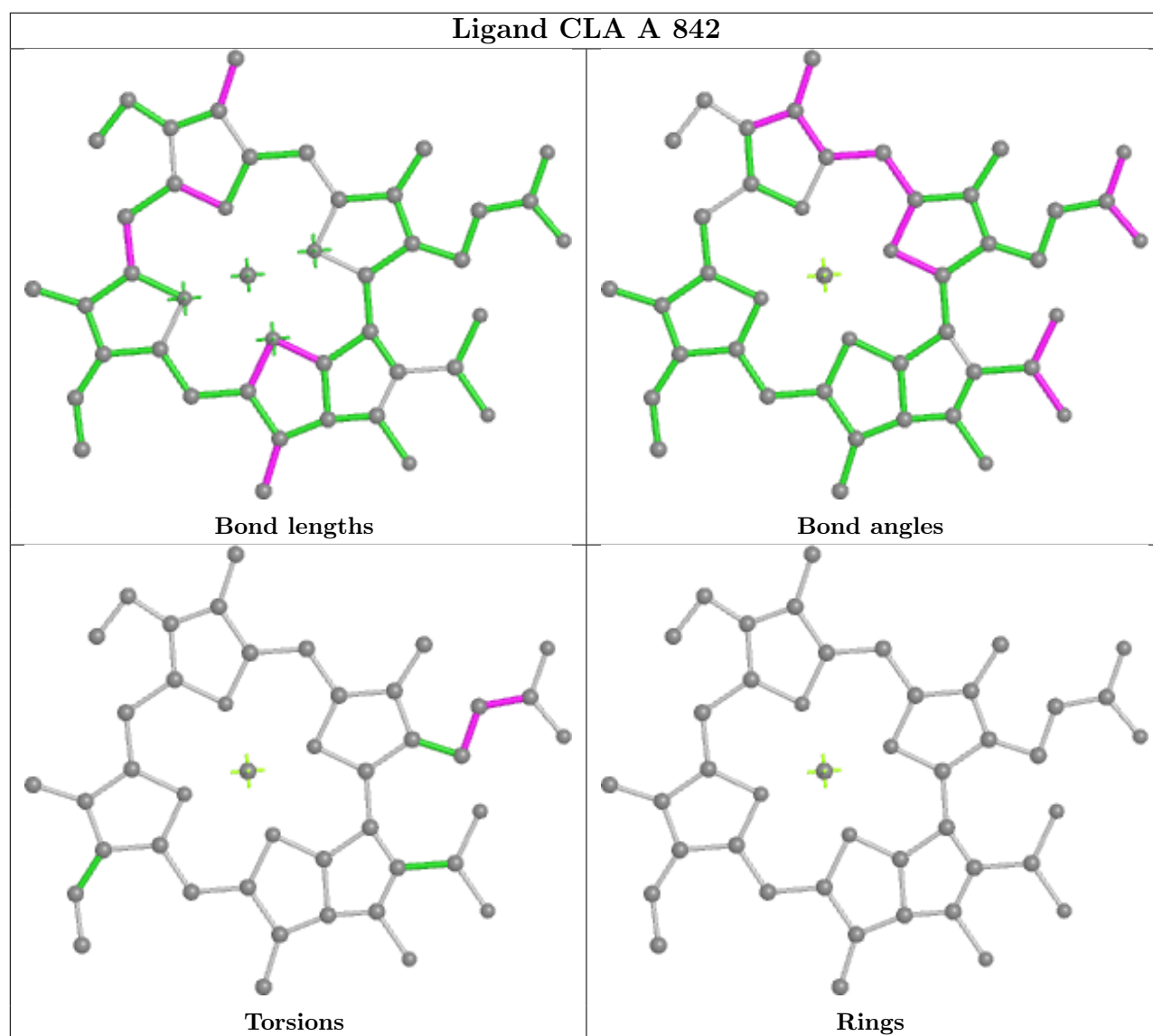
Rings

## Ligand CLA 5 601

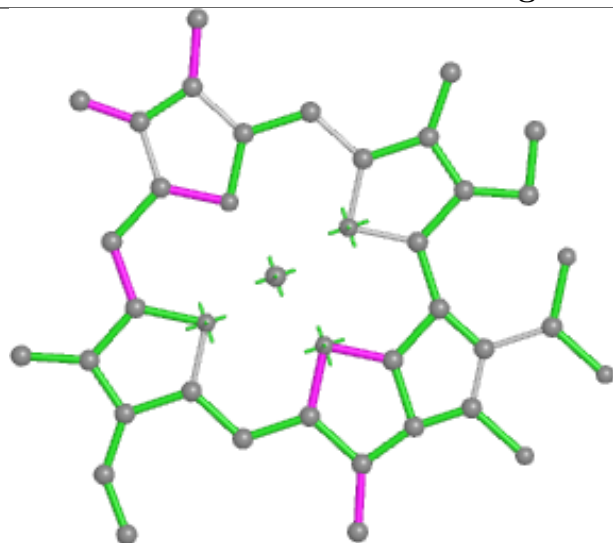


## Ligand CLA B 830

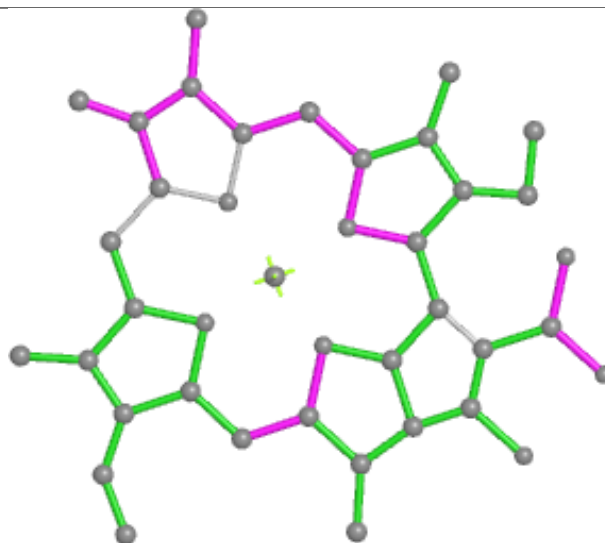




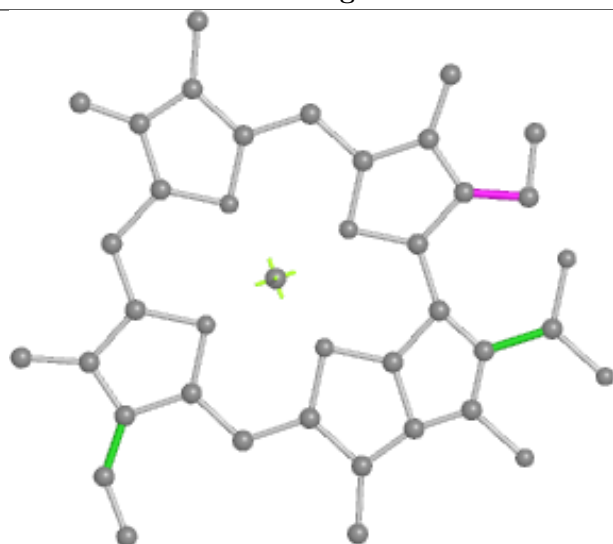
## Ligand CLA 3 607



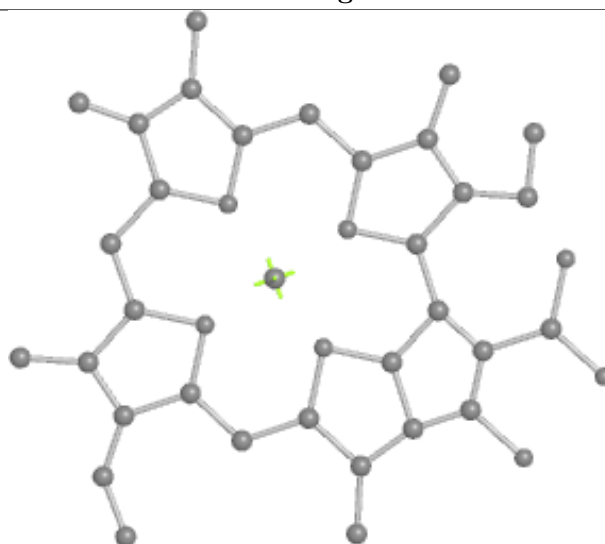
Bond lengths



Bond angles

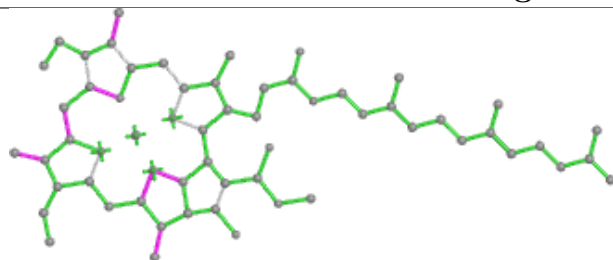


Torsions

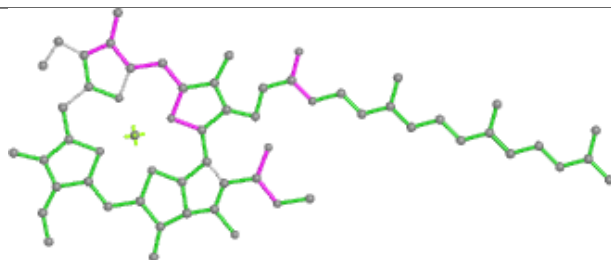


Rings

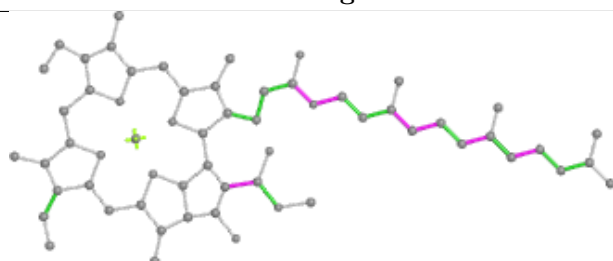
## Ligand CLA B 815



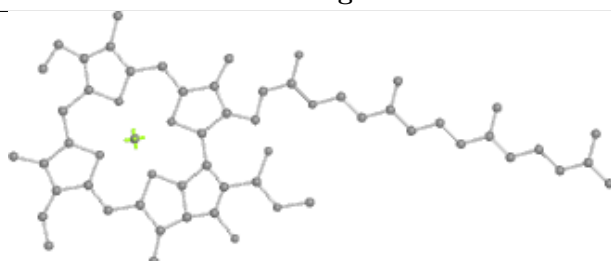
Bond lengths



Bond angles

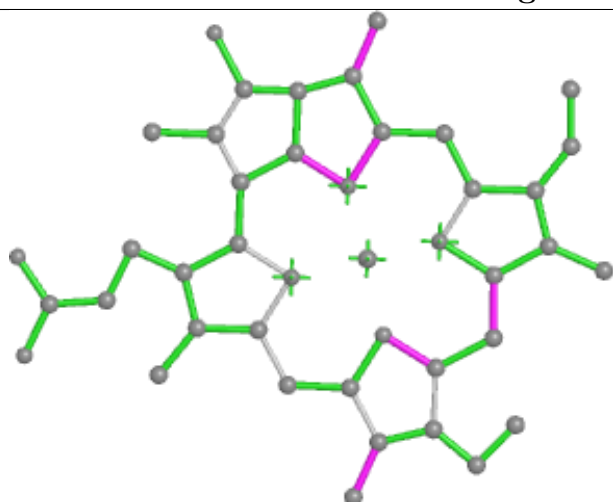


Torsions

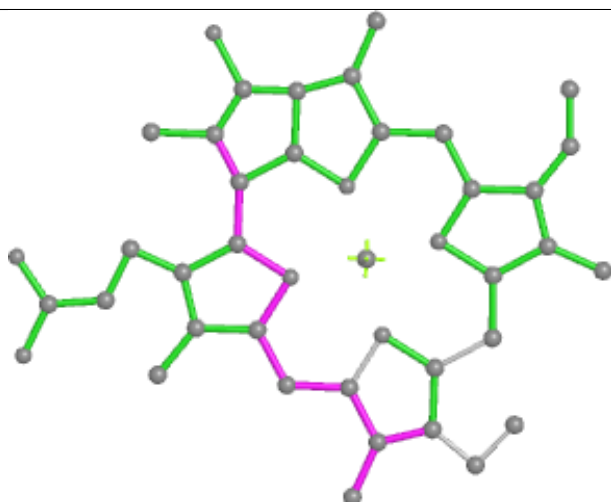


Rings

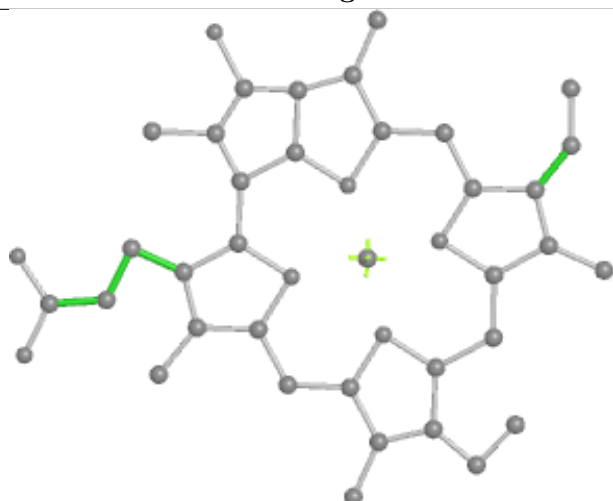
## Ligand CLA 2 611



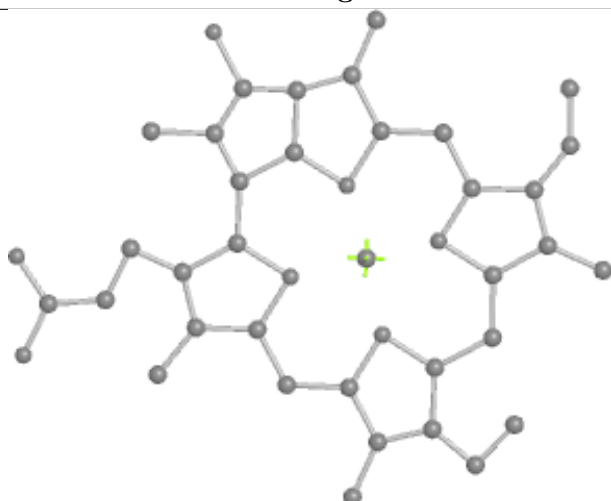
Bond lengths



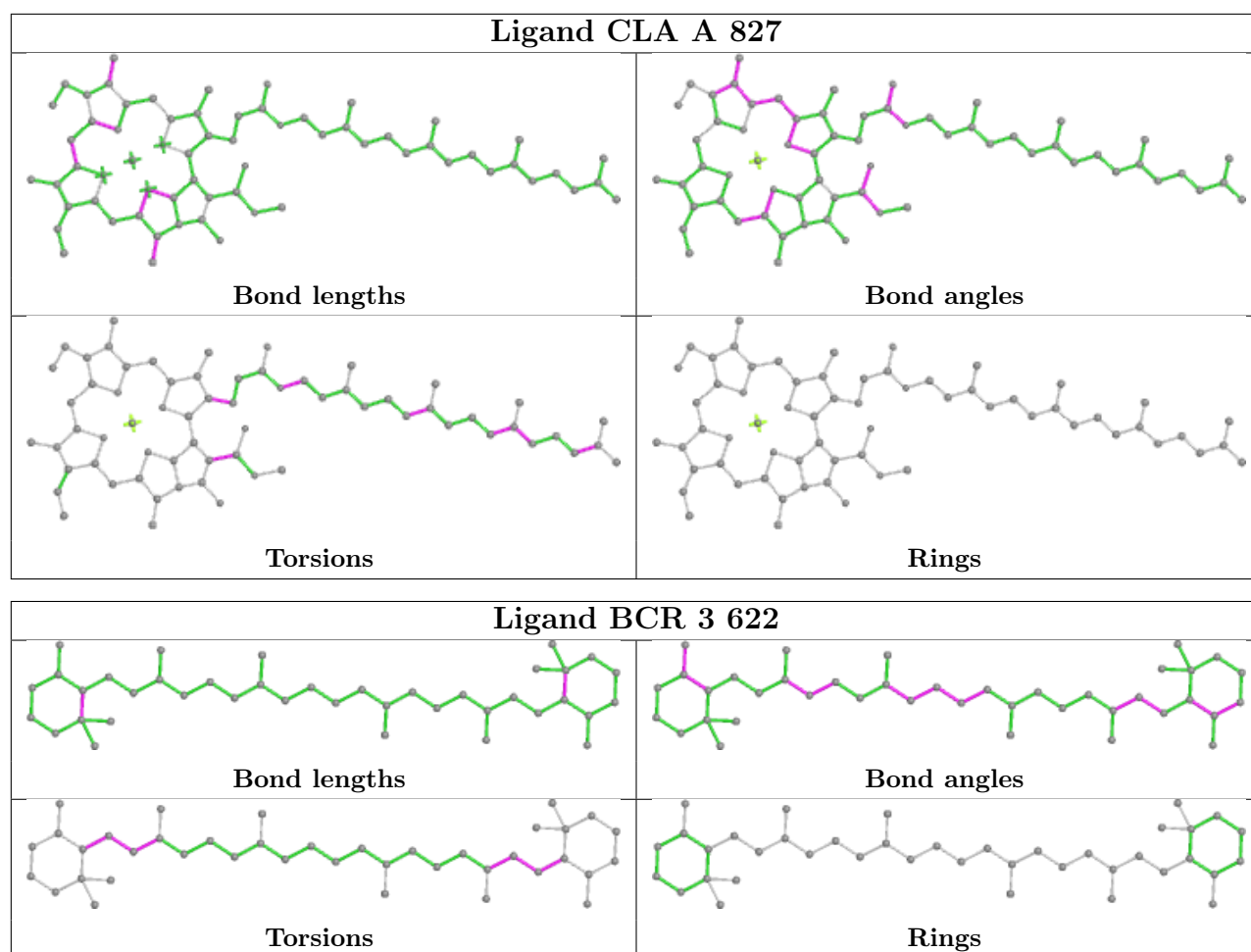
Bond angles



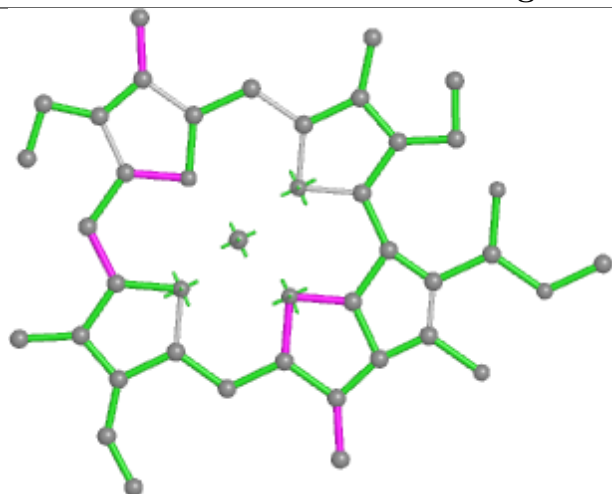
Torsions



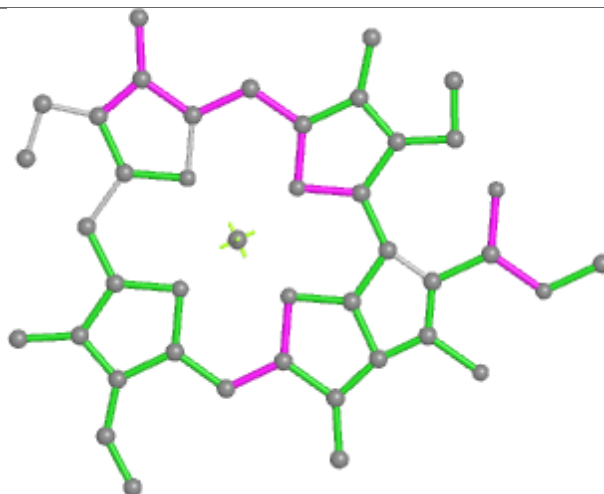
Rings



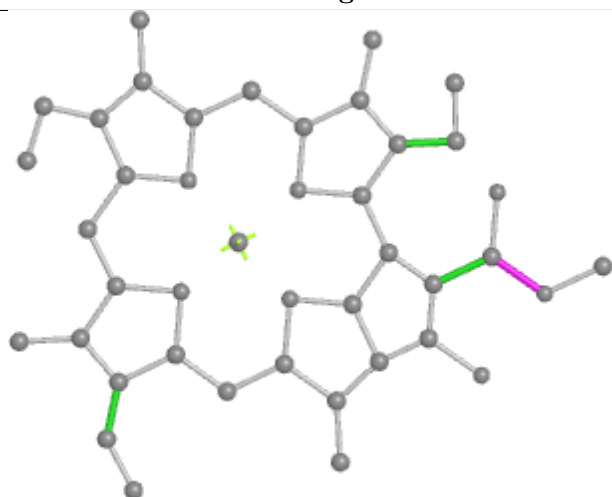
## Ligand CLA 2 614



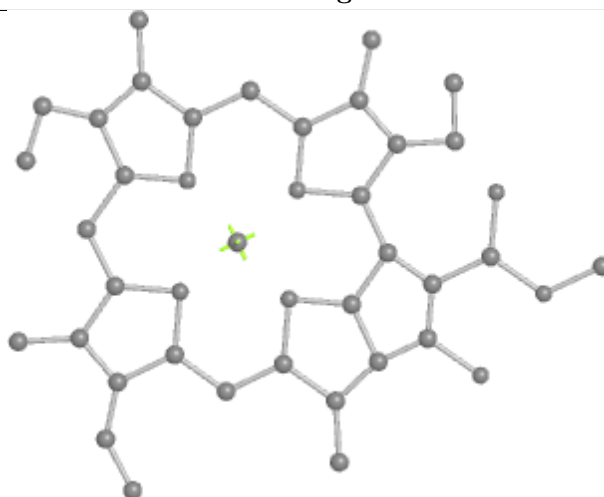
Bond lengths



Bond angles



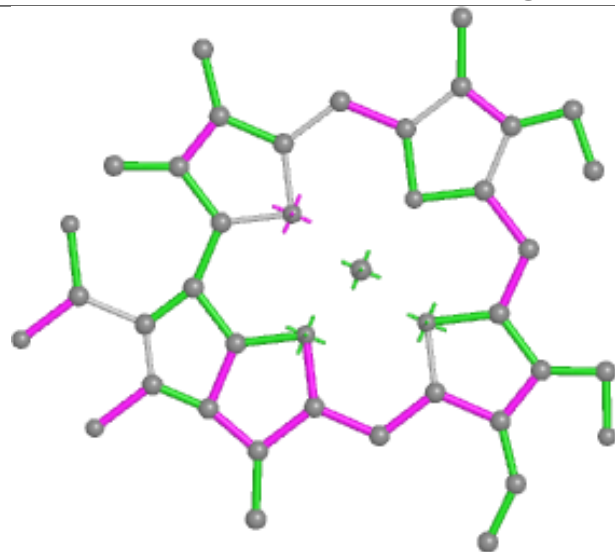
Torsions



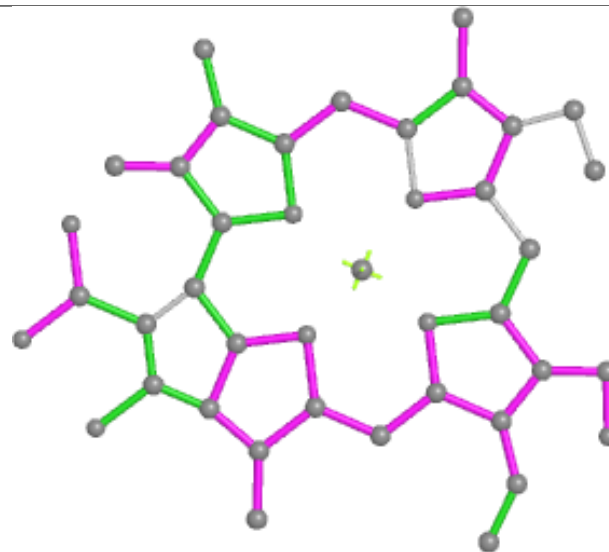
Rings



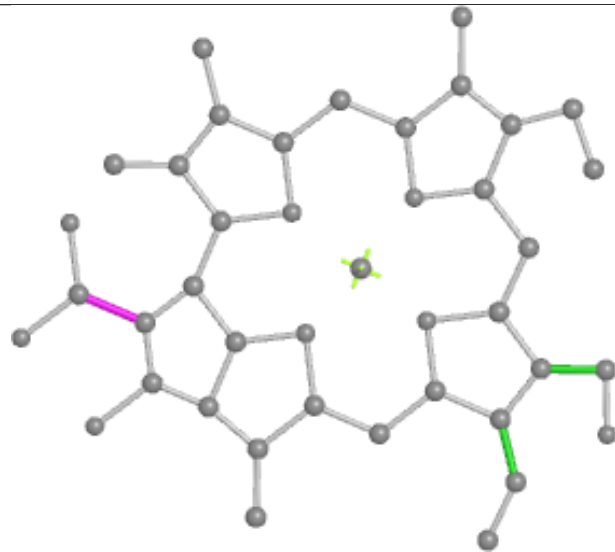
## Ligand CHL 2 608



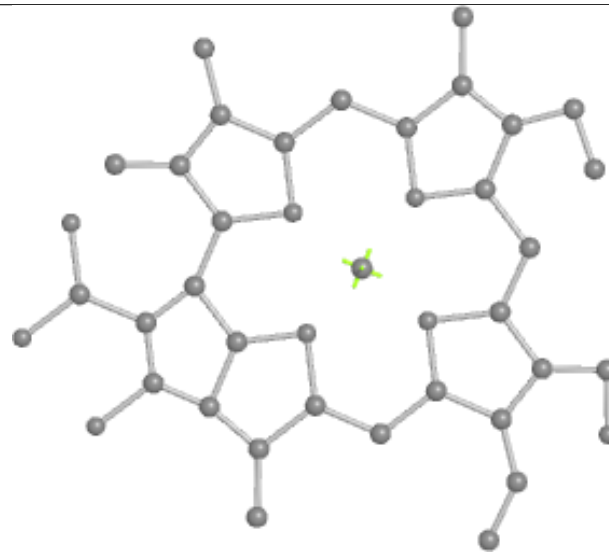
Bond lengths



Bond angles

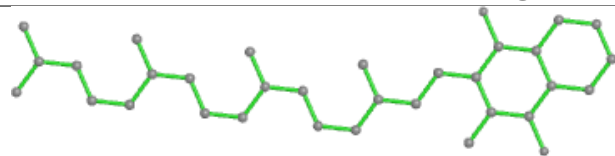


Torsions

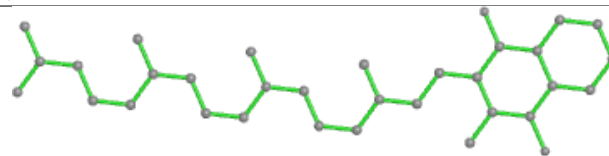


Rings

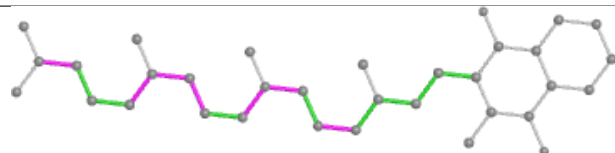
## Ligand PQN B 842



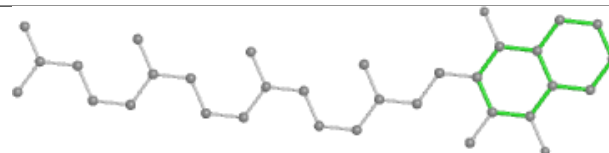
Bond lengths



Bond angles

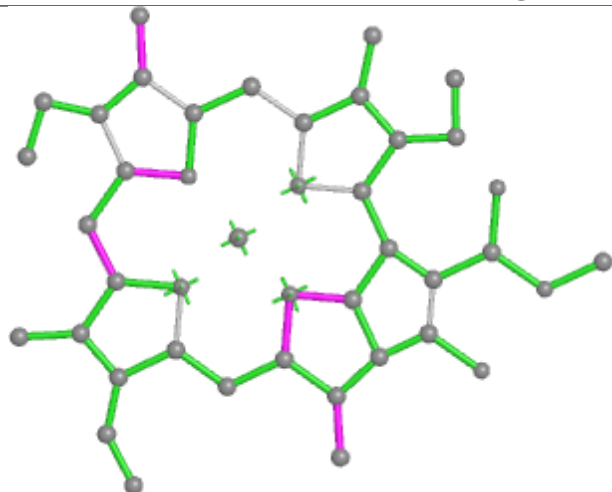


Torsions

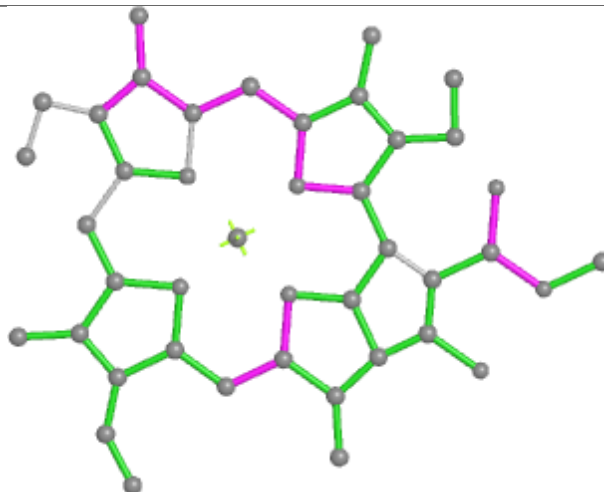


Rings

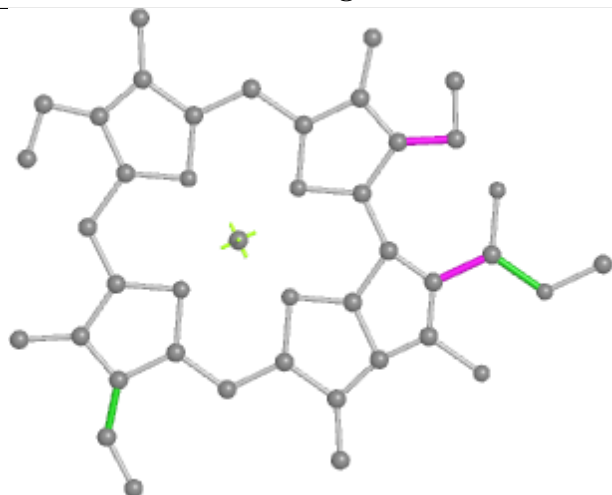
## Ligand CLA A 816



Bond lengths



Bond angles

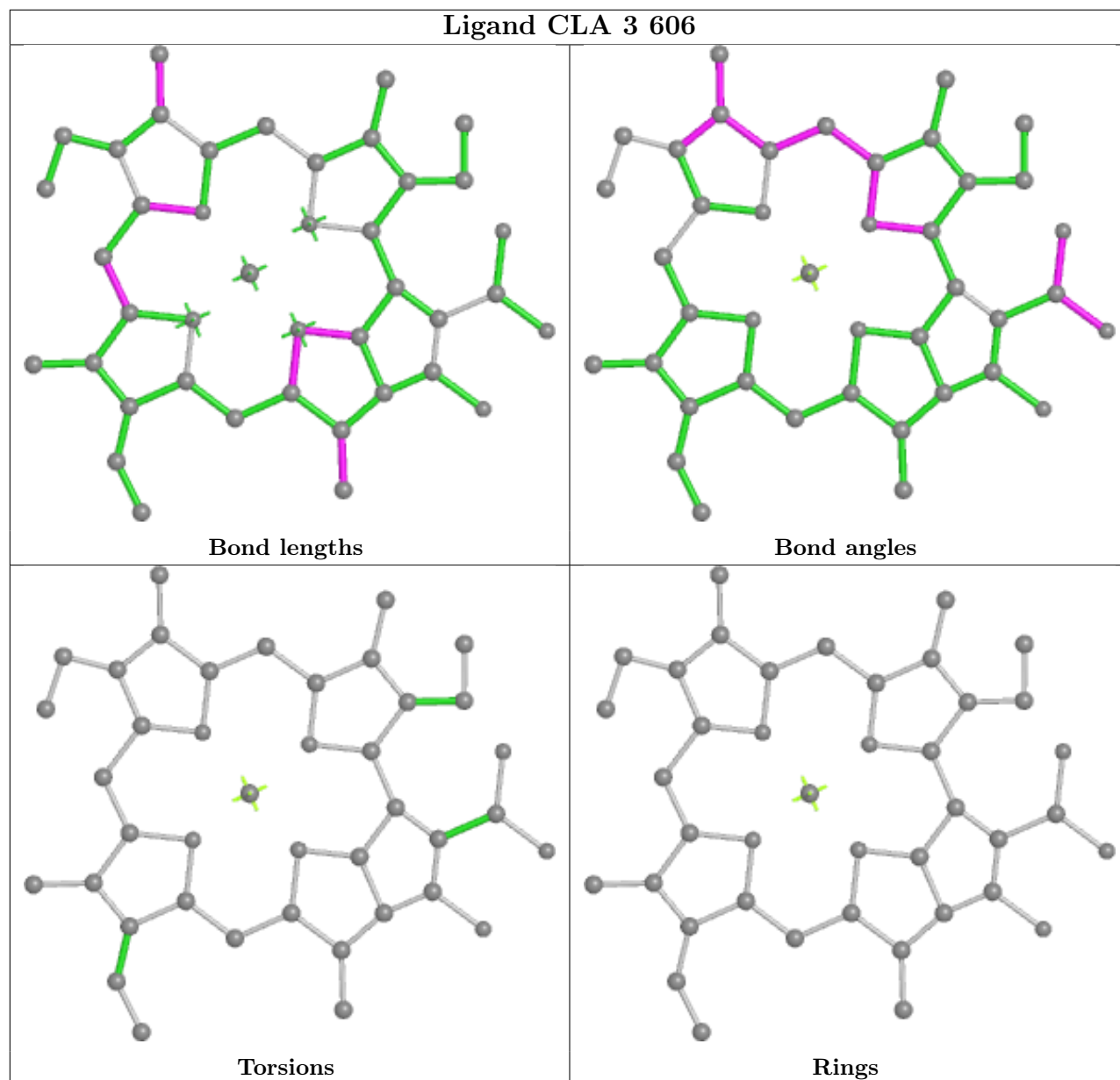


Torsions

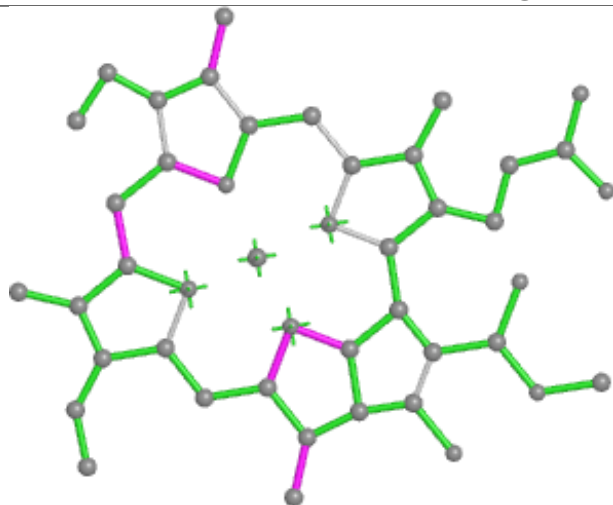


Rings

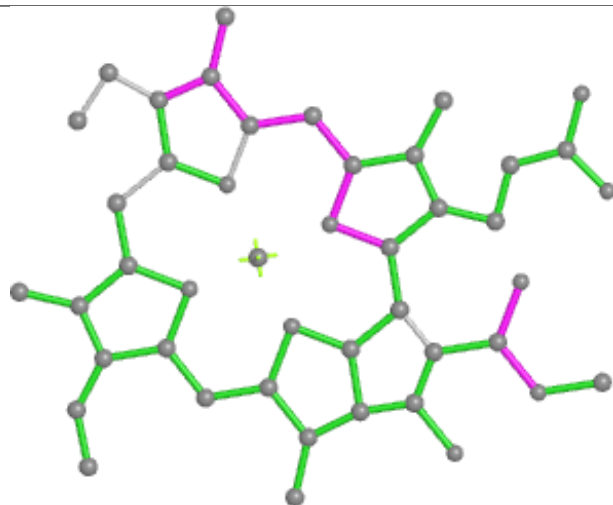
## Ligand CLA 3 606



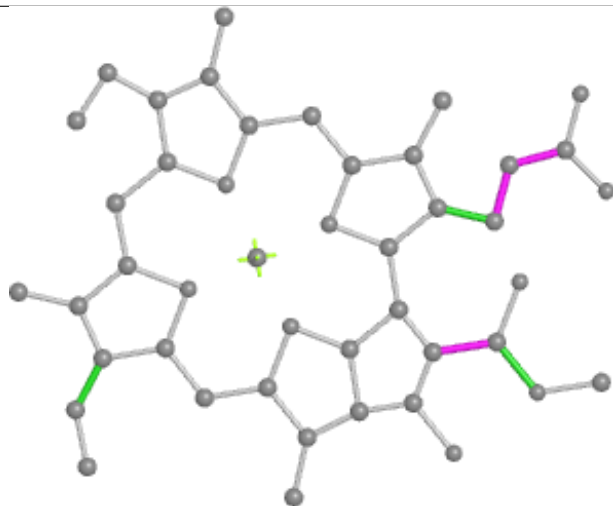
## Ligand CLA F 305



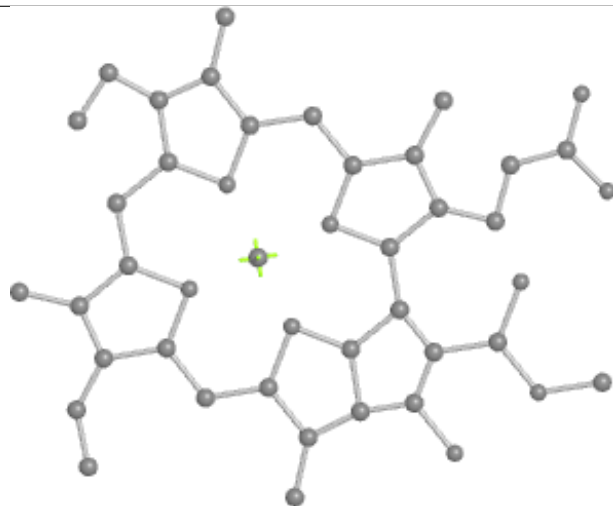
Bond lengths



Bond angles

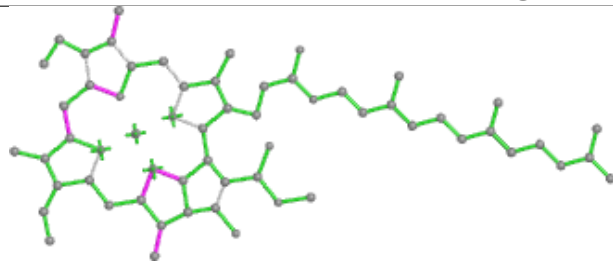


Torsions

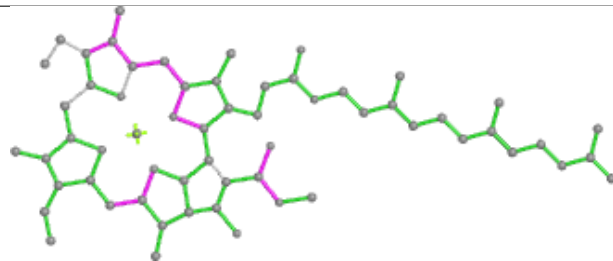


Rings

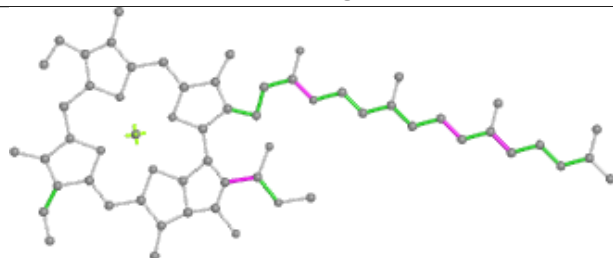
## Ligand CLA B 836



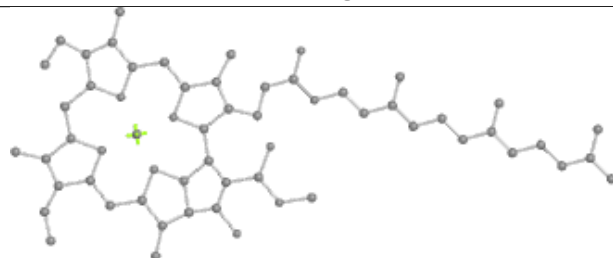
Bond lengths



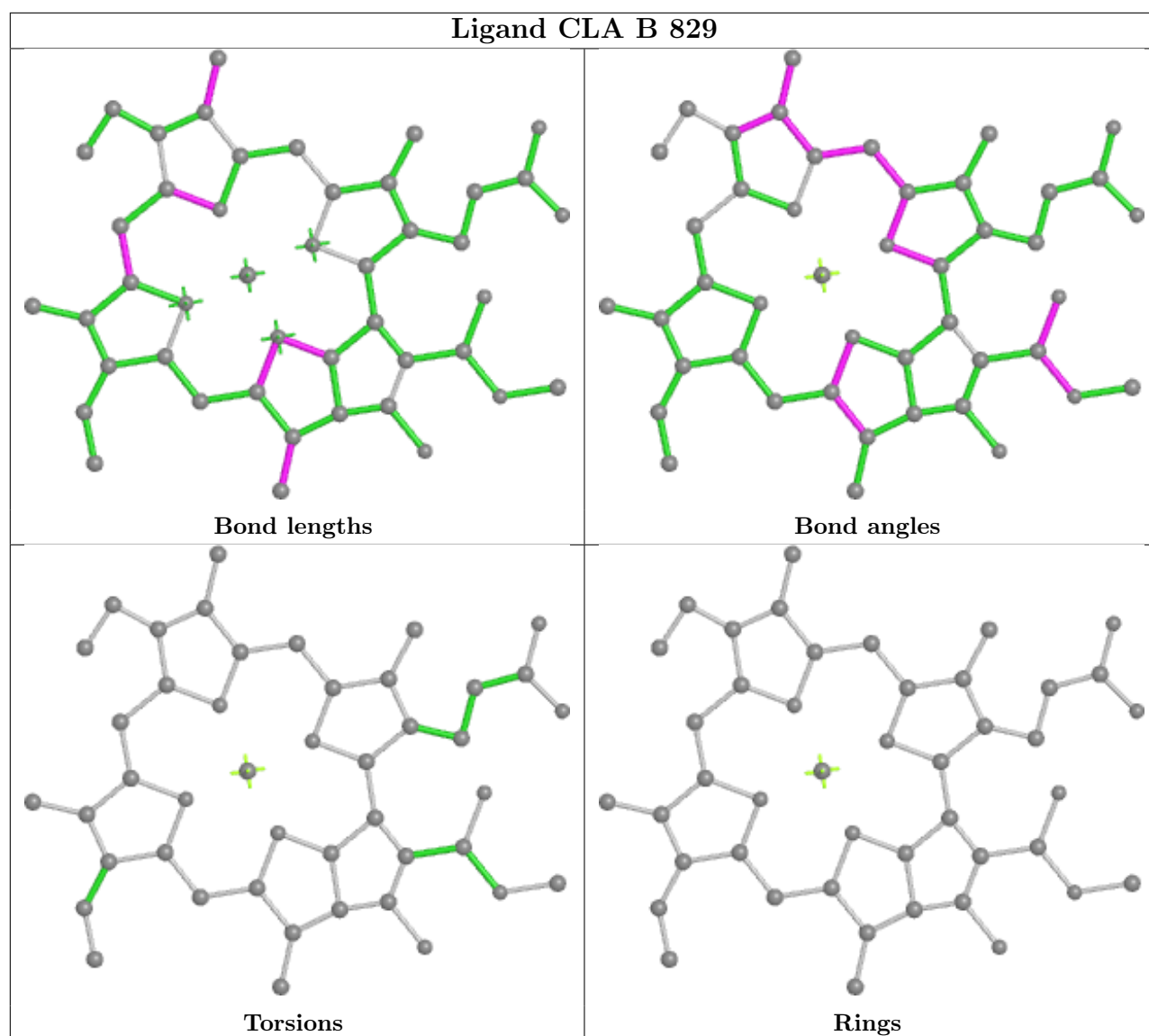
Bond angles

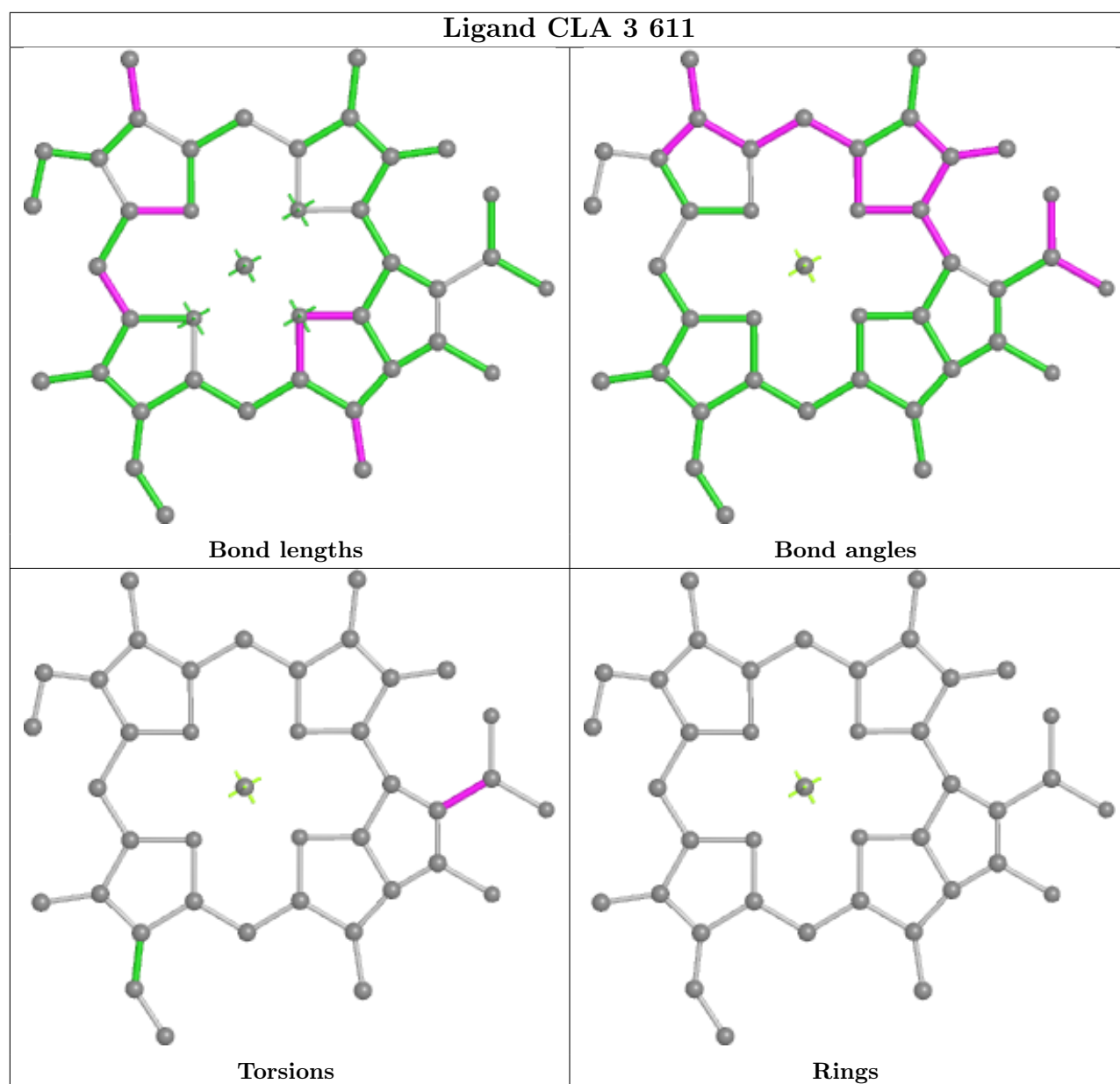


Torsions

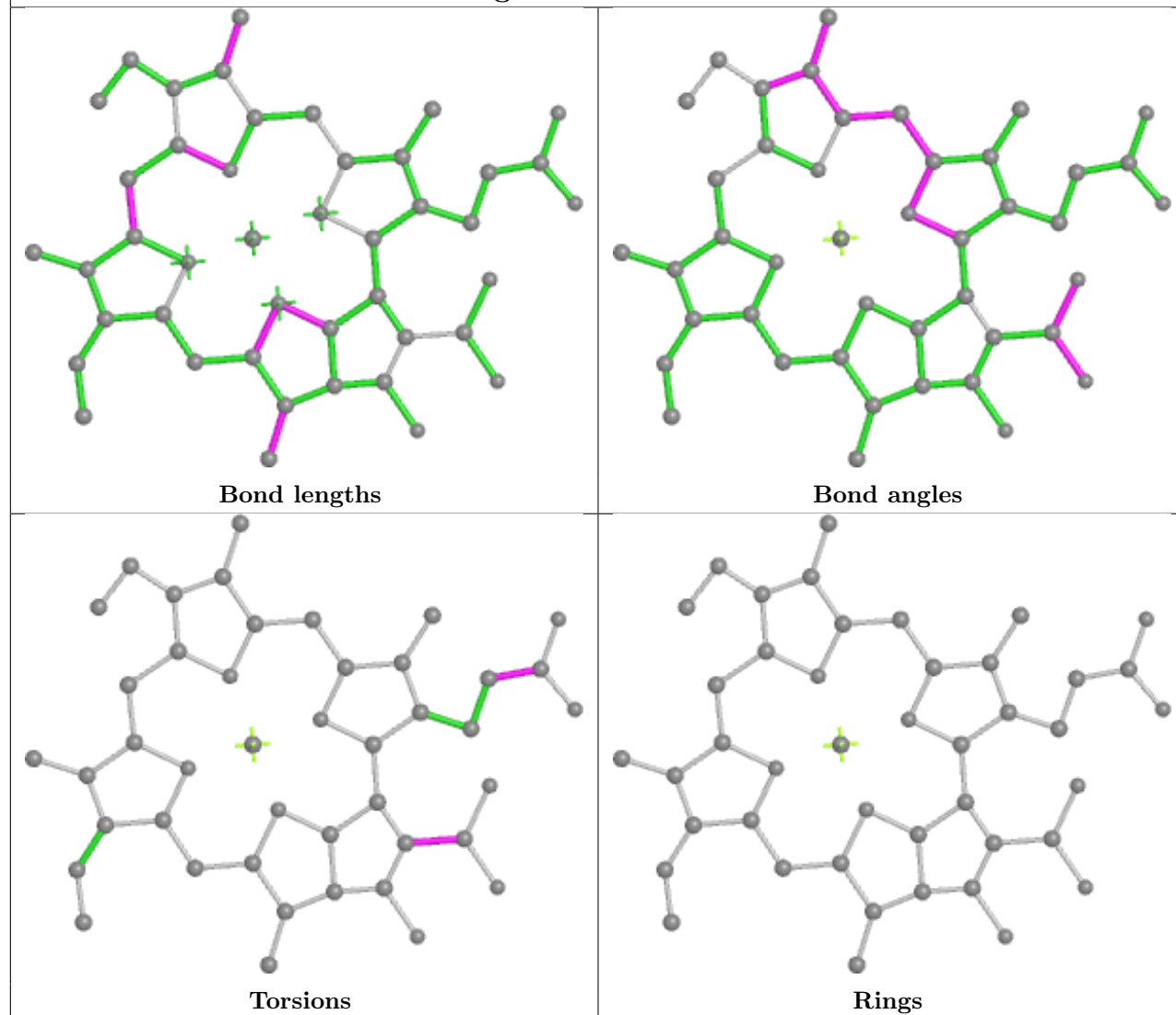


Rings

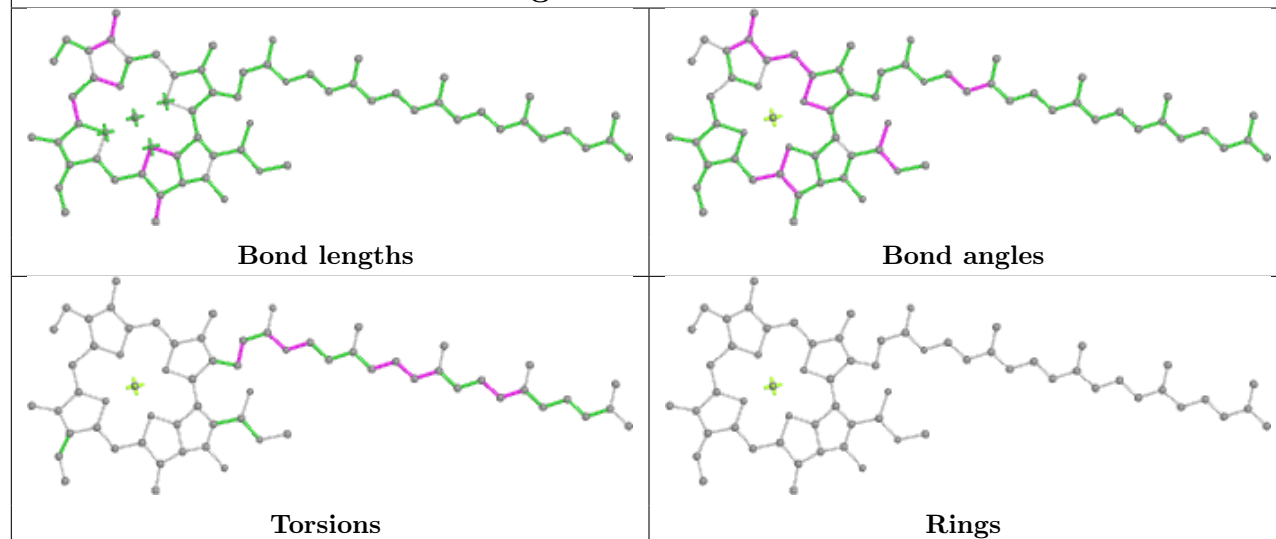




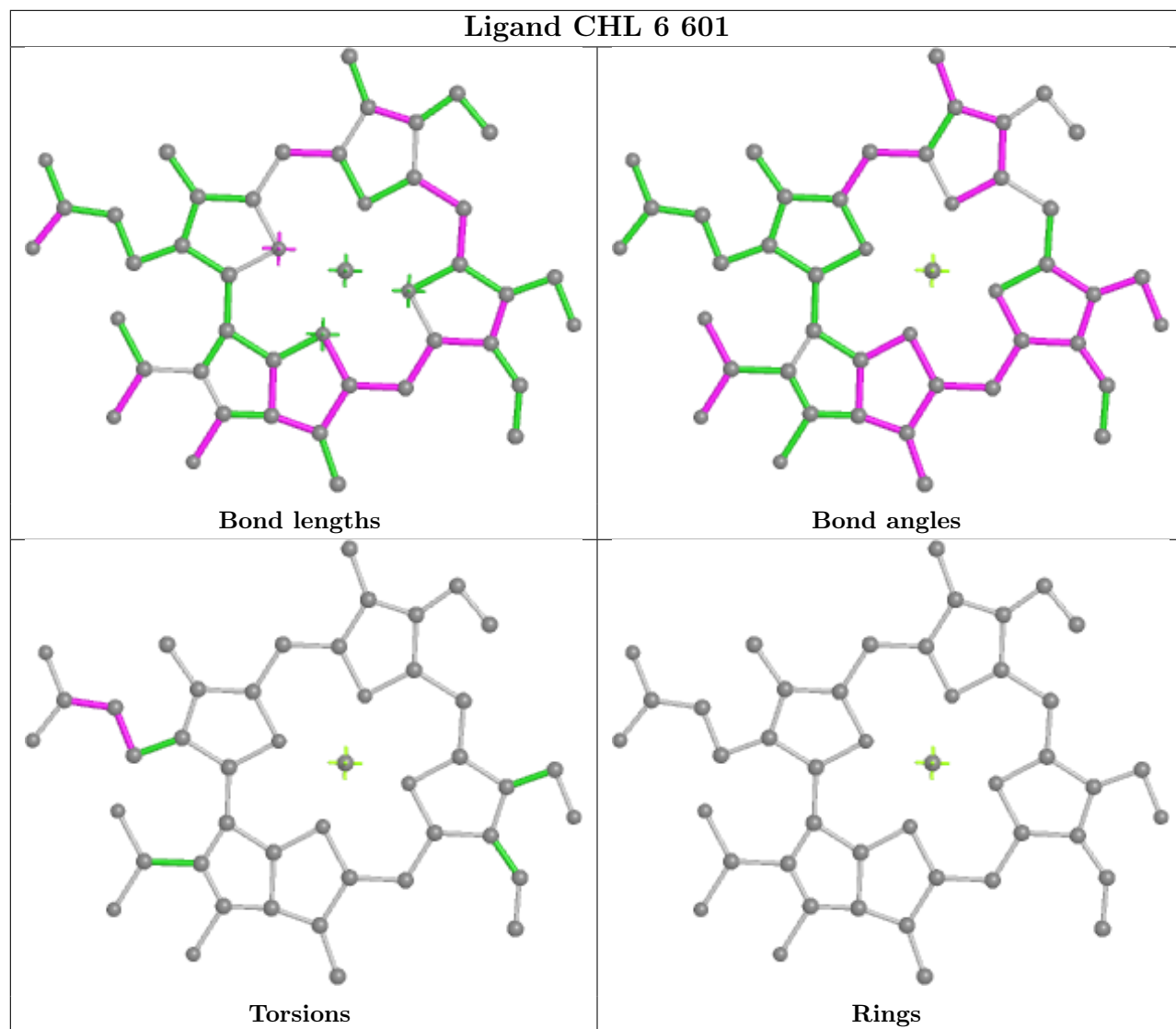
## Ligand CLA 5 603



## Ligand CLA A 843

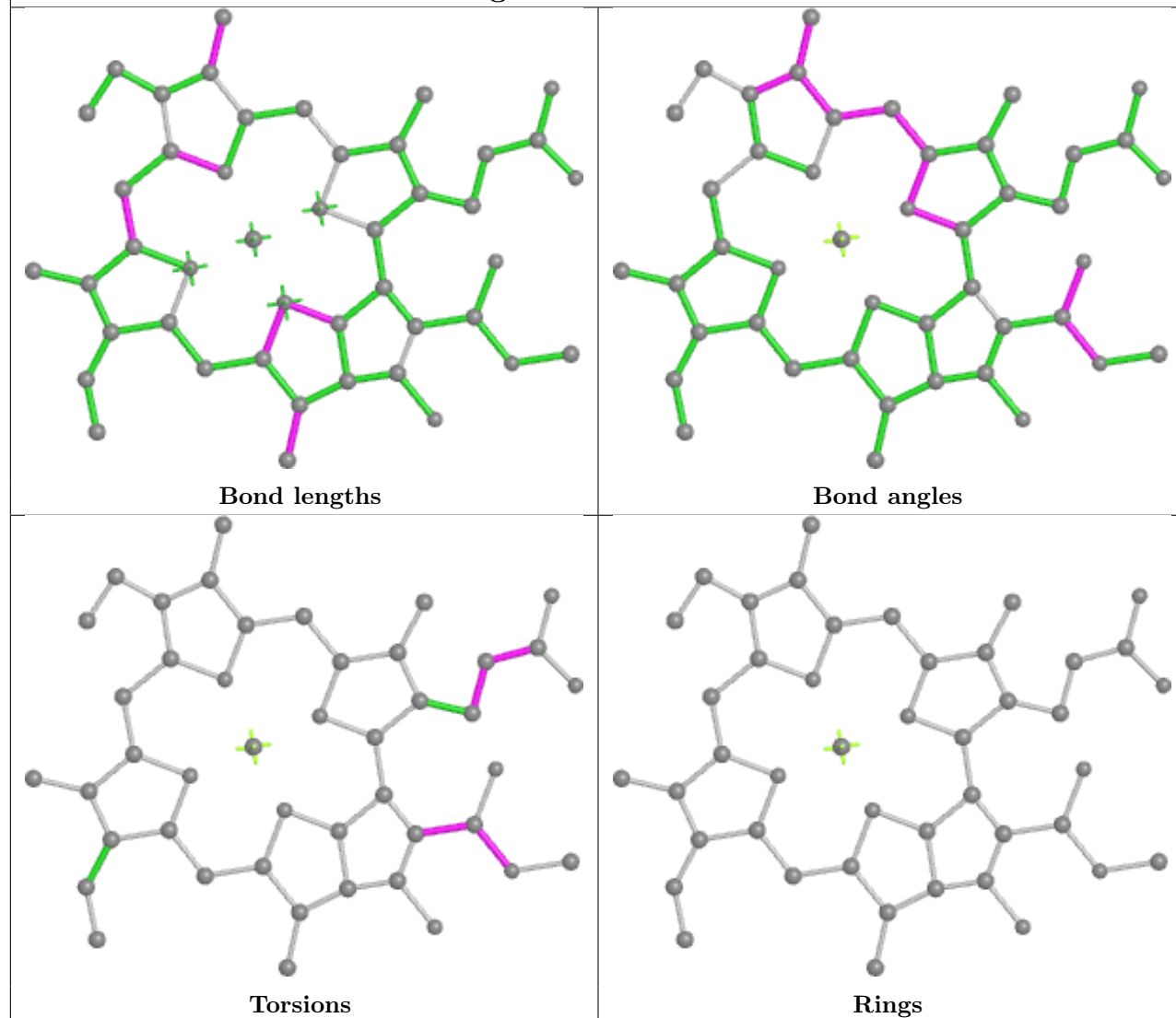


## Ligand CHL 6 601

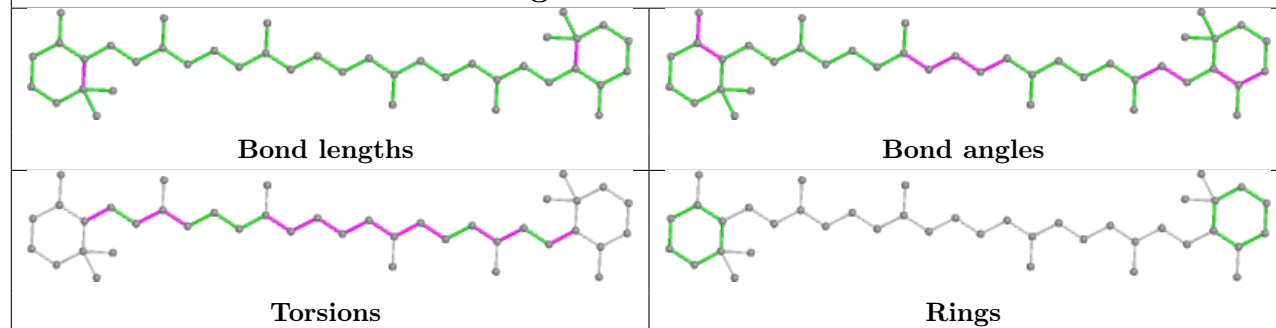


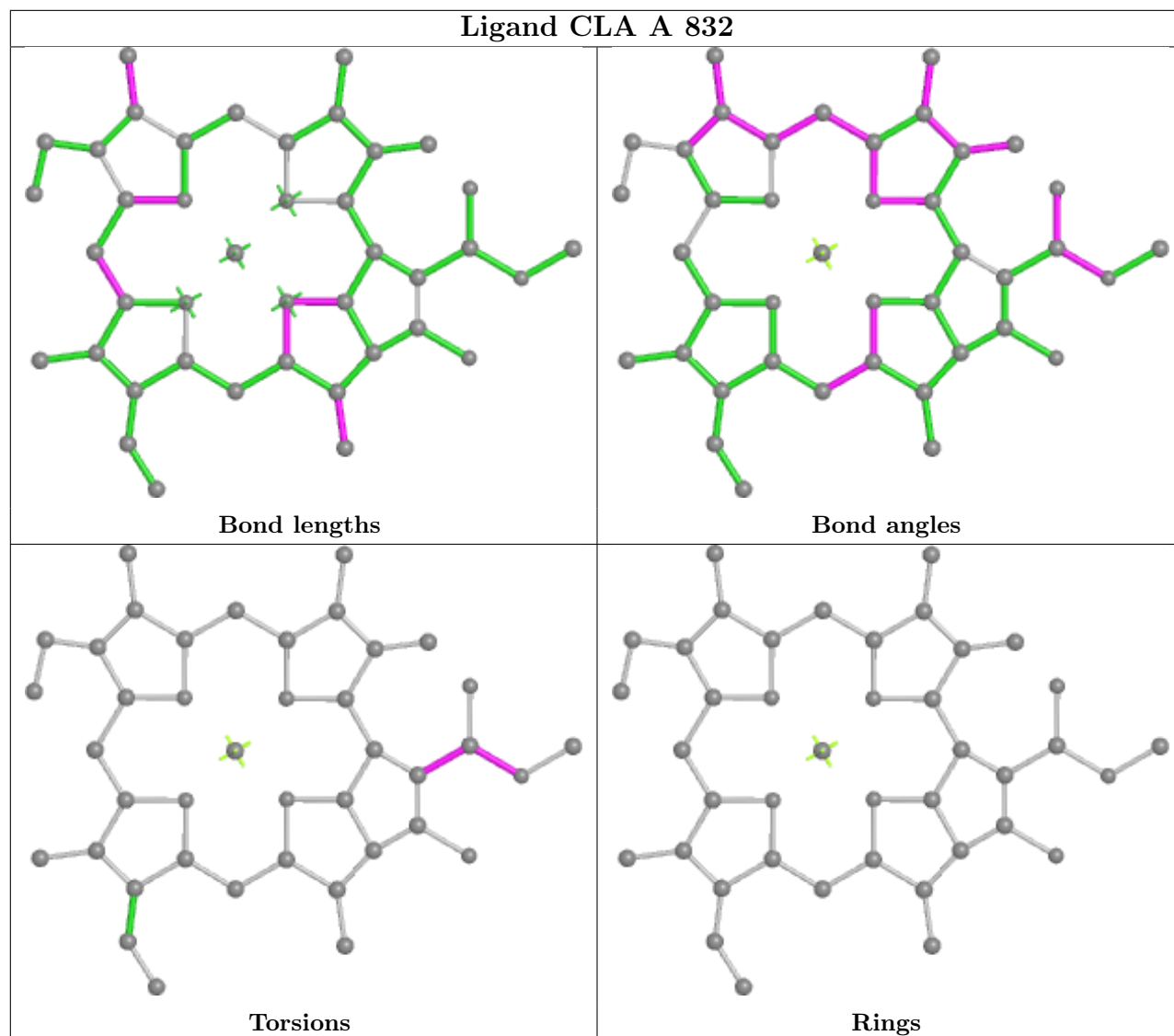
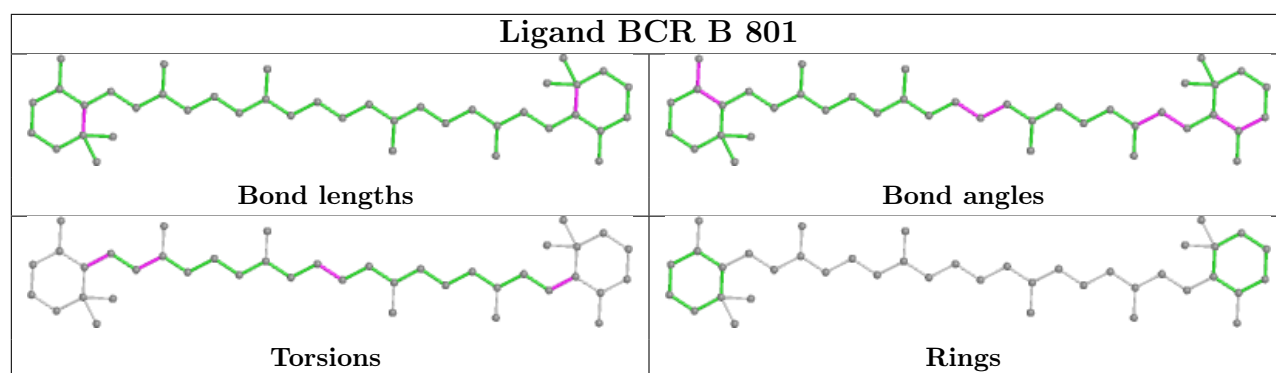


## Ligand CLA A 802

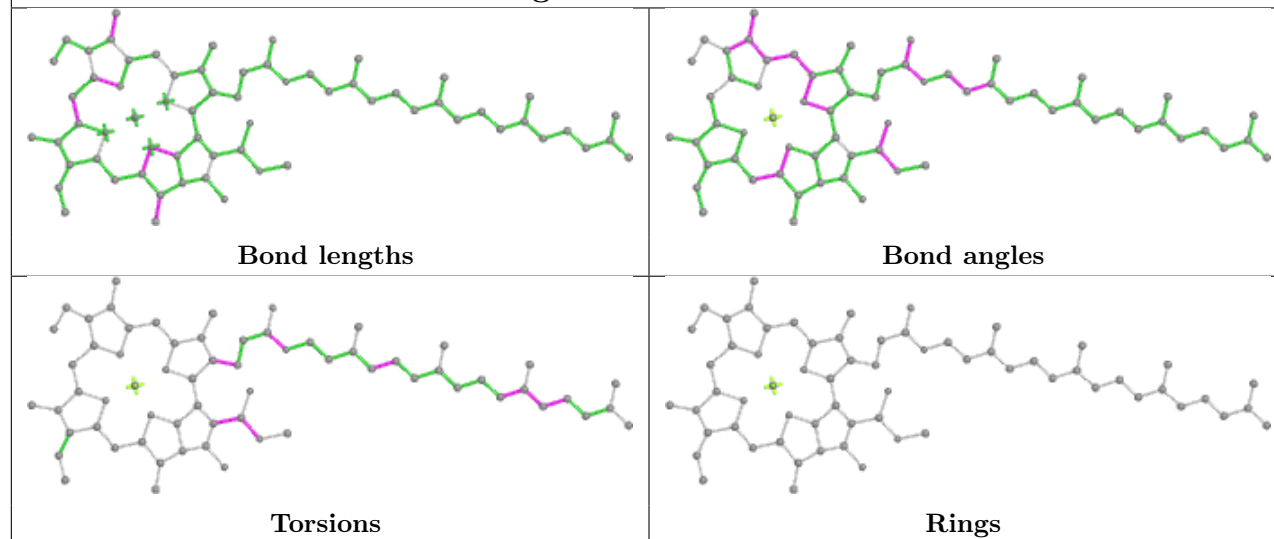


## Ligand BCR B 845

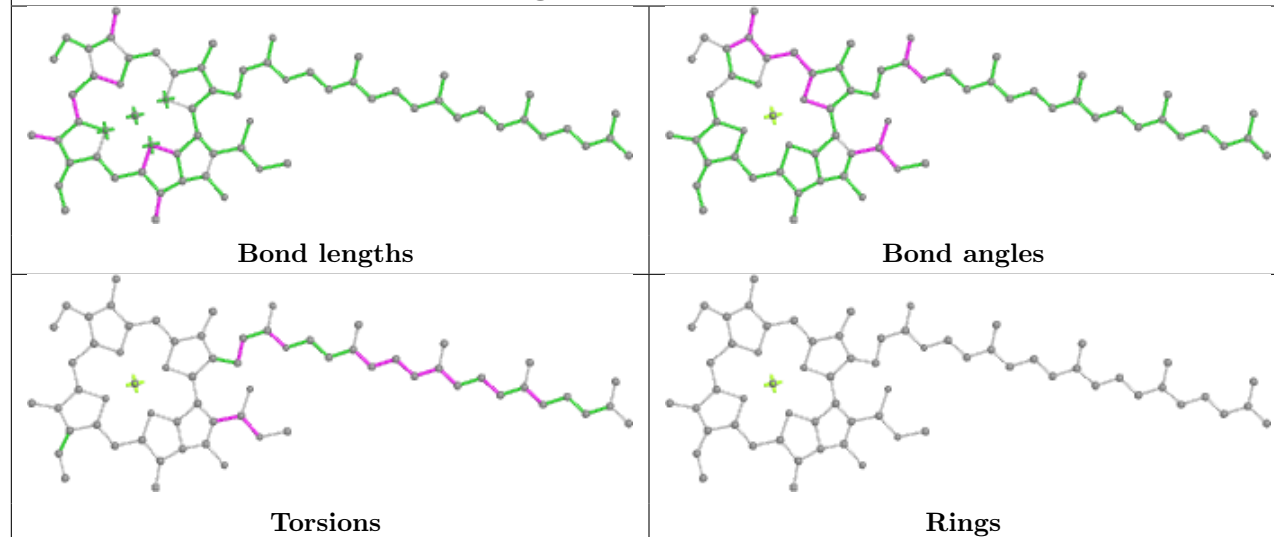




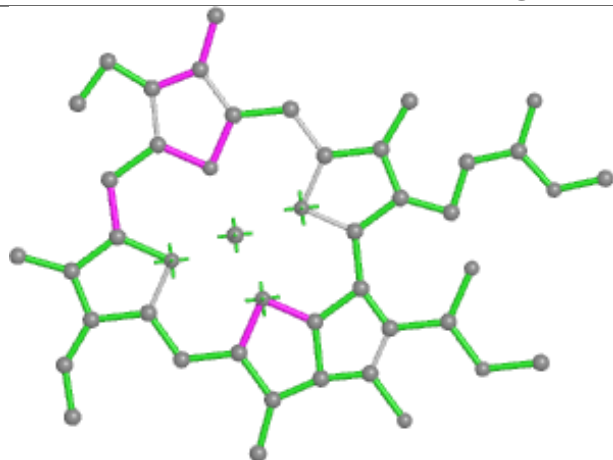
## Ligand CLA B 841



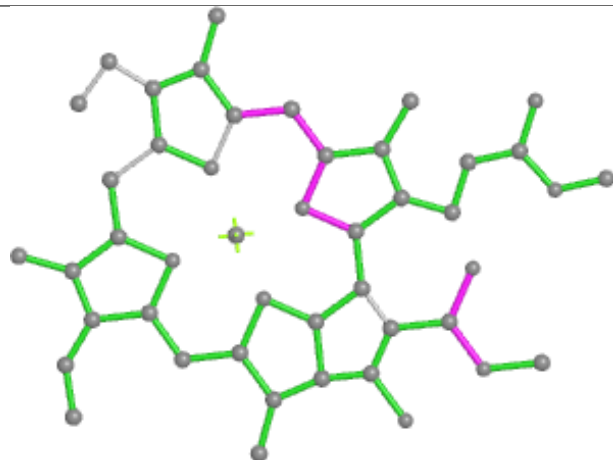
## Ligand CLA A 818



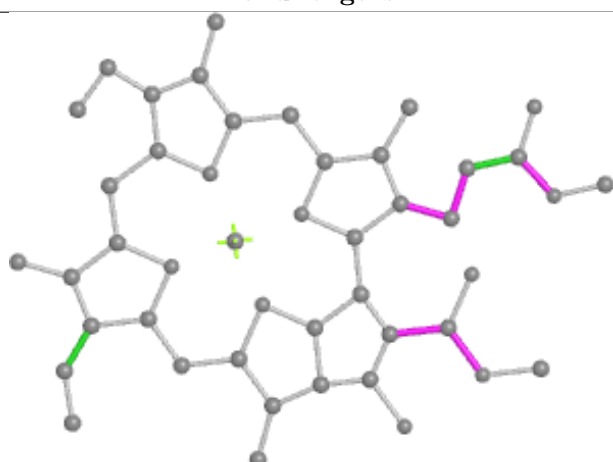
## Ligand CLA K 201



Bond lengths



Bond angles

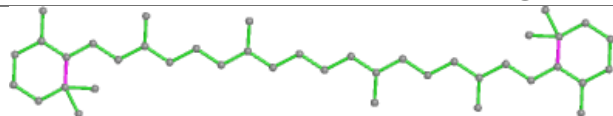


Torsions

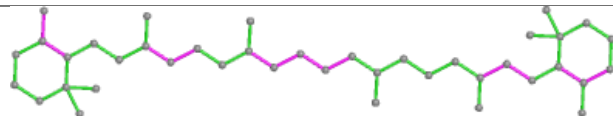


Rings

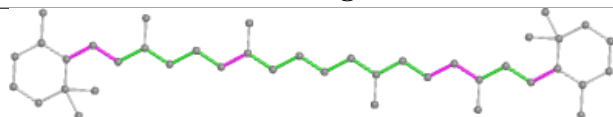
## Ligand BCR 2 621



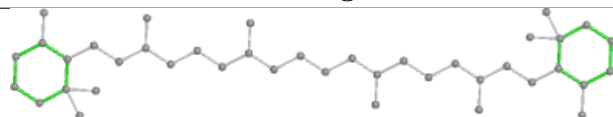
Bond lengths



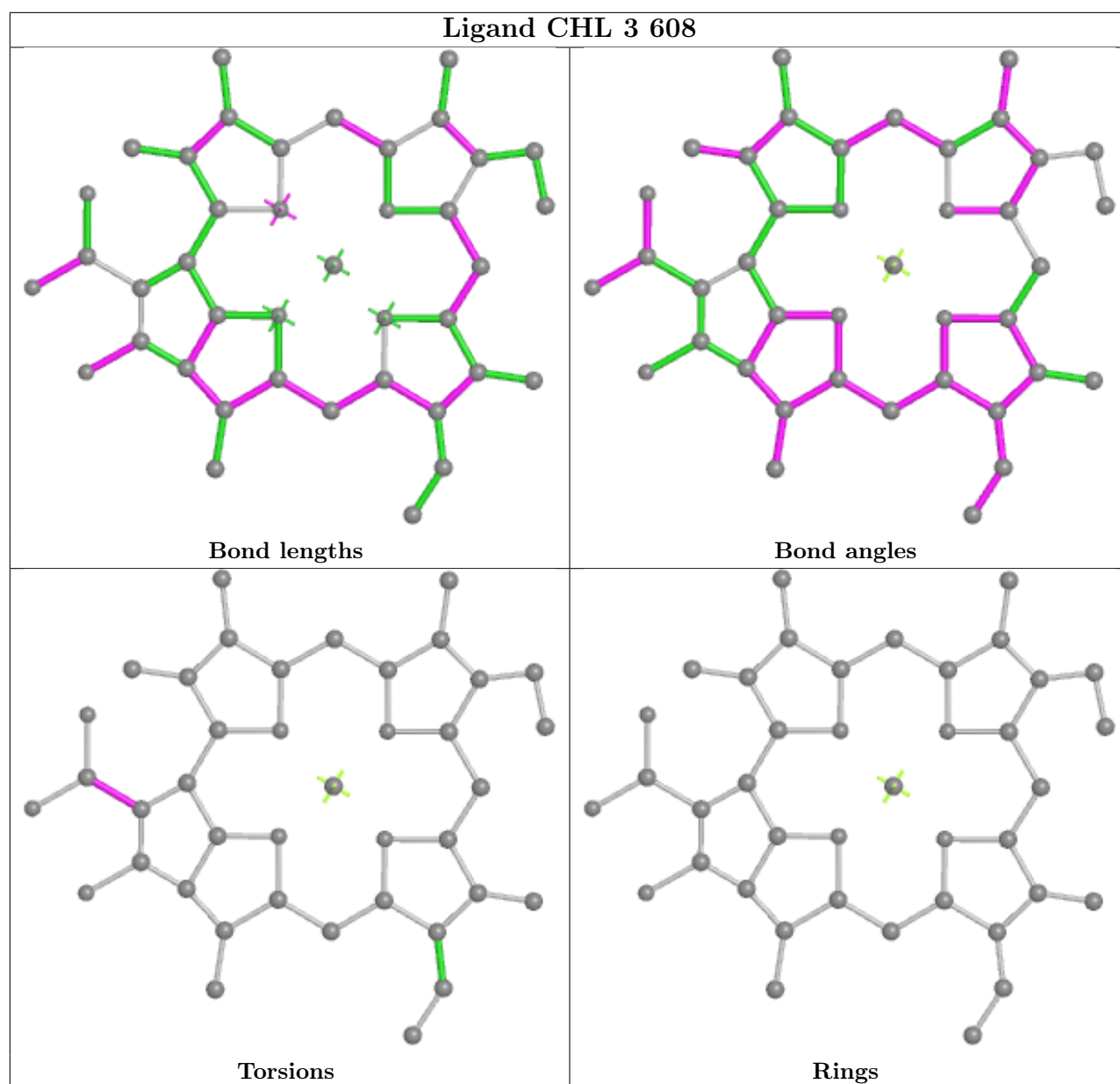
Bond angles

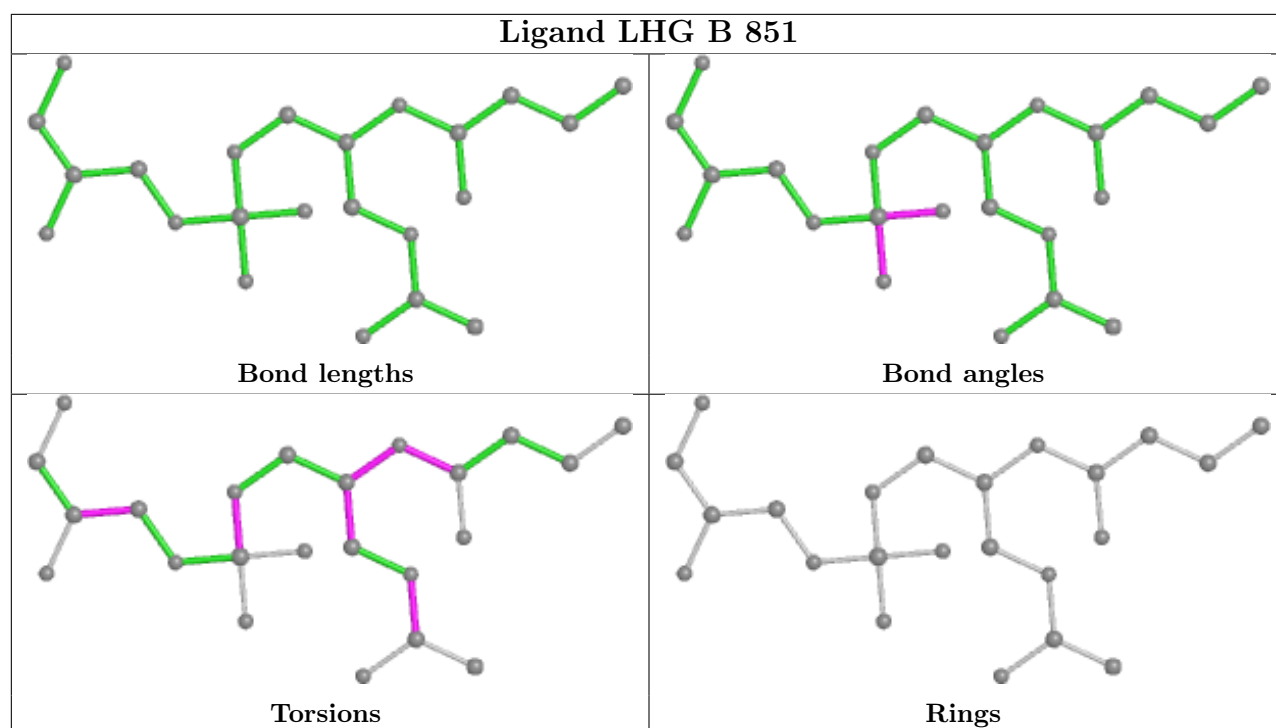


Torsions

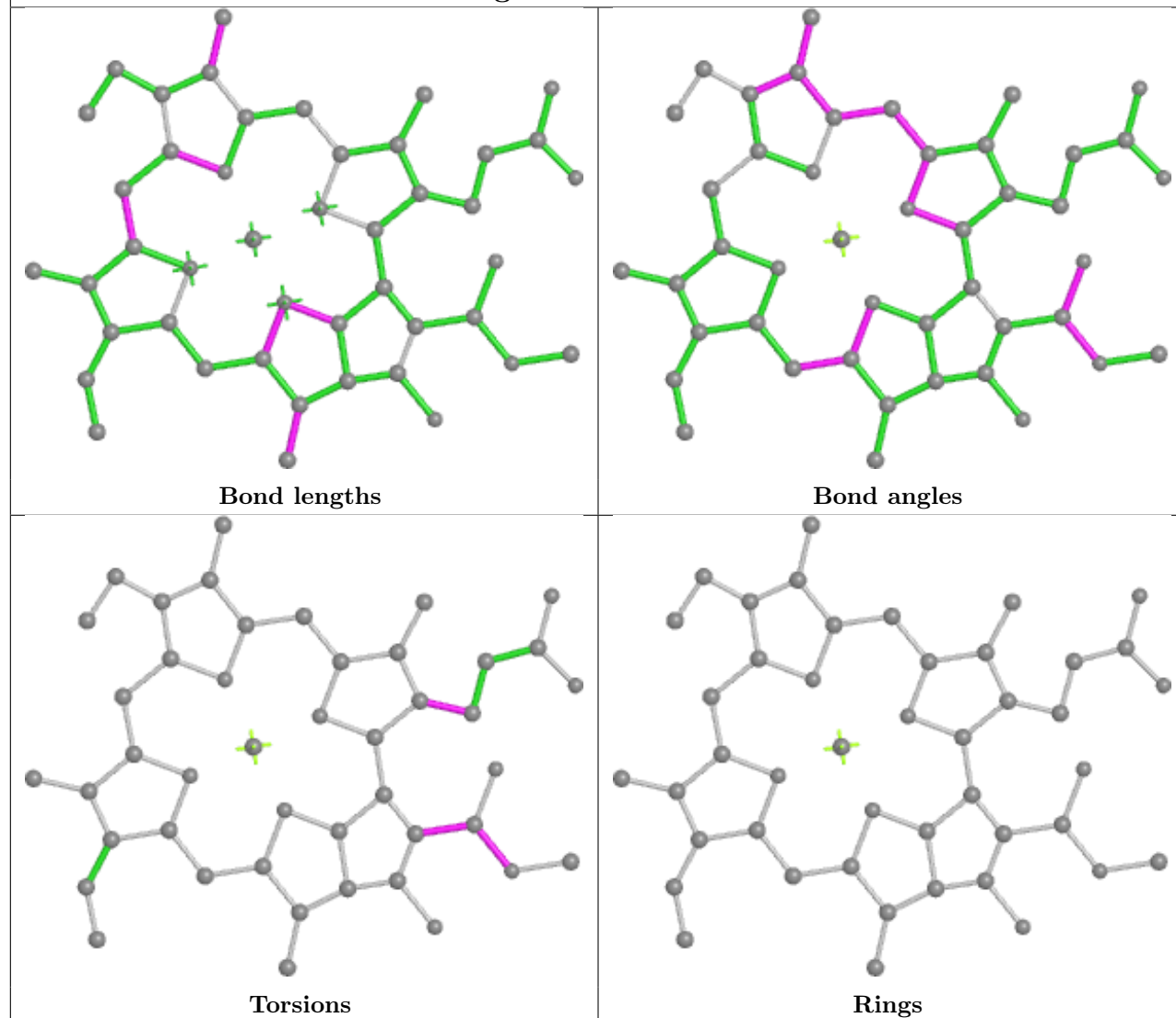


Rings

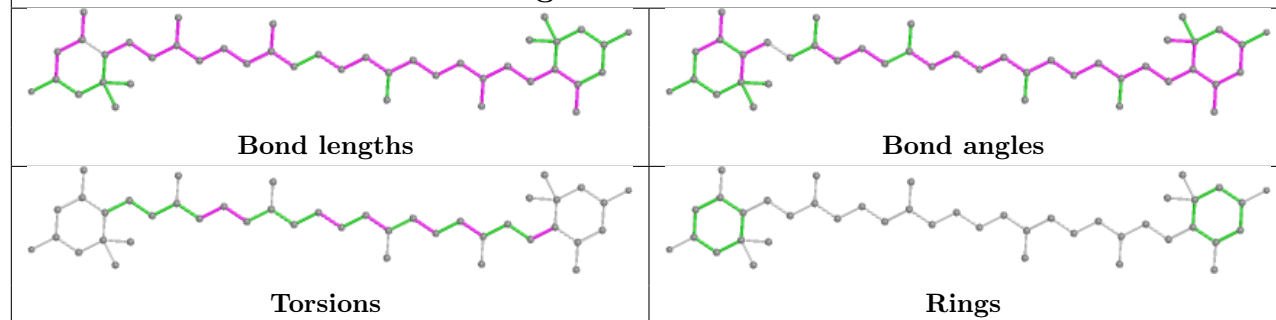




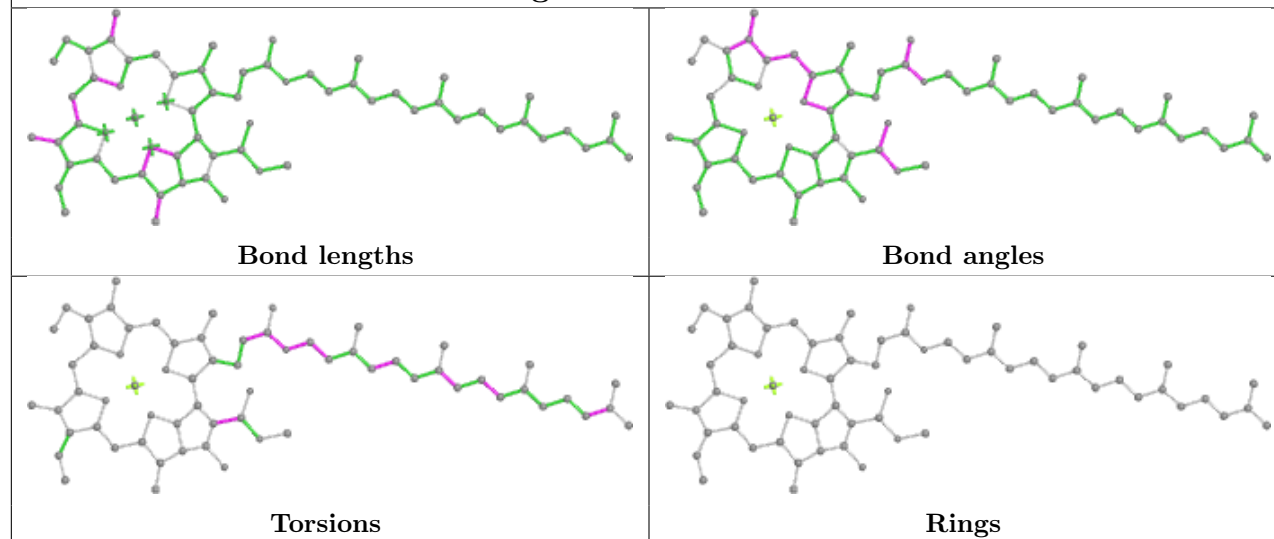
## Ligand CLA 2 602



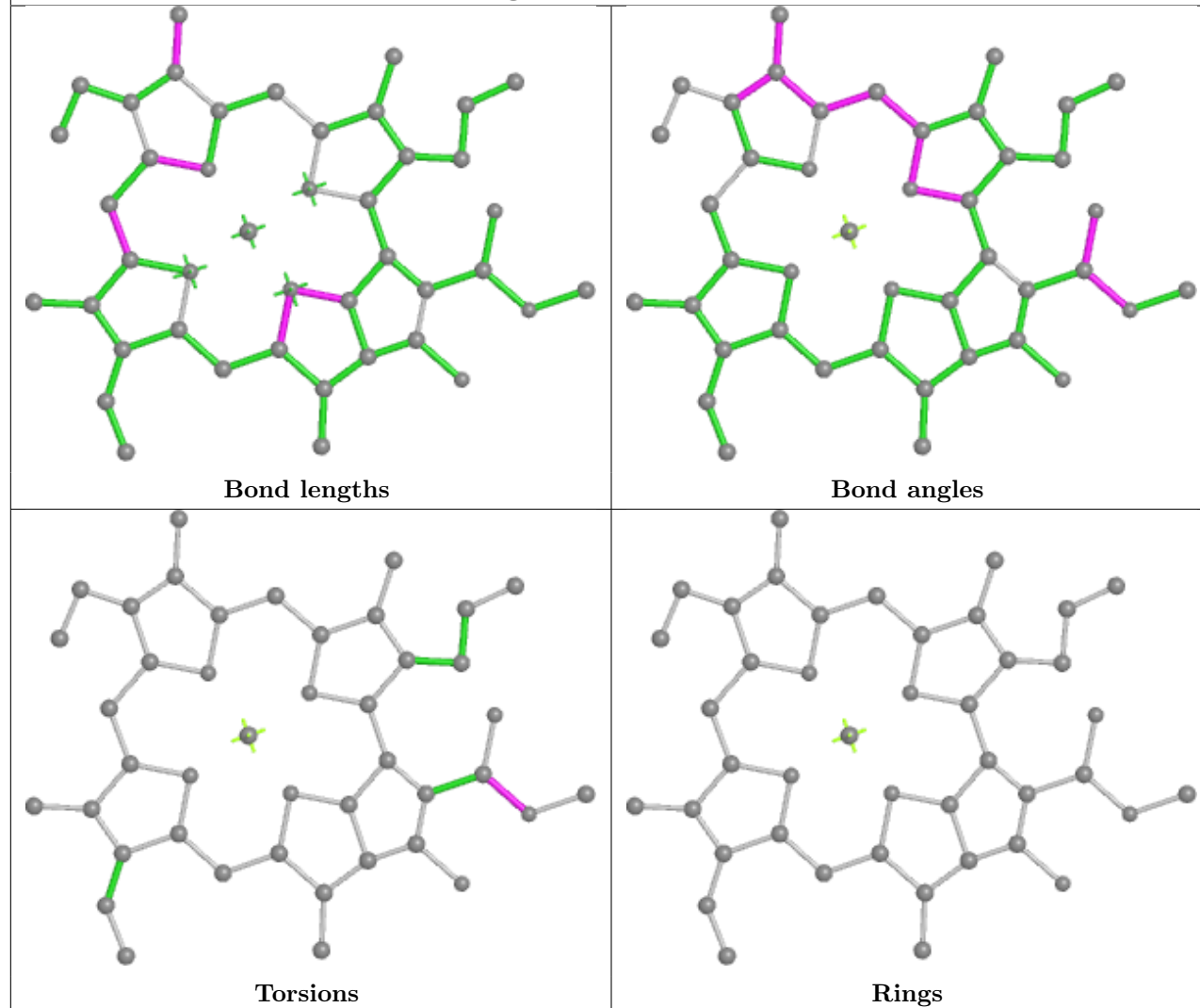
## Ligand LUT 5 619



## Ligand CLA A 806

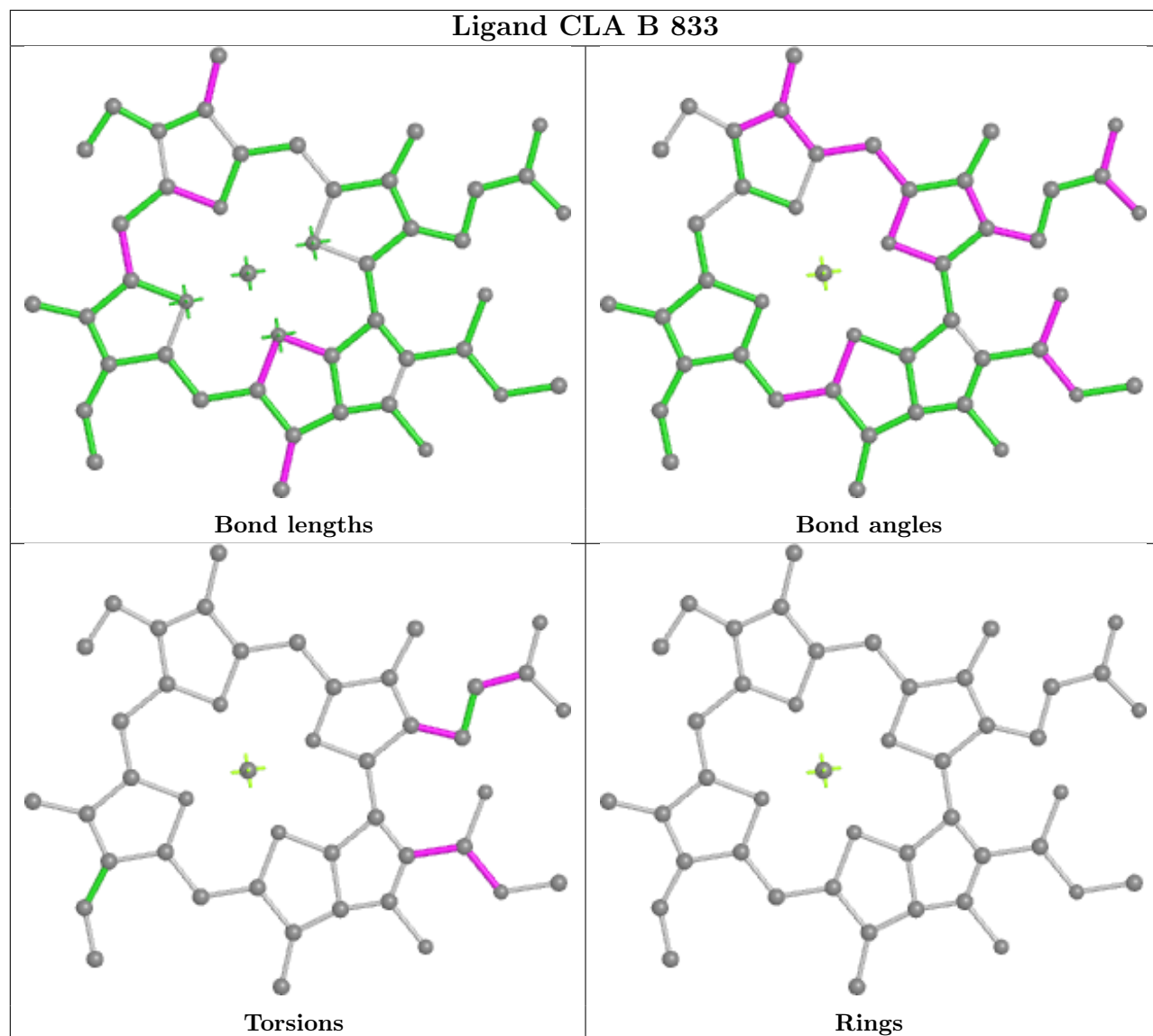


## Ligand CLA 3 612

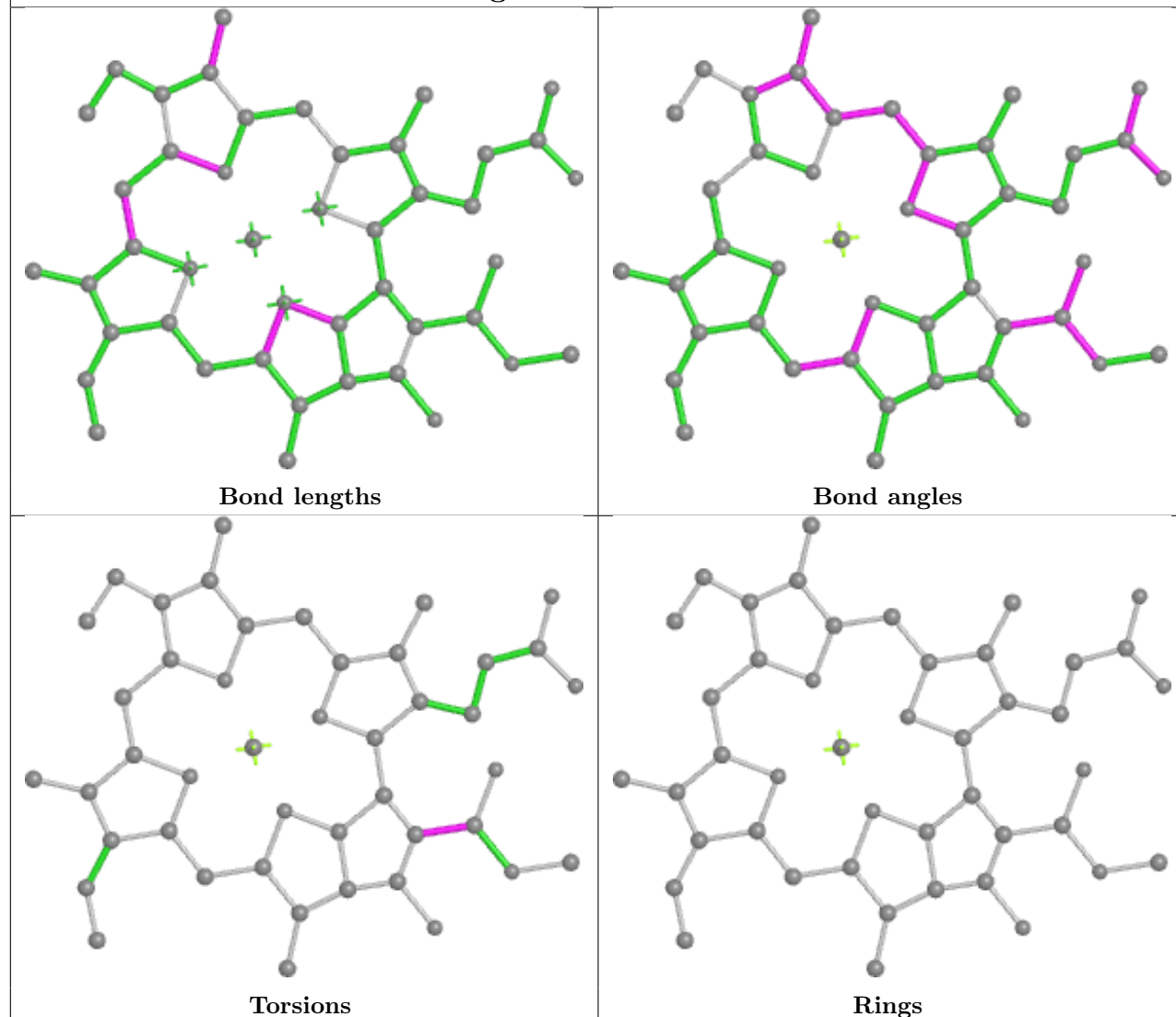




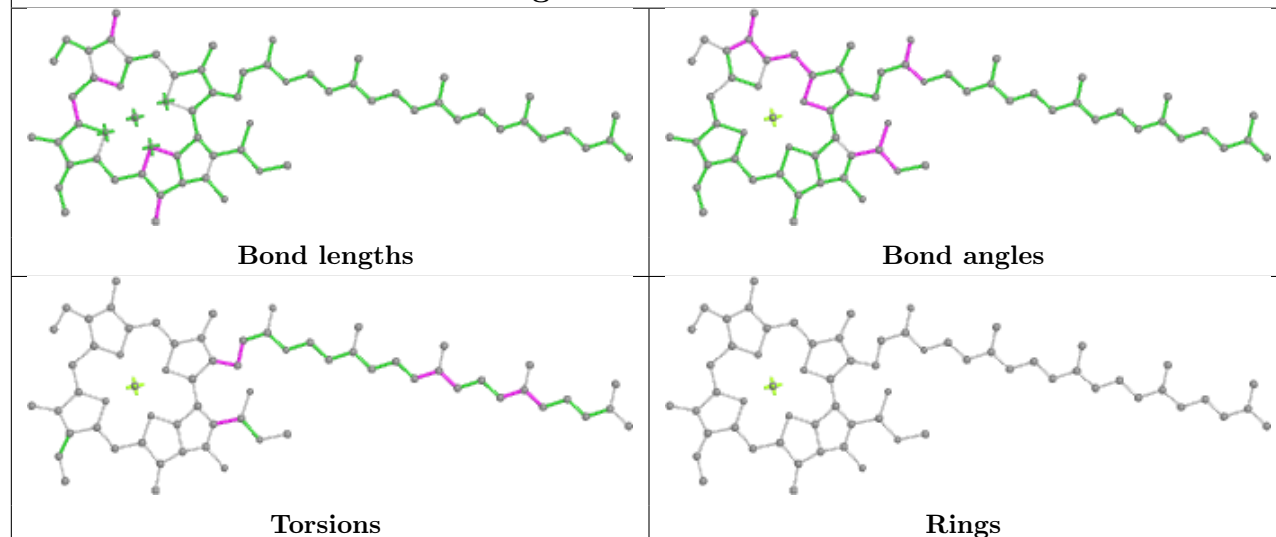
## Ligand CLA B 833



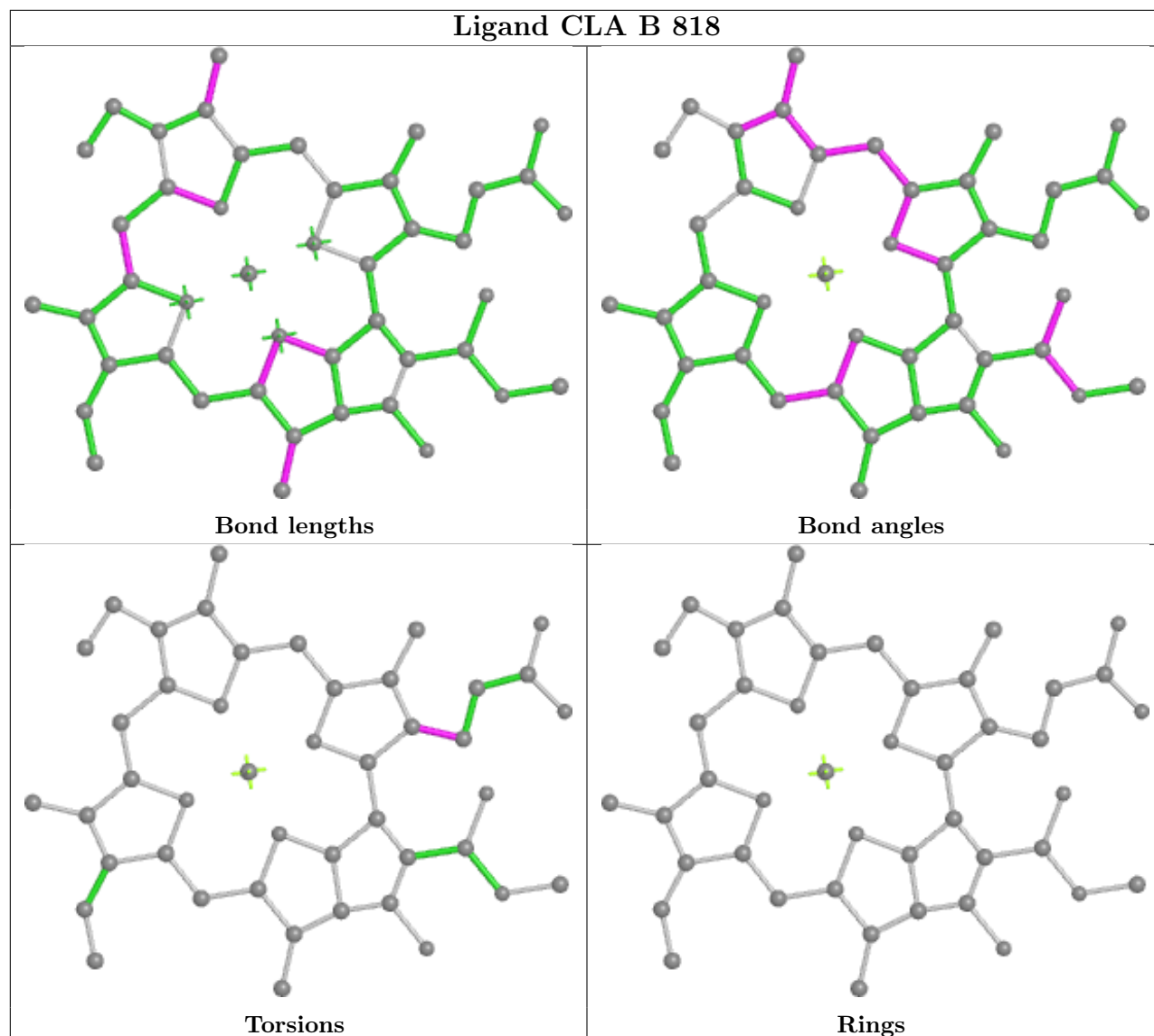
## Ligand CLA A 837



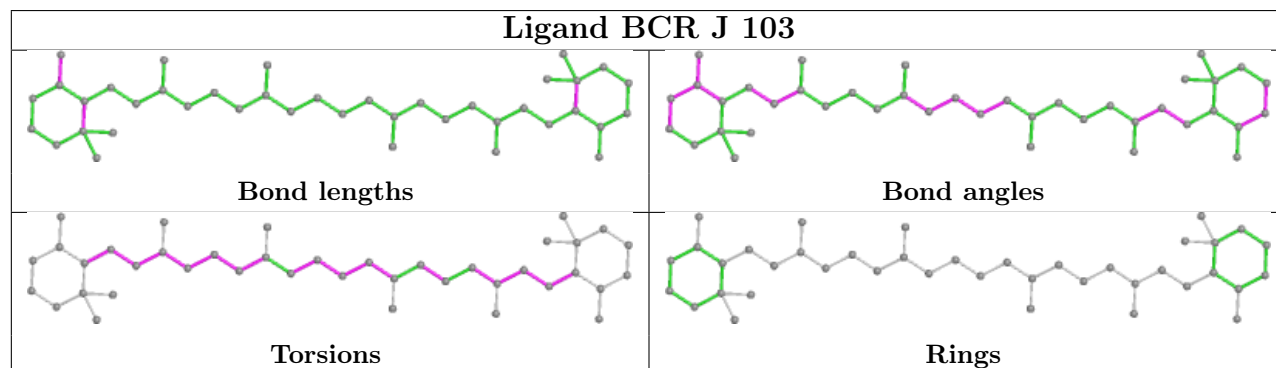
## Ligand CLA B 805

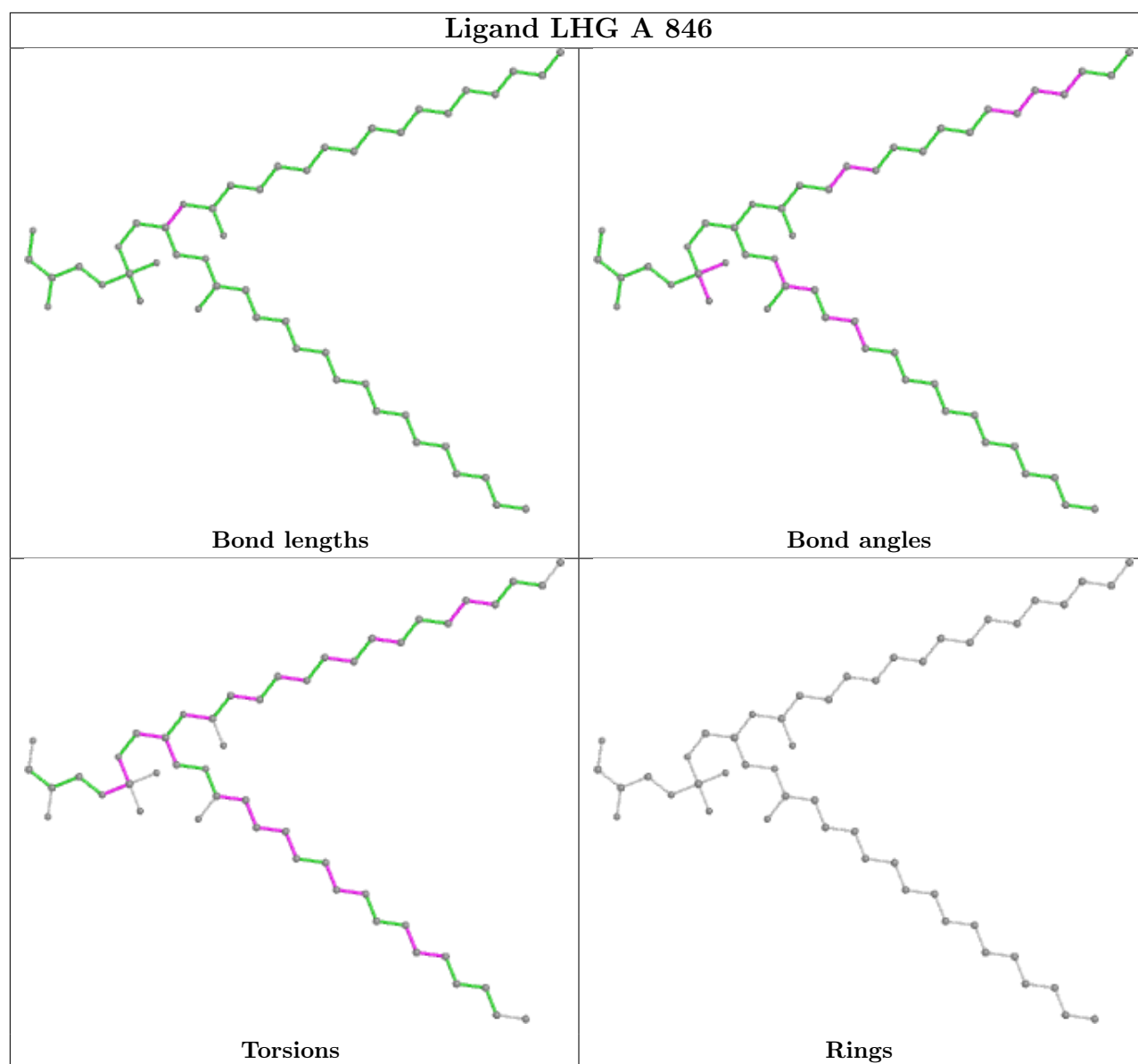


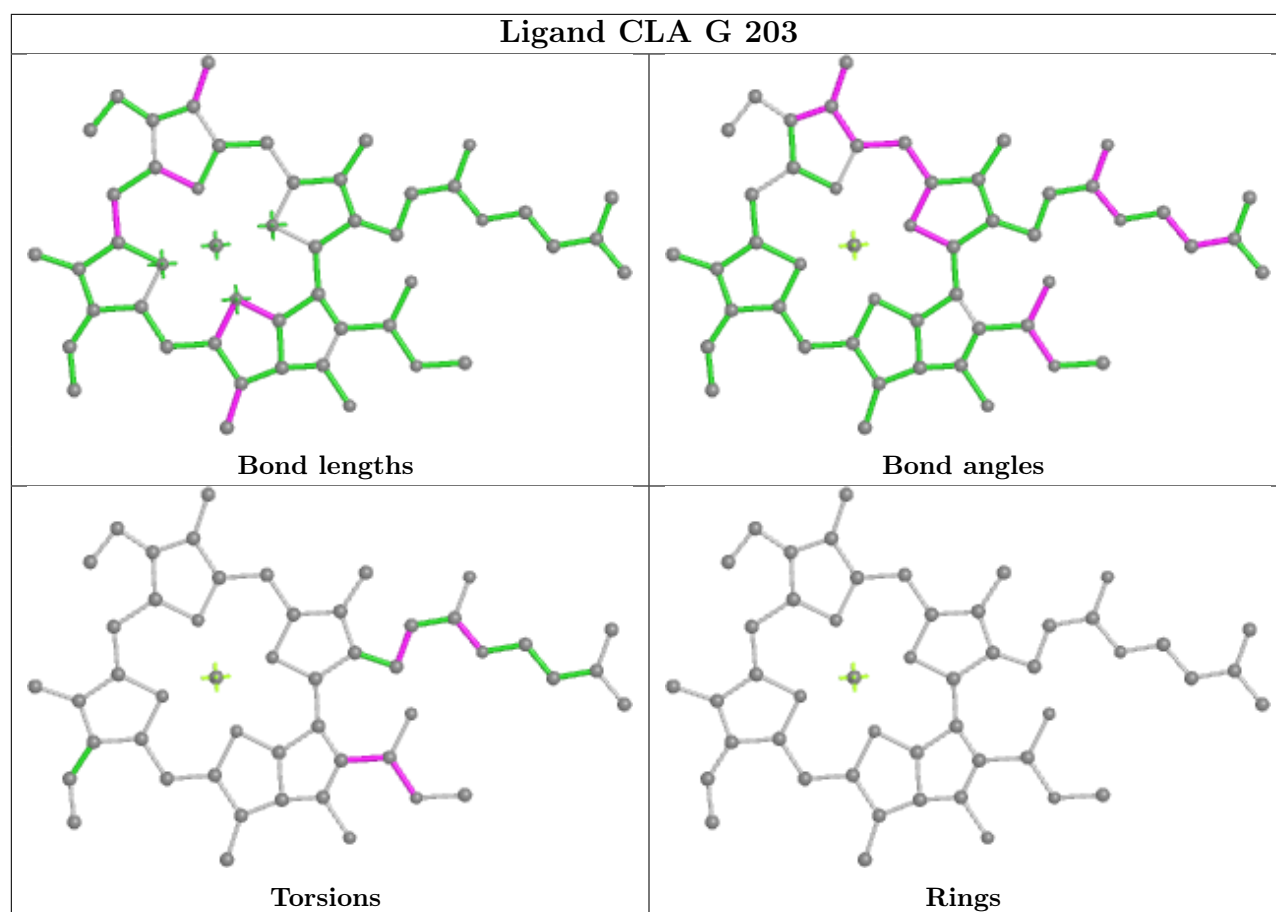
## Ligand CLA B 818

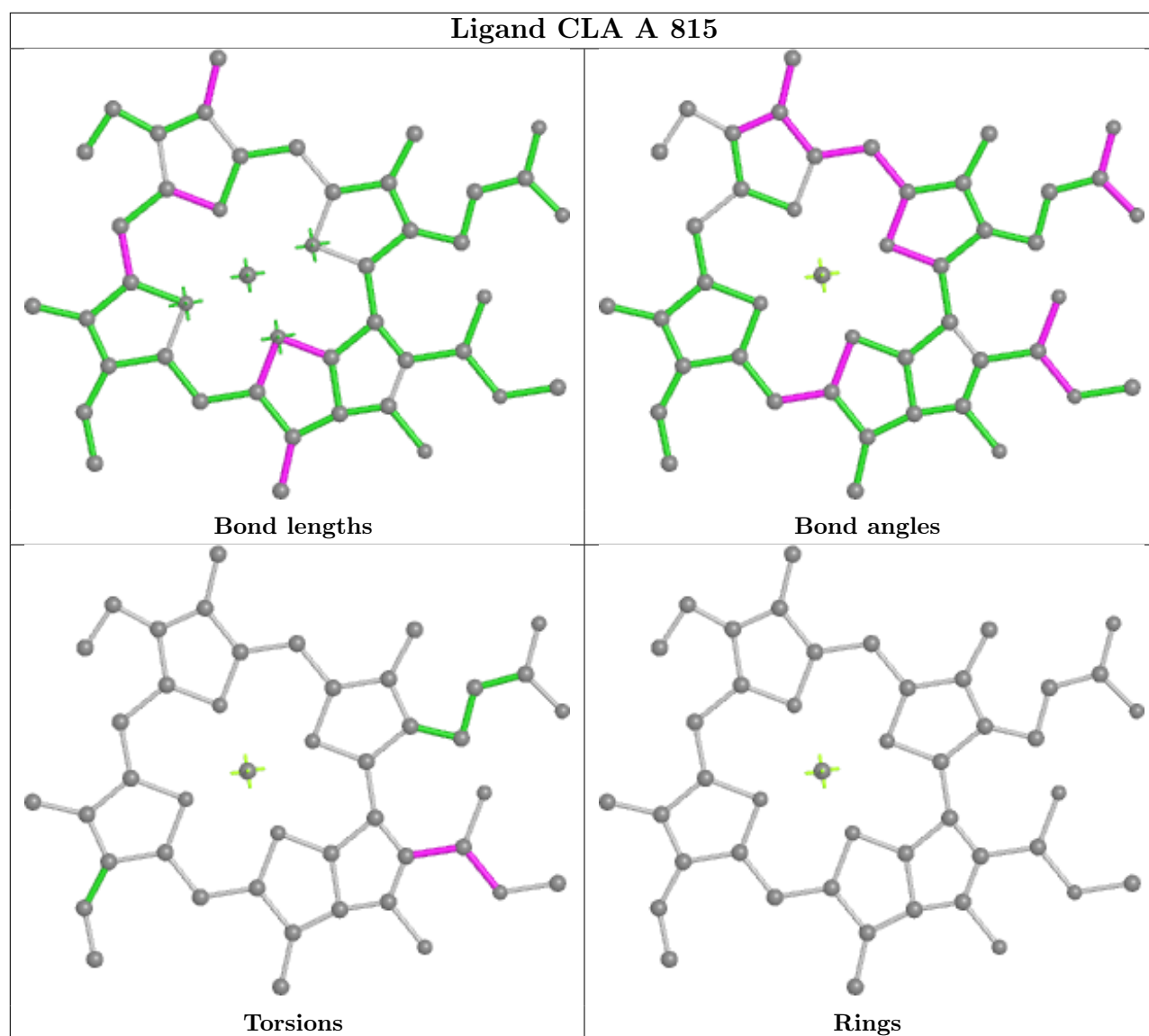


## Ligand BCR J 103

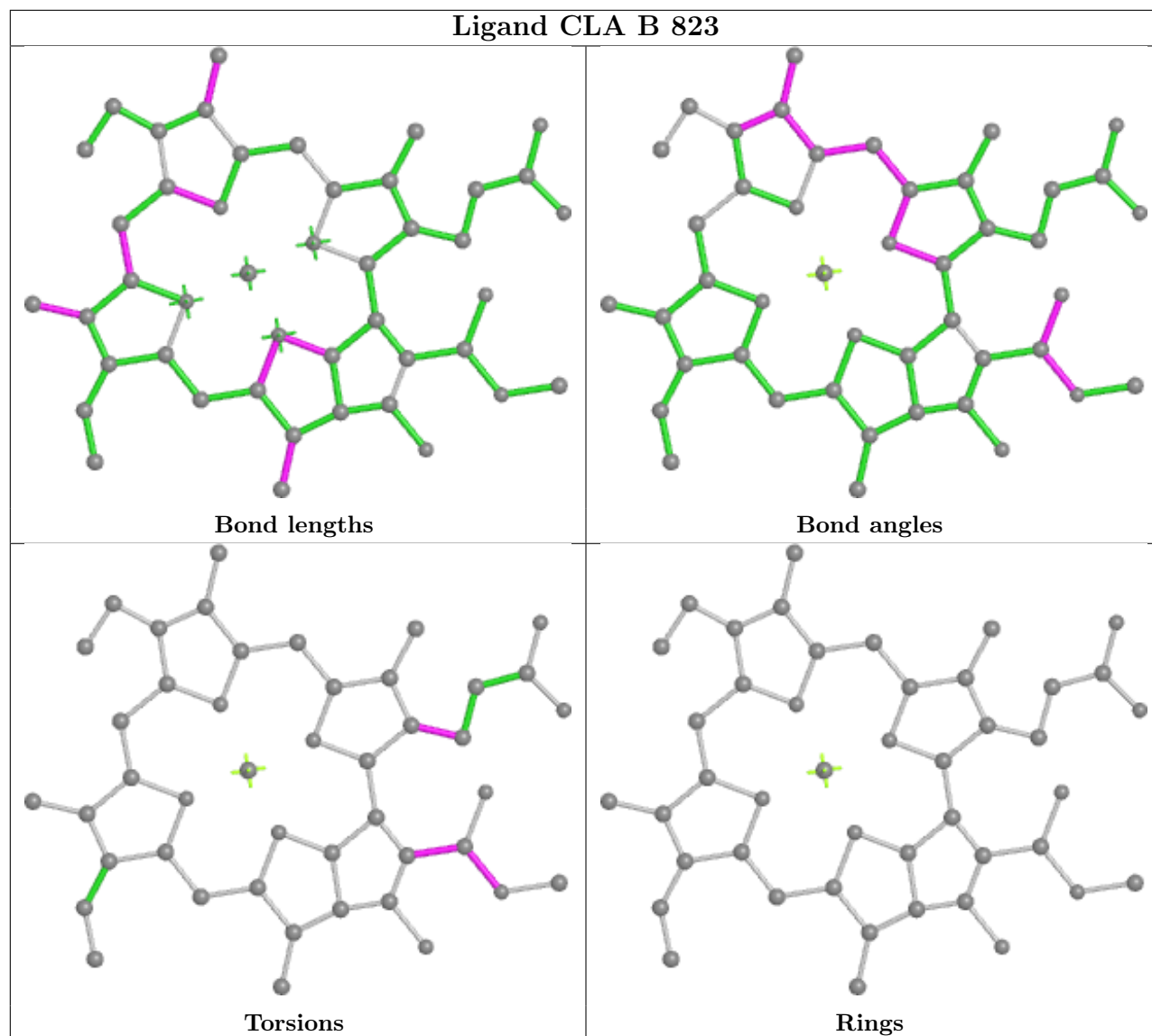




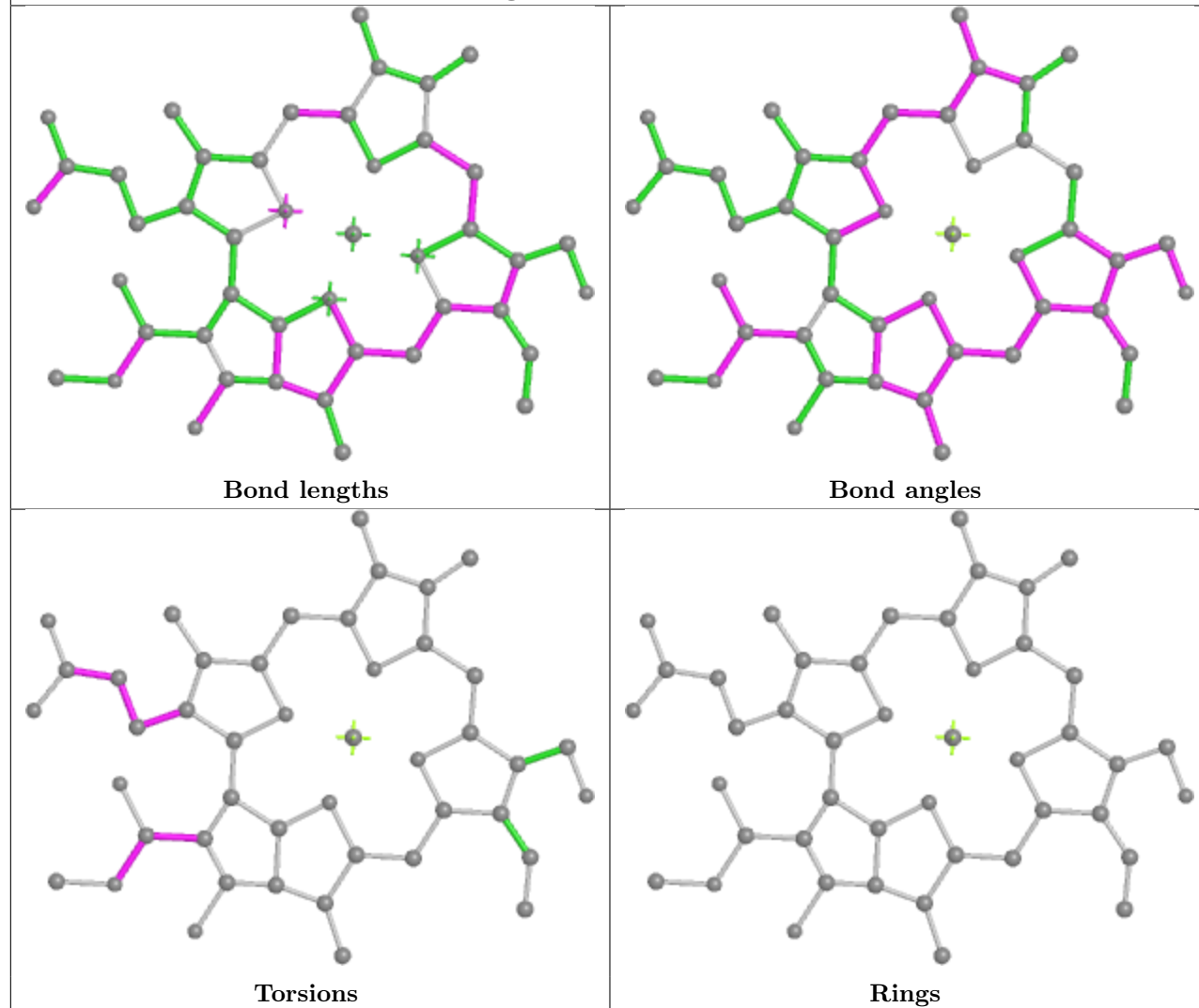




## Ligand CLA B 823

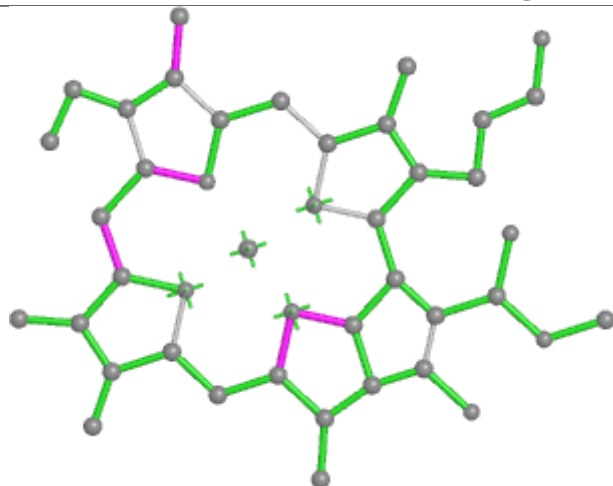


## Ligand CHL 2 601

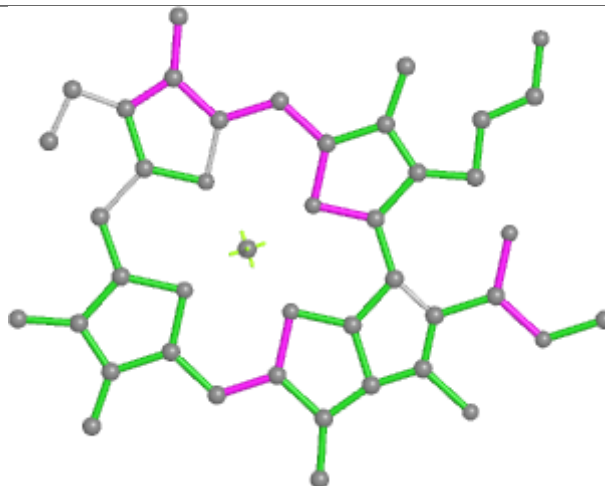




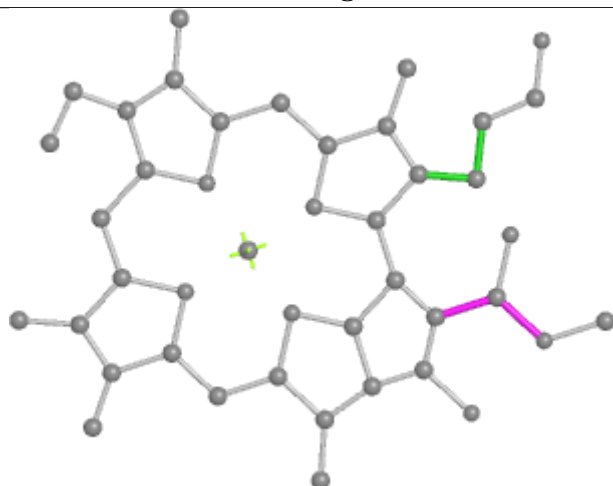
## Ligand CLA 5 604



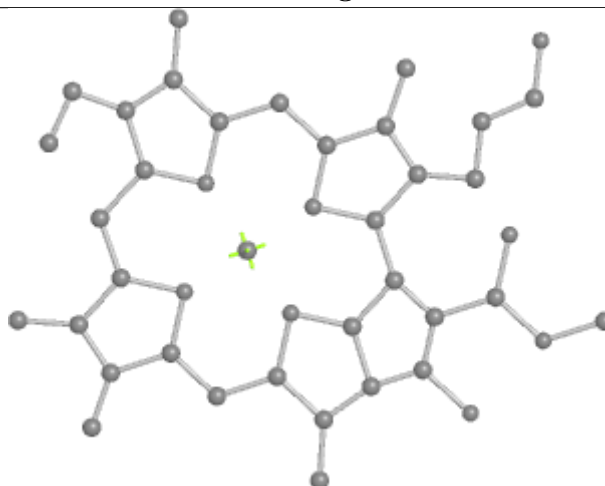
Bond lengths



Bond angles

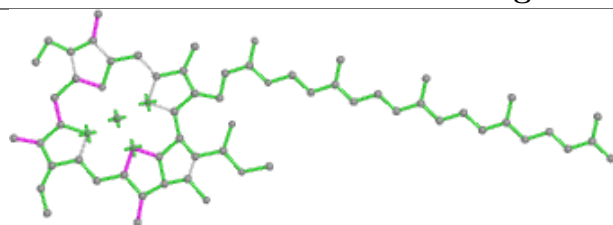


Torsions

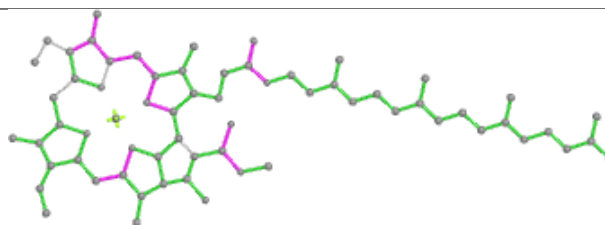


Rings

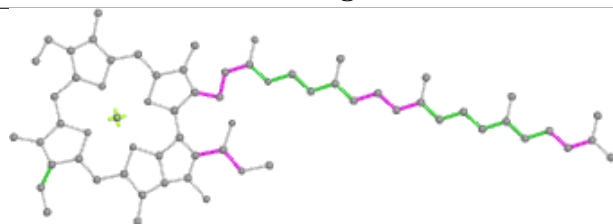
## Ligand CLA A 814



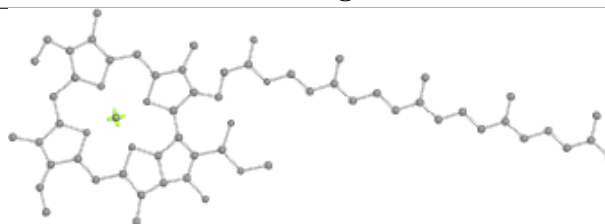
Bond lengths



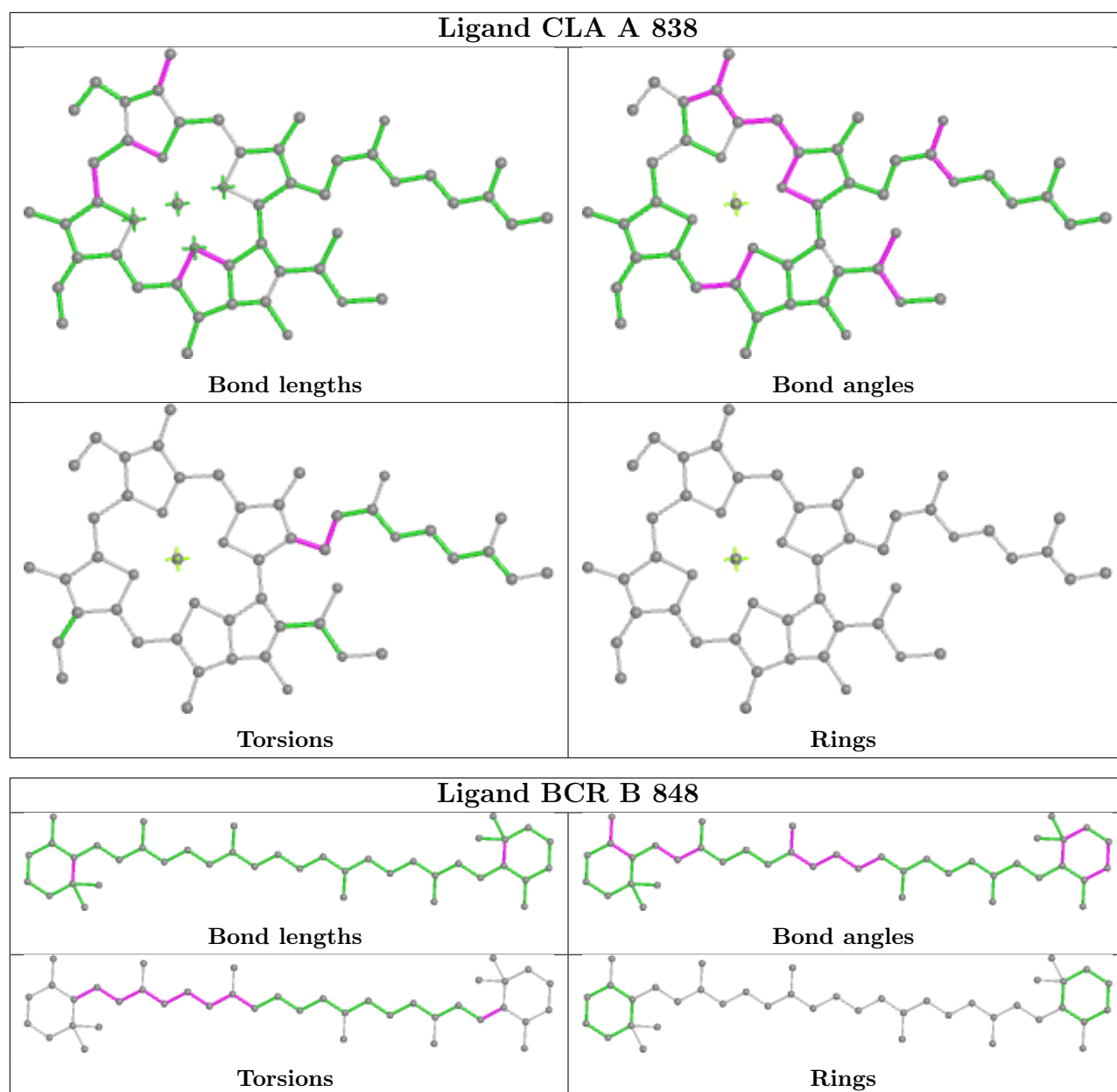
Bond angles



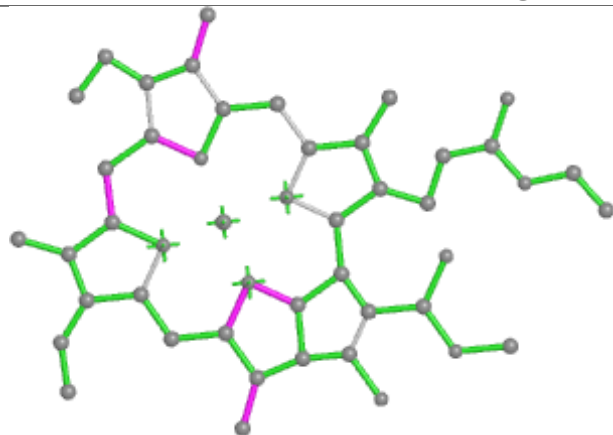
Torsions



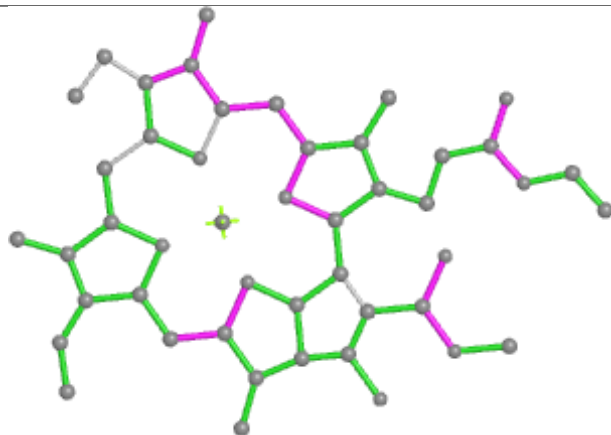
Rings



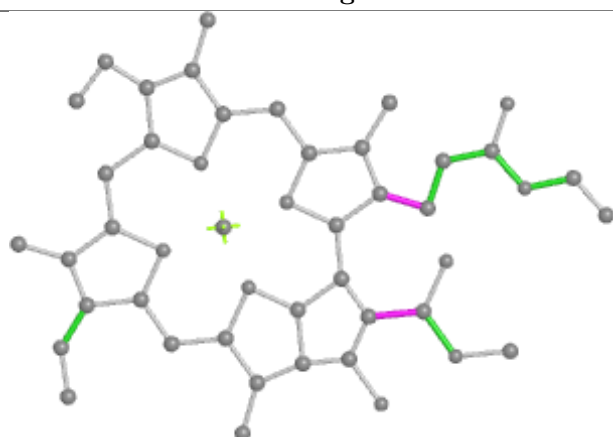
## Ligand CLA B 838



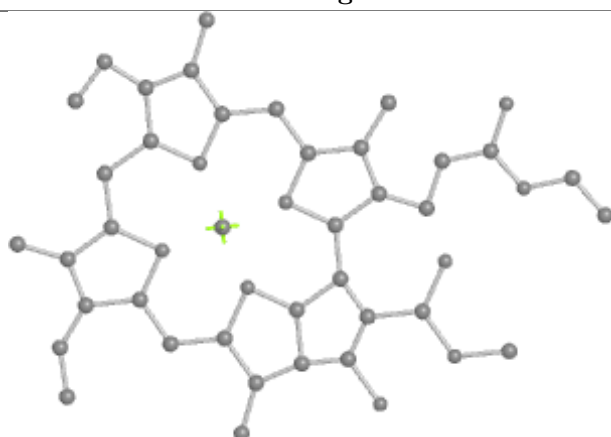
Bond lengths



Bond angles

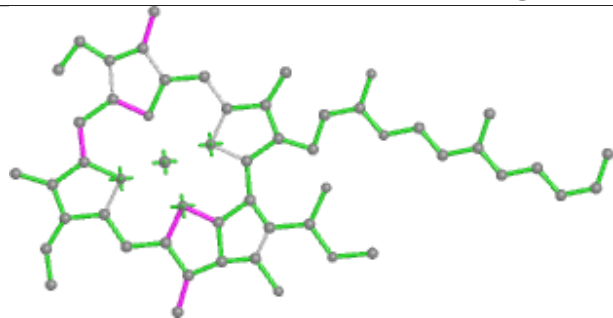


Torsions

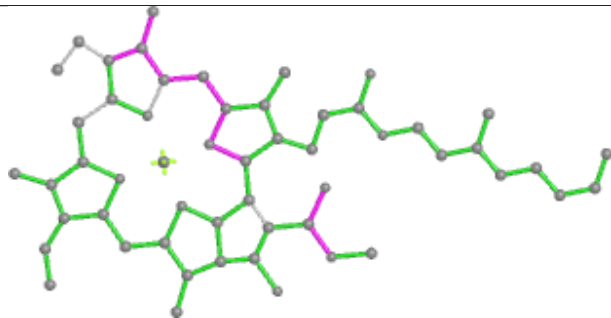


Rings

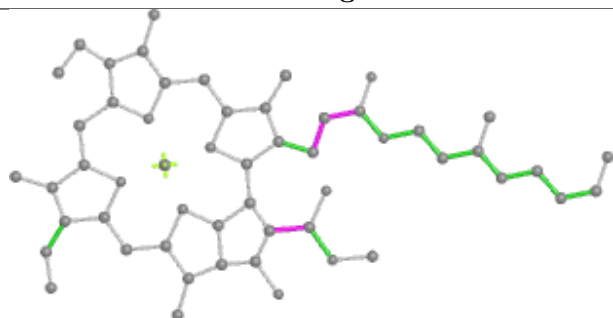
## Ligand CLA A 813



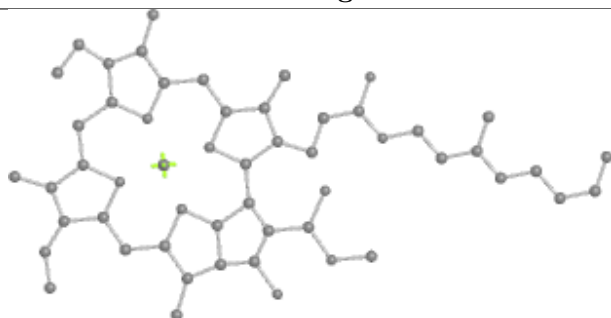
Bond lengths



Bond angles

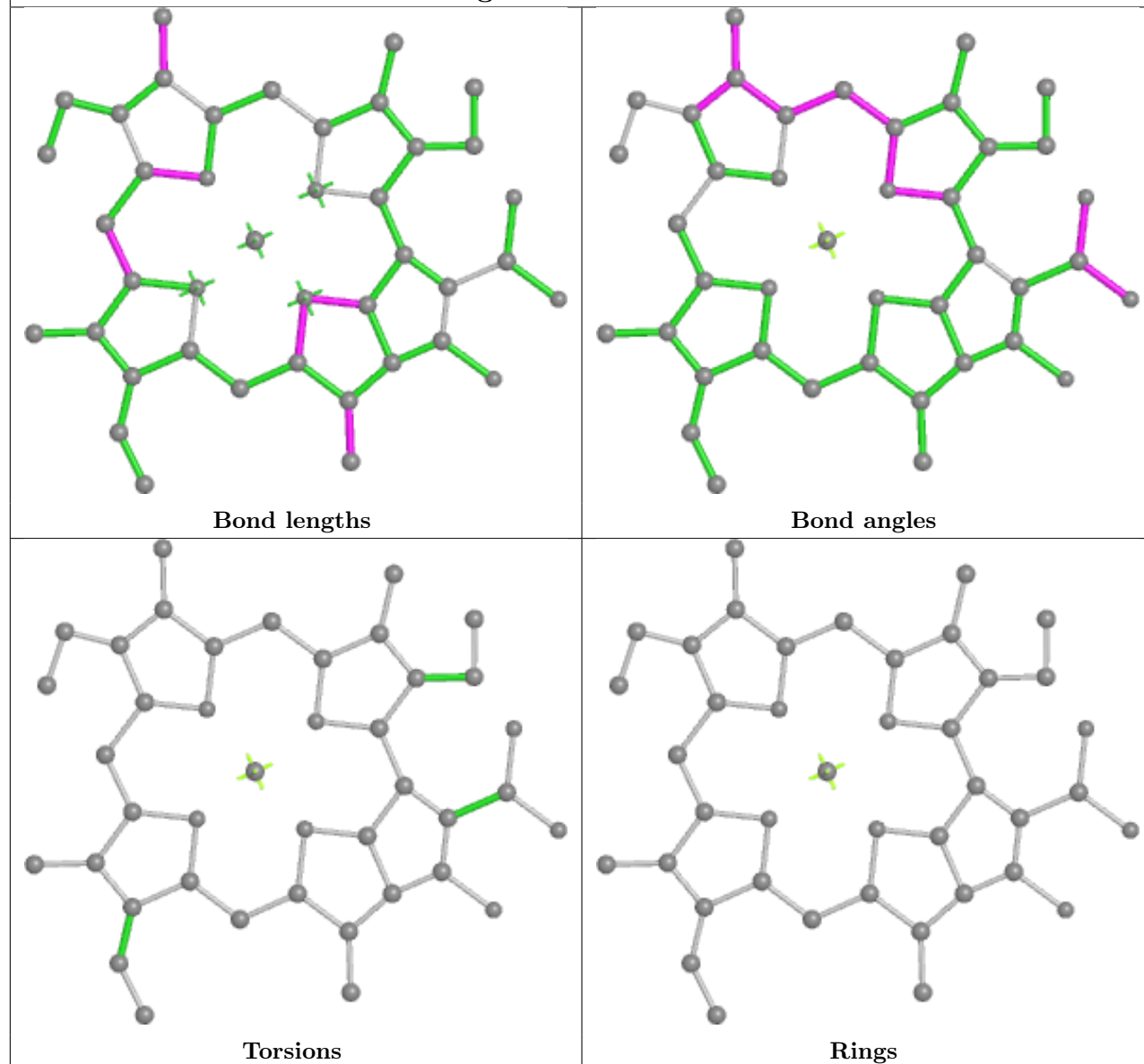


Torsions

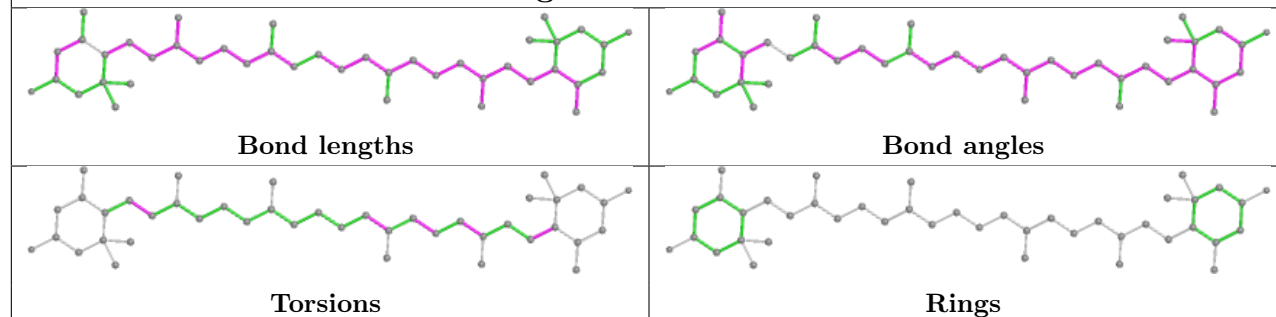


Rings

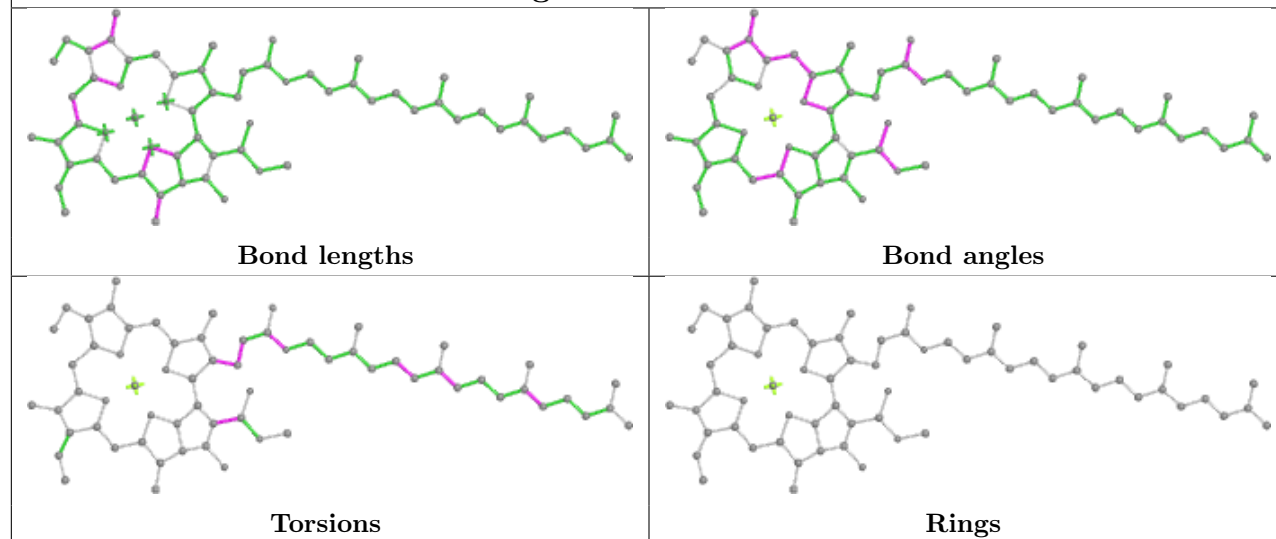
## Ligand CLA B 839



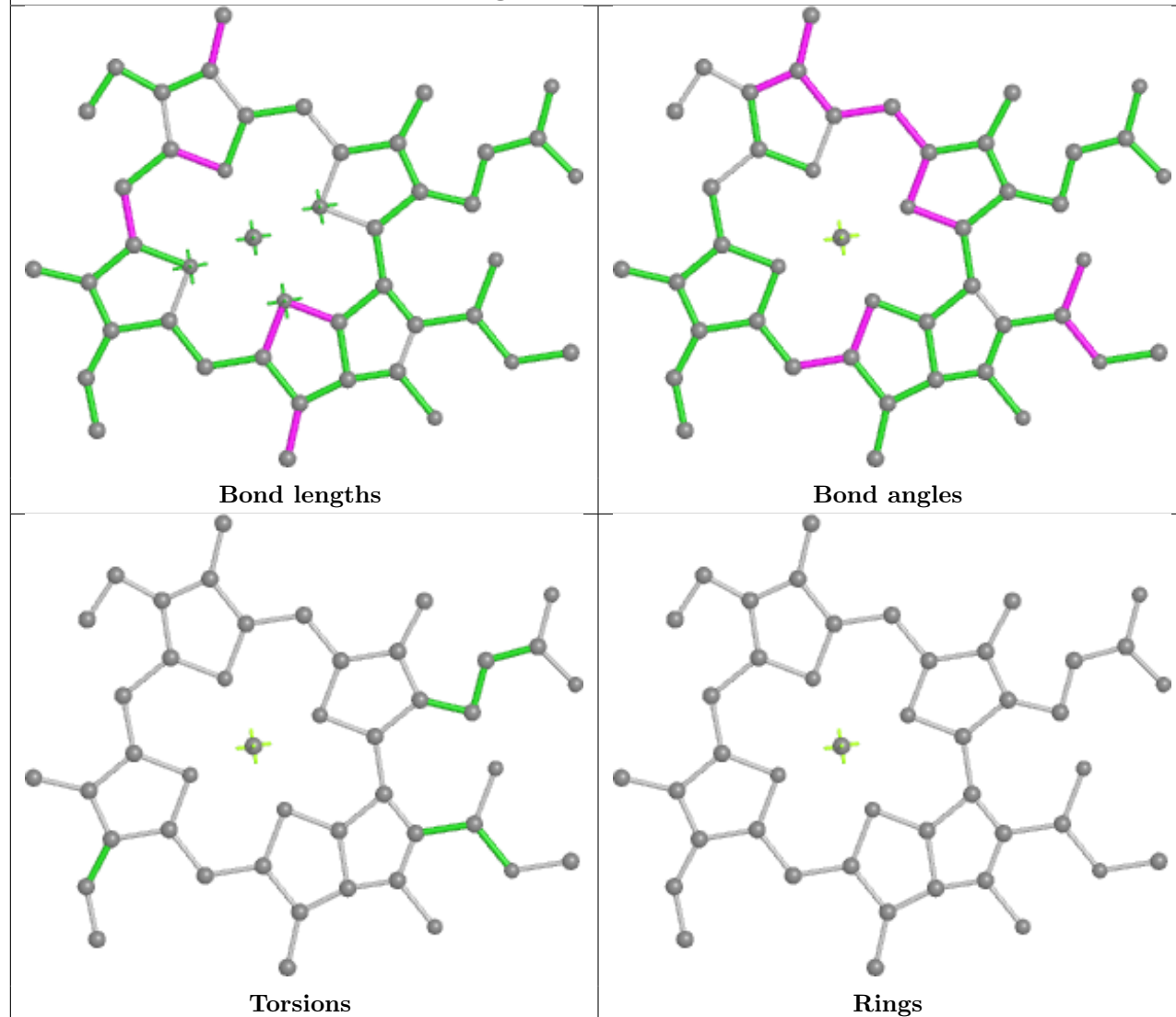
## Ligand LUT 3 618

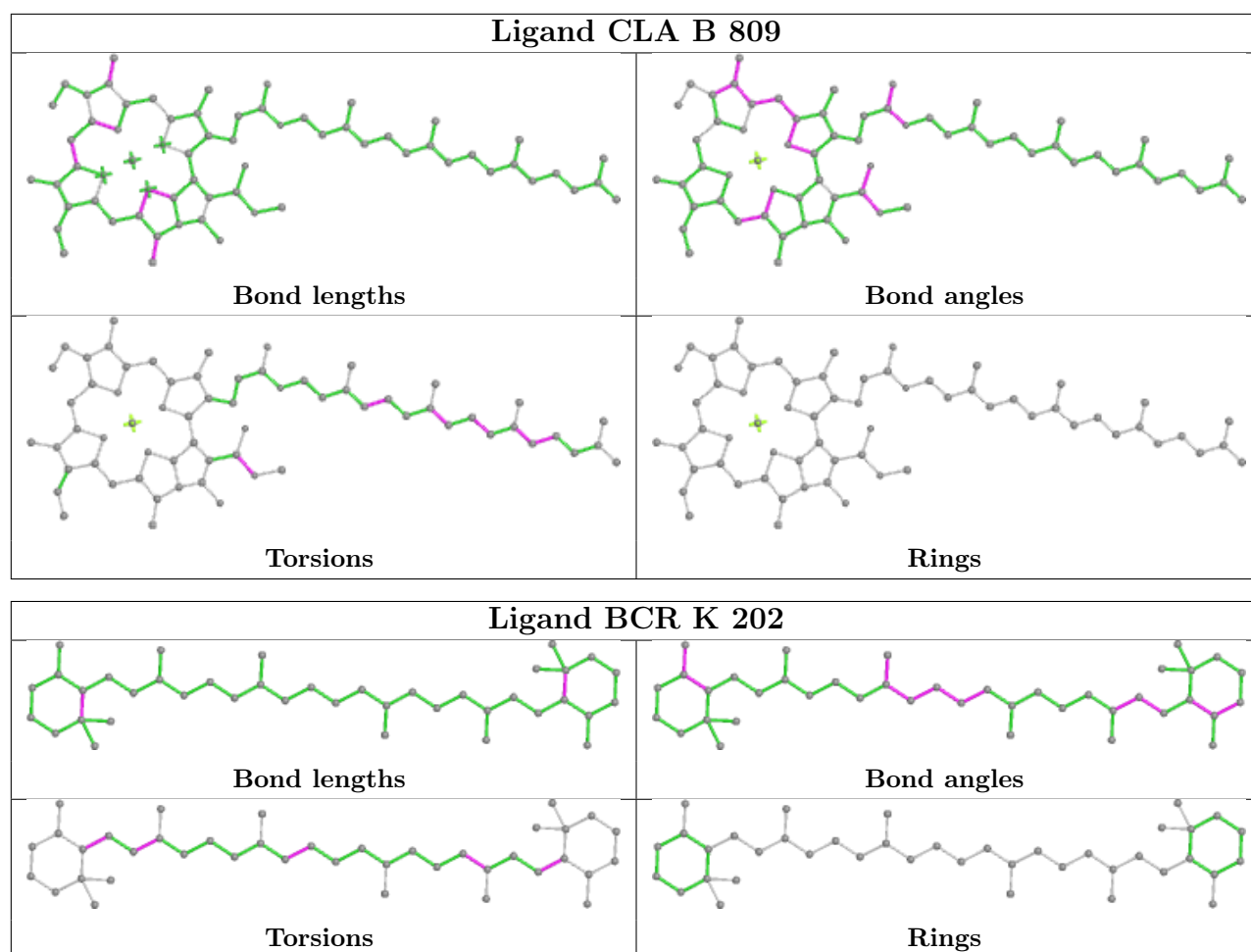


## Ligand CLA B 828

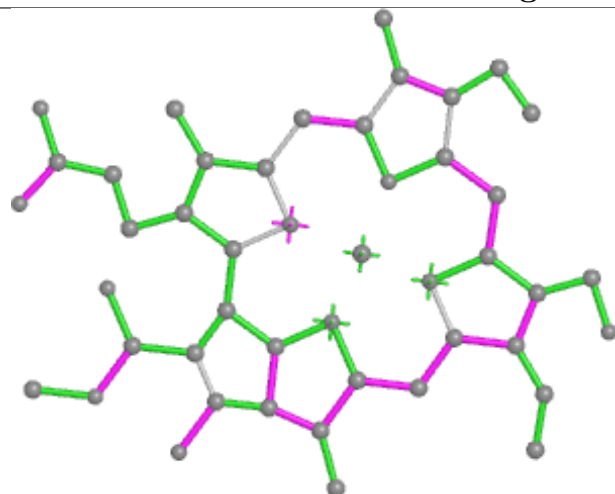


## Ligand CLA L 303

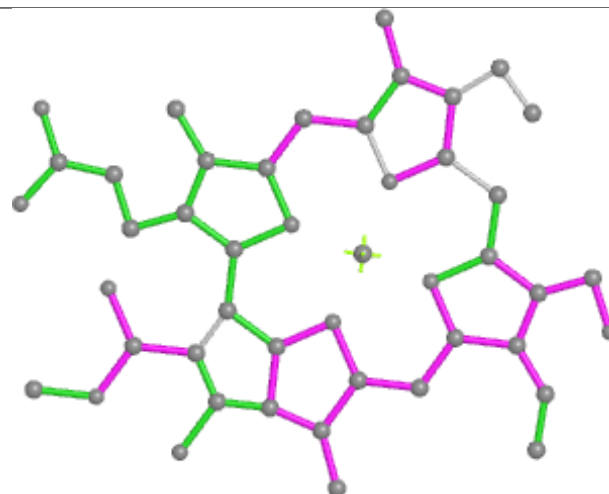




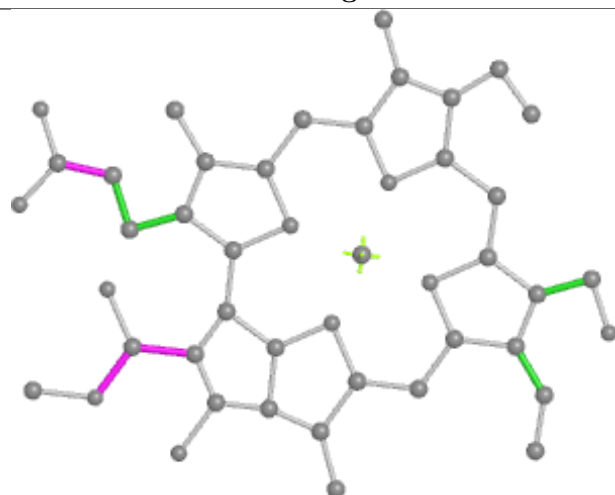
## Ligand CHL 2 616



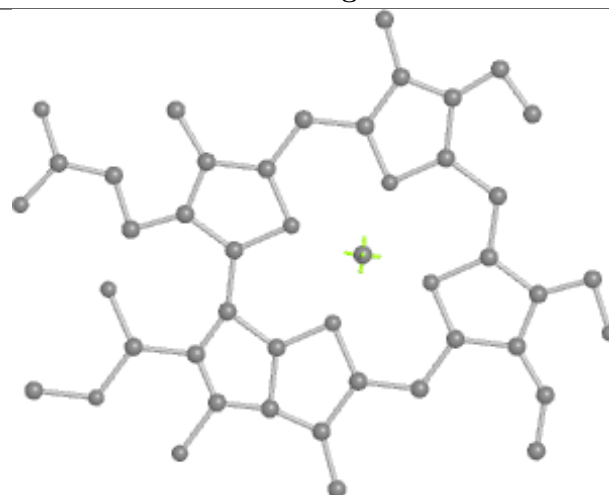
Bond lengths



Bond angles

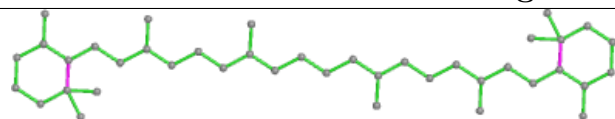


Torsions

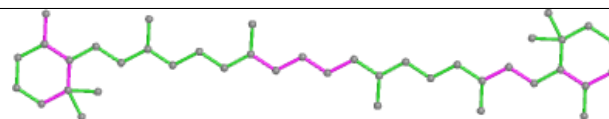


Rings

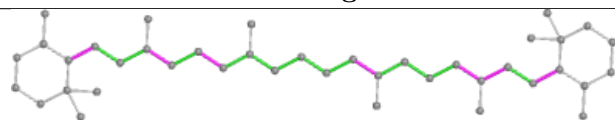
## Ligand BCR L 301



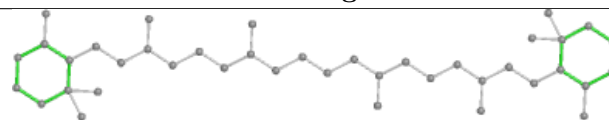
Bond lengths



Bond angles

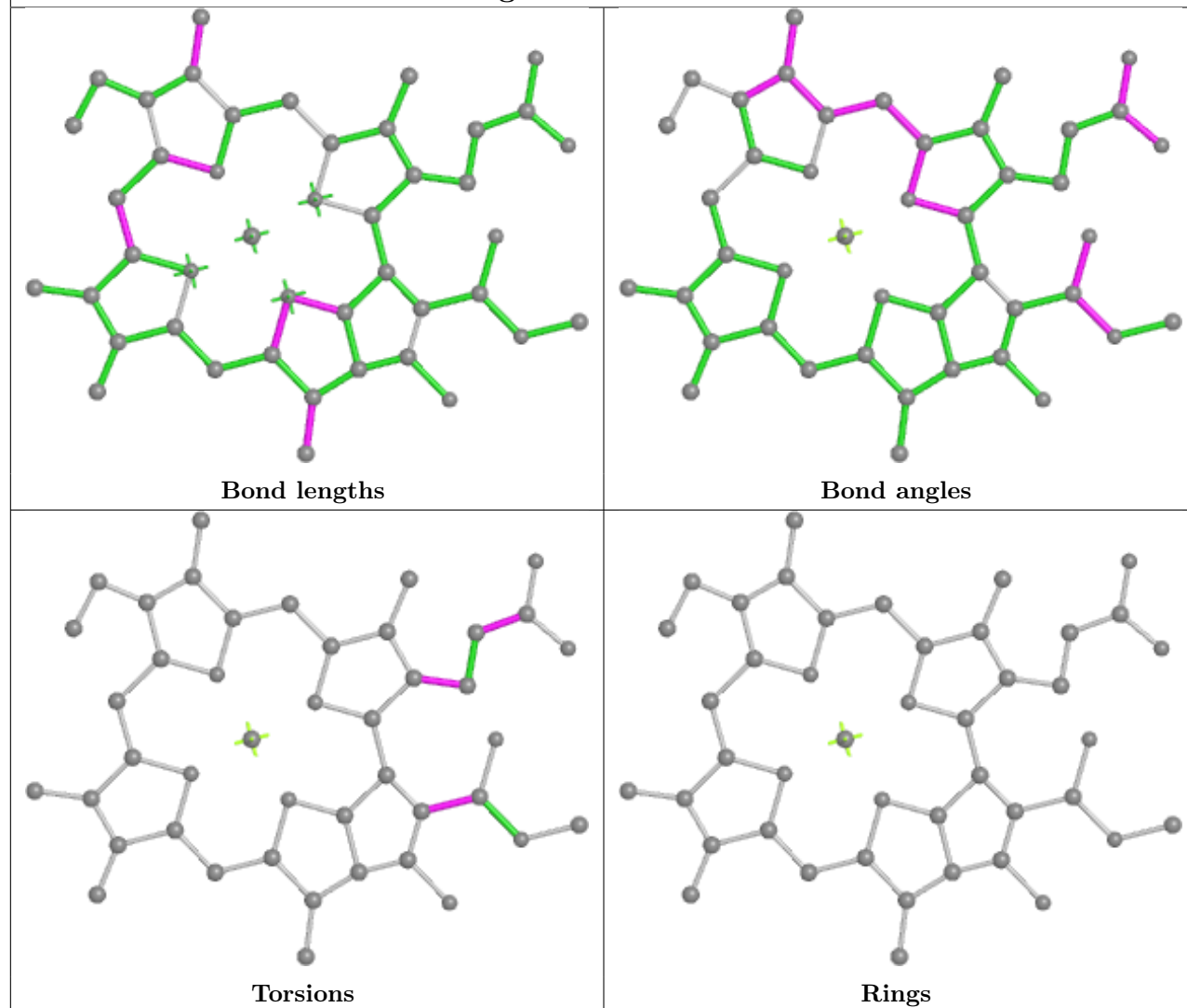


Torsions

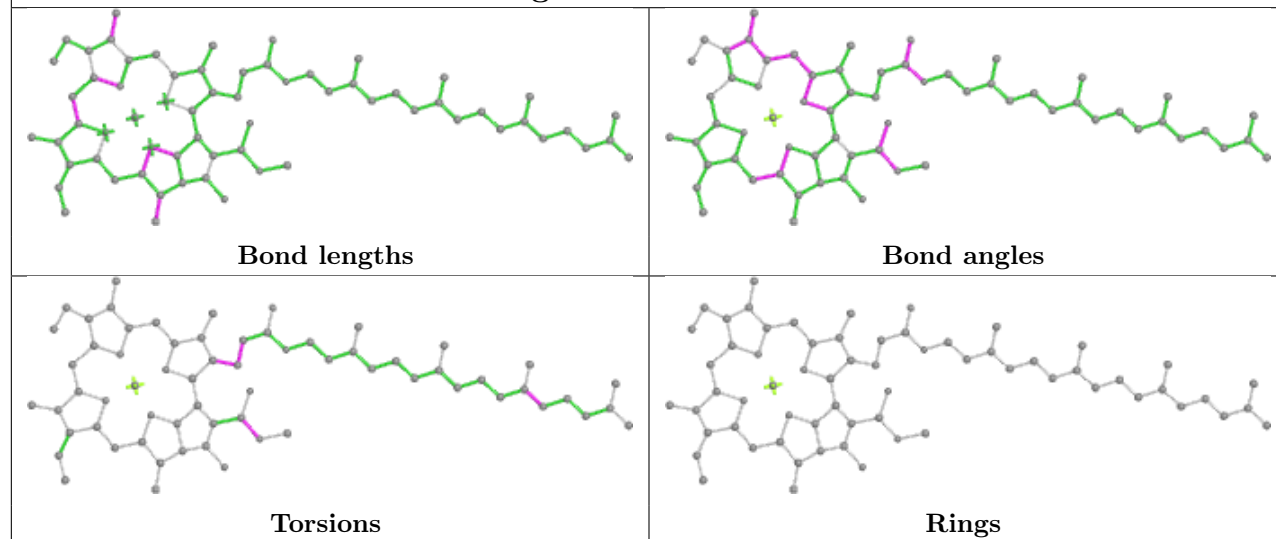


Rings

## Ligand CLA 5 612

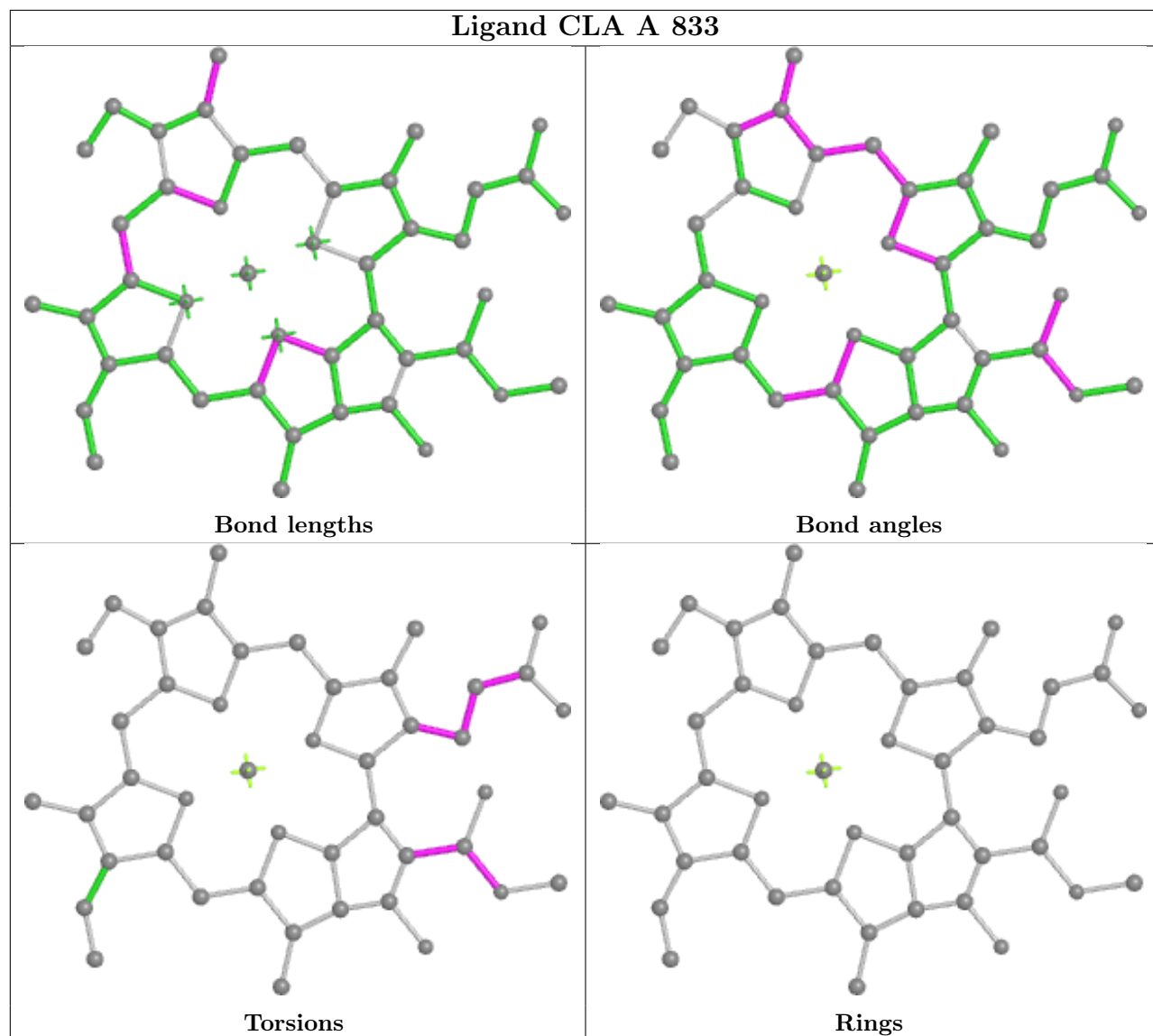


## Ligand CLA A 803

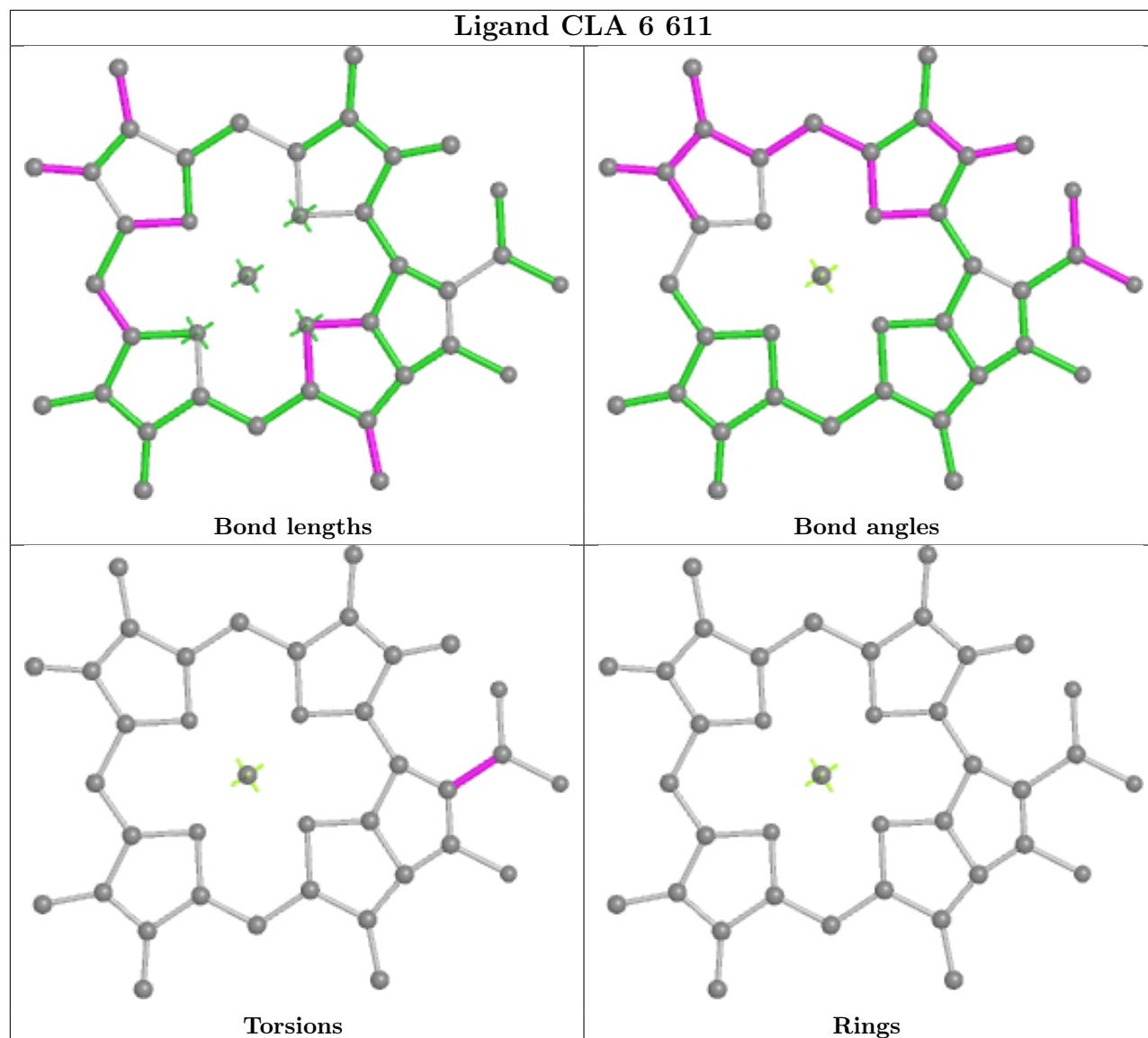




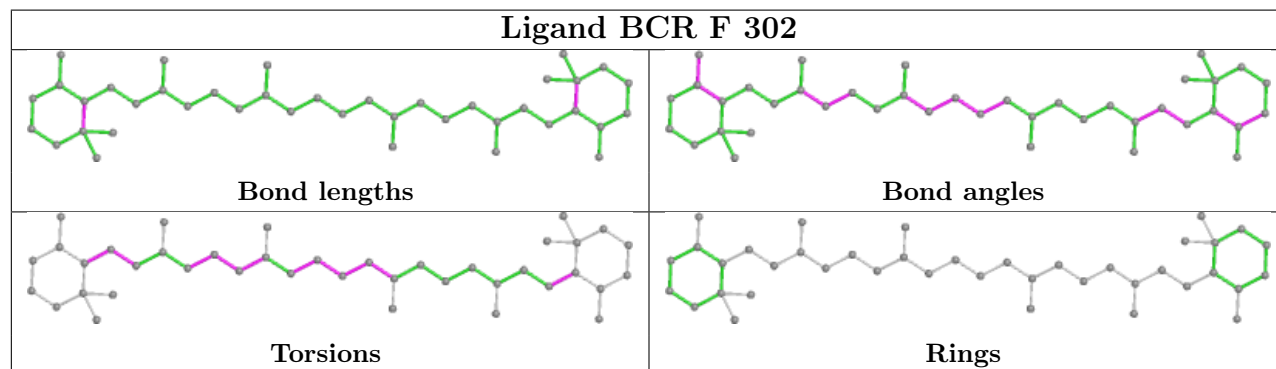
## Ligand CLA A 833



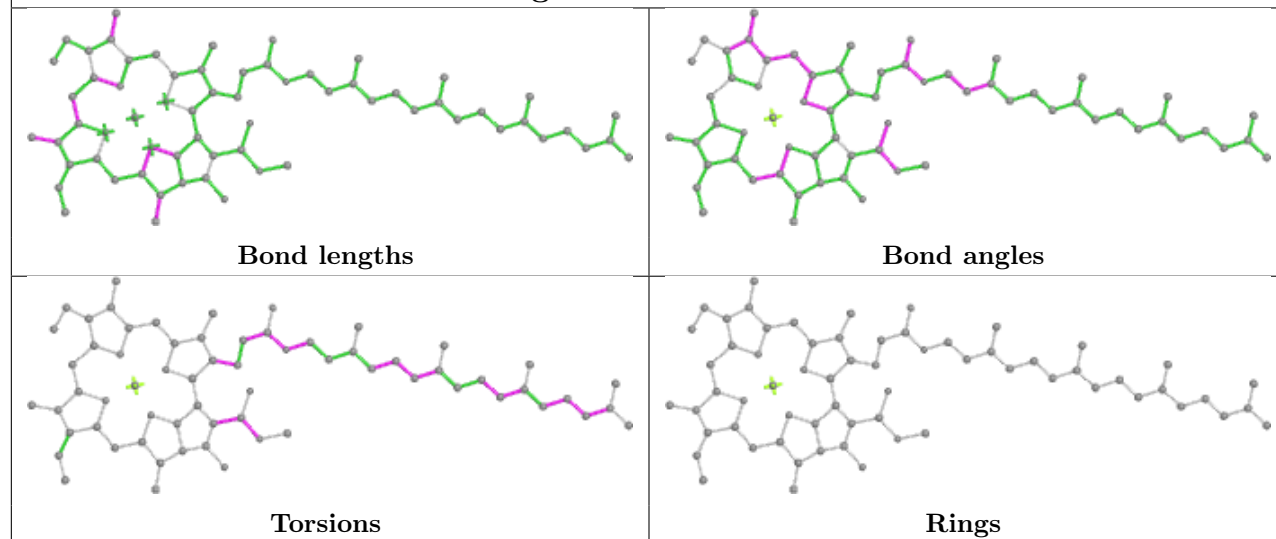
## Ligand CLA 6 611



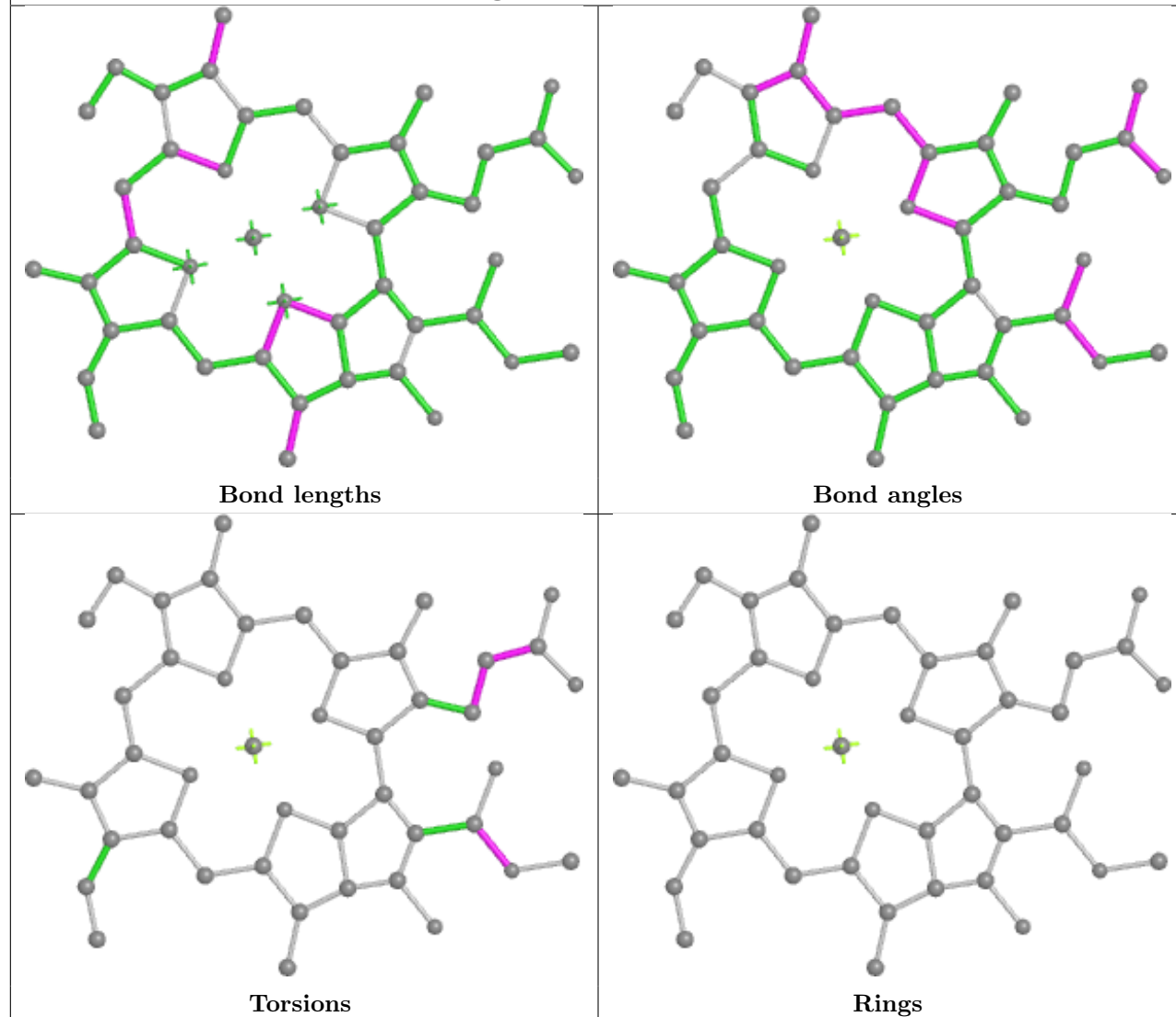
## Ligand BCR F 302

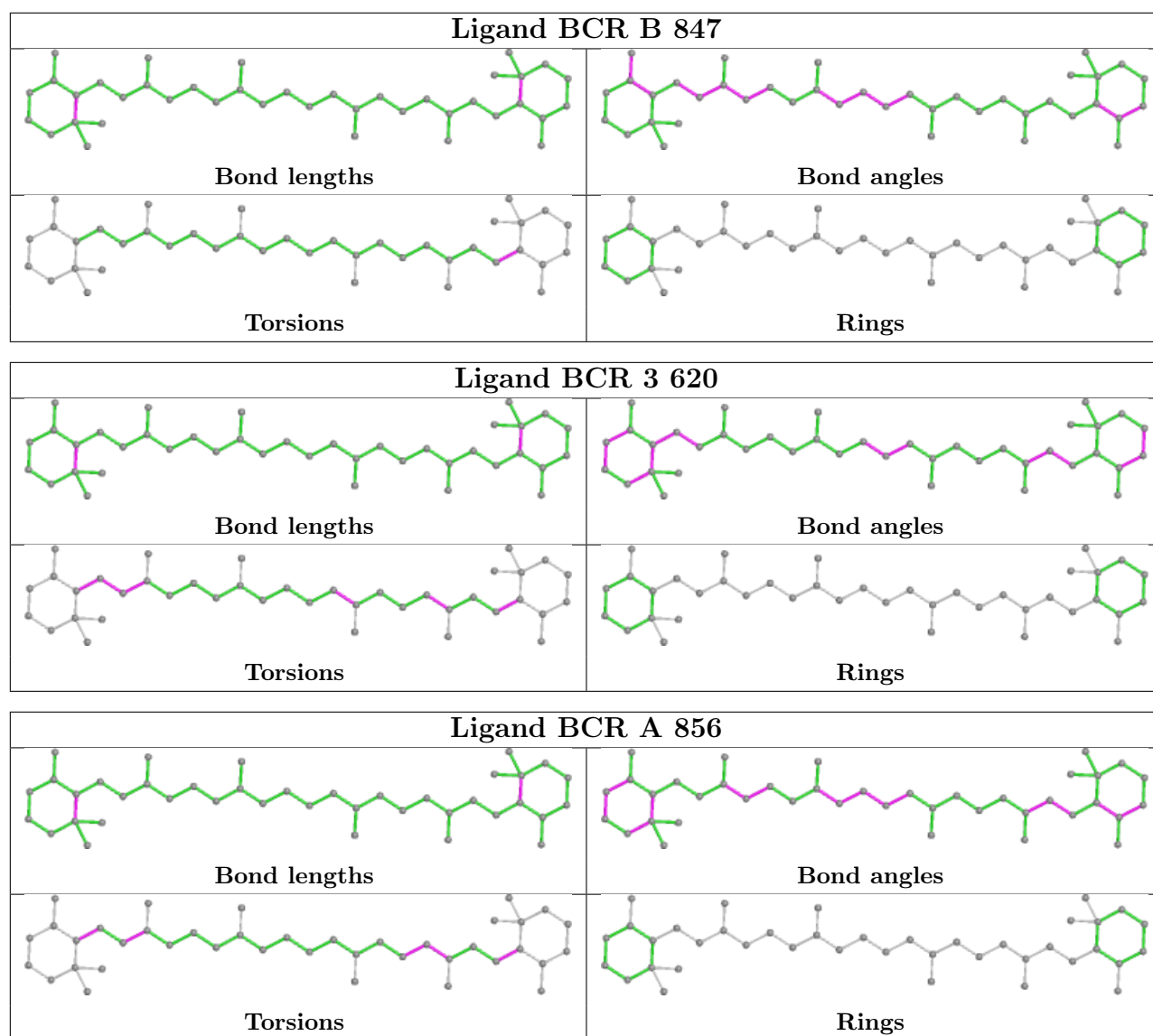


## Ligand CLA A 829

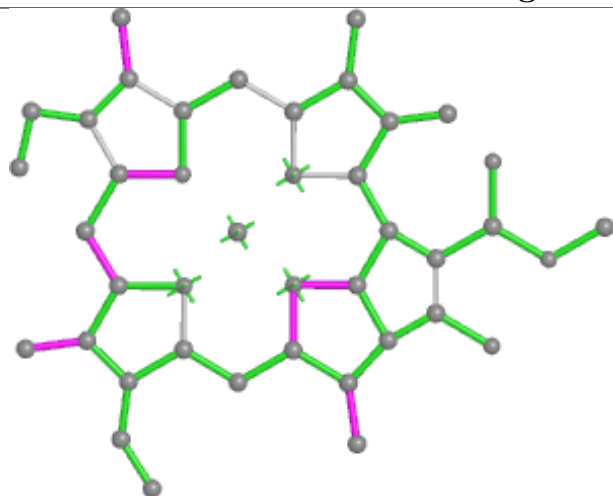


## Ligand CLA K 206

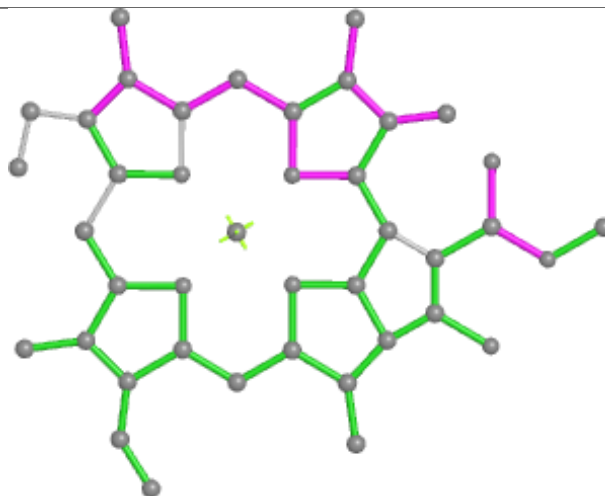




## Ligand CLA 3 610



Bond lengths



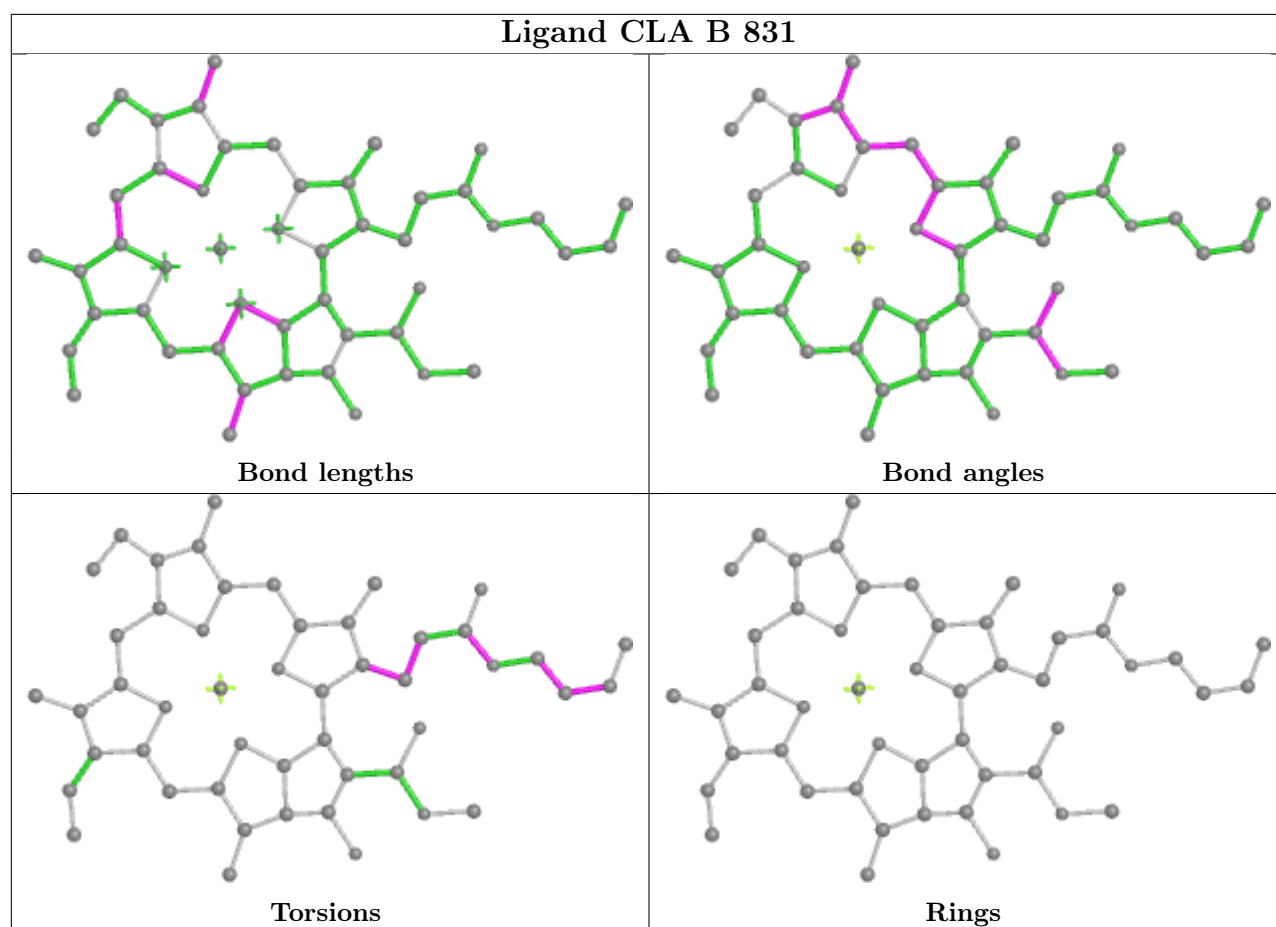
Bond angles



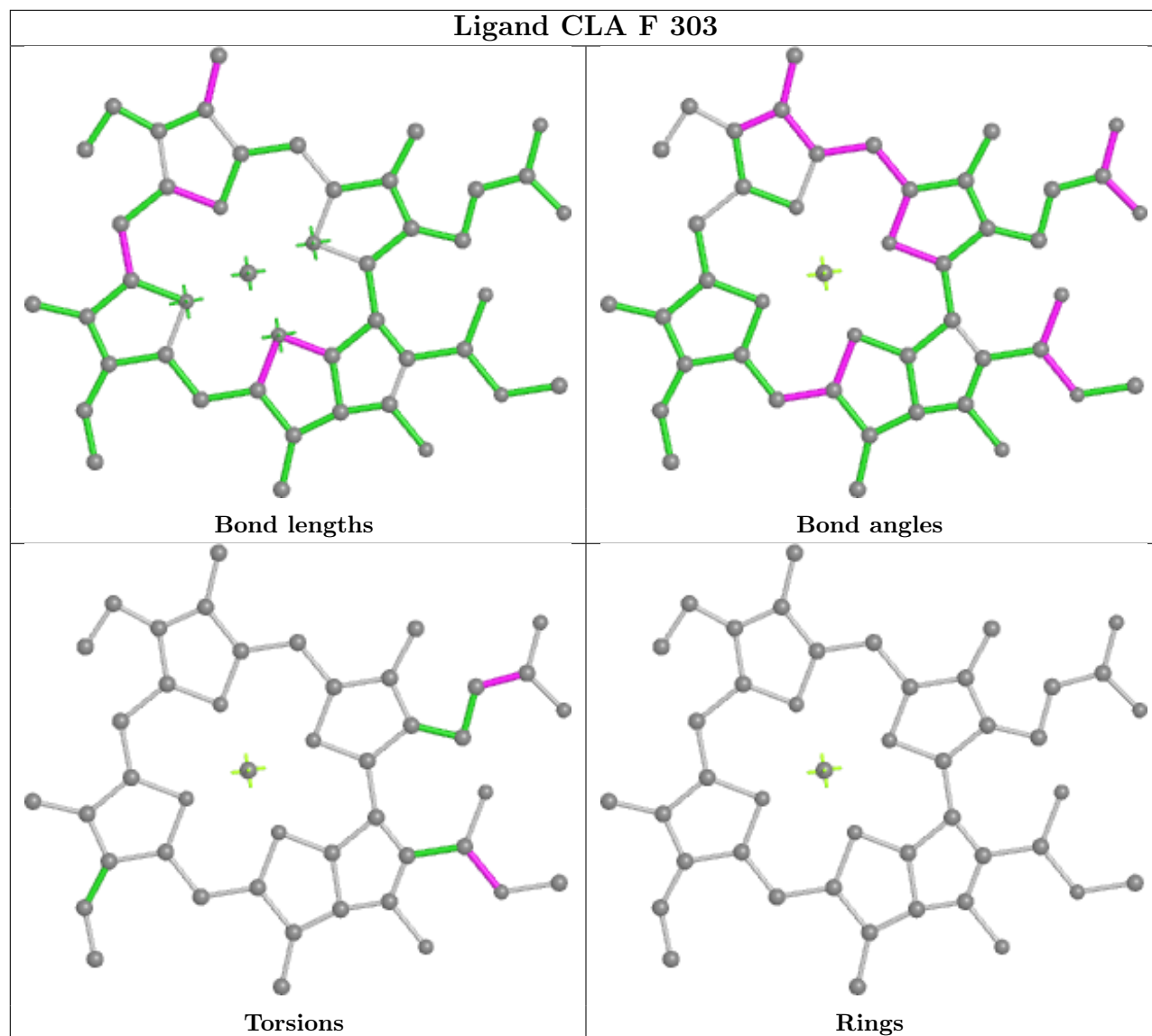
Torsions

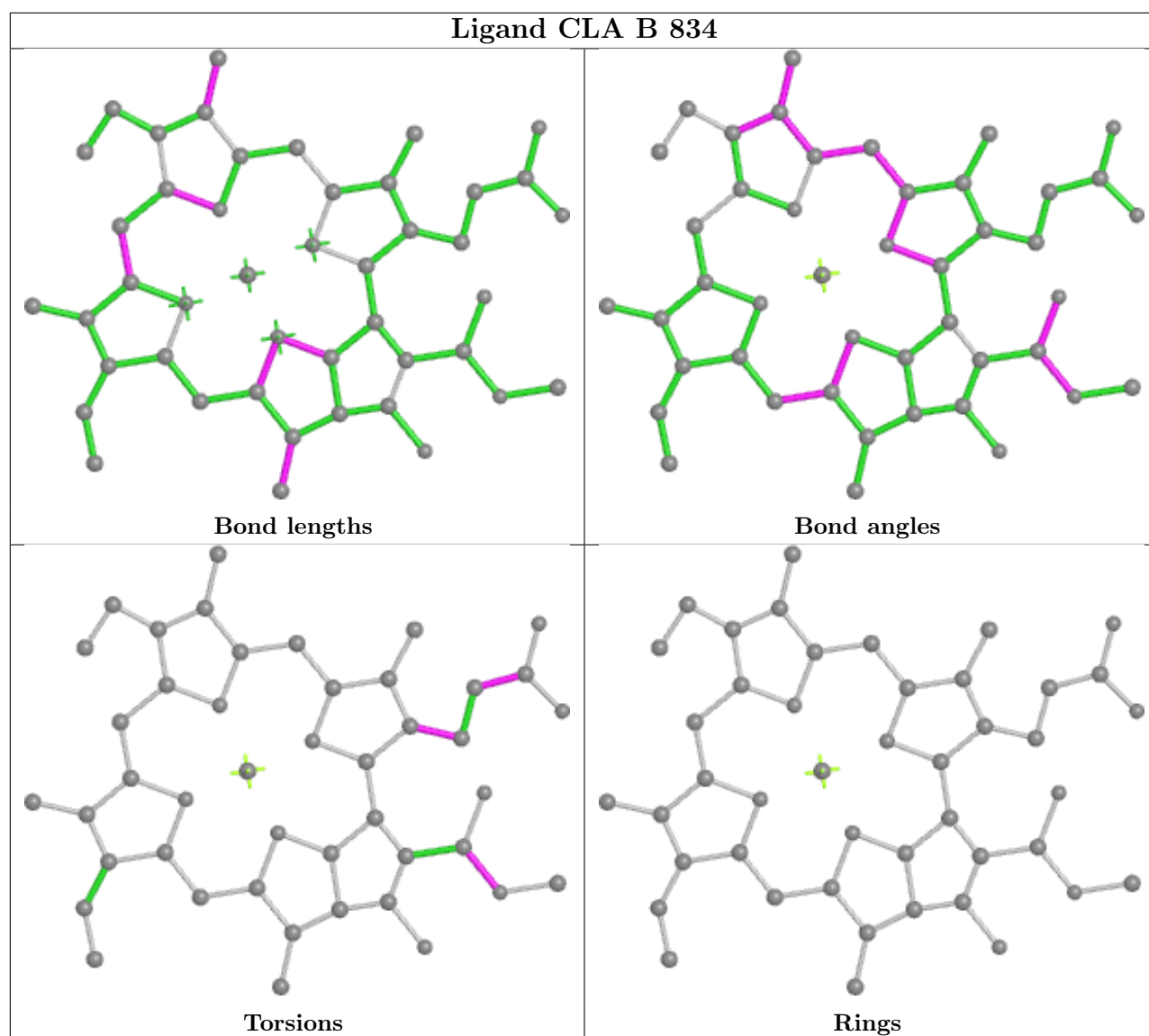


Rings



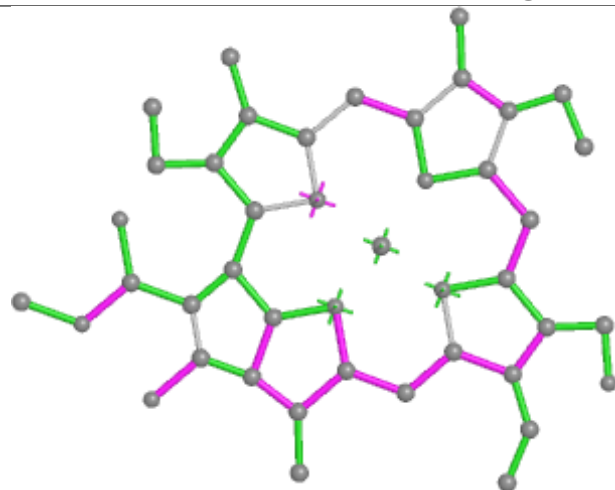
## Ligand CLA F 303



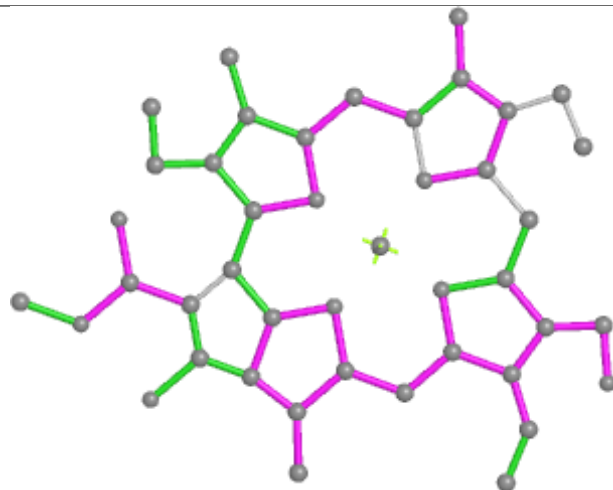




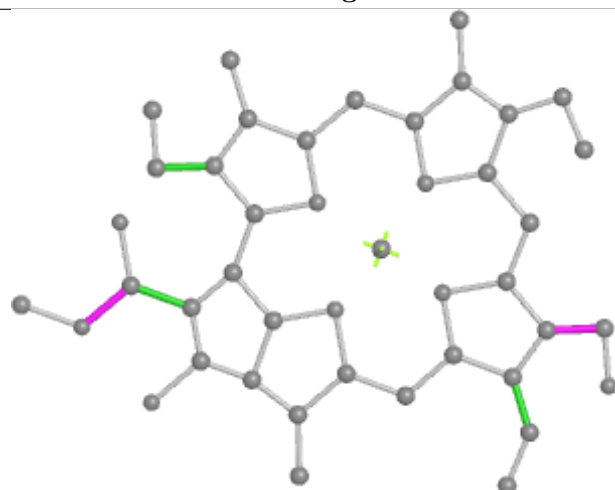
## Ligand CHL 2 607



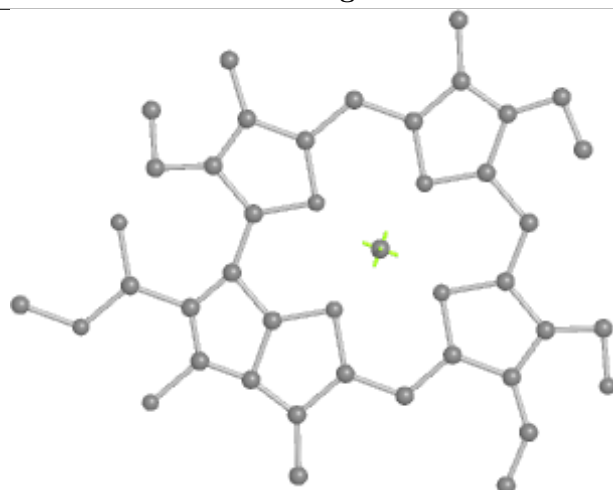
Bond lengths



Bond angles

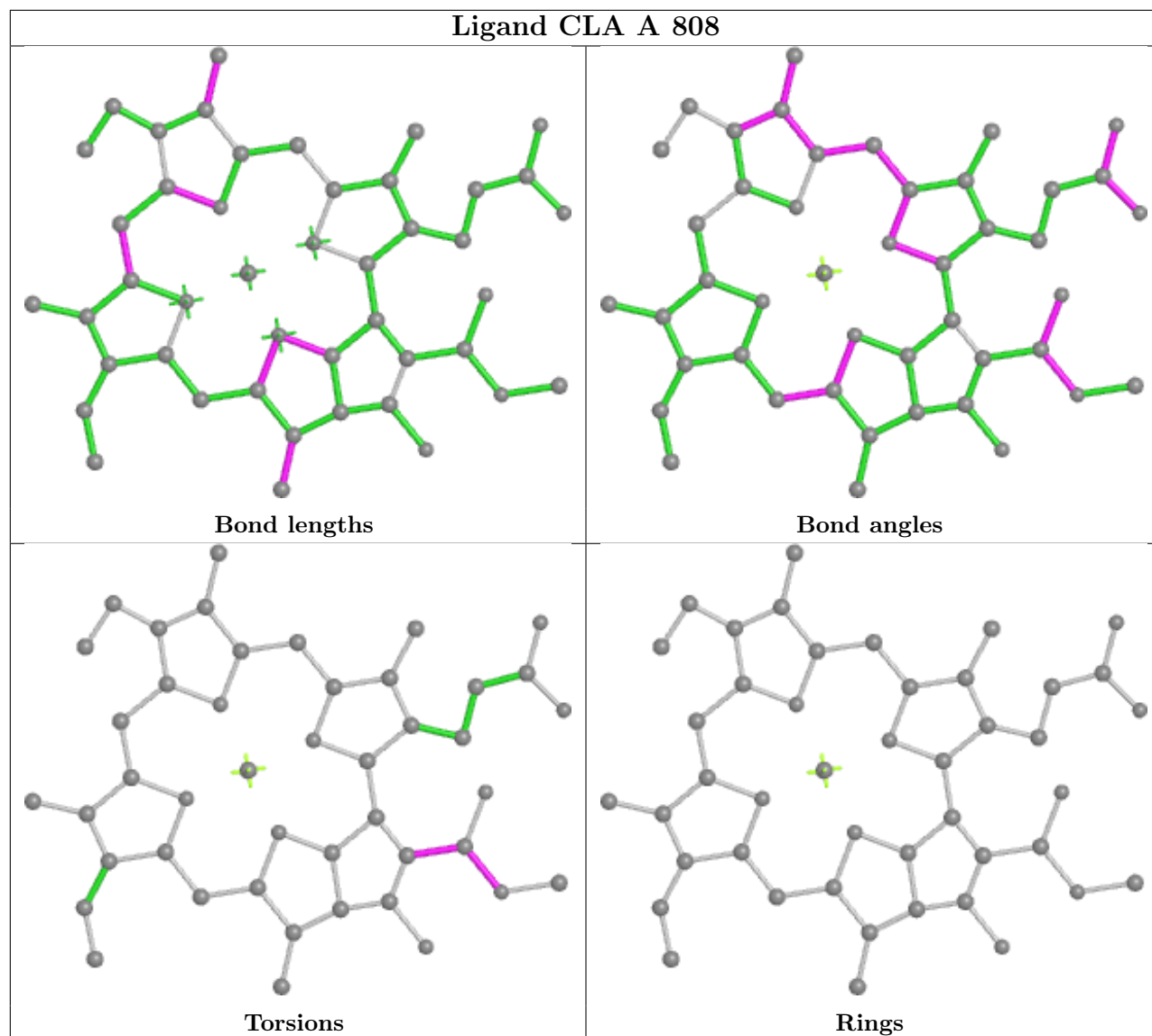


Torsions

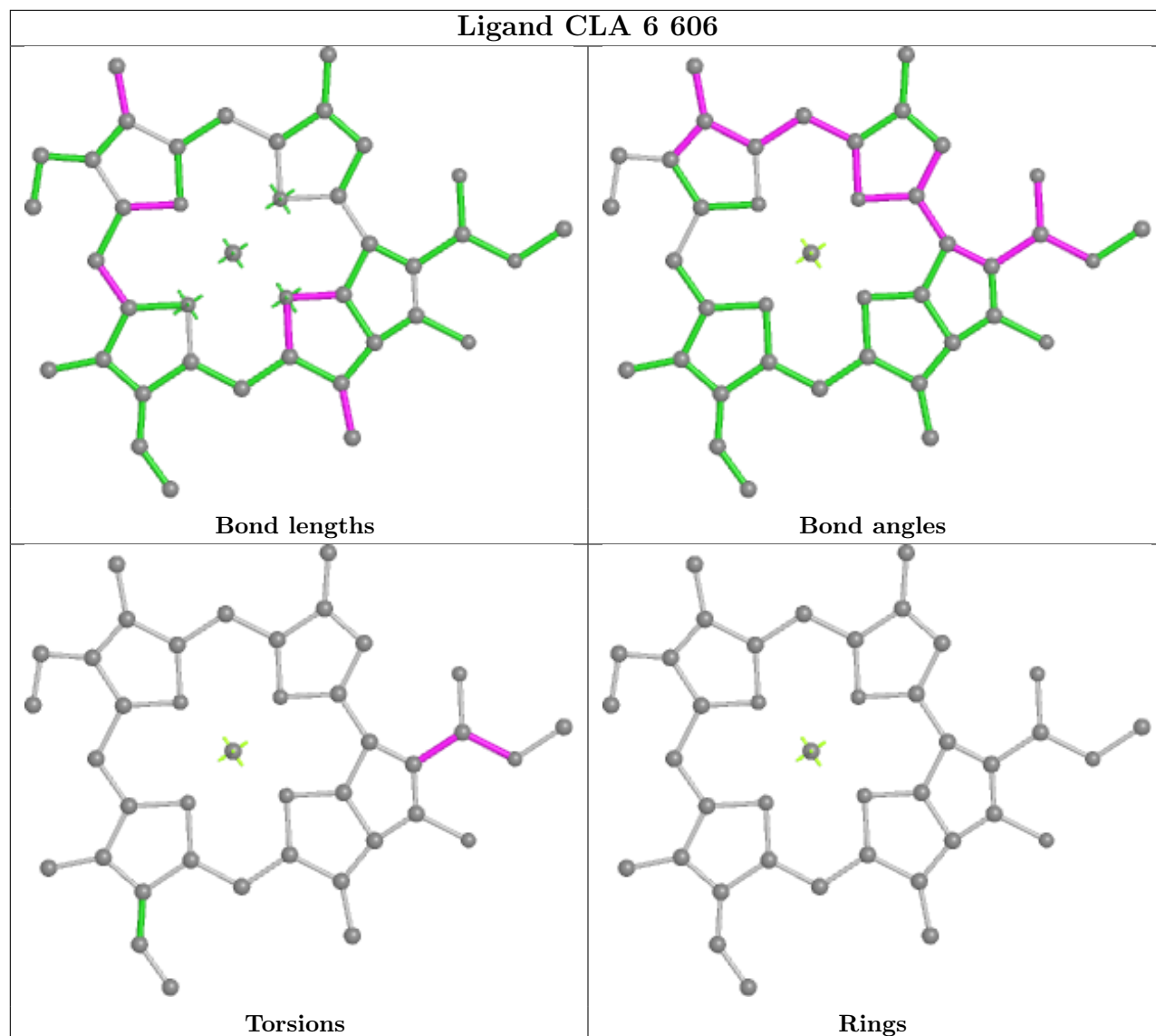


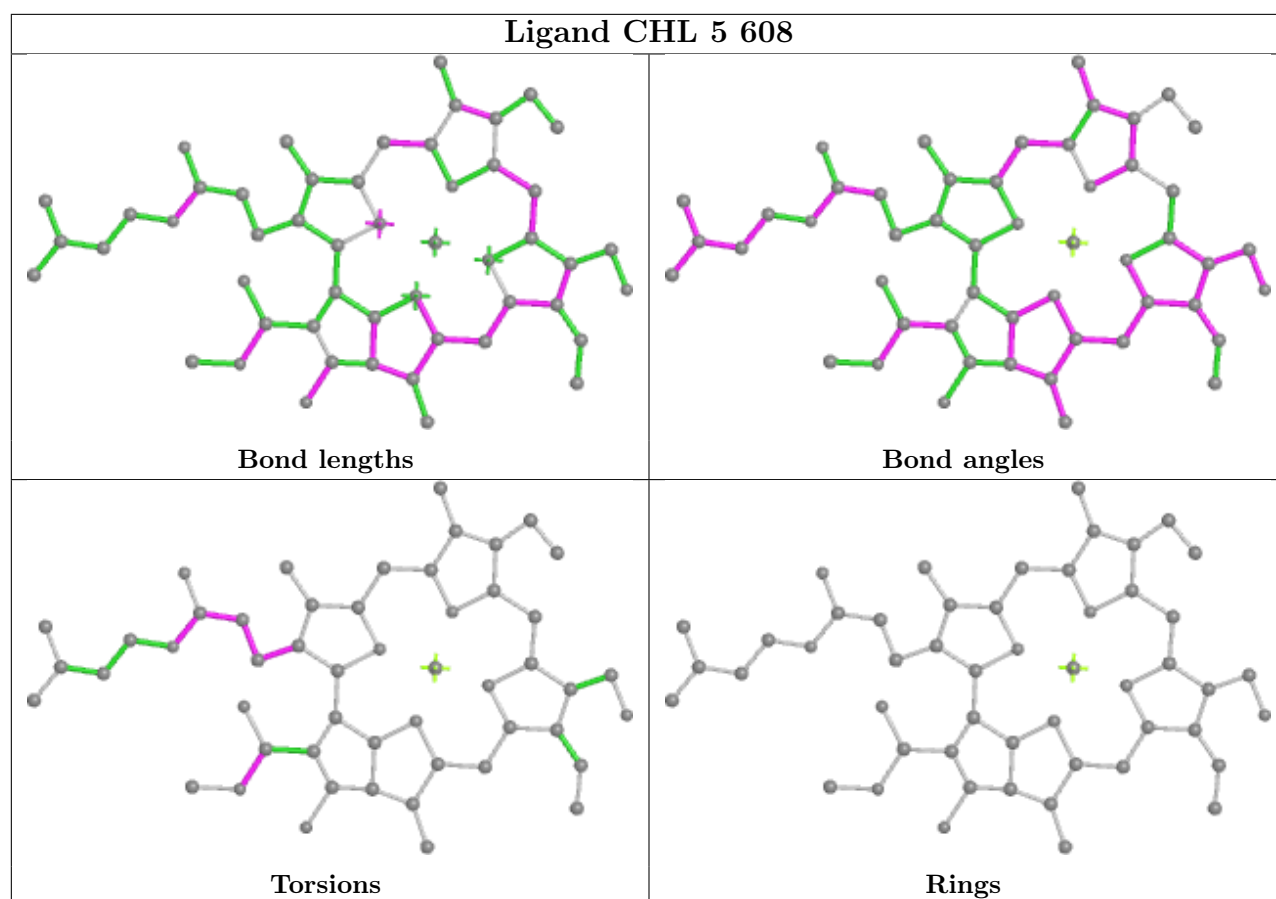
Rings

## Ligand CLA A 808

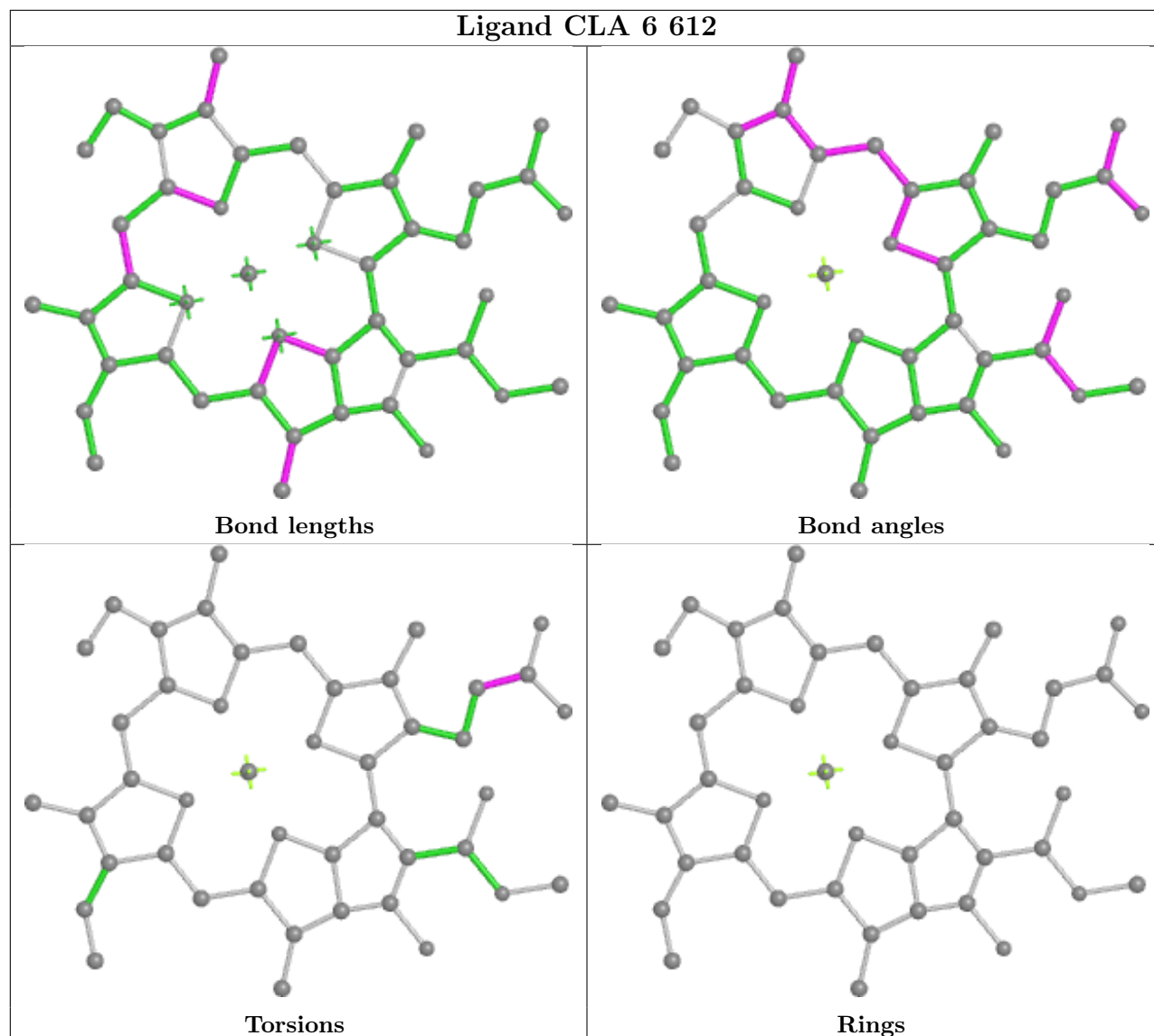


## Ligand CLA 6 606

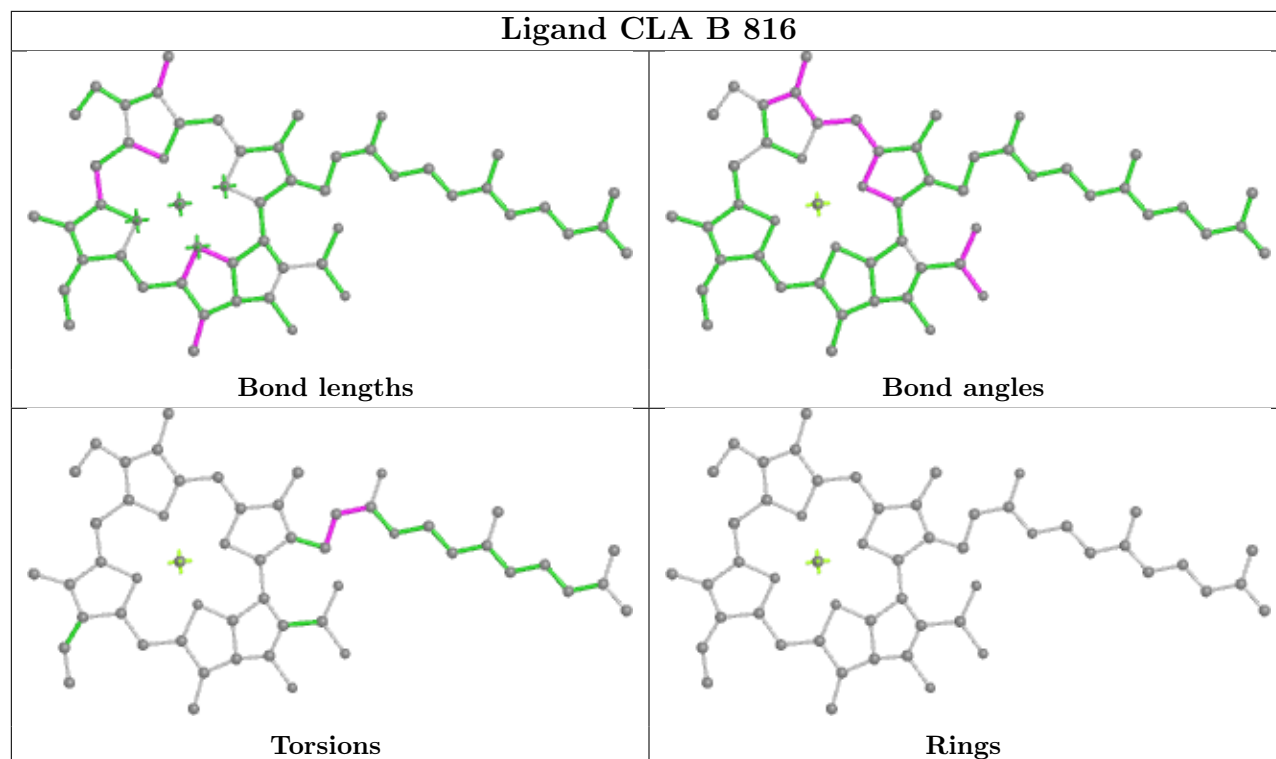




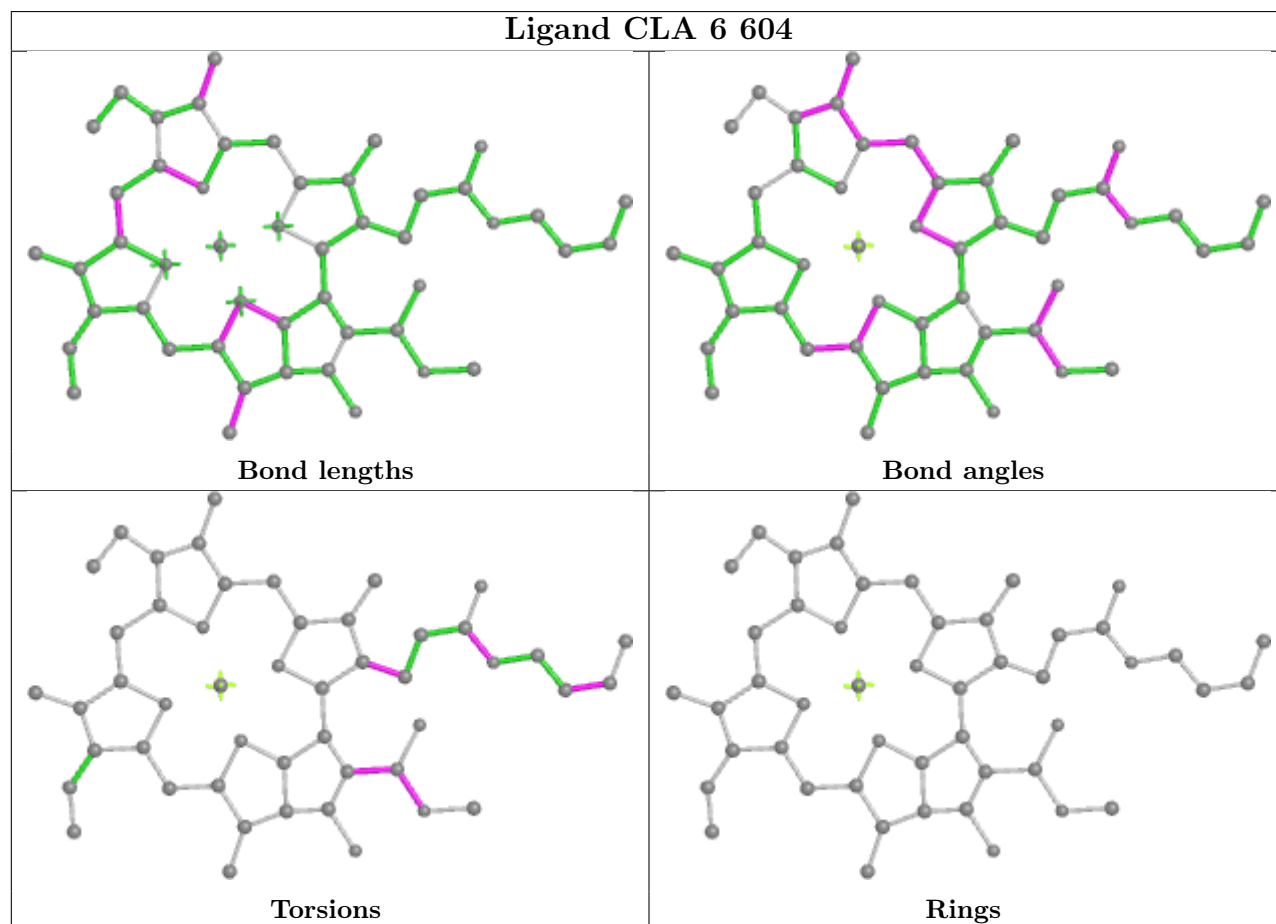
## Ligand CLA 6 612

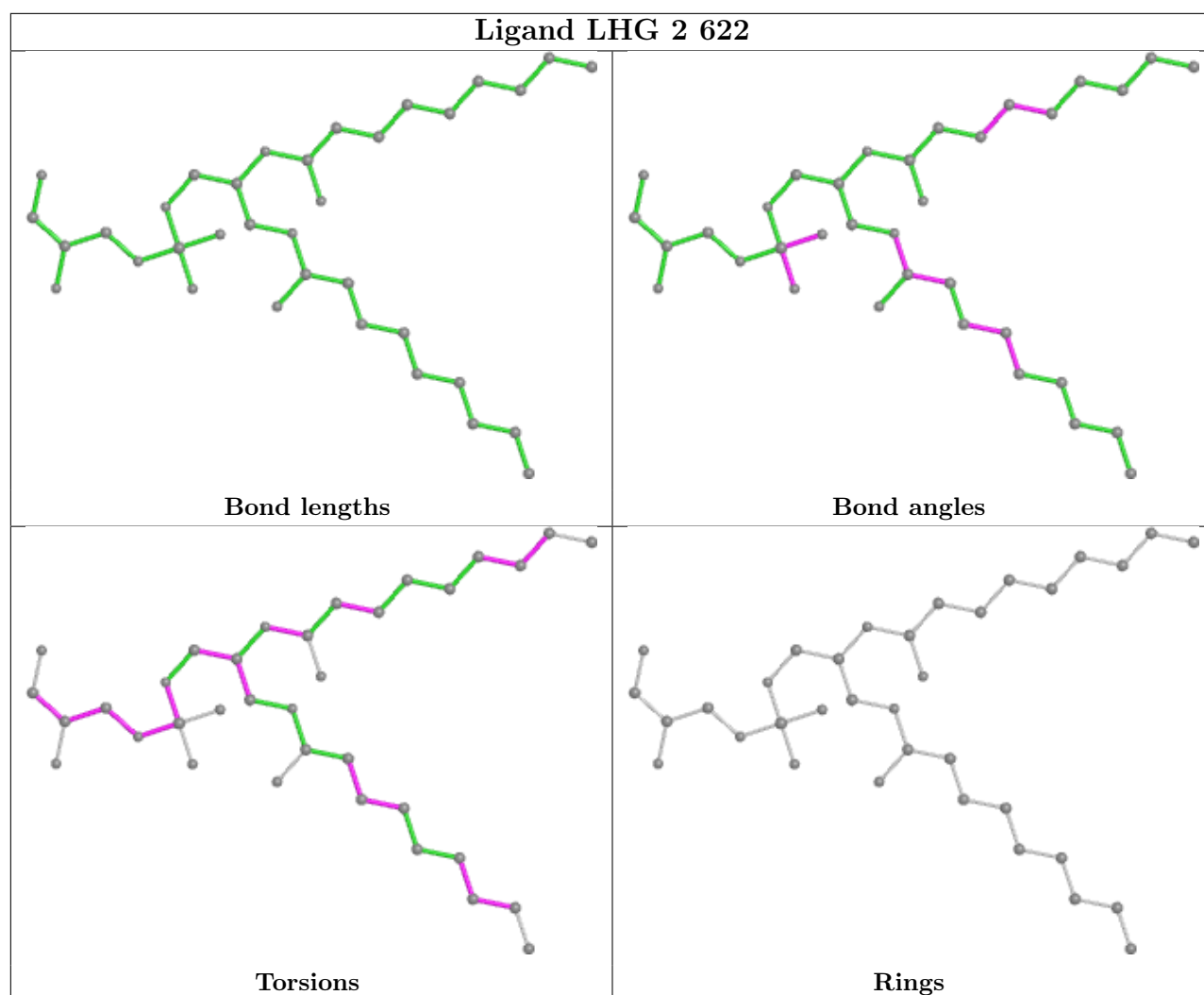


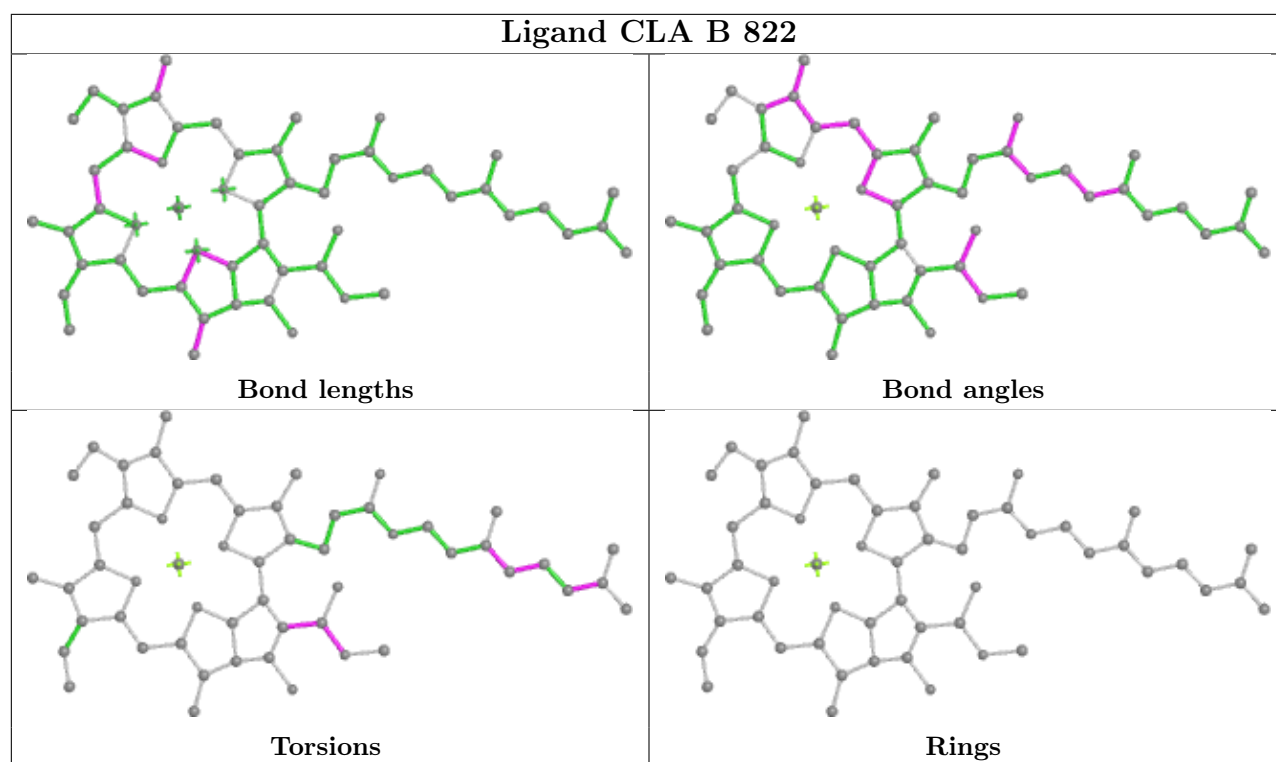
## Ligand CLA B 816



## Ligand CLA 6 604

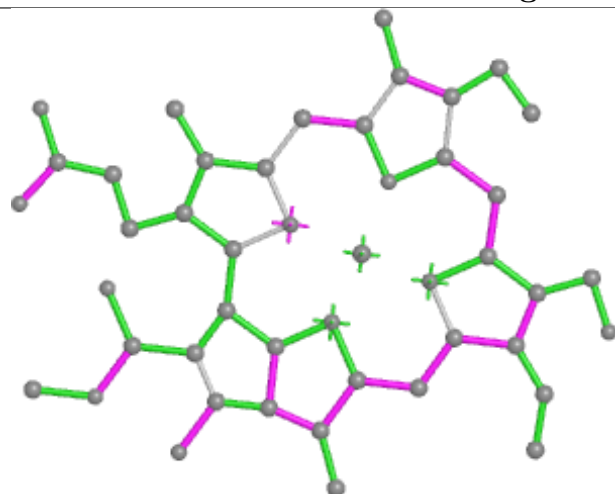




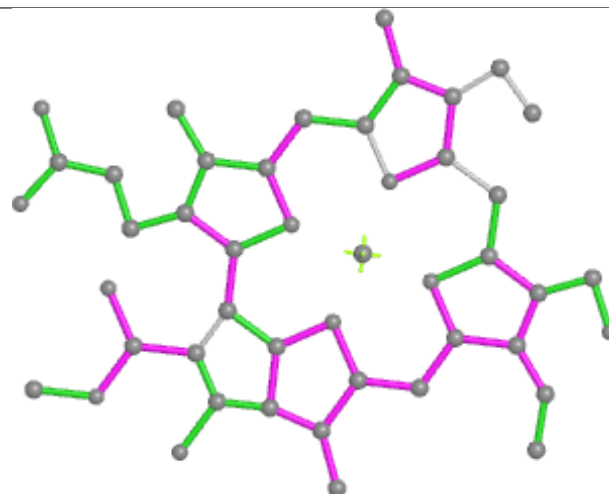




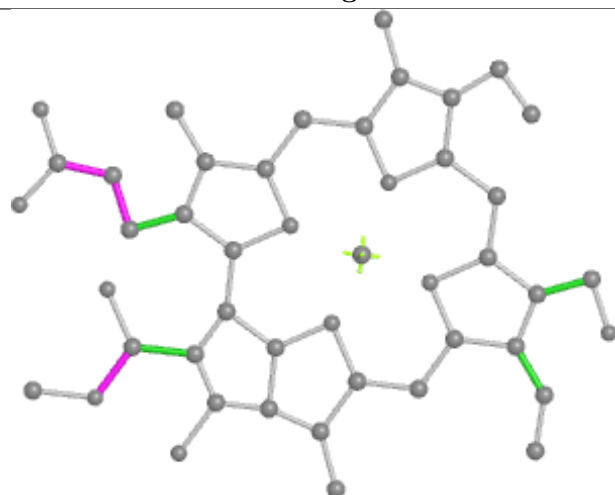
## Ligand CHL 2 606



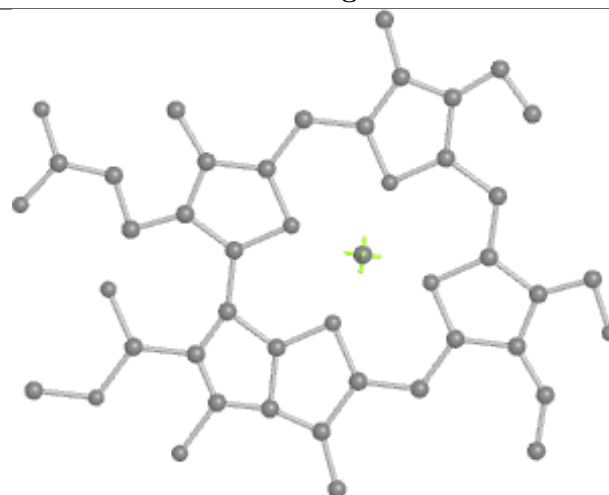
Bond lengths



Bond angles

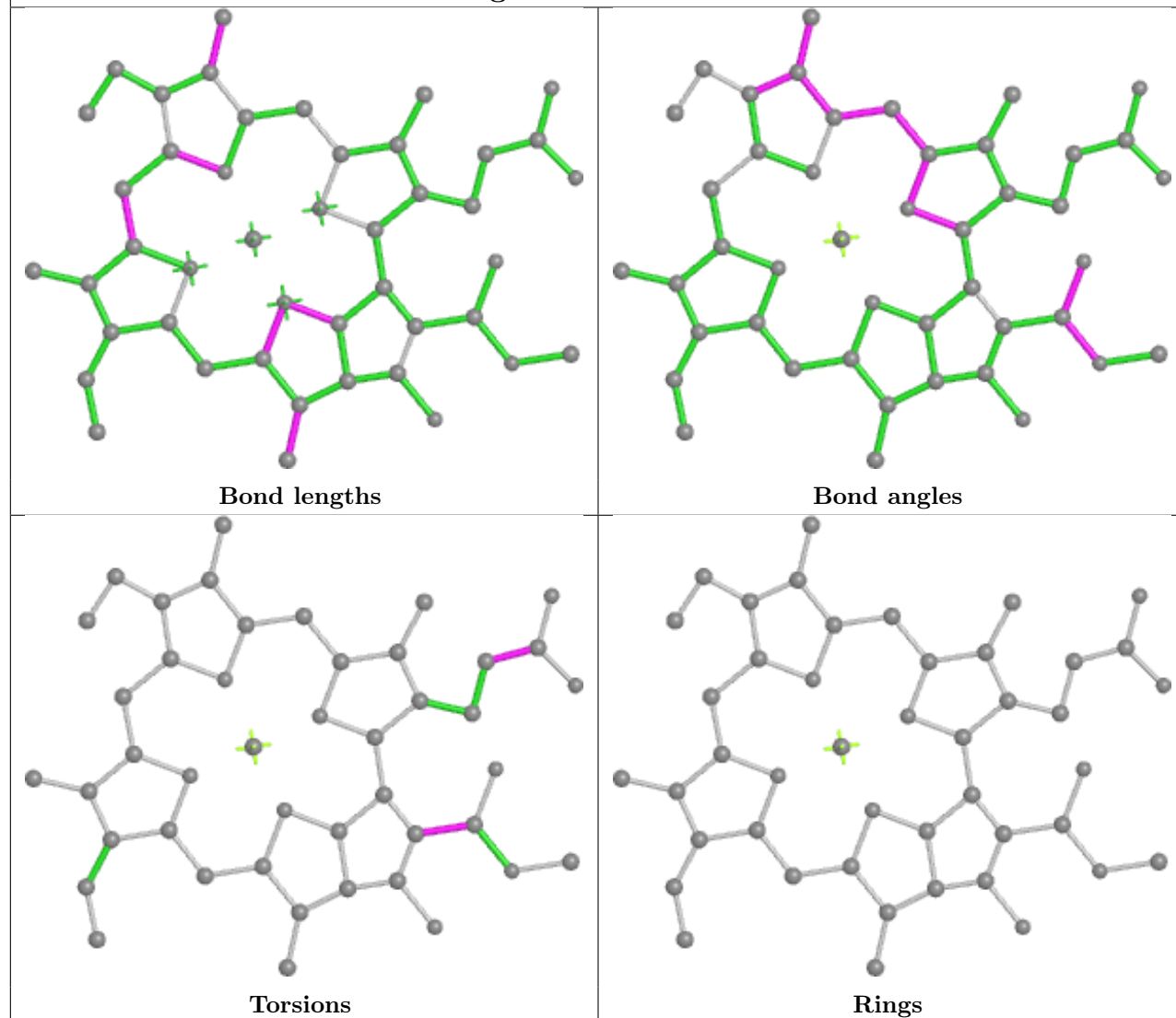


Torsions

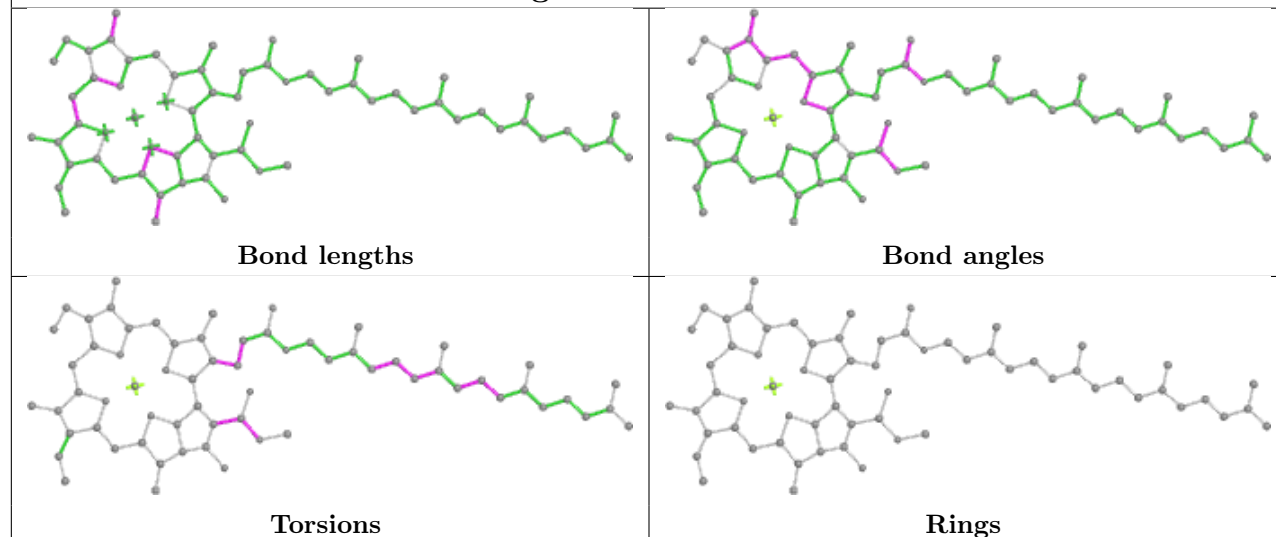


Rings

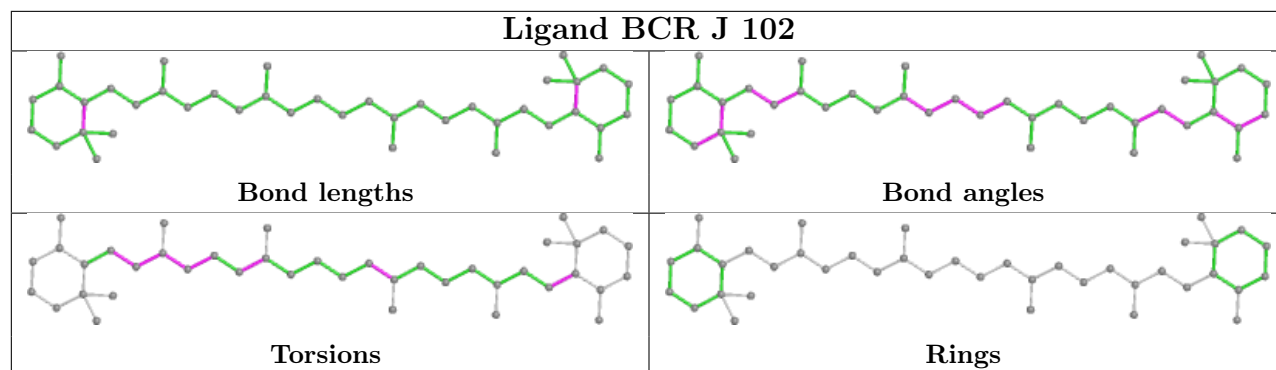
## Ligand CLA A 840



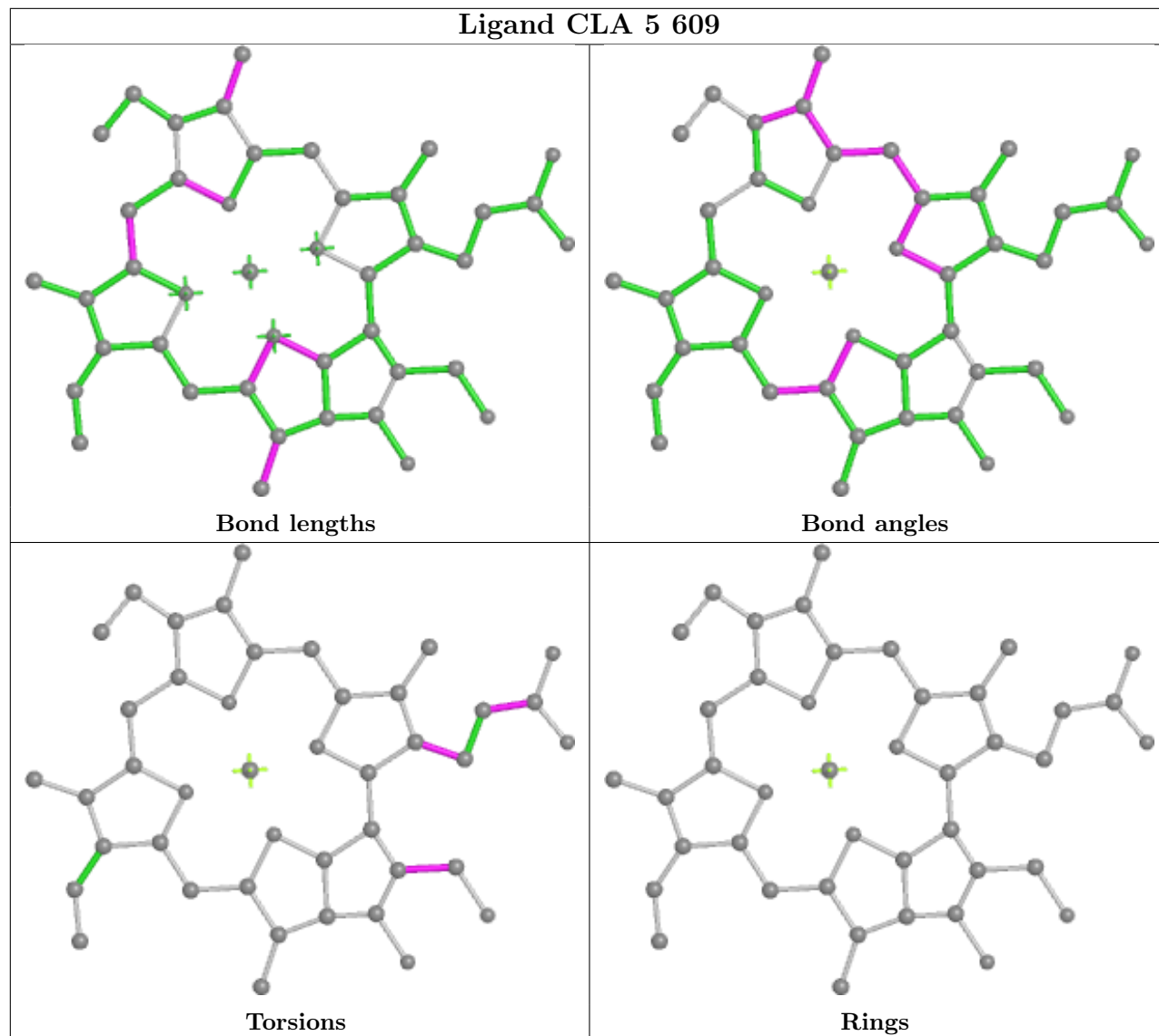
## Ligand CLA A 834



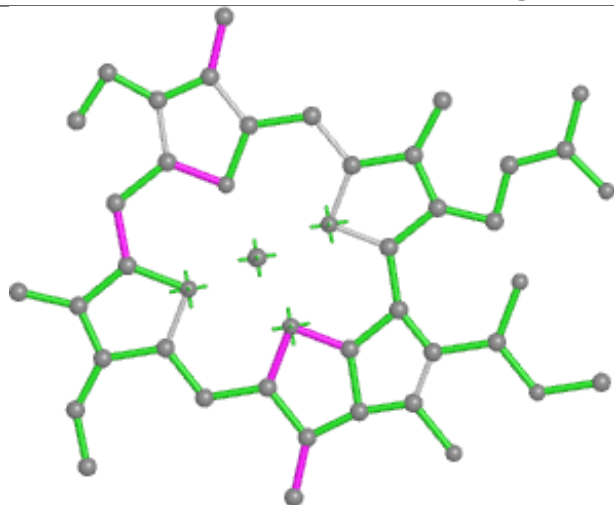
## Ligand BCR J 102



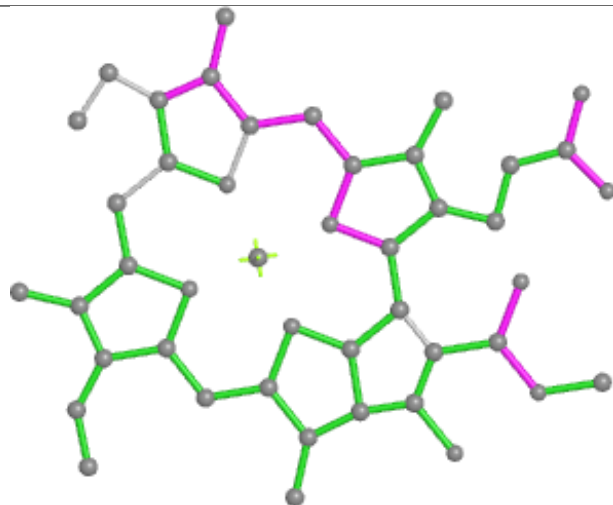
## Ligand CLA 5 609



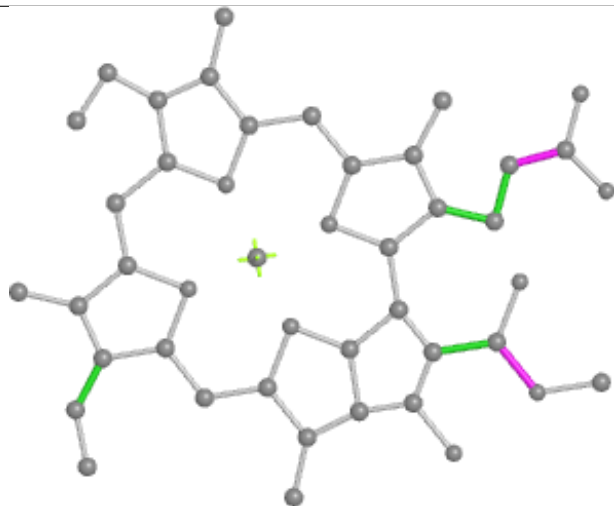
## Ligand CLA K 203



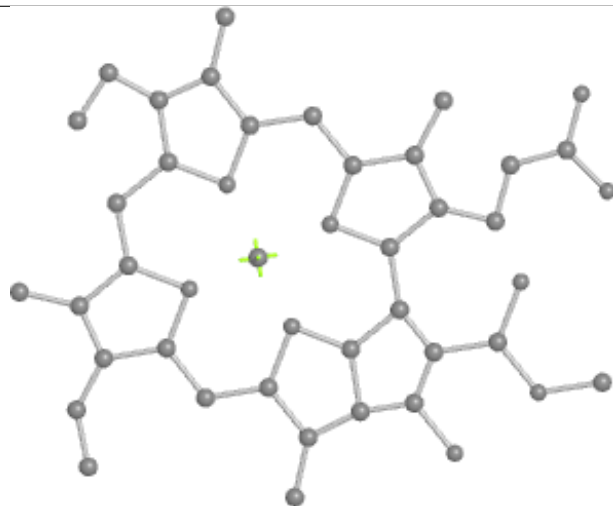
Bond lengths



Bond angles

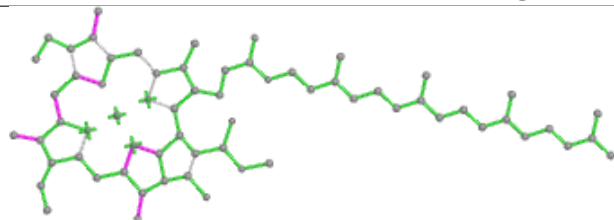


Torsions

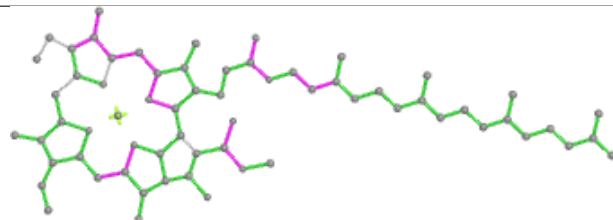


Rings

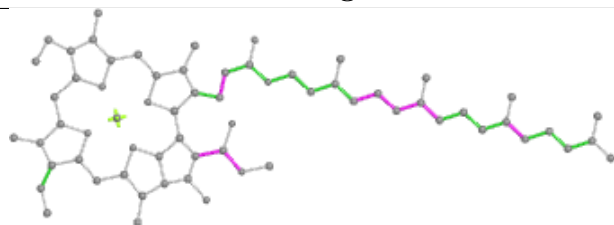
## Ligand CLA A 841



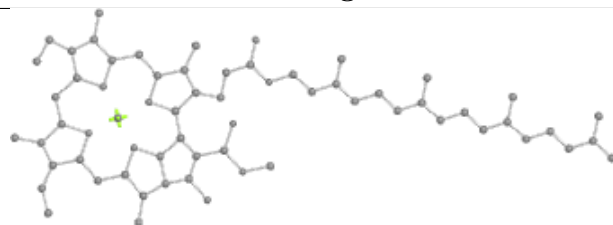
Bond lengths



Bond angles

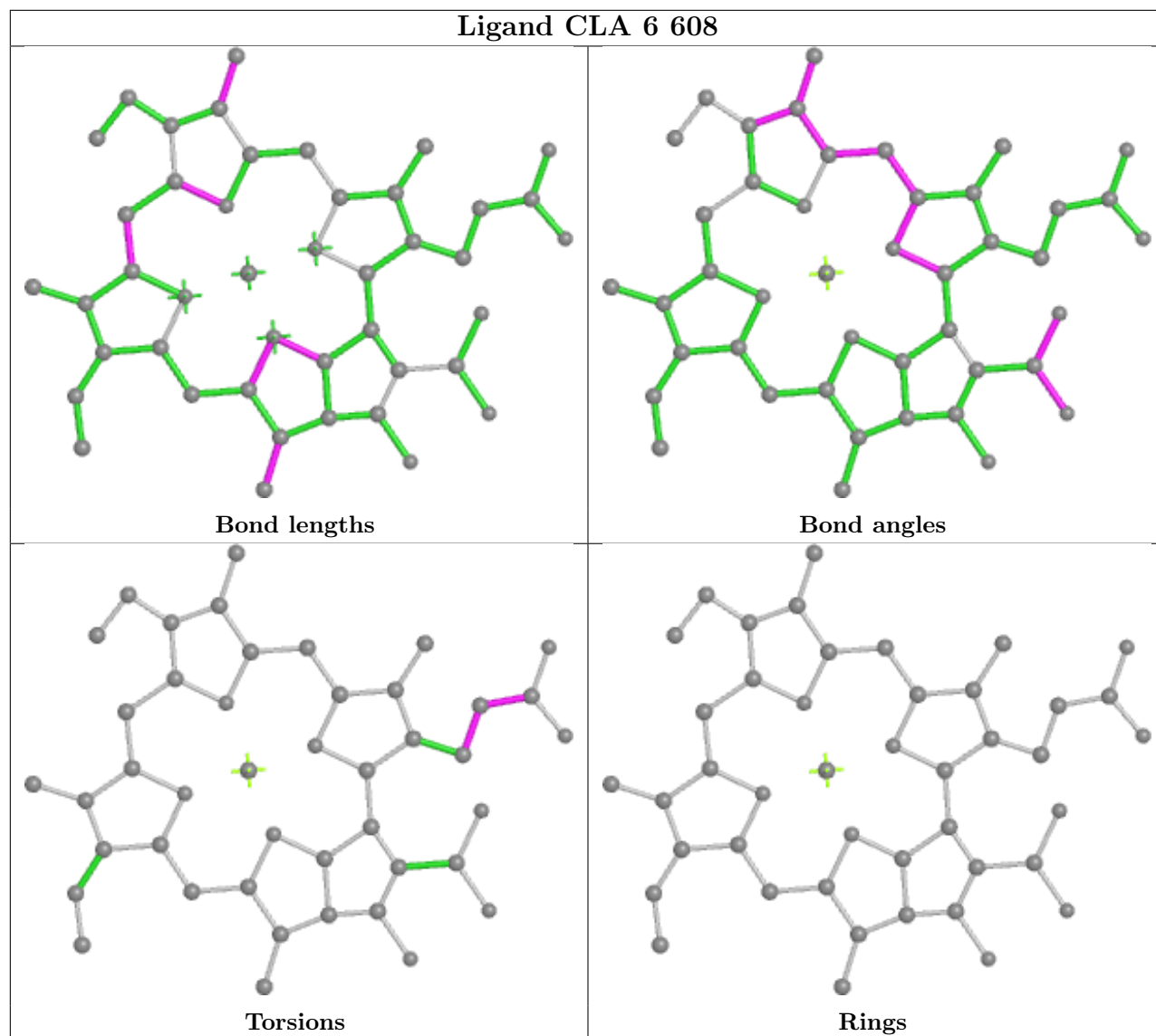


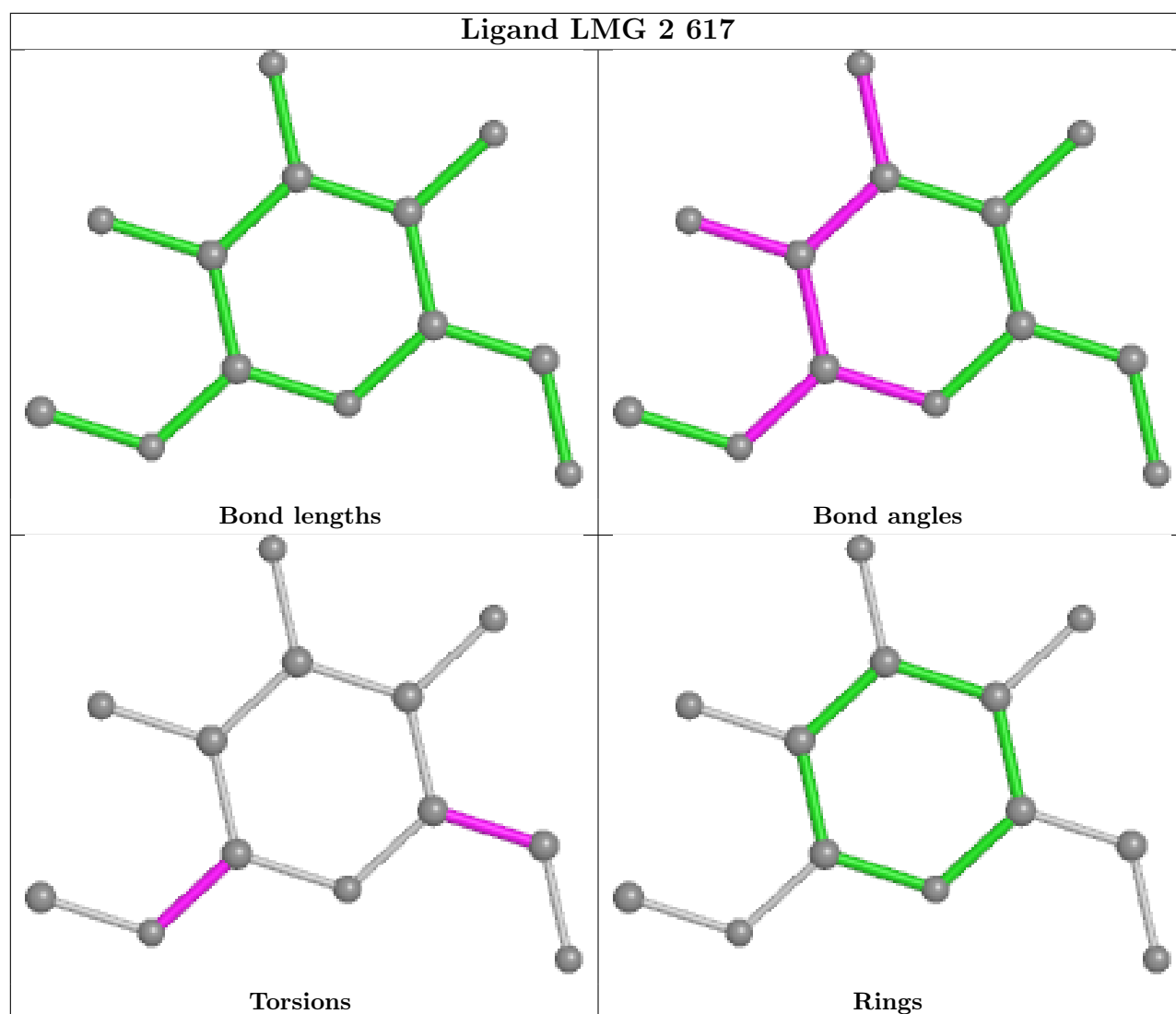
Torsions



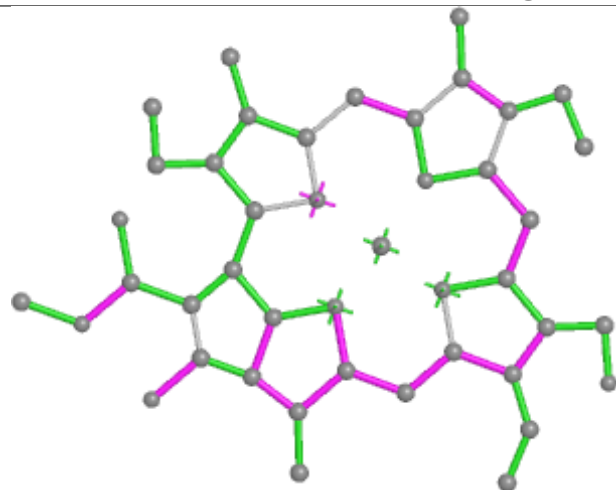
Rings

## Ligand CLA 6 608

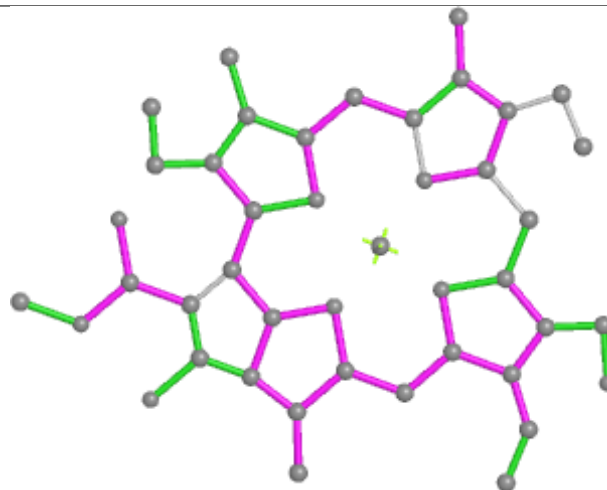




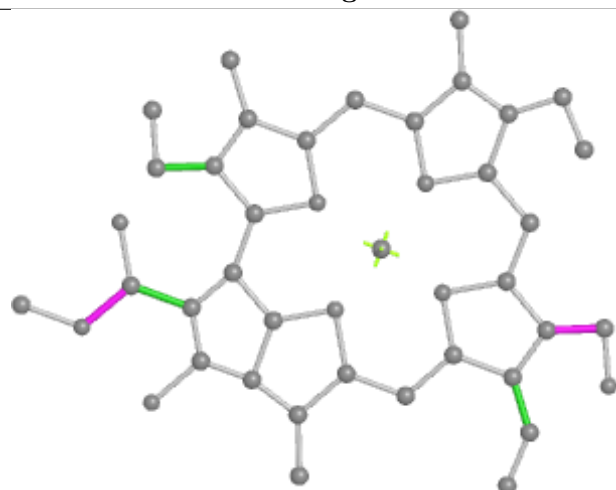
## Ligand CHL 5 615



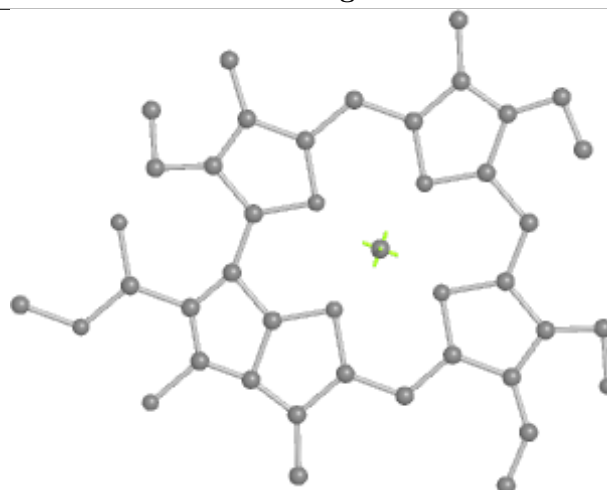
Bond lengths



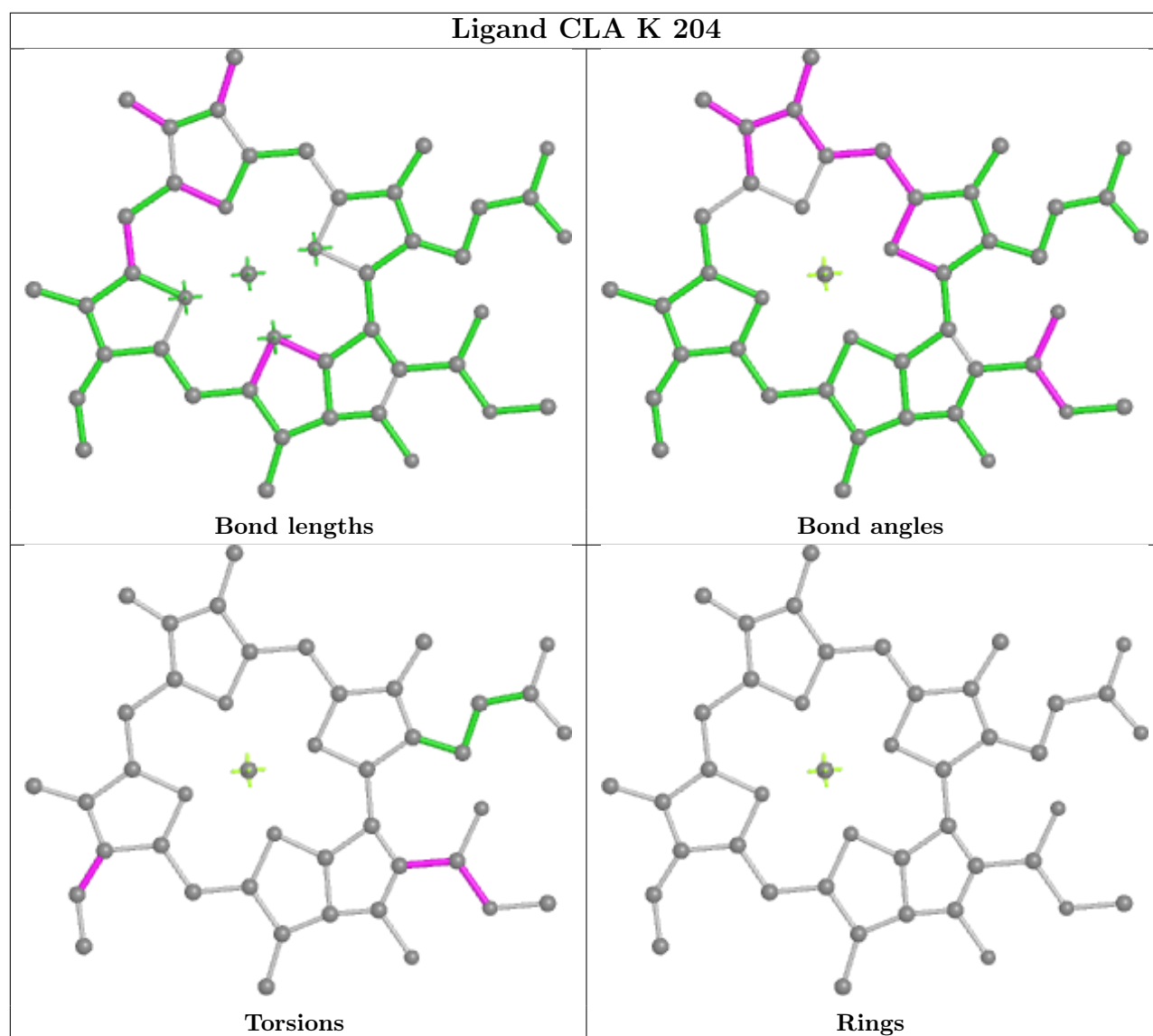
Bond angles



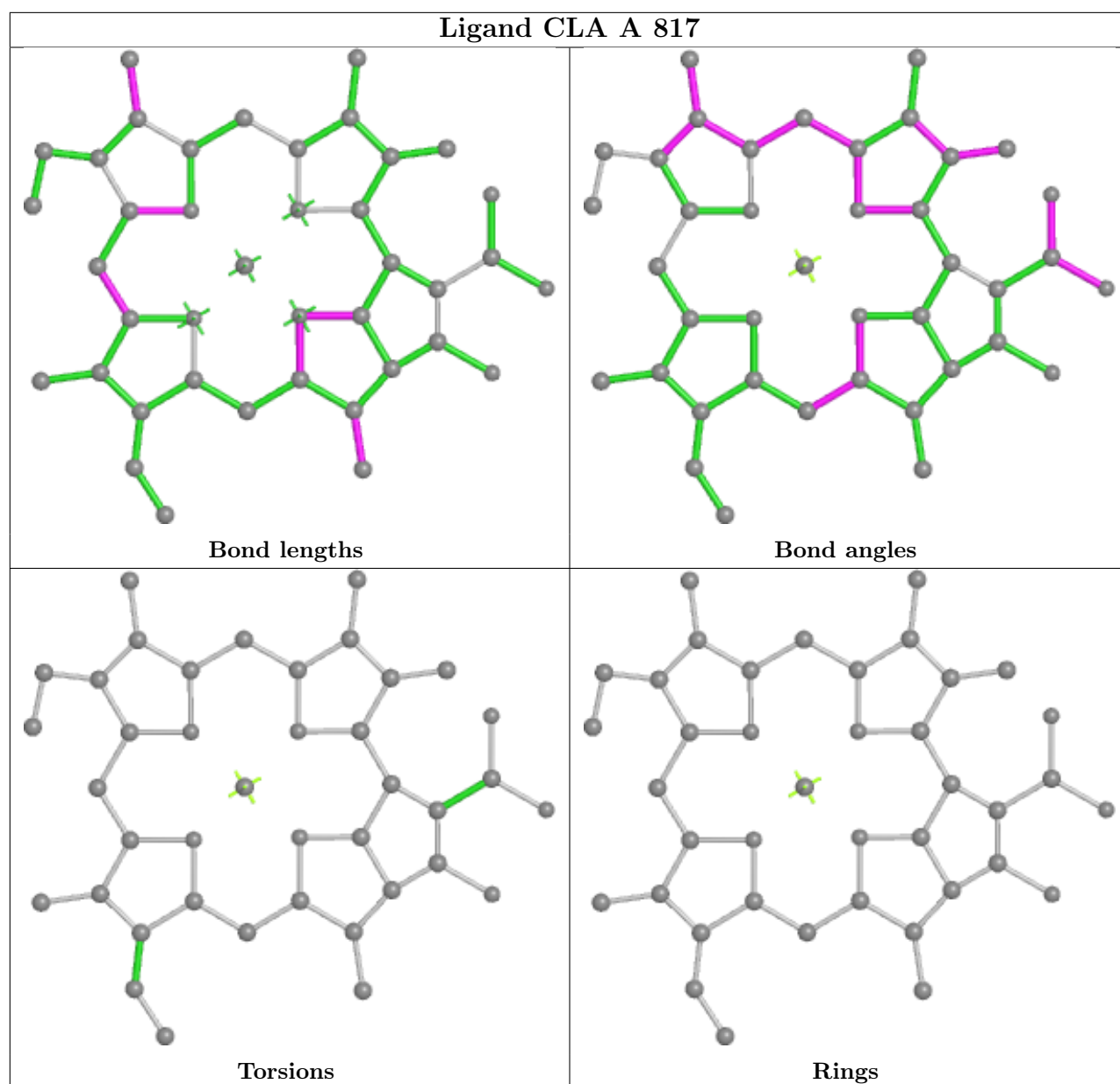
Torsions

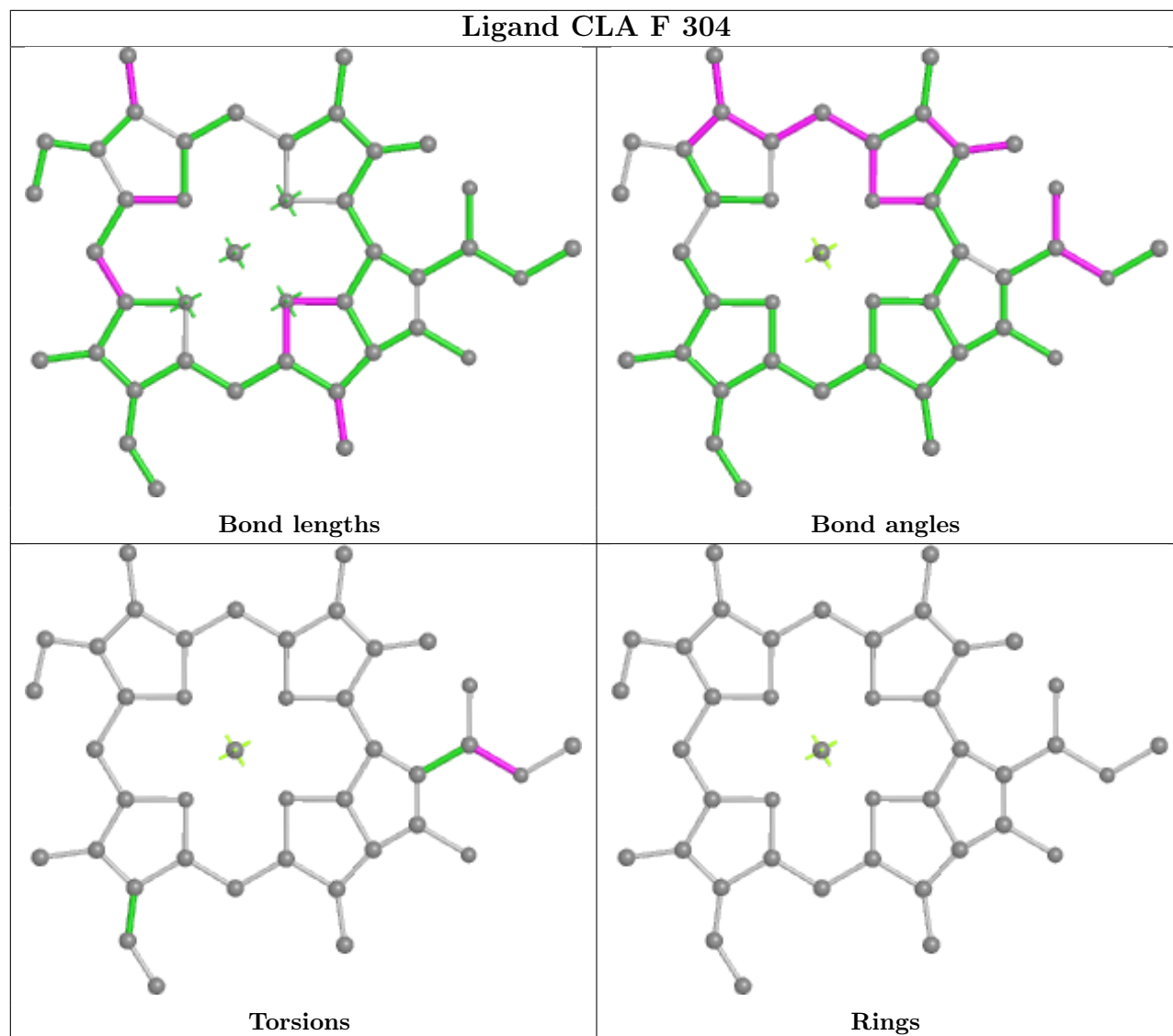


Rings

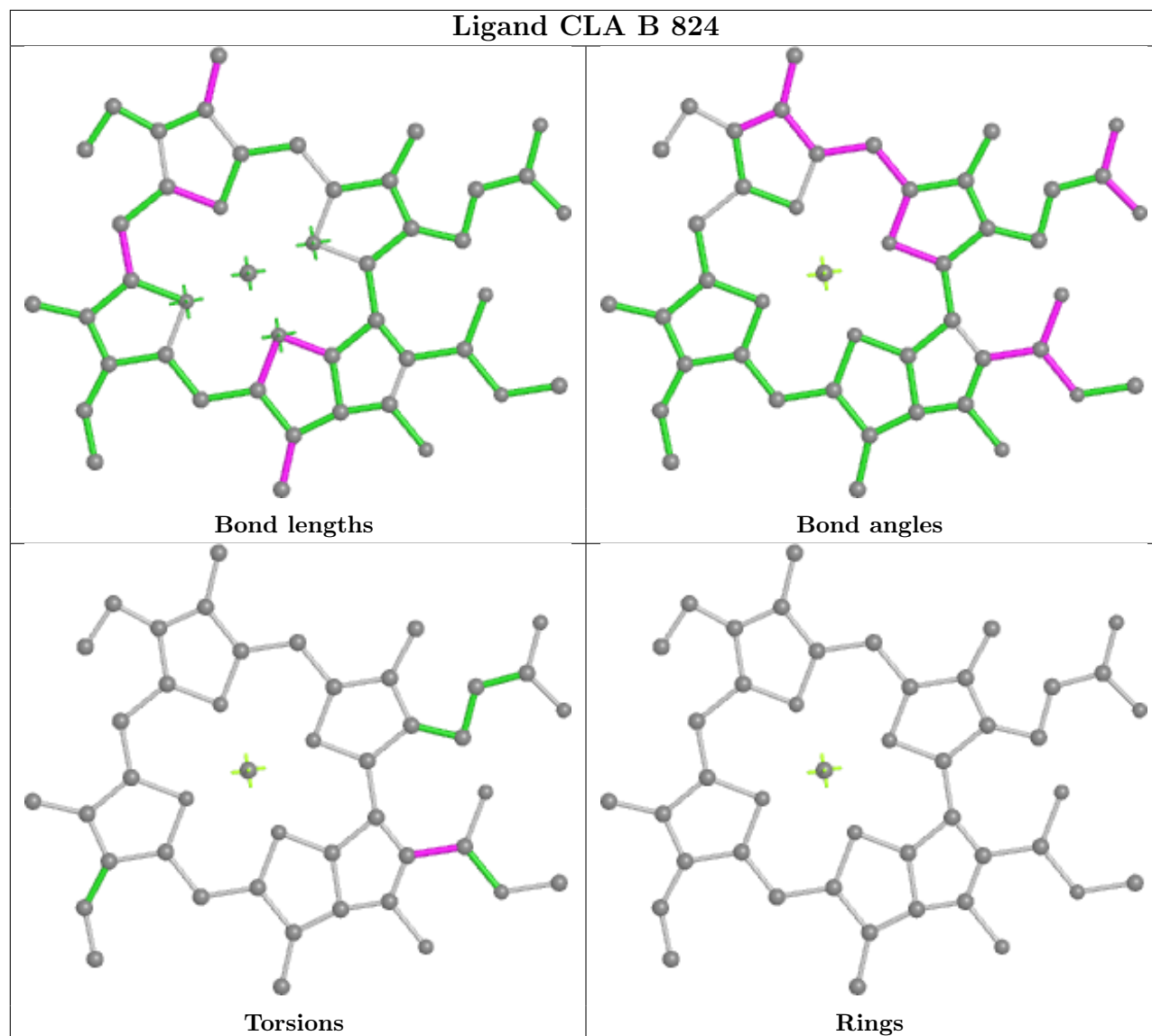




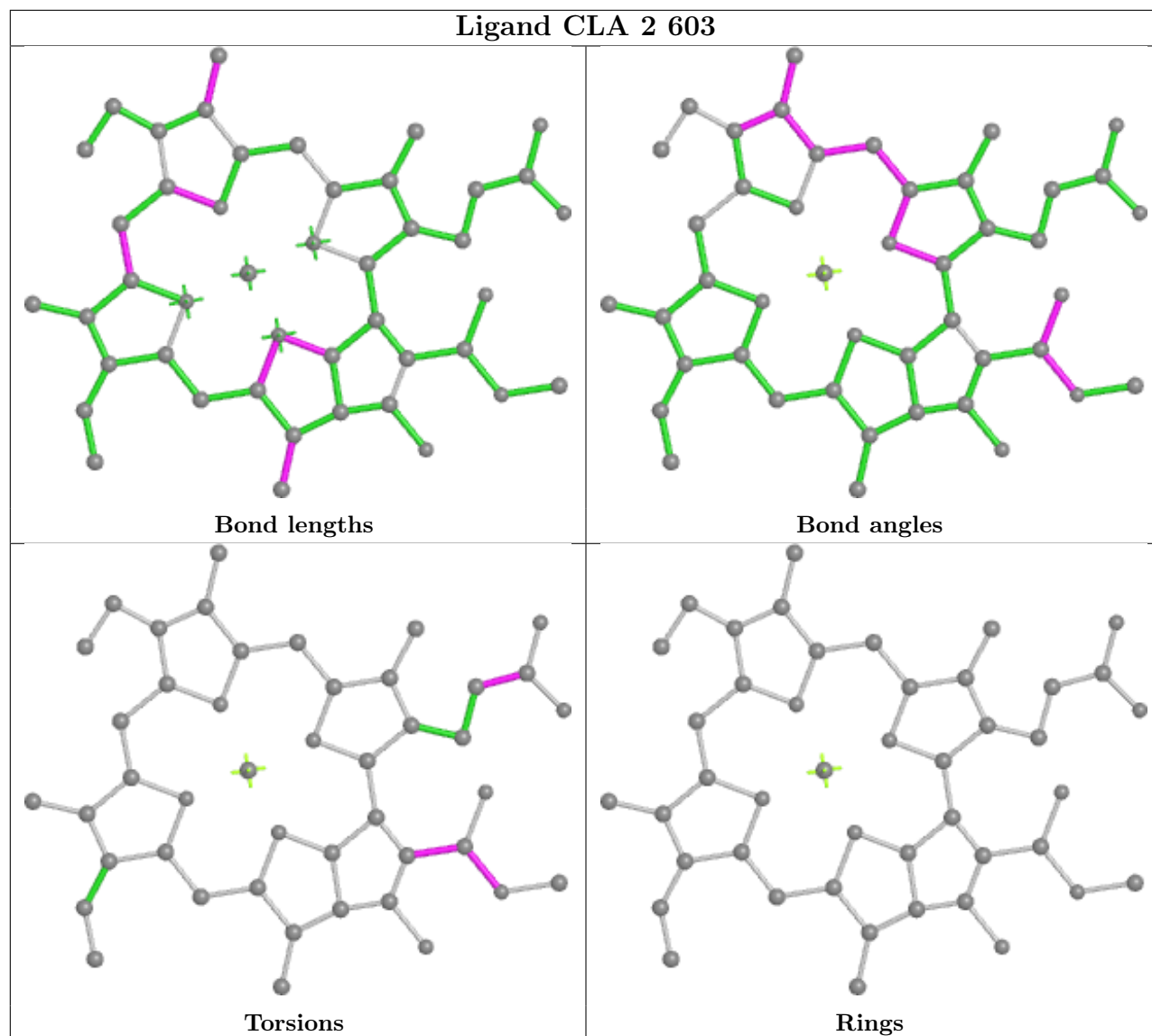




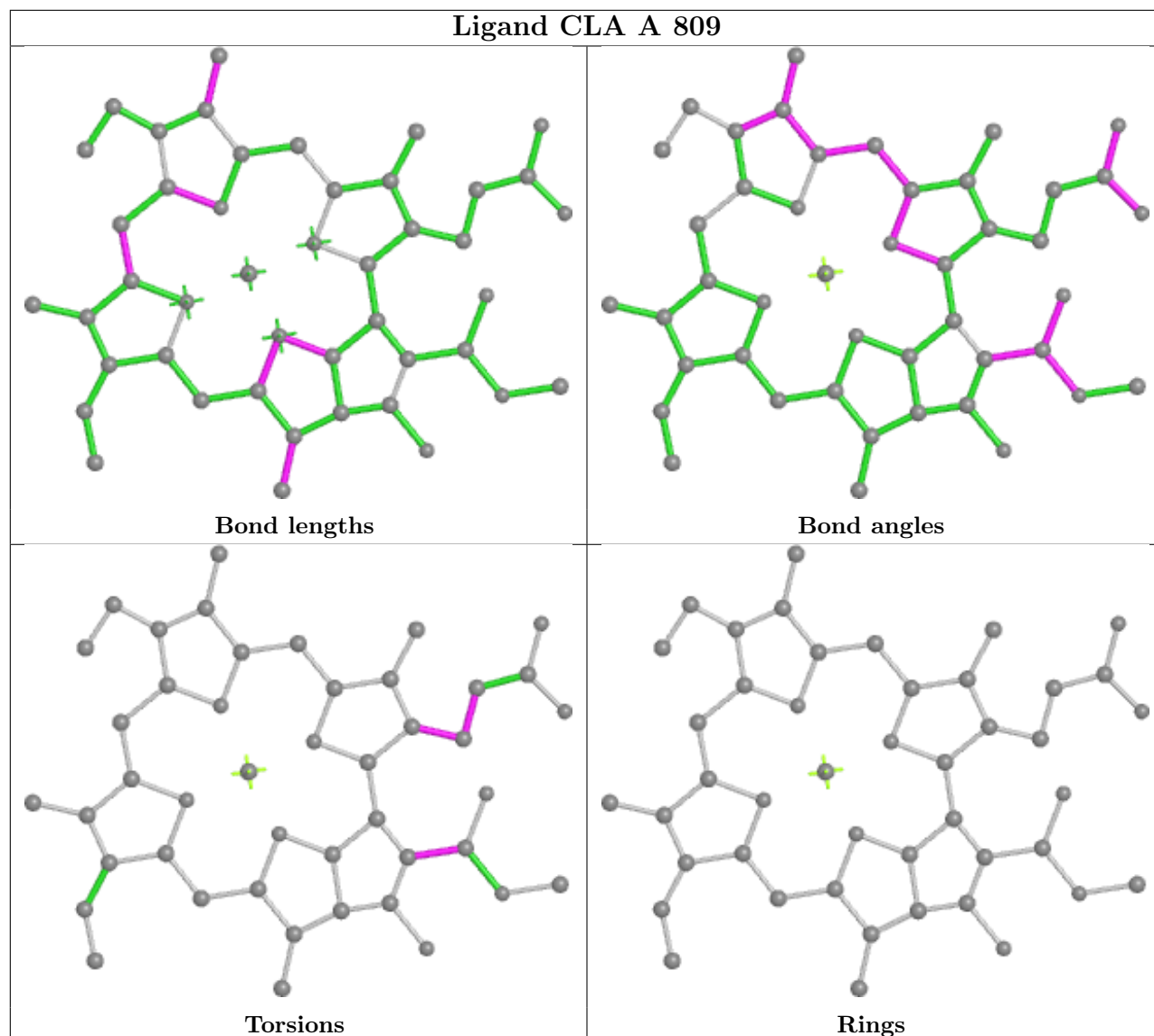
## Ligand CLA B 824



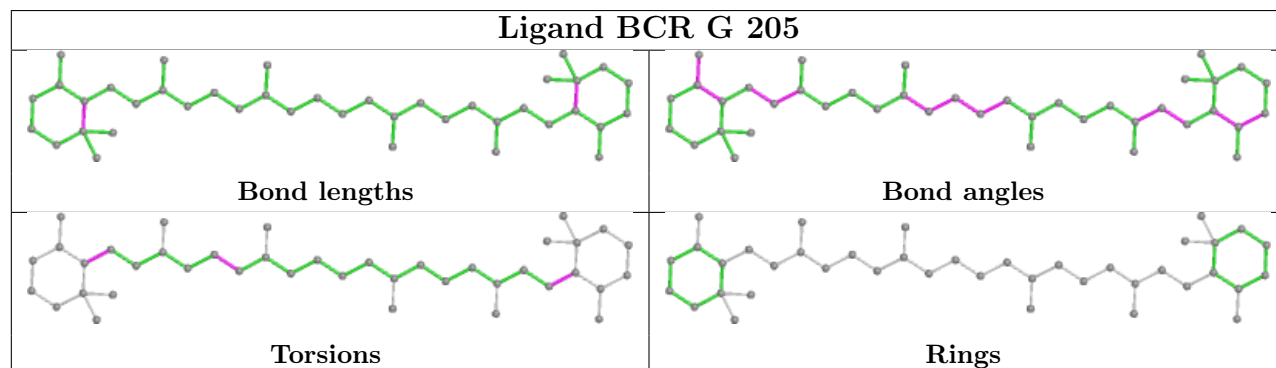
## Ligand CLA 2 603

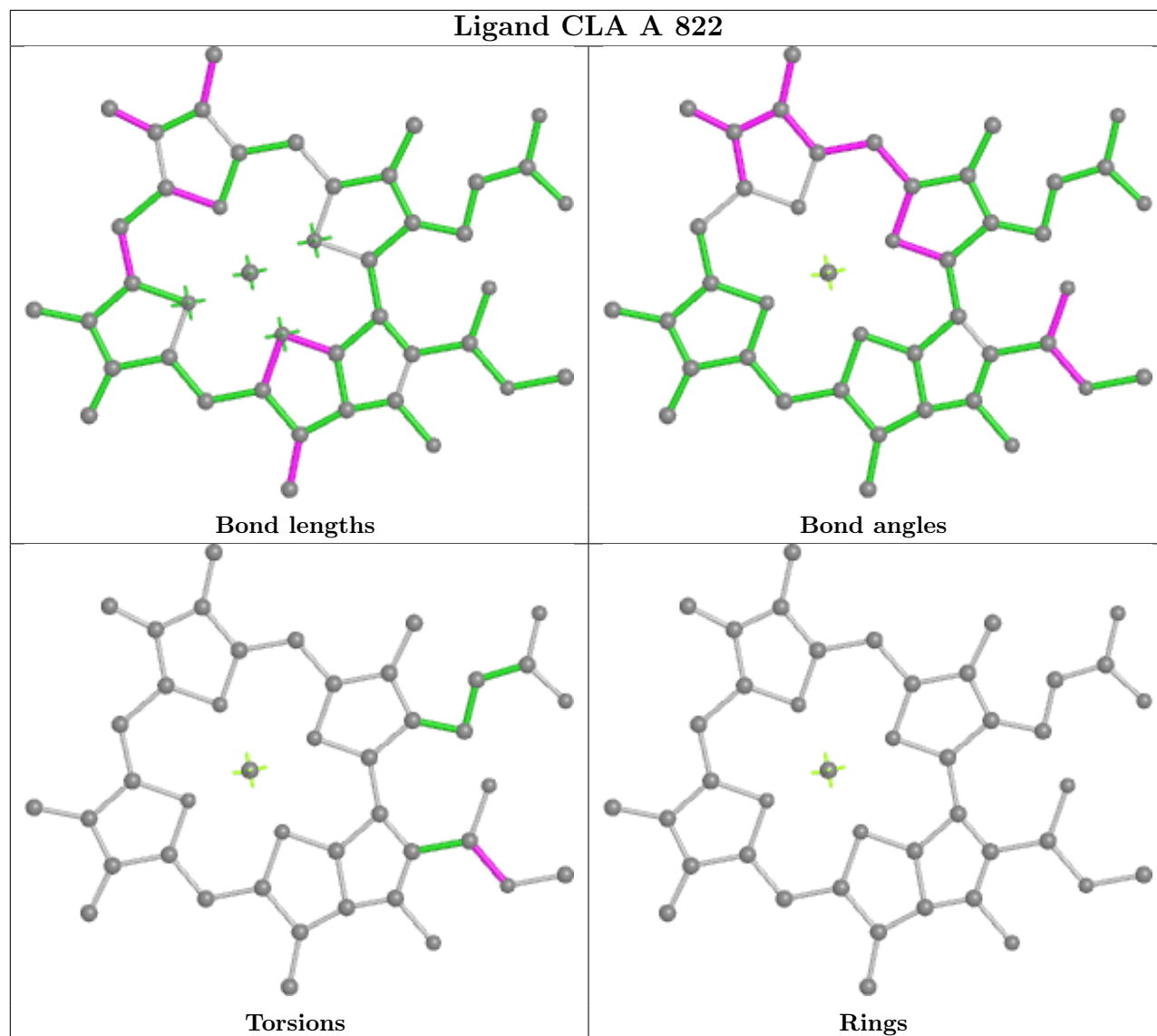
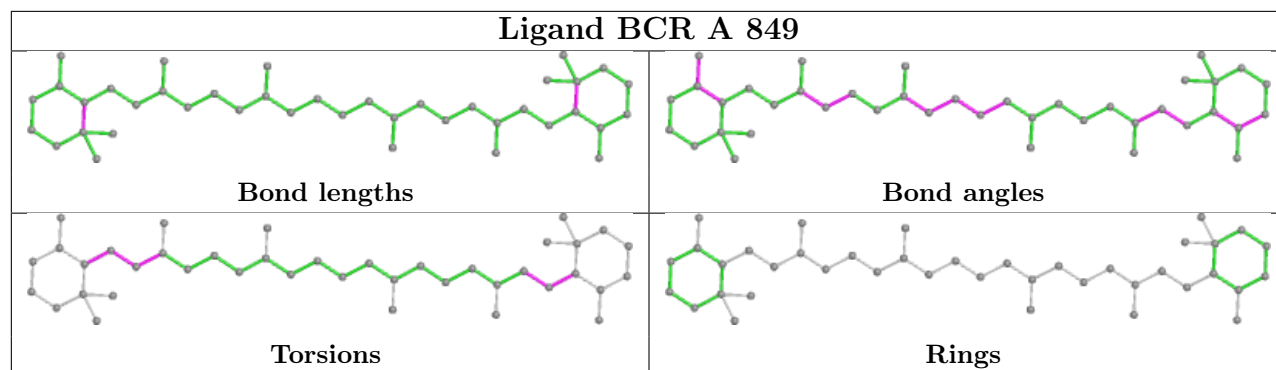


## Ligand CLA A 809

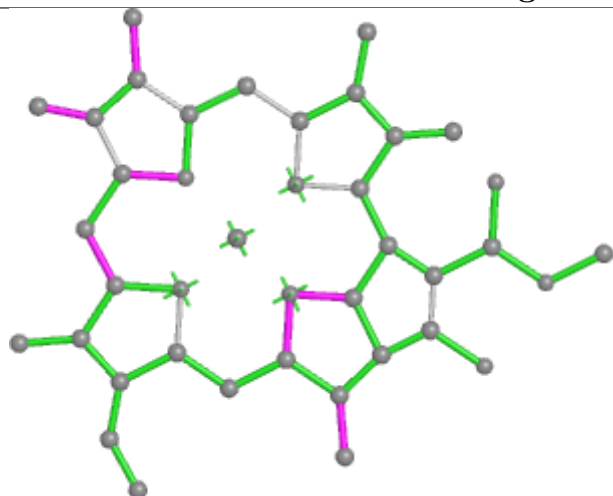


## Ligand BCR G 205

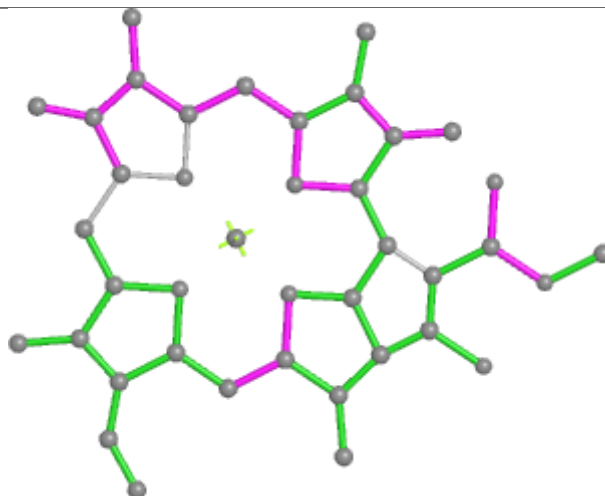




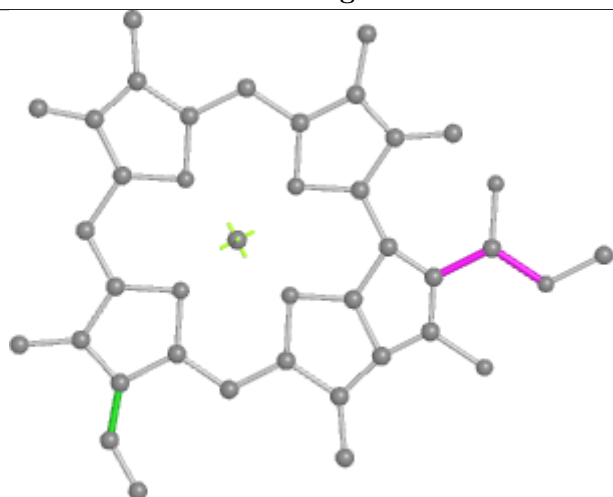
## Ligand CLA 6 609



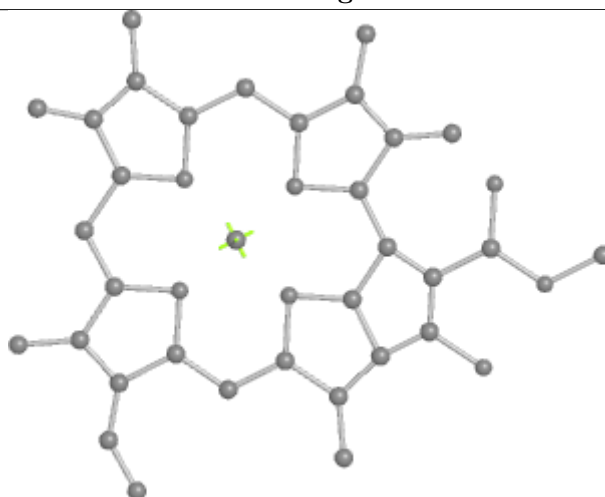
Bond lengths



Bond angles

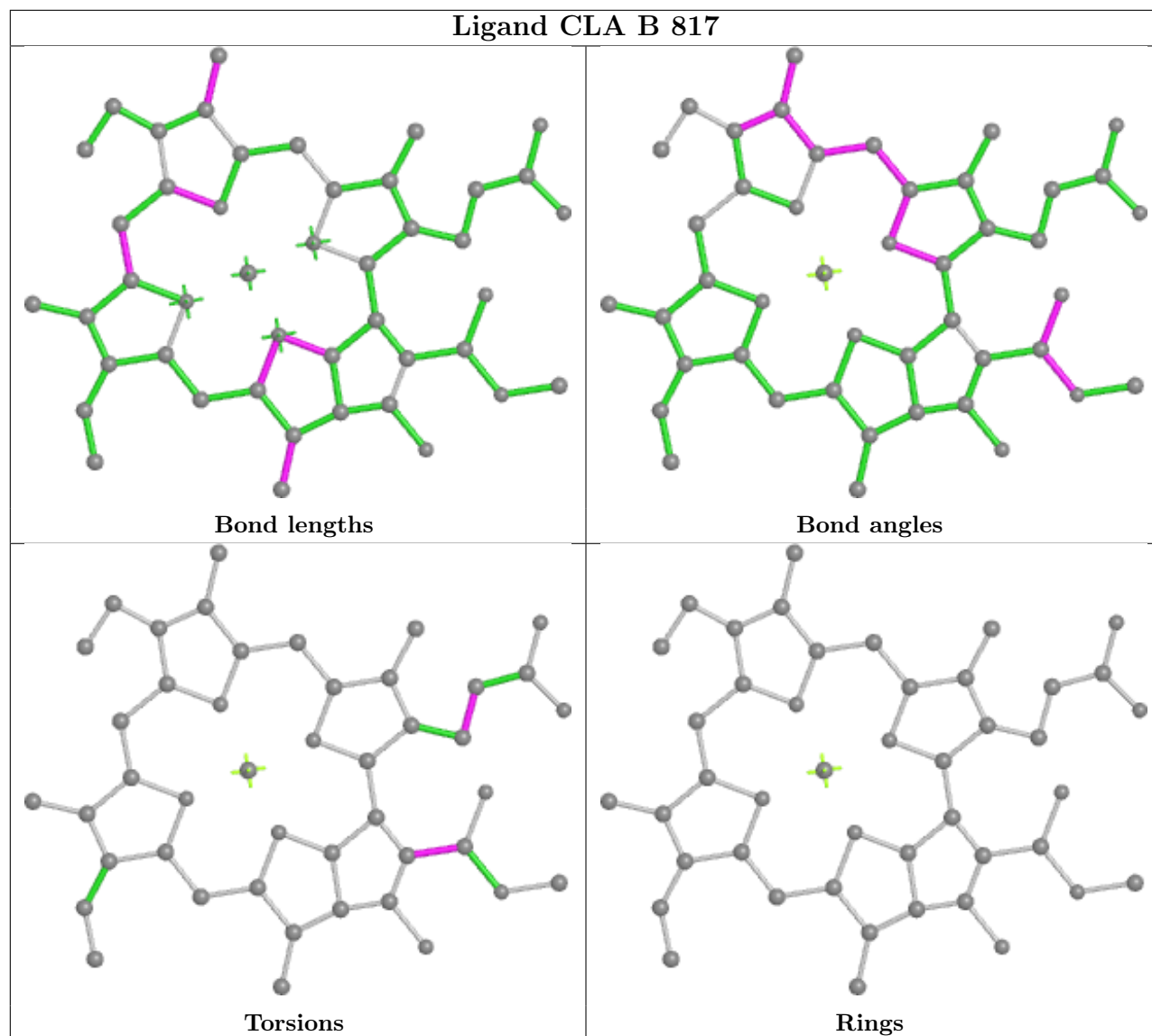


Torsions

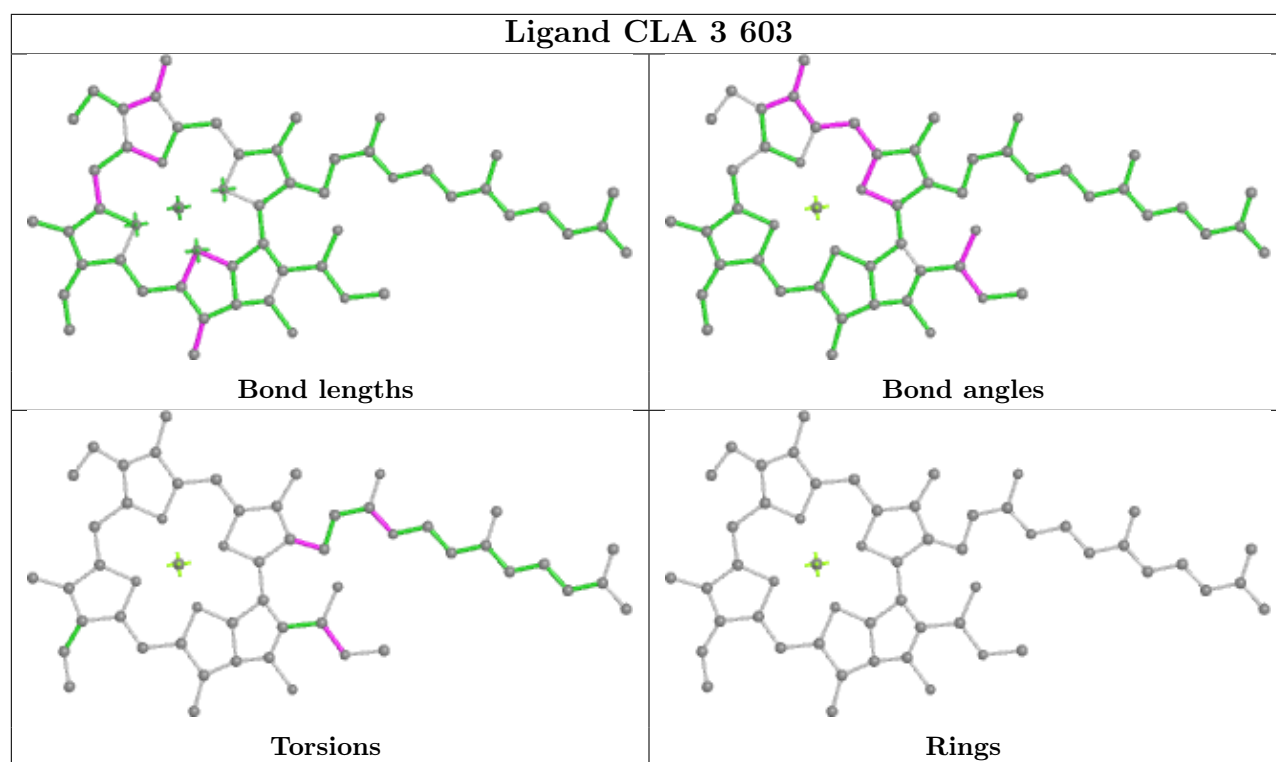


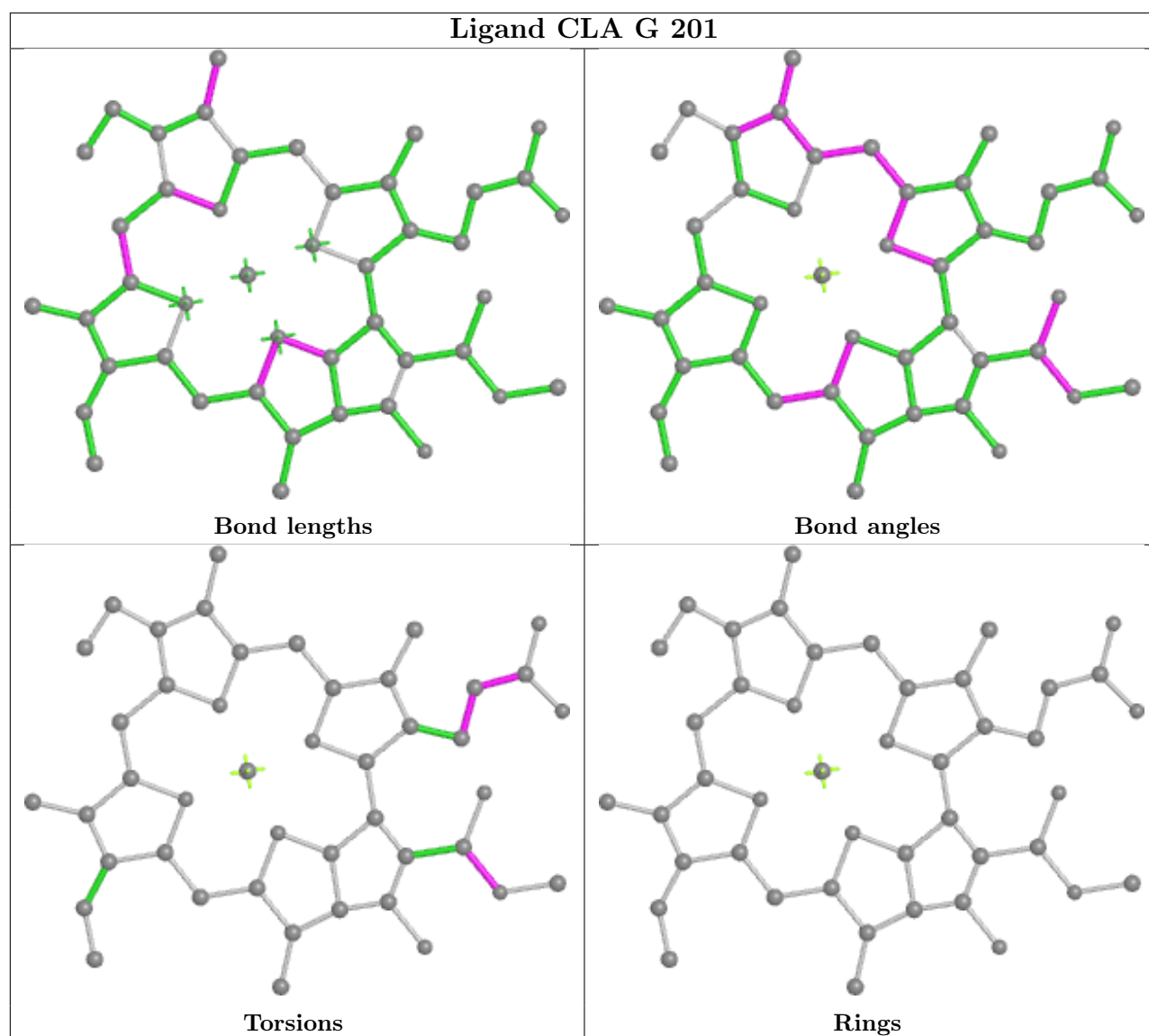
Rings

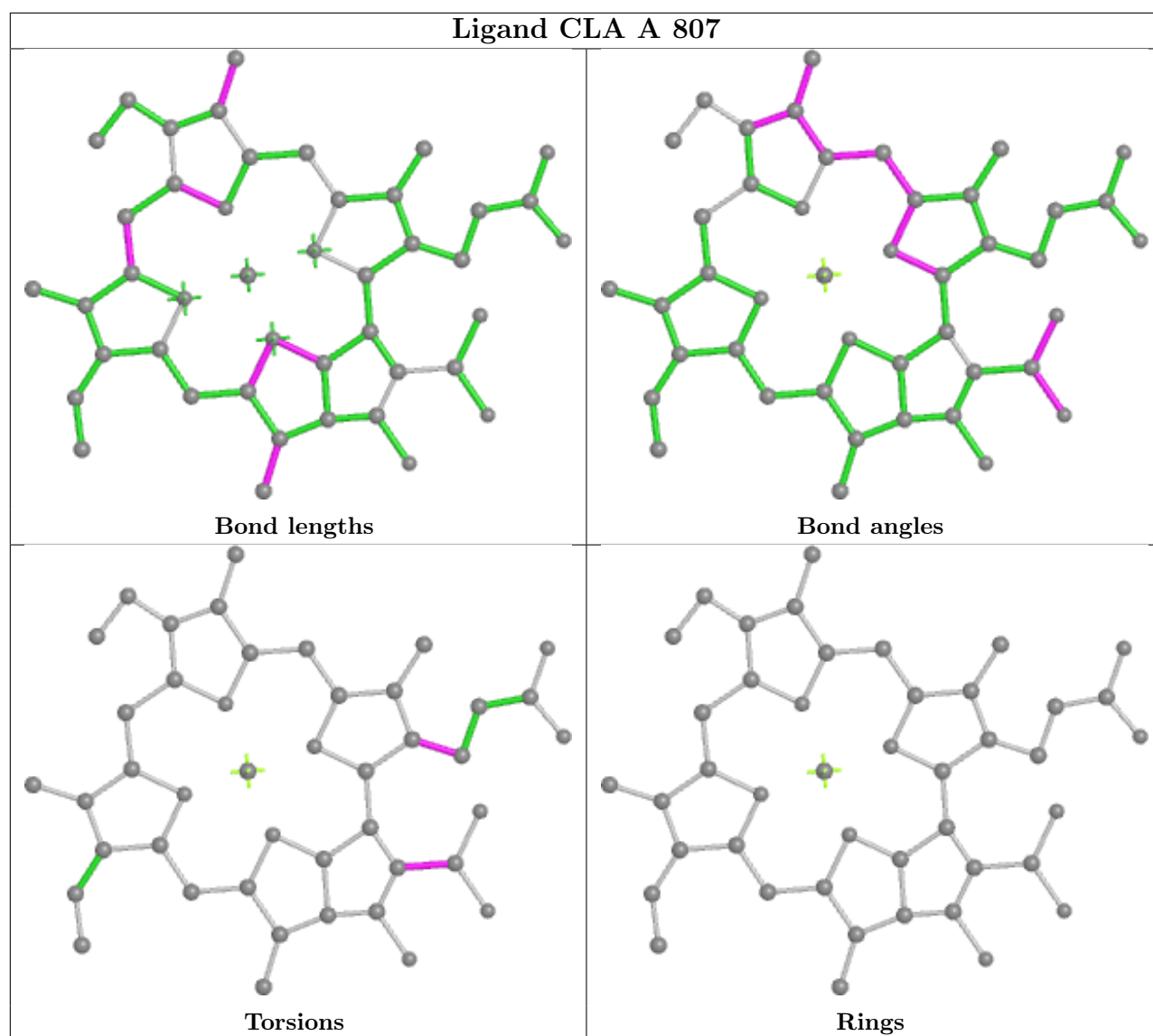
## Ligand CLA B 817



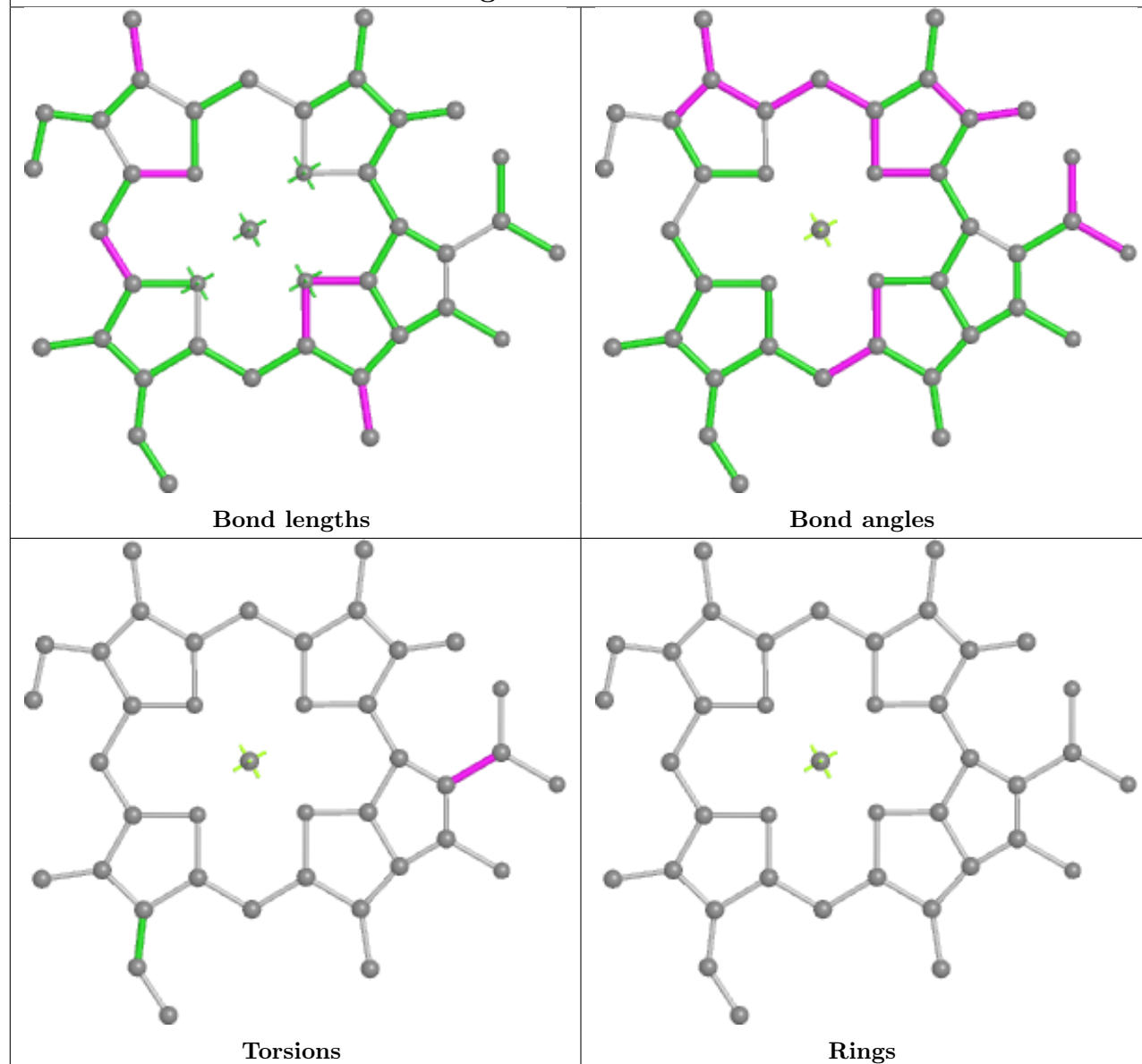




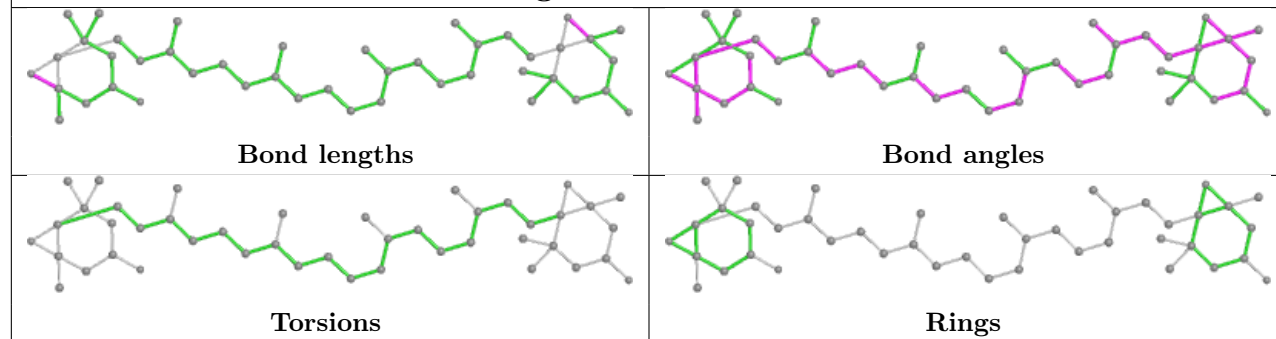




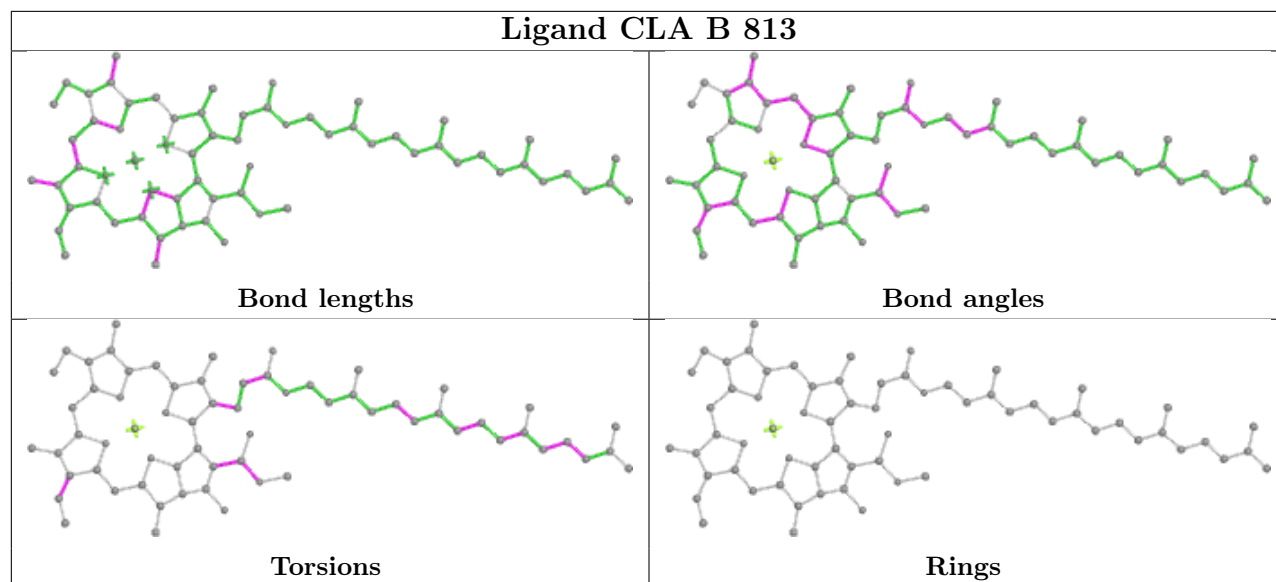
## Ligand CLA 3 617



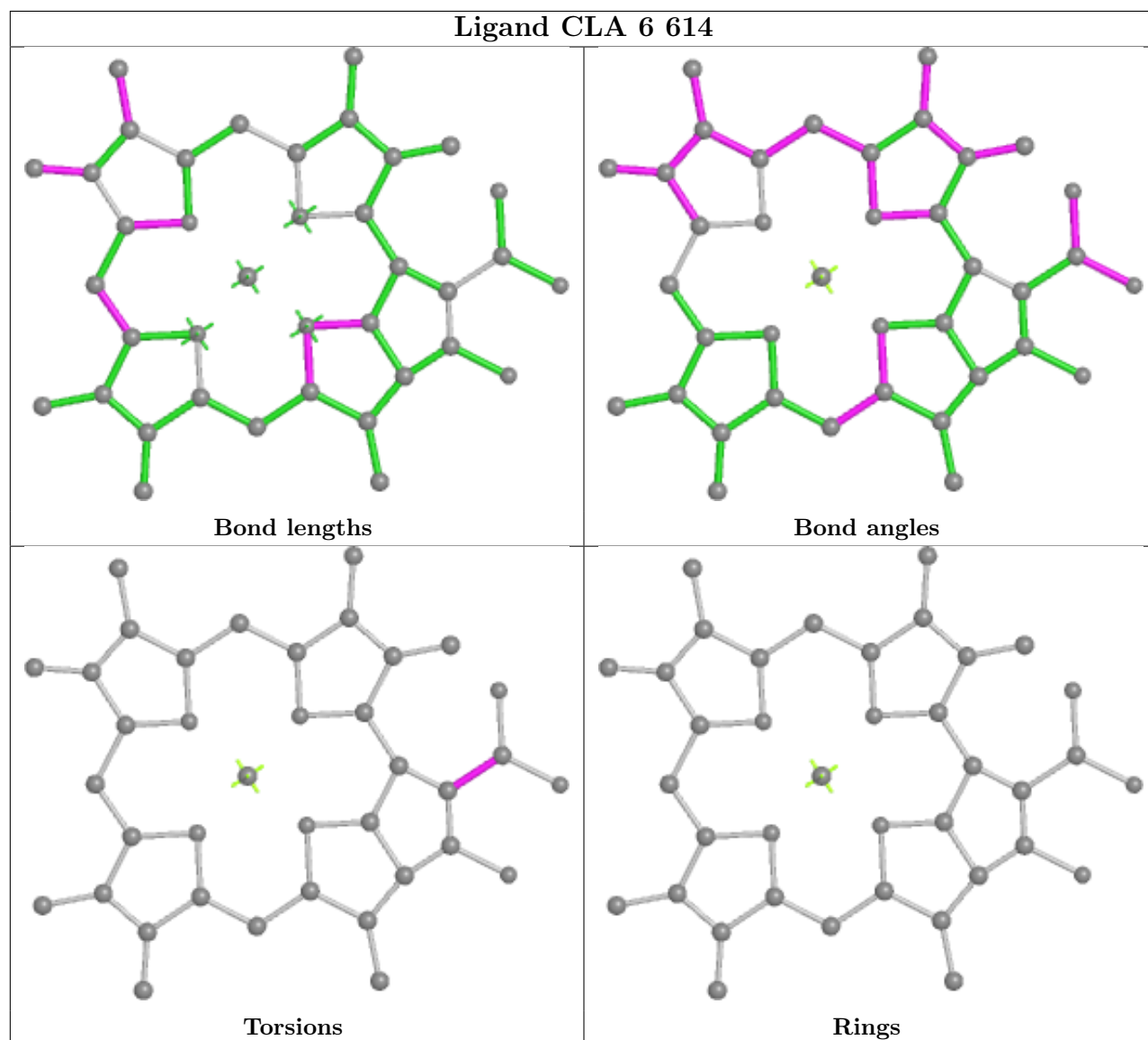
## Ligand XAT 3 619



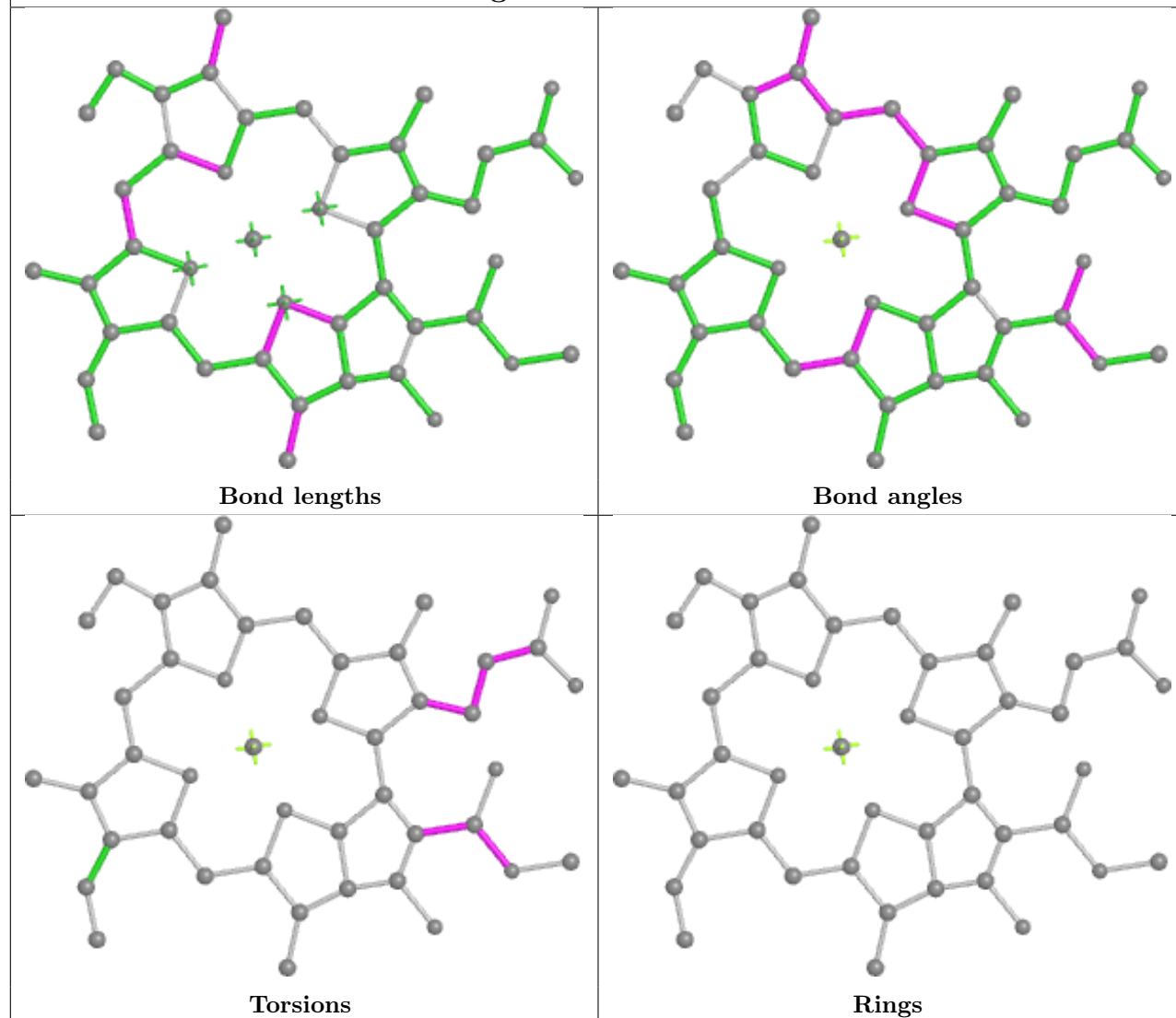
## Ligand CLA B 813



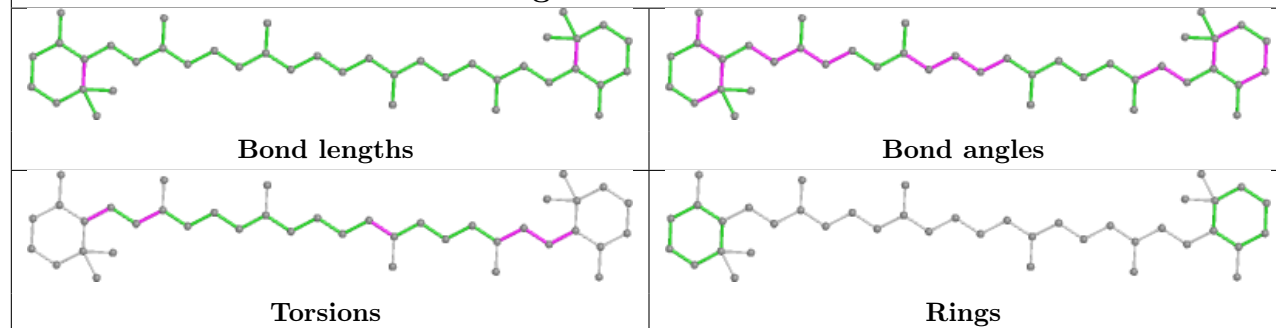
## Ligand CLA 6 614

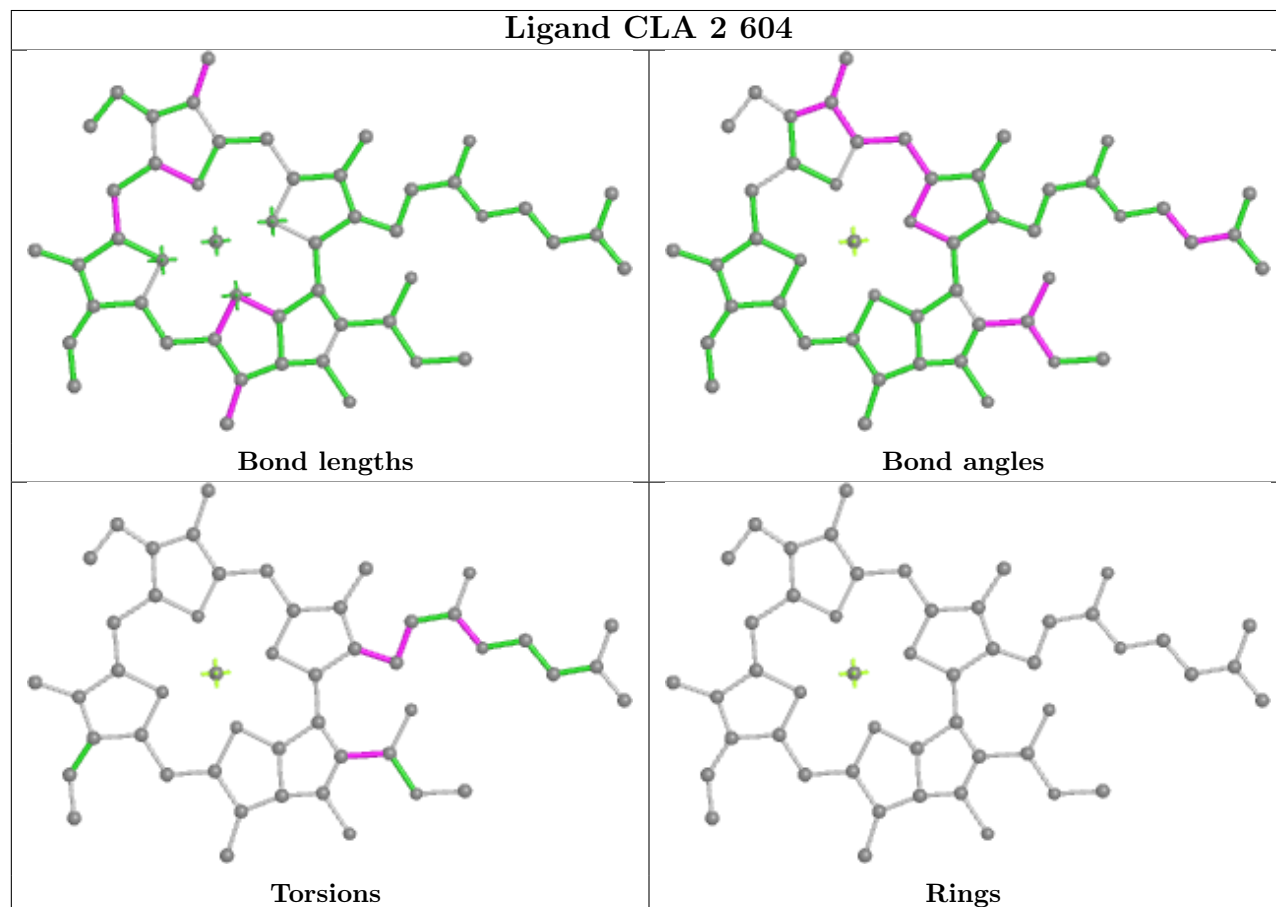
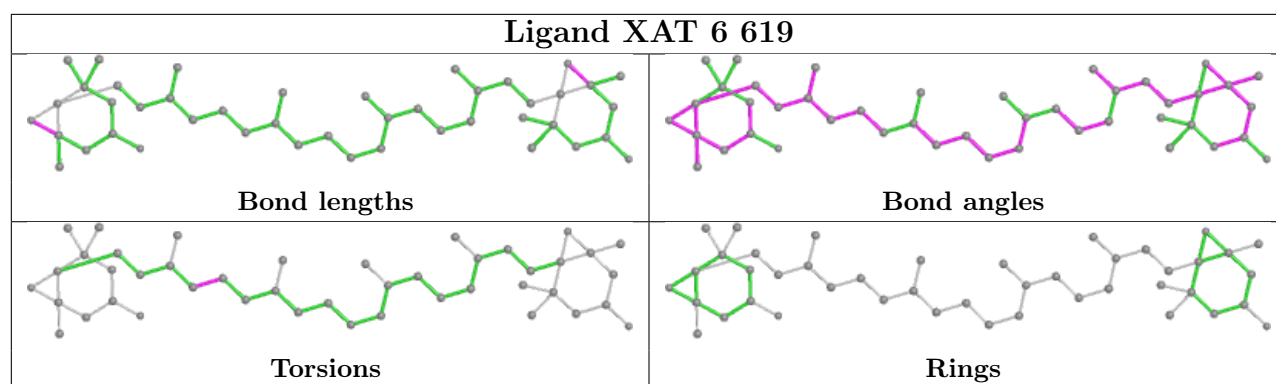


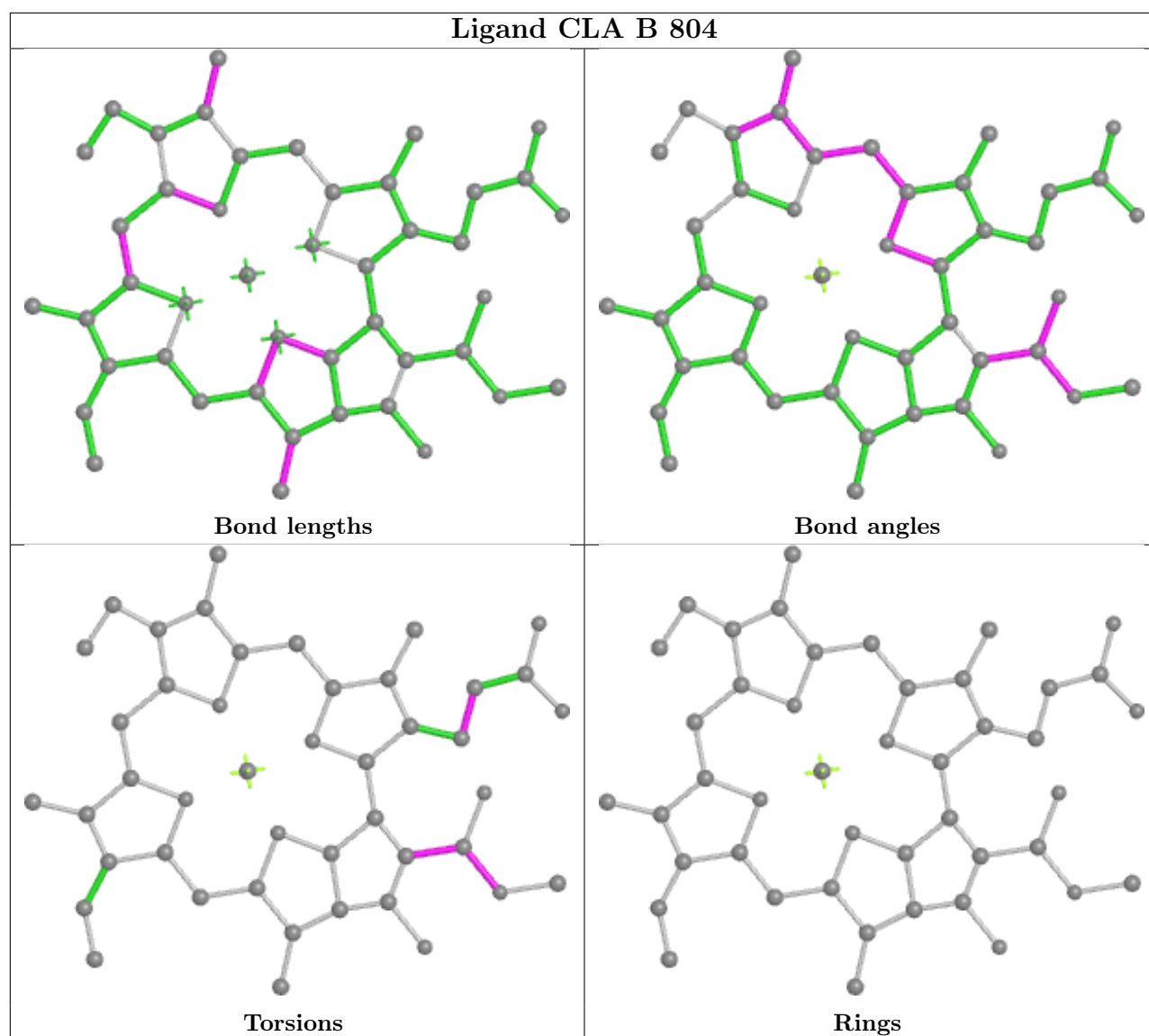
## Ligand CLA B 835



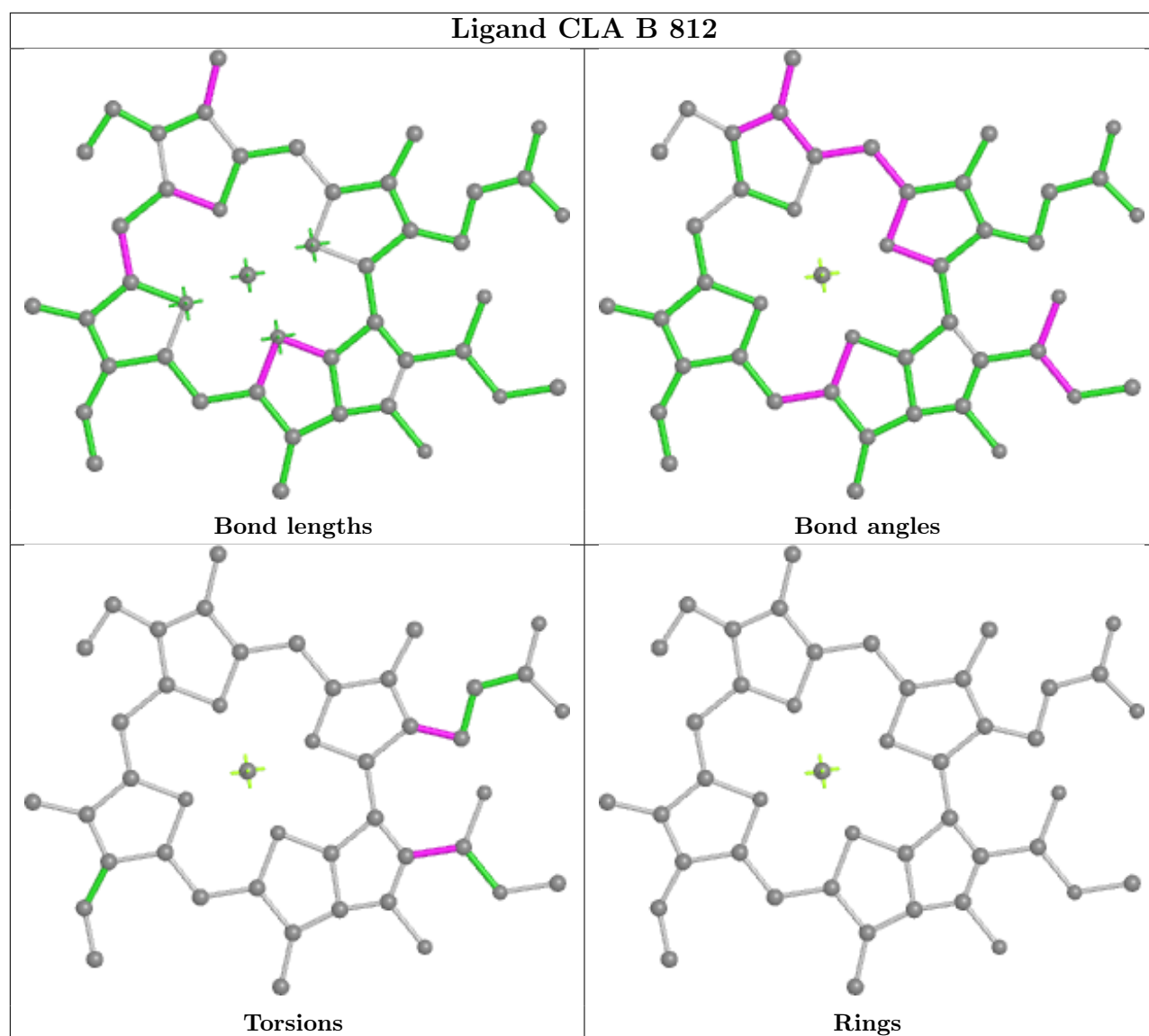
## Ligand BCR L 305



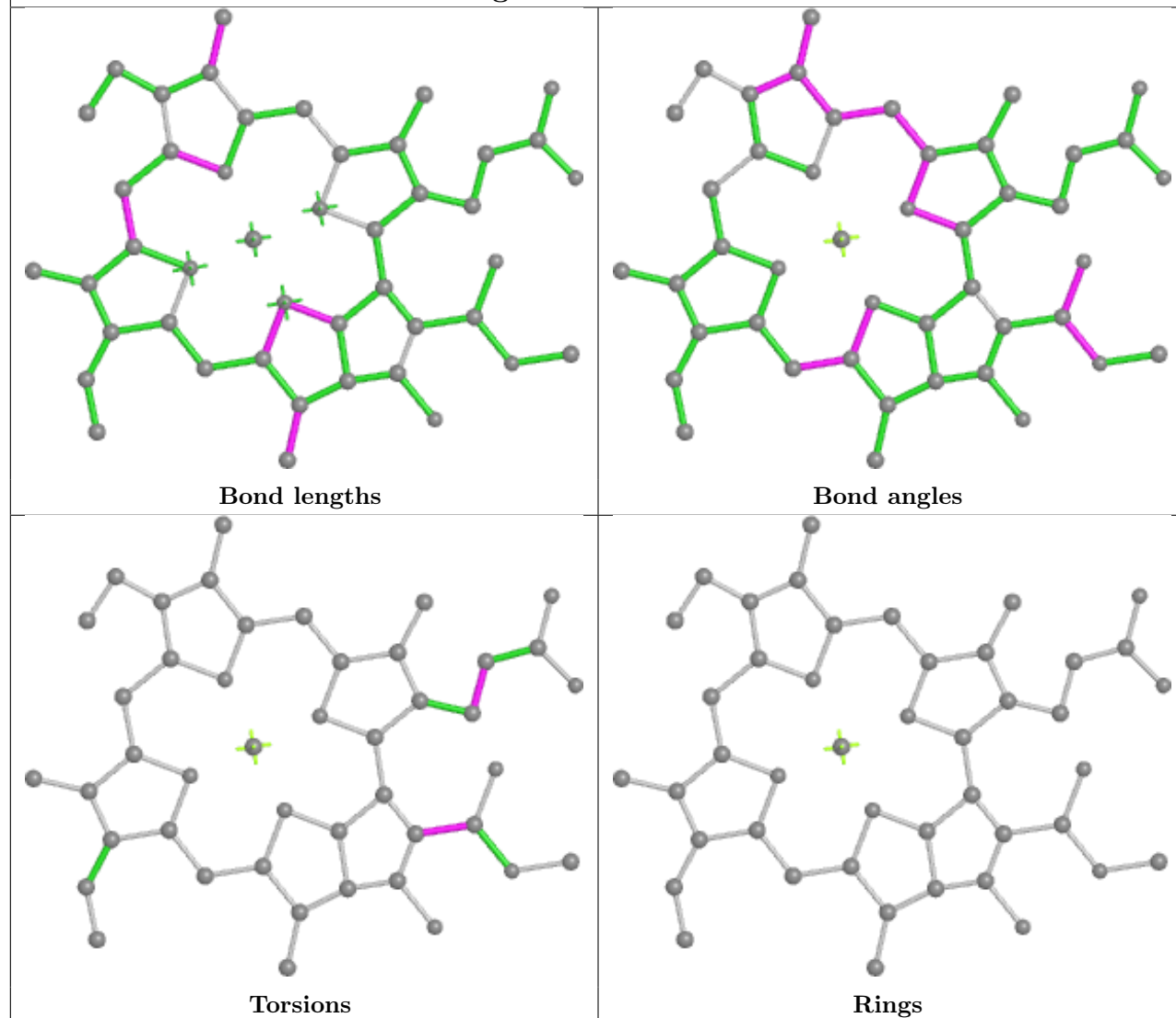




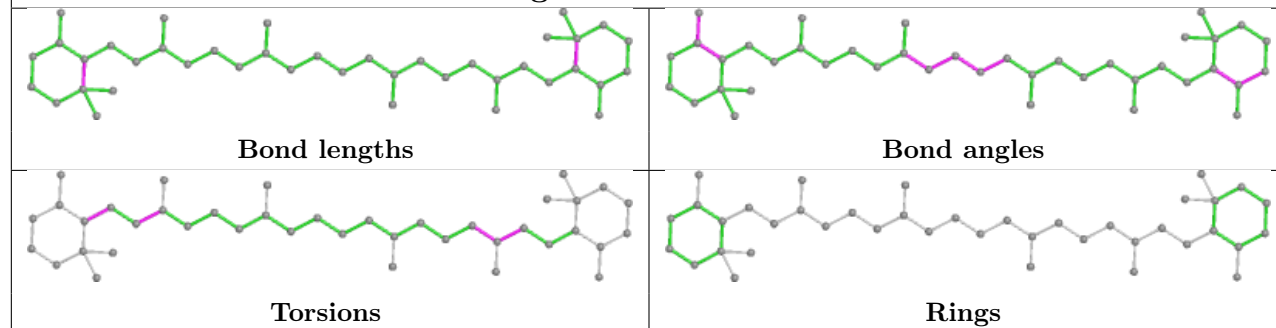




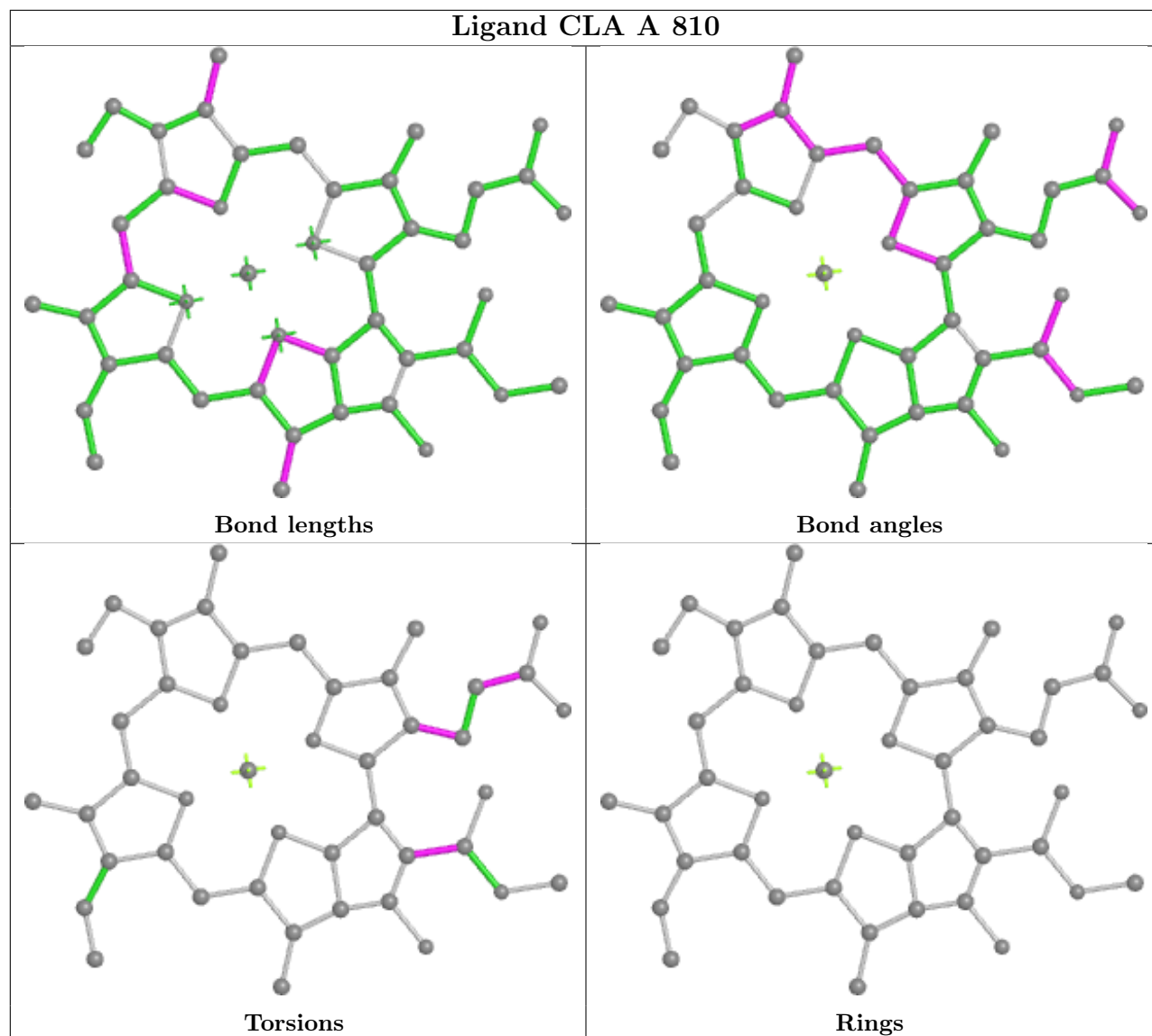
## Ligand CLA L 302



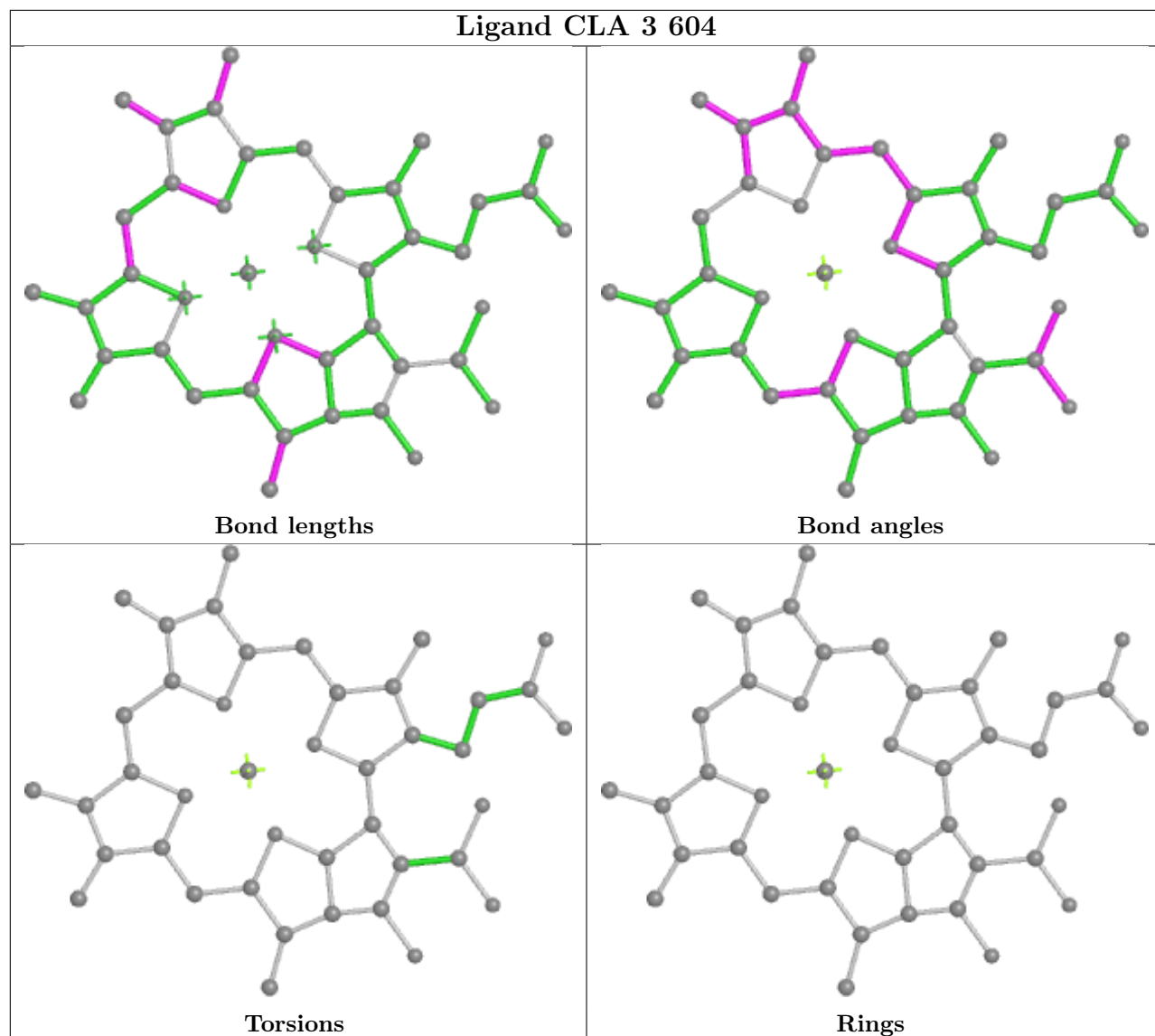
## Ligand BCR B 844



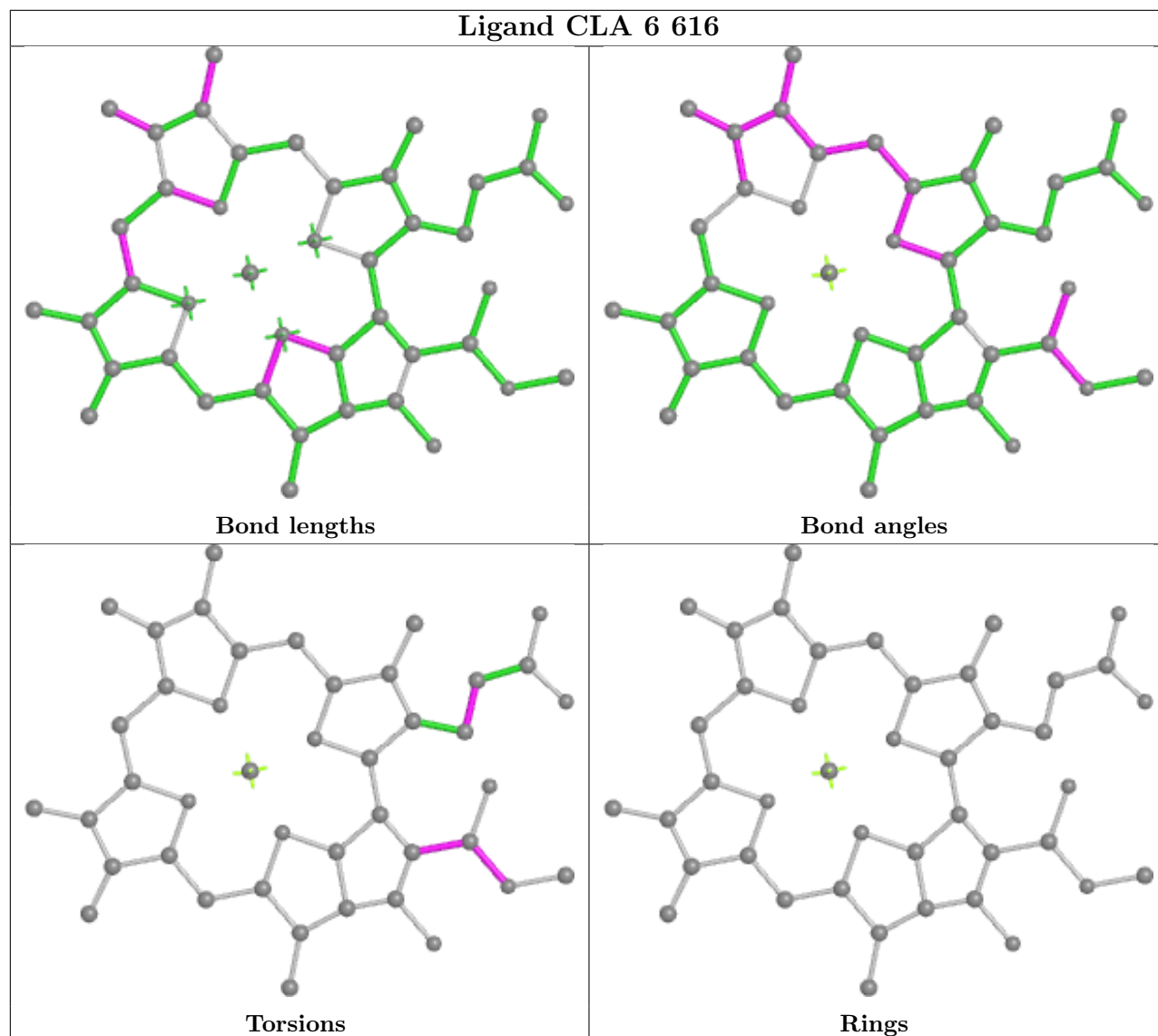
## Ligand CLA A 810



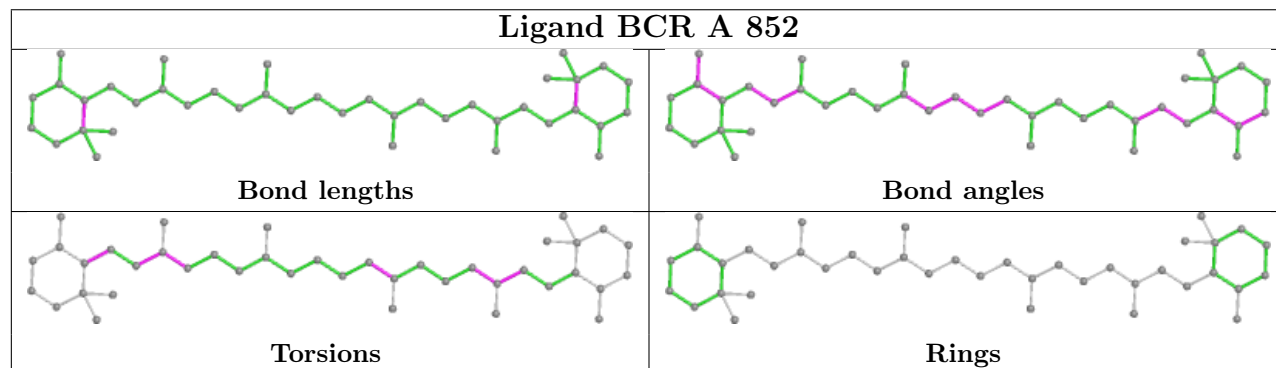
## Ligand CLA 3 604

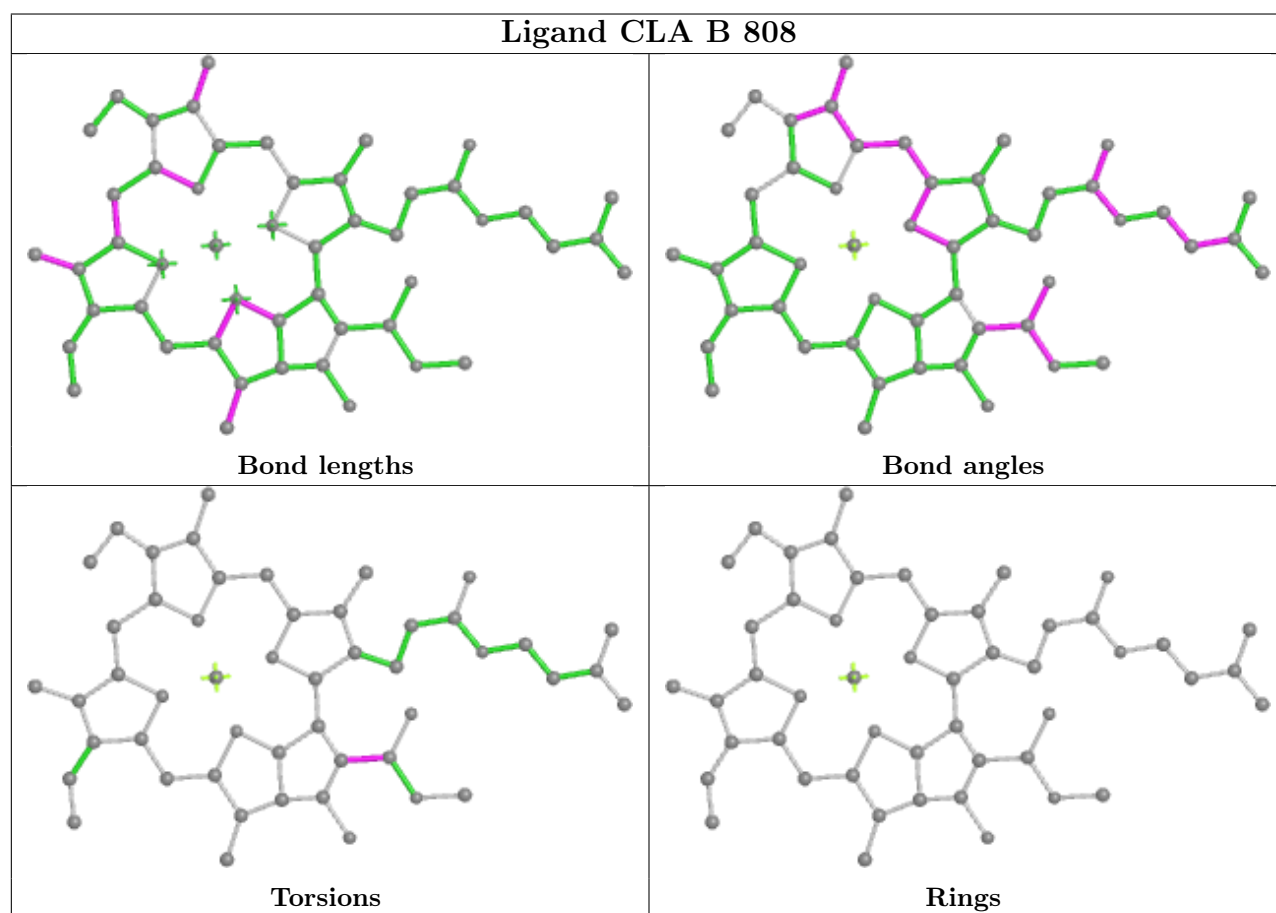
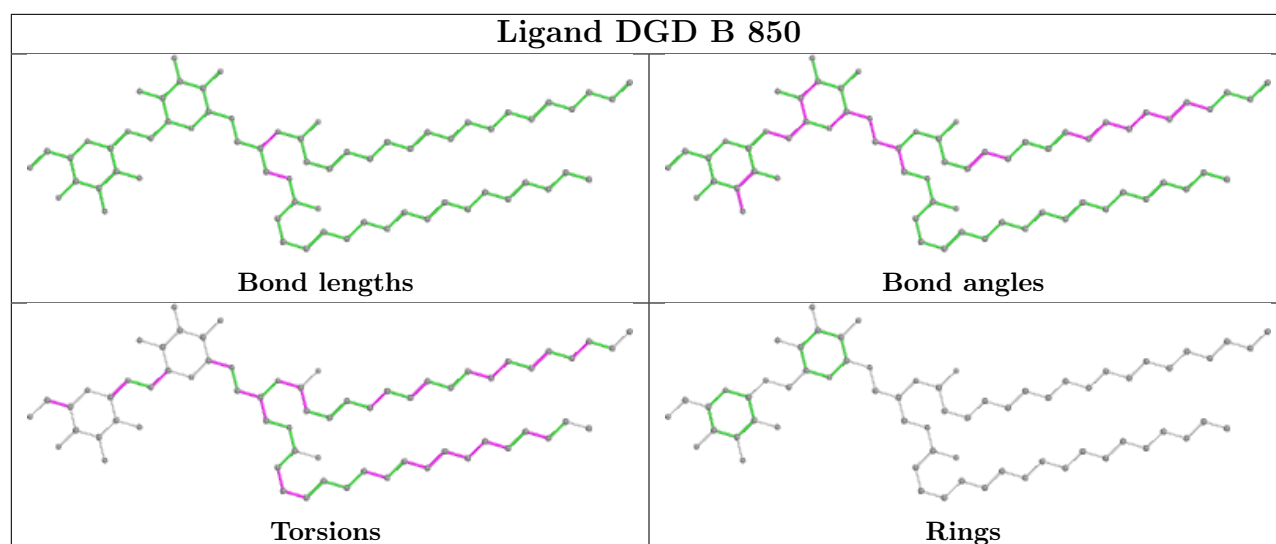


## Ligand CLA 6 616

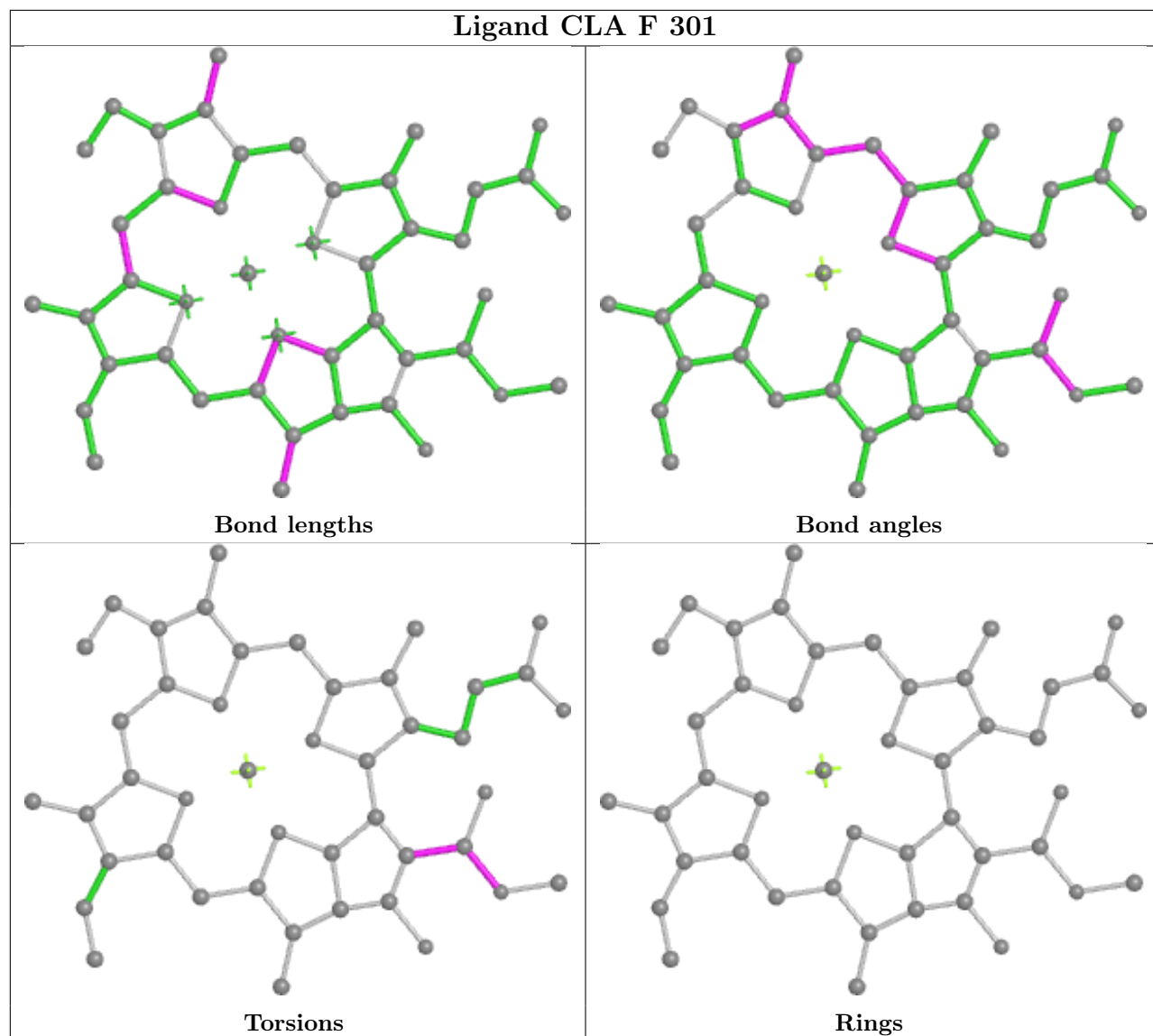


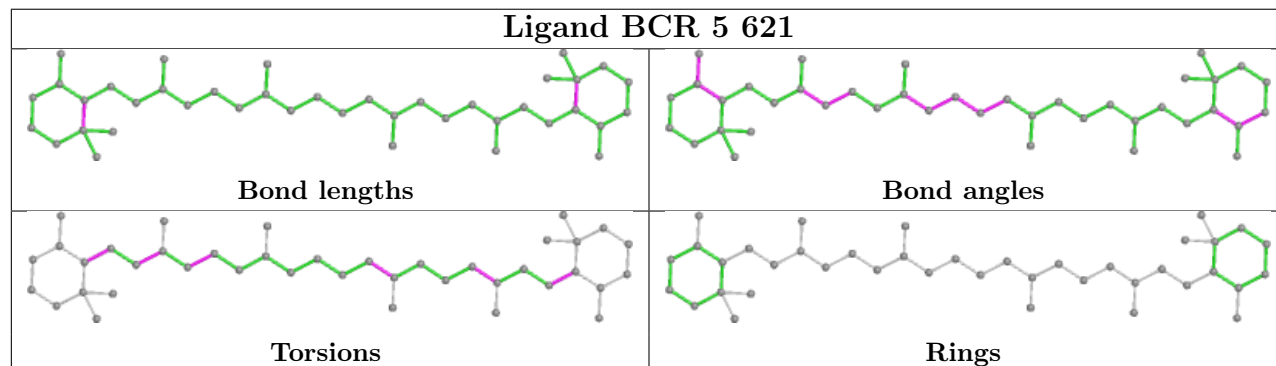
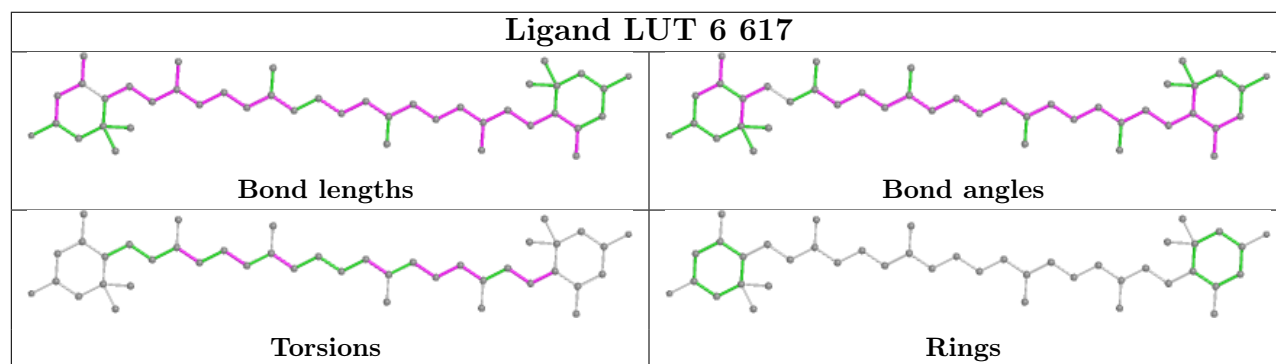
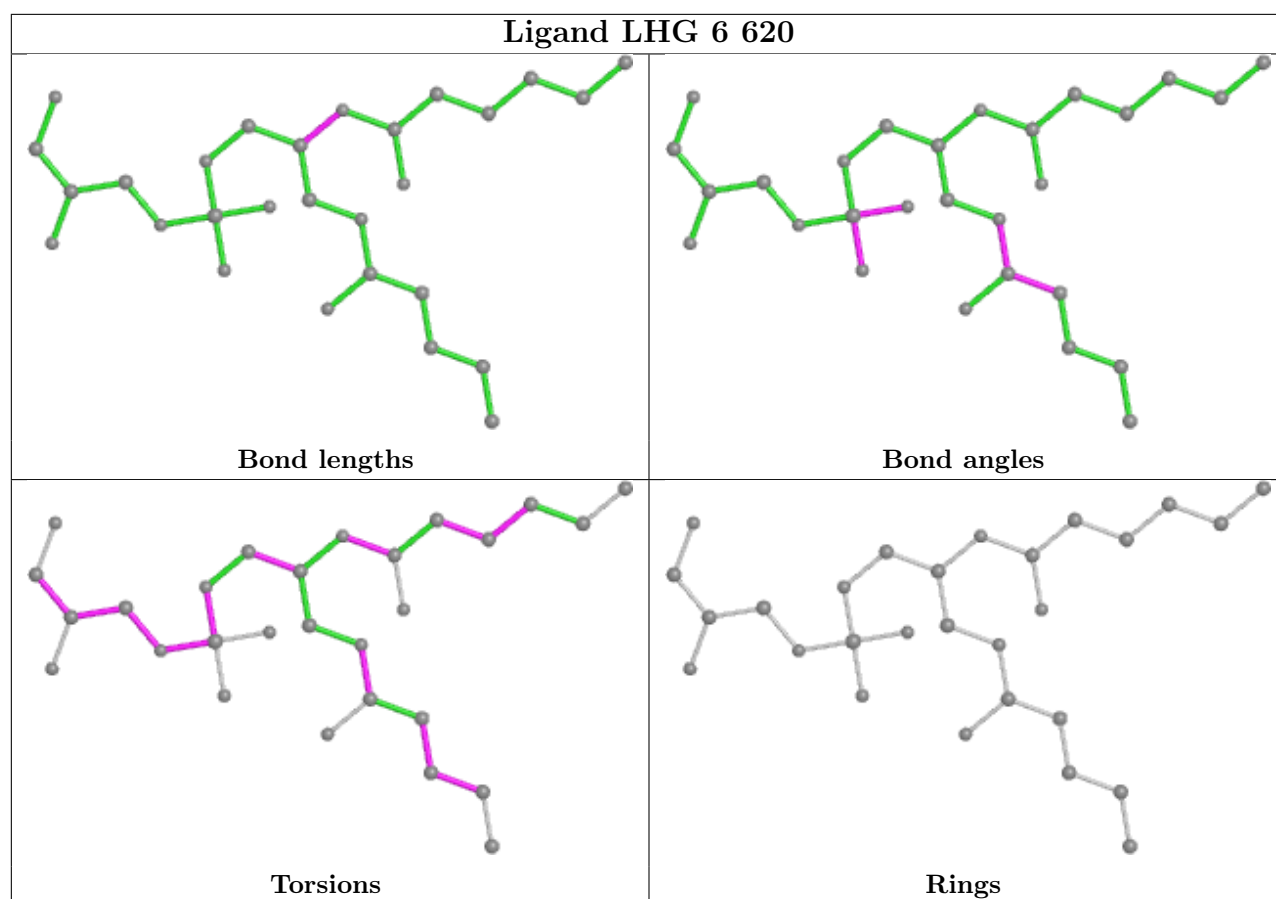
## Ligand BCR A 852



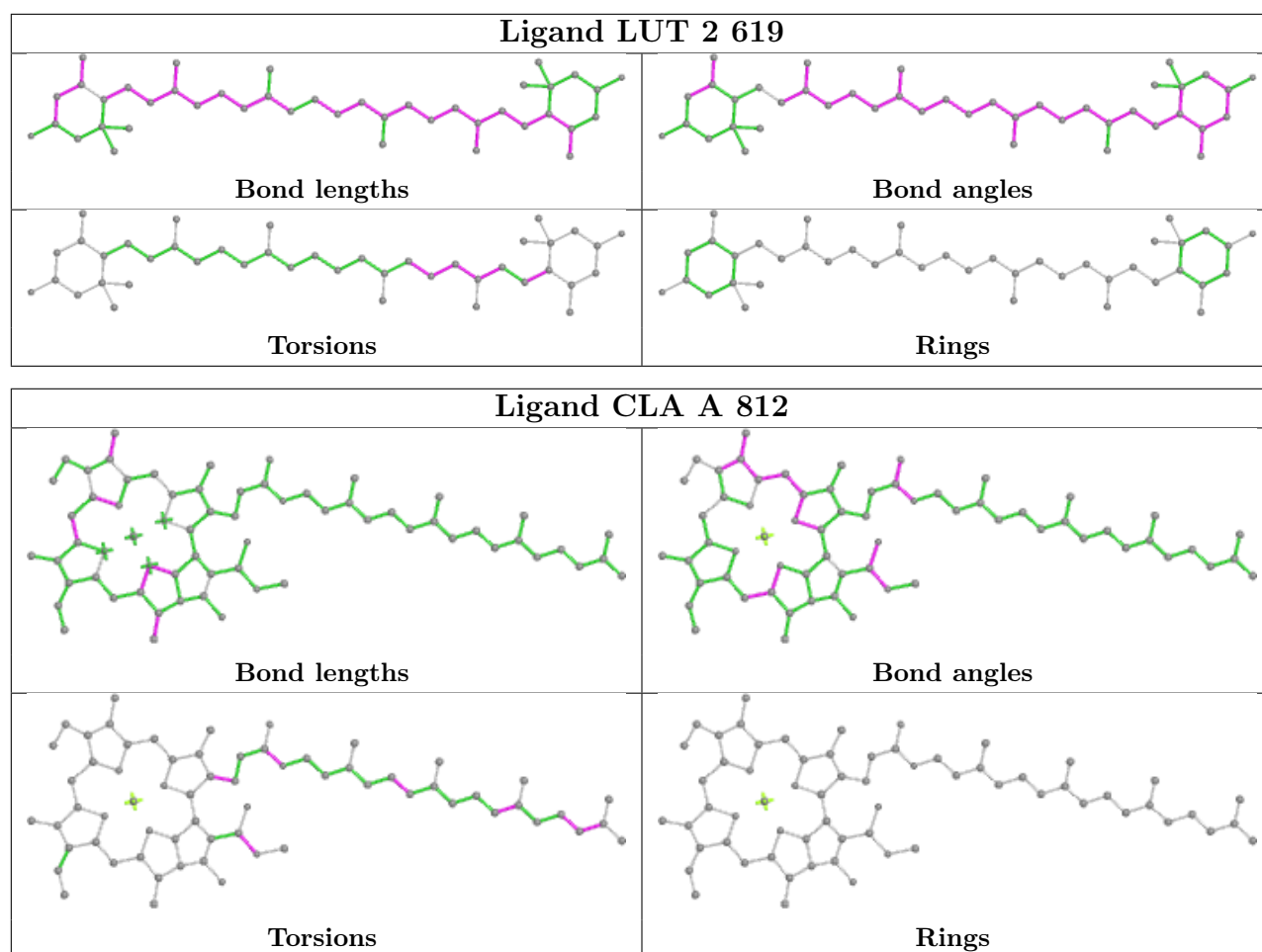


## Ligand CLA F 301









## 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 ⓘ

This section contains visualisations of the EMDB entry EMD-0821. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections ⓘ

This section was not generated.

### 6.2 Central slices ⓘ

This section was not generated.

### 6.3 Largest variance slices ⓘ

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views ⓘ

This section was not generated.

### 6.6 Mask visualisation ⓘ

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit ⓘ

This section was not generated.