



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 8AM5 / pdb\_00008am5  
EMDB ID : EMD-15522  
Title : RCII/PSI complex, class 3  
Authors : Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.;  
Sazanov, L.A.; Komenda, J.  
Deposited on : 2022-08-02  
Resolution : 3.10 Å (reported)  
Based on initial models : 2XBG, 5OY0, 6WJ6

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

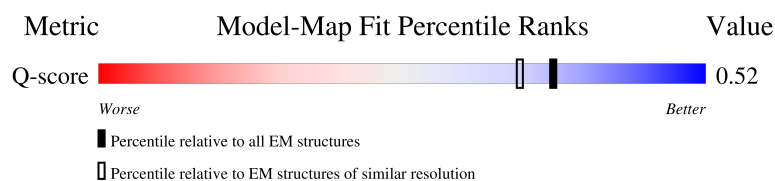
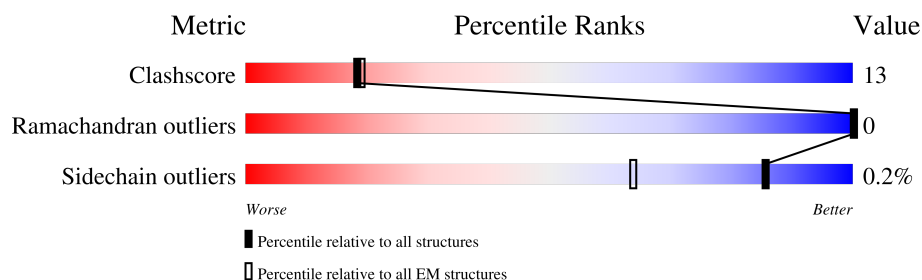
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14724 ( 2.60 - 3.60 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 344    |                  |
| 2   | D     | 336    |                  |
| 3   | E     | 81     |                  |
| 4   | F     | 44     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | I     | 38     |                  |
| 6   | S     | 342    |                  |
| 7   | a     | 751    |                  |
| 8   | b     | 731    |                  |
| 9   | c     | 81     |                  |
| 10  | d     | 141    |                  |
| 11  | e     | 74     |                  |
| 12  | f     | 165    |                  |
| 13  | i     | 40     |                  |
| 14  | j     | 40     |                  |
| 15  | k     | 86     |                  |
| 16  | l     | 157    |                  |
| 17  | m     | 31     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 19  | CLA  | A     | 402 | X         | -        | -       | -                |
| 19  | CLA  | A     | 403 | X         | -        | -       | -                |
| 19  | CLA  | A     | 405 | X         | -        | -       | -                |
| 19  | CLA  | A     | 407 | X         | -        | -       | -                |
| 19  | CLA  | D     | 402 | X         | -        | -       | -                |
| 19  | CLA  | D     | 403 | X         | -        | -       | -                |
| 19  | CLA  | a     | 802 | X         | -        | -       | -                |
| 19  | CLA  | a     | 803 | X         | -        | -       | -                |
| 19  | CLA  | a     | 804 | X         | -        | -       | -                |
| 19  | CLA  | a     | 805 | X         | -        | -       | -                |
| 19  | CLA  | a     | 806 | X         | -        | -       | -                |
| 19  | CLA  | a     | 807 | X         | -        | -       | -                |
| 19  | CLA  | a     | 808 | X         | -        | -       | -                |
| 19  | CLA  | a     | 809 | X         | -        | -       | -                |
| 19  | CLA  | a     | 810 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 19  | CLA  | a     | 811 | X         | -        | -       | -                |
| 19  | CLA  | a     | 812 | X         | -        | -       | -                |
| 19  | CLA  | a     | 813 | X         | -        | -       | -                |
| 19  | CLA  | a     | 815 | X         | -        | -       | -                |
| 19  | CLA  | a     | 816 | X         | -        | -       | -                |
| 19  | CLA  | a     | 817 | X         | -        | -       | -                |
| 19  | CLA  | a     | 818 | X         | -        | -       | -                |
| 19  | CLA  | a     | 819 | X         | -        | -       | -                |
| 19  | CLA  | a     | 820 | X         | -        | -       | -                |
| 19  | CLA  | a     | 821 | X         | -        | -       | -                |
| 19  | CLA  | a     | 822 | X         | -        | -       | -                |
| 19  | CLA  | a     | 823 | X         | -        | -       | -                |
| 19  | CLA  | a     | 824 | X         | -        | -       | -                |
| 19  | CLA  | a     | 825 | X         | -        | -       | -                |
| 19  | CLA  | a     | 826 | X         | -        | -       | -                |
| 19  | CLA  | a     | 827 | X         | -        | -       | -                |
| 19  | CLA  | a     | 828 | X         | -        | -       | -                |
| 19  | CLA  | a     | 829 | X         | -        | -       | -                |
| 19  | CLA  | a     | 830 | X         | -        | -       | -                |
| 19  | CLA  | a     | 831 | X         | -        | -       | -                |
| 19  | CLA  | a     | 832 | X         | -        | -       | -                |
| 19  | CLA  | a     | 833 | X         | -        | -       | -                |
| 19  | CLA  | a     | 834 | X         | -        | -       | -                |
| 19  | CLA  | a     | 835 | X         | -        | -       | -                |
| 19  | CLA  | a     | 836 | X         | -        | -       | -                |
| 19  | CLA  | a     | 837 | X         | -        | -       | -                |
| 19  | CLA  | a     | 838 | X         | -        | -       | -                |
| 19  | CLA  | a     | 839 | X         | -        | -       | -                |
| 19  | CLA  | a     | 840 | X         | -        | -       | -                |
| 19  | CLA  | a     | 841 | X         | -        | -       | -                |
| 19  | CLA  | a     | 842 | X         | -        | -       | -                |
| 19  | CLA  | a     | 843 | X         | -        | -       | -                |
| 19  | CLA  | a     | 856 | X         | -        | -       | -                |
| 19  | CLA  | a     | 857 | X         | -        | -       | -                |
| 19  | CLA  | a     | 860 | X         | -        | -       | -                |
| 19  | CLA  | b     | 801 | X         | -        | -       | -                |
| 19  | CLA  | b     | 802 | X         | -        | -       | -                |
| 19  | CLA  | b     | 803 | X         | -        | -       | -                |
| 19  | CLA  | b     | 804 | X         | -        | -       | -                |
| 19  | CLA  | b     | 805 | X         | -        | -       | -                |
| 19  | CLA  | b     | 806 | X         | -        | -       | -                |
| 19  | CLA  | b     | 807 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 19  | CLA  | b     | 808 | X         | -        | -       | -                |
| 19  | CLA  | b     | 809 | X         | -        | -       | -                |
| 19  | CLA  | b     | 810 | X         | -        | -       | -                |
| 19  | CLA  | b     | 811 | X         | -        | -       | -                |
| 19  | CLA  | b     | 812 | X         | -        | -       | -                |
| 19  | CLA  | b     | 813 | X         | -        | -       | -                |
| 19  | CLA  | b     | 814 | X         | -        | -       | -                |
| 19  | CLA  | b     | 815 | X         | -        | -       | -                |
| 19  | CLA  | b     | 816 | X         | -        | -       | -                |
| 19  | CLA  | b     | 817 | X         | -        | -       | -                |
| 19  | CLA  | b     | 818 | X         | -        | -       | -                |
| 19  | CLA  | b     | 819 | X         | -        | -       | -                |
| 19  | CLA  | b     | 820 | X         | -        | -       | -                |
| 19  | CLA  | b     | 821 | X         | -        | -       | -                |
| 19  | CLA  | b     | 822 | X         | -        | -       | -                |
| 19  | CLA  | b     | 823 | X         | -        | -       | -                |
| 19  | CLA  | b     | 824 | X         | -        | -       | -                |
| 19  | CLA  | b     | 825 | X         | -        | -       | -                |
| 19  | CLA  | b     | 826 | X         | -        | -       | -                |
| 19  | CLA  | b     | 827 | X         | -        | -       | -                |
| 19  | CLA  | b     | 828 | X         | -        | -       | -                |
| 19  | CLA  | b     | 829 | X         | -        | -       | -                |
| 19  | CLA  | b     | 830 | X         | -        | -       | -                |
| 19  | CLA  | b     | 831 | X         | -        | -       | -                |
| 19  | CLA  | b     | 832 | X         | -        | -       | -                |
| 19  | CLA  | b     | 833 | X         | -        | -       | -                |
| 19  | CLA  | b     | 834 | X         | -        | -       | -                |
| 19  | CLA  | b     | 835 | X         | -        | -       | -                |
| 19  | CLA  | b     | 836 | X         | -        | -       | -                |
| 19  | CLA  | b     | 837 | X         | -        | -       | -                |
| 19  | CLA  | b     | 838 | X         | -        | -       | -                |
| 19  | CLA  | b     | 839 | X         | -        | -       | -                |
| 19  | CLA  | b     | 840 | X         | -        | -       | -                |
| 19  | CLA  | f     | 201 | X         | -        | -       | -                |
| 19  | CLA  | f     | 203 | X         | -        | -       | -                |
| 19  | CLA  | f     | 204 | X         | -        | -       | -                |
| 19  | CLA  | j     | 103 | X         | -        | -       | -                |
| 19  | CLA  | j     | 104 | X         | -        | -       | -                |
| 19  | CLA  | k     | 101 | X         | -        | -       | -                |
| 19  | CLA  | k     | 102 | X         | -        | -       | -                |
| 19  | CLA  | l     | 202 | X         | -        | -       | -                |
| 19  | CLA  | l     | 203 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 19  | CLA  | l     | 204 | X         | -        | -       | -                |
| 23  | CL0  | a     | 801 | X         | -        | -       | -                |

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 32746 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 II protein D1 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 290      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2256  | 1484 | 367 | 390 | 15 |         |       |

- Molecule 2 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | D     | 278      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2188  | 1465 | 351 | 360 | 12 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| D     | -5      | MET      | -      | initiating methionine | UNP P09192 |
| D     | -4      | HIS      | -      | expression tag        | UNP P09192 |
| D     | -3      | HIS      | -      | expression tag        | UNP P09192 |
| D     | -2      | HIS      | -      | expression tag        | UNP P09192 |
| D     | -1      | HIS      | -      | expression tag        | UNP P09192 |
| D     | 0       | HIS      | -      | expression tag        | UNP P09192 |
| D     | 1       | HIS      | -      | expression tag        | UNP P09192 |

- Molecule 3 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | E     | 37       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 301   | 206 | 44 | 50 | 1 |         |       |

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4   | F     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 222   | 149 | 39 | 33 | 1 |         |       |

- Molecule 5 is a protein called Photosystem II reaction center protein I.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | I     | 29       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 229   | 159 | 33 | 37 |         |       |

- Molecule 6 is a protein called Photosystem II assembly lipoprotein Ycf48.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | S     | 303      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2328  | 1481 | 393 | 451 | 3 |         |       |

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | a     | 741      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5795  | 3797 | 984 | 987 | 27 |         |       |

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | b     | 729      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5770  | 3798 | 967 | 990 | 15 |         |       |

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | c     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 600   | 369 | 103 | 117 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | d     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1087  | 688 | 188 | 208 | 3 |         |       |

- Molecule 11 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 11  | e     | 69       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 538   | 337 | 95 | 106 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | f     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 715 | 184 | 204 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | i     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 311   | 209 | 44 | 55 | 3 |         |       |

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | j     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 319   | 215 | 47 | 54 | 3 |         |       |

- Molecule 15 is a protein called Photosystem I reaction center subunit PsaK 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | k     | 75       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 524   | 343 | 87 | 90 | 4 |         |       |

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | l     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1069  | 697 | 173 | 197 | 2 |         |       |

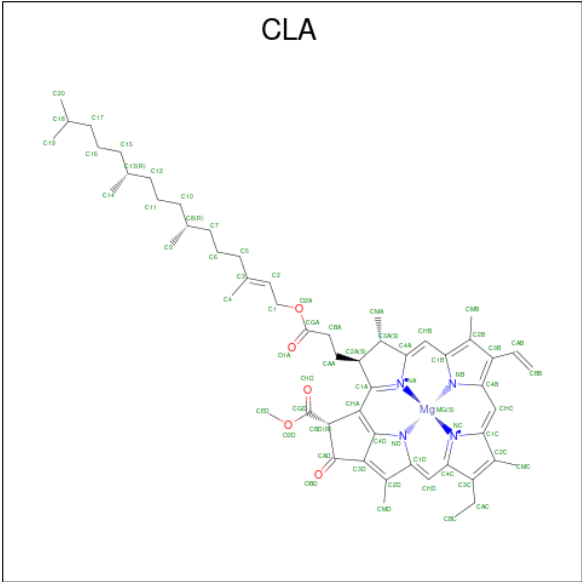
- Molecule 17 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | m     | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 238   | 159 | 36 | 42 | 1 |         |       |

- Molecule 18 is FE (II) ION (CCD ID: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 18  | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | D     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 19  | D     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>56 | C<br>46 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 19  | 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 |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 56    | 46 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 57    | 47 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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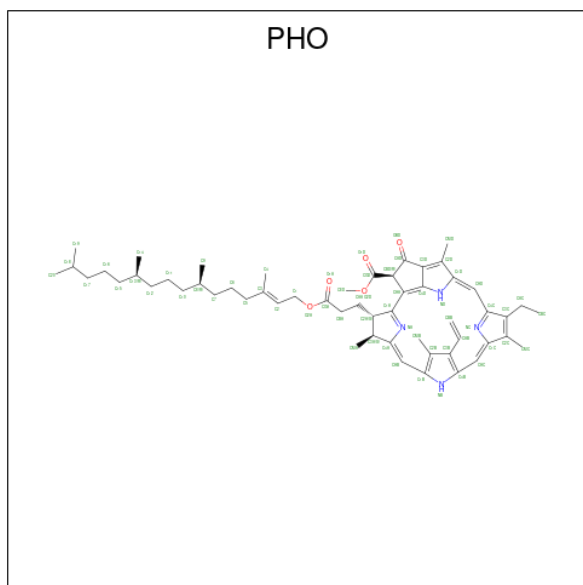
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | f     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 19  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 46    | 36 | 1  | 4 | 5 |         |
| 19  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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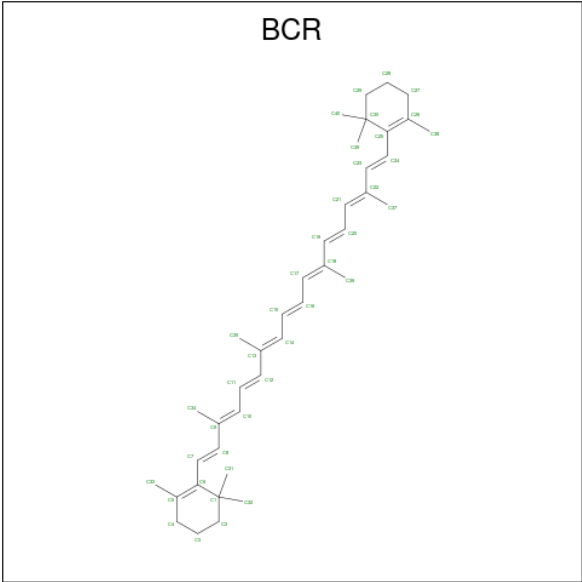
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 19  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | 1     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 52    | 42 | 1  | 4 | 5 |         |

- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 20  | A     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |
| 20  | D     | 1        | Total | C  | N | O | 0       |
|     |       |          | 64    | 55 | 4 | 5 |         |

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



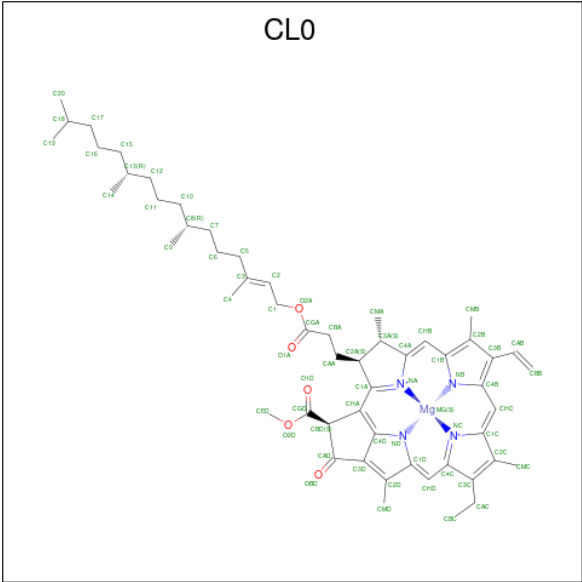
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | A     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | a     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 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 |         |
| 21  | a     | 1        | Total | C  | 0       |
|     |       |          | 25    | 25 |         |
| 21  | a     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | b     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 21  | f     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 21  | i     | 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  | k     | 1        | Total C<br>40 40 | 0       |
| 21  | l     | 1        | Total C<br>40 40 | 0       |

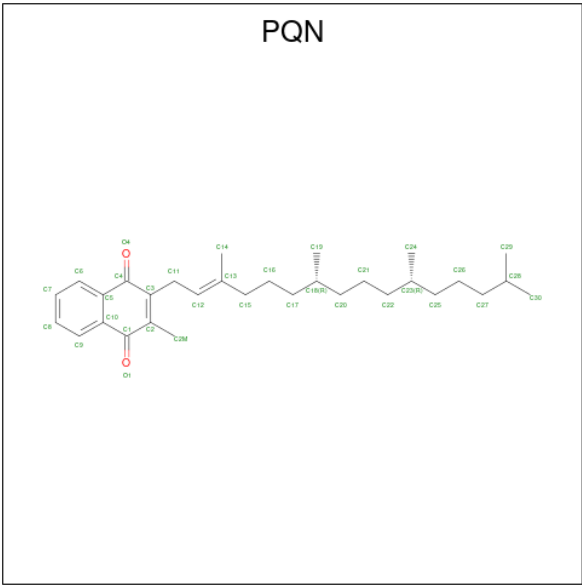
- # HEM

- Molecule 23 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



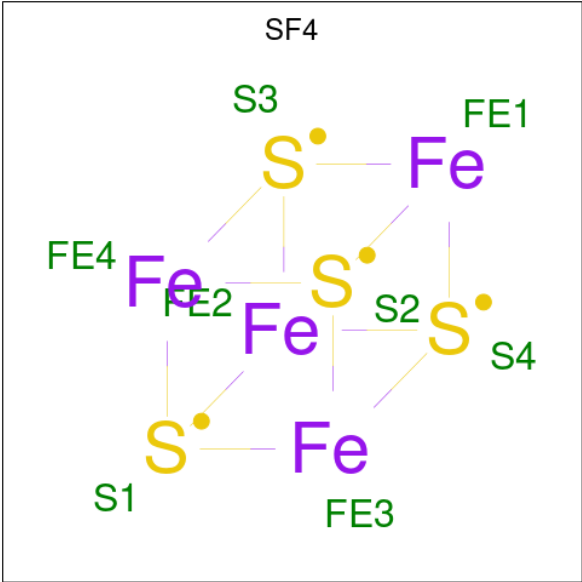
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 23  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



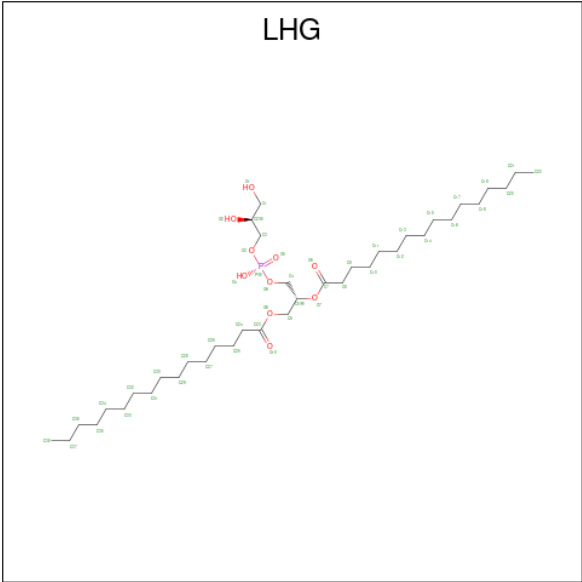
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 24  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 33 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

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



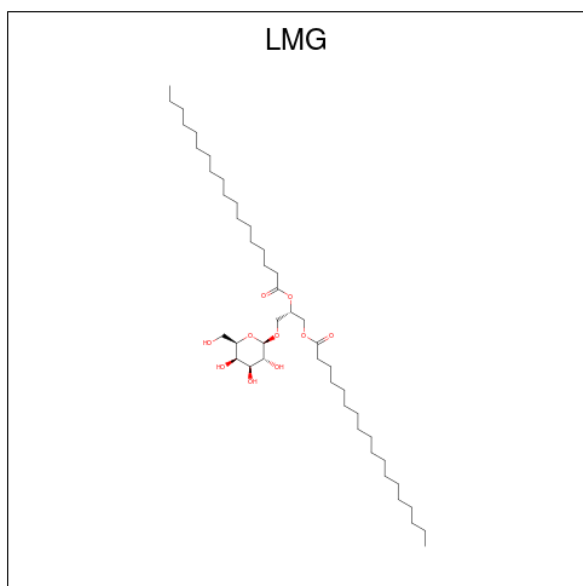
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 25  | a     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 25  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 25  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



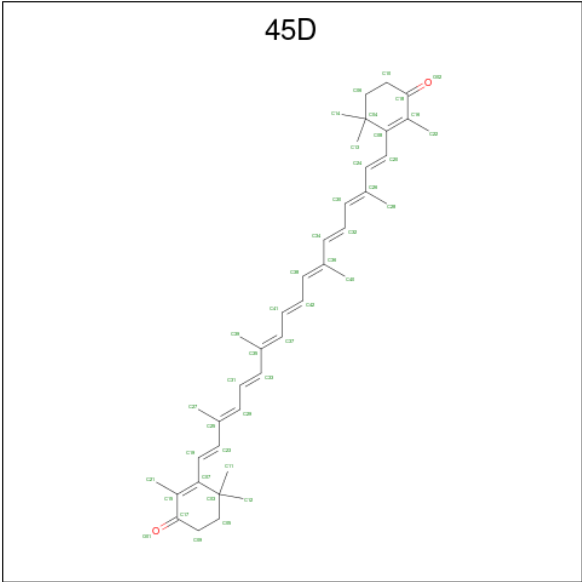
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 26  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 38    | 27 | 10 | 1 |         |
| 26  | f     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



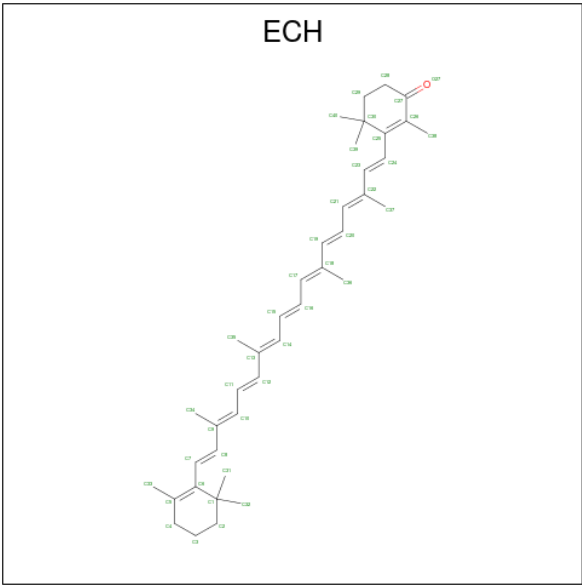
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 27  | a     | 1        | Total | C  | O  | 0       |
|     |       |          | 40    | 30 | 10 |         |
| 27  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 27  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 27  | l     | 1        | Total | C  | O  | 0       |
|     |       |          | 50    | 40 | 10 |         |

- Molecule 28 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula:  $C_{40}H_{52}O_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 28  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

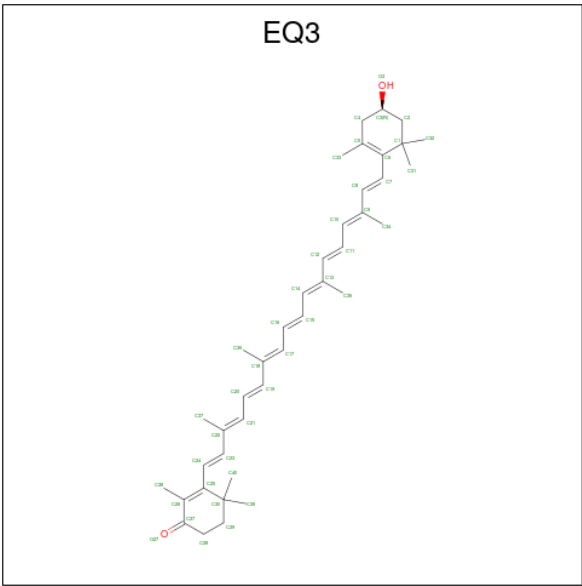
- Molecule 29 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C<sub>40</sub>H<sub>54</sub>O).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |
| 29  | m     | 1        | Total | C  | O | 0       |
|     |       |          | 41    | 40 | 1 |         |

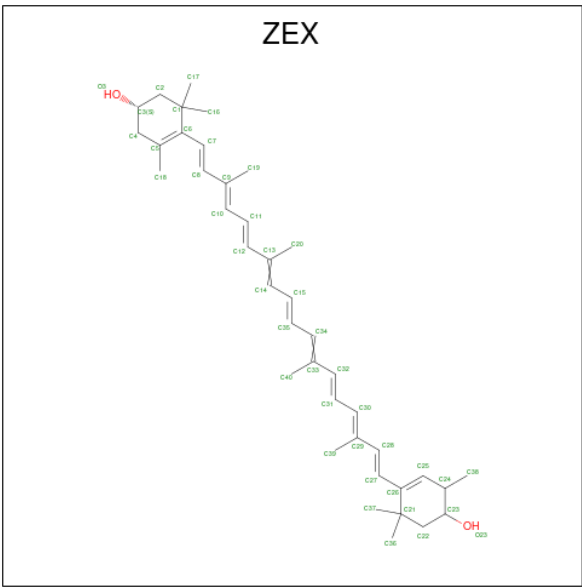
- Molecule 30 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula:

C<sub>40</sub>H<sub>54</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 30  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 31 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



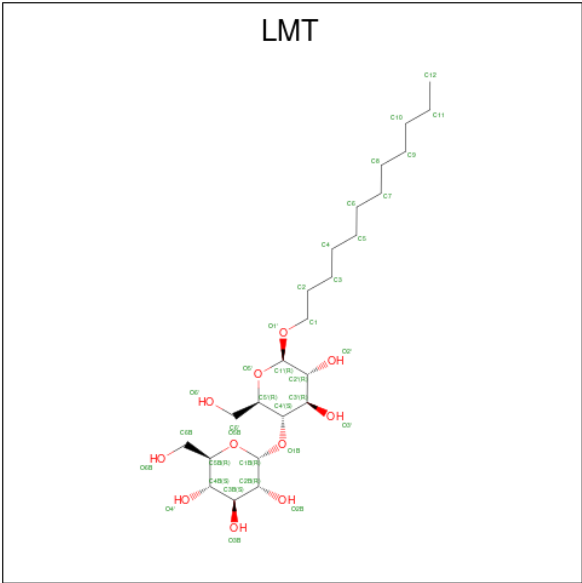
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 31  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 31  | f     | 1        | Total | C  | O | 0       |
|     |       |          | 42    | 40 | 2 |         |

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).

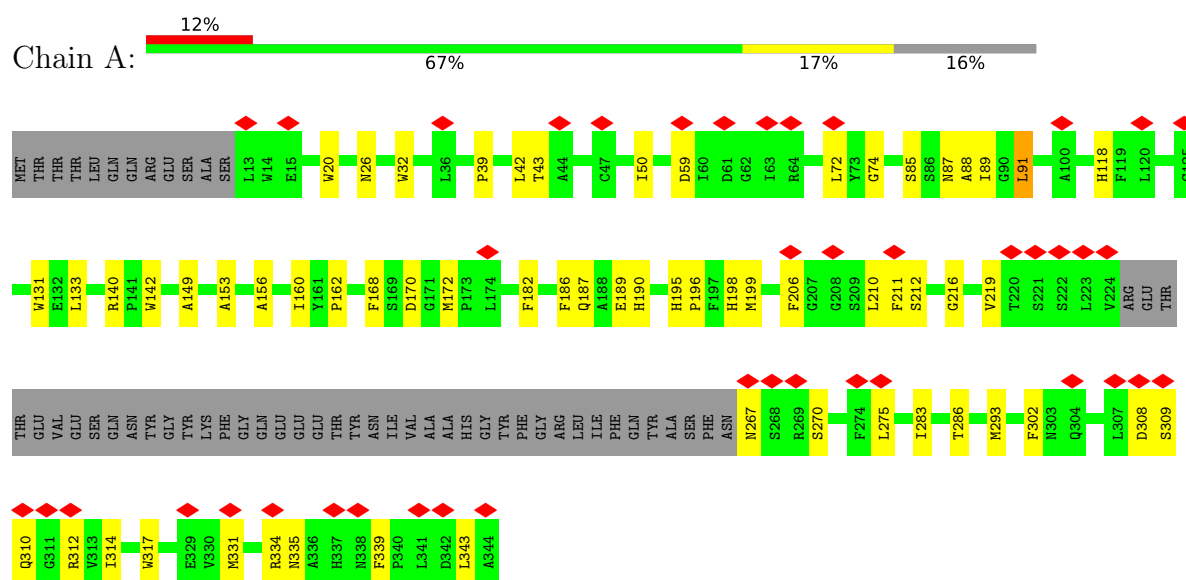


| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 32  | j     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 24 | 11 |         |

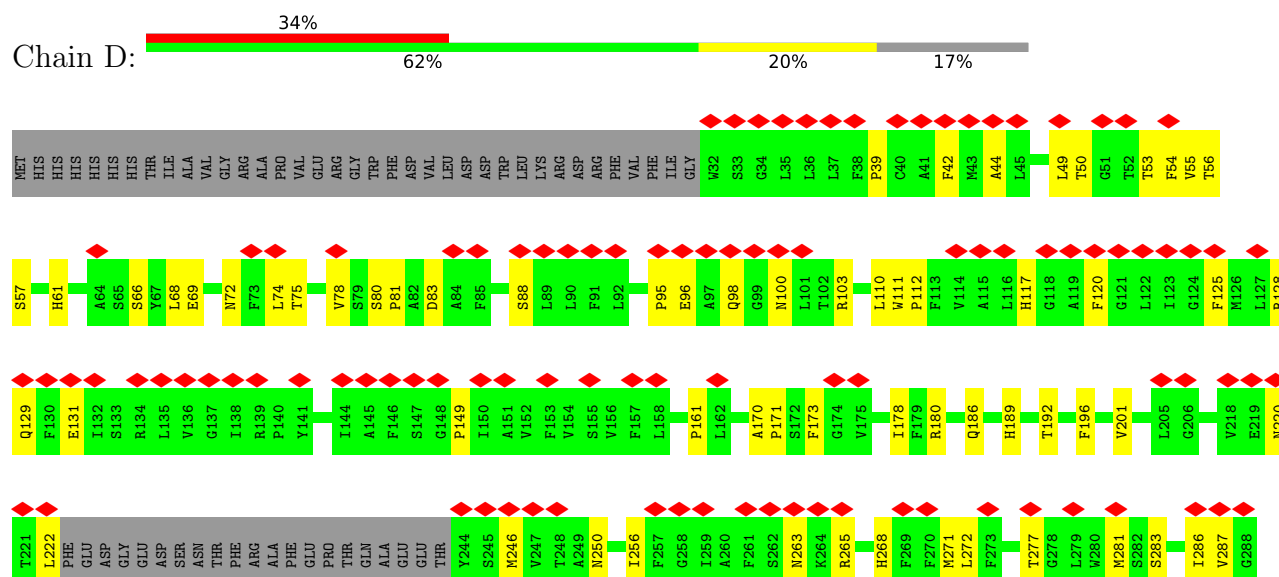
### 3 Residue-property plots

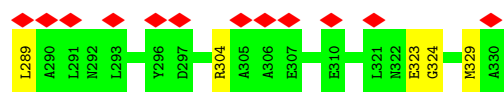
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Photosystem II protein D1 2

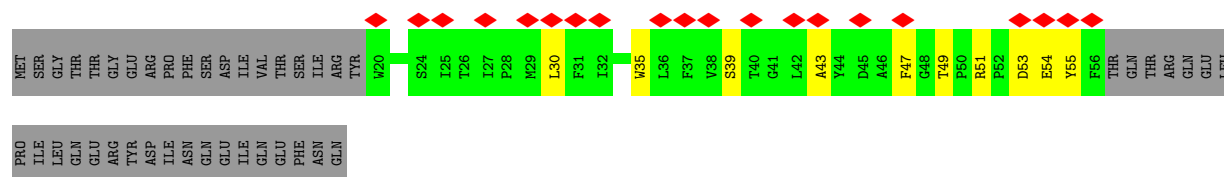
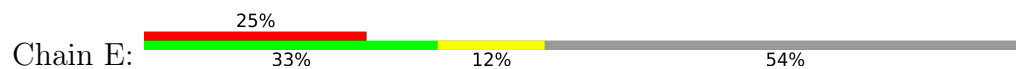


#### • Molecule 2: Photosystem II D2 protein

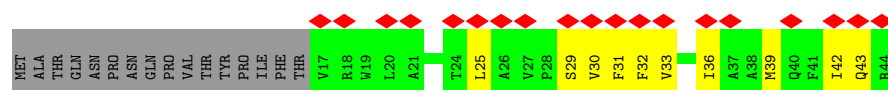




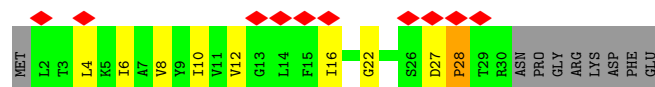
• Molecule 3: Cytochrome b559 subunit alpha



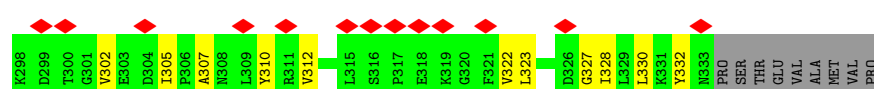
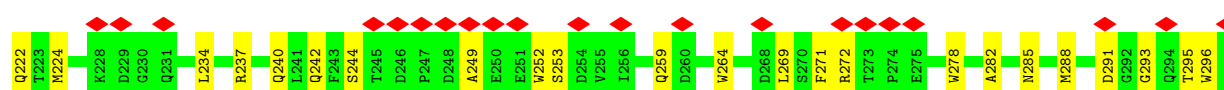
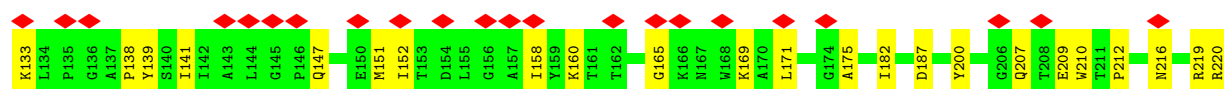
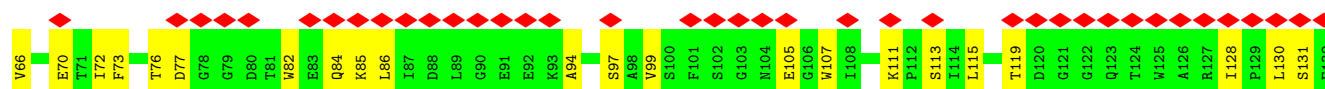
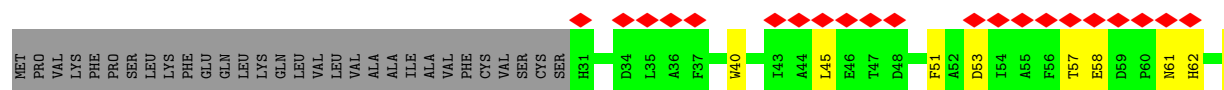
• Molecule 4: Cytochrome b559 subunit beta



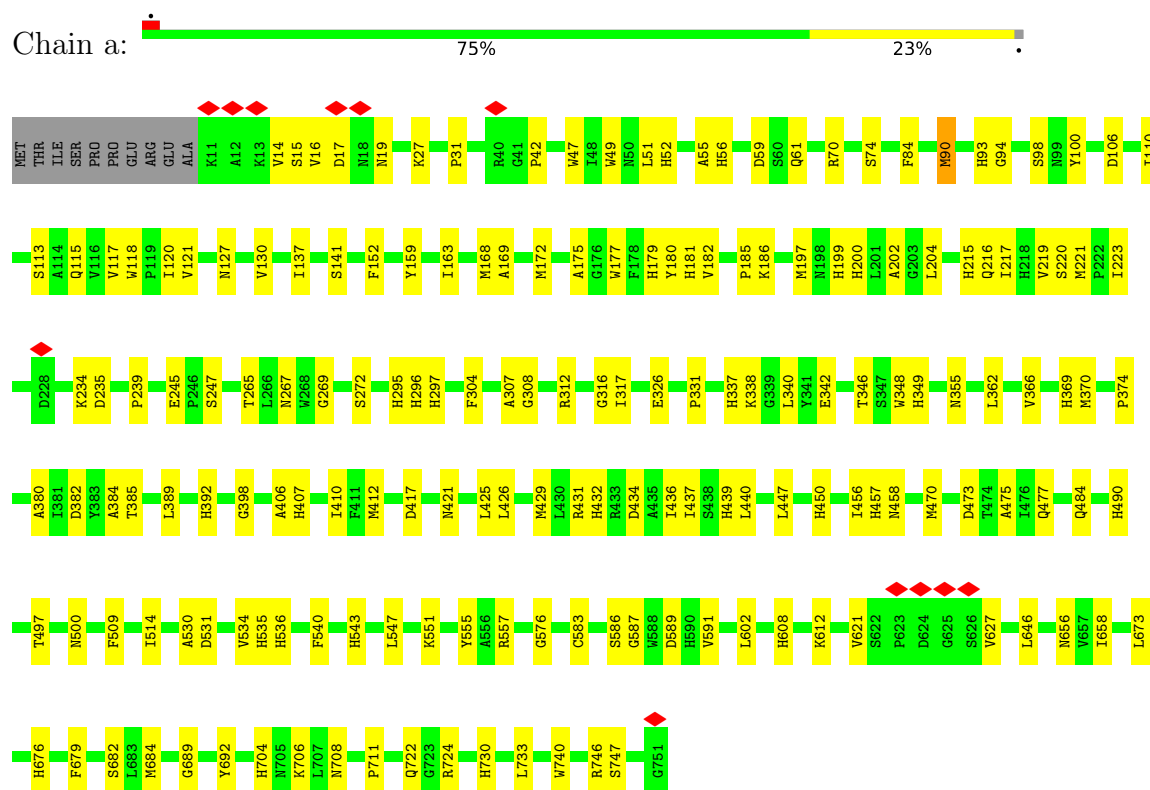
• Molecule 5: Photosystem II reaction center protein I



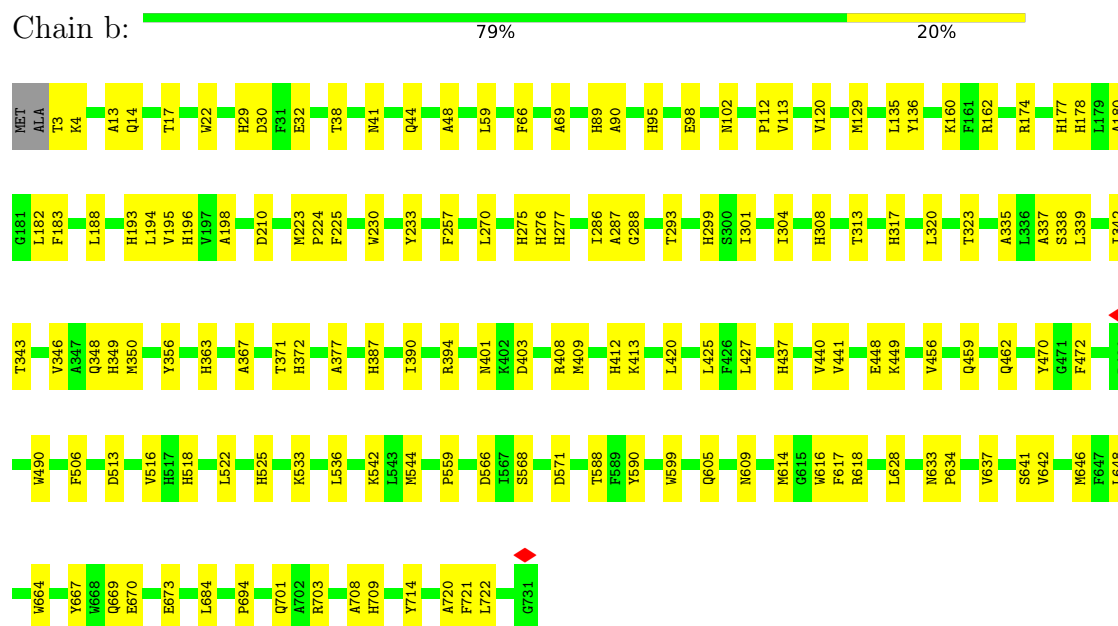
• Molecule 6: Photosystem II assembly lipoprotein Ycf48



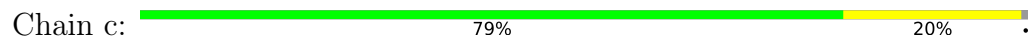
- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2



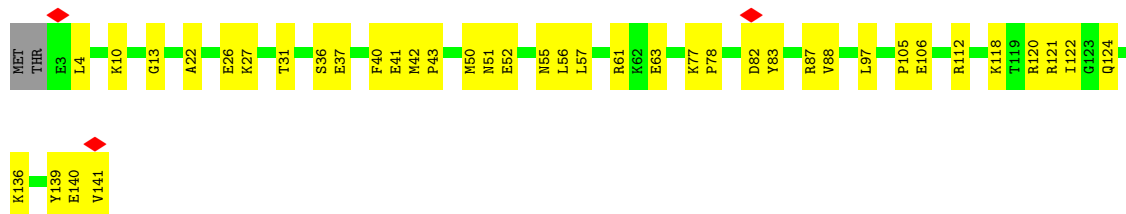
- Molecule 9: Photosystem I iron-sulfur center





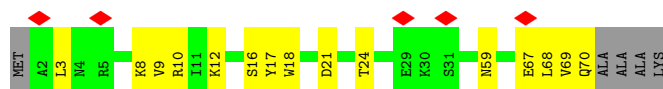
- Molecule 10: Photosystem I reaction center subunit II

Chain d: 70% 28%



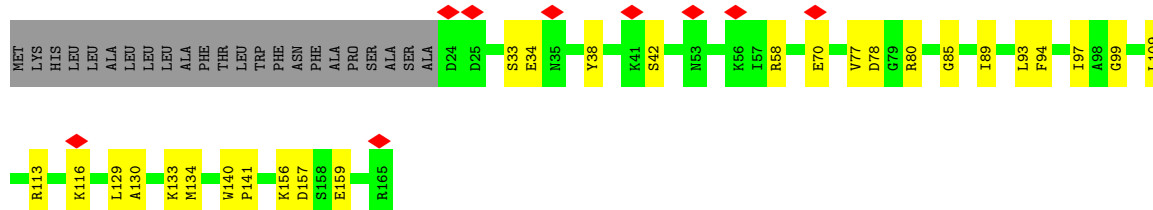
- Molecule 11: Photosystem I reaction center subunit IV

Chain e: 7% 73% 20% 7%



- Molecule 12: Photosystem I reaction center subunit III

Chain f: 5% 70% 16% 14%



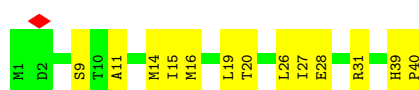
- Molecule 13: Photosystem I reaction center subunit VIII

Chain i: 10% 75% 25%

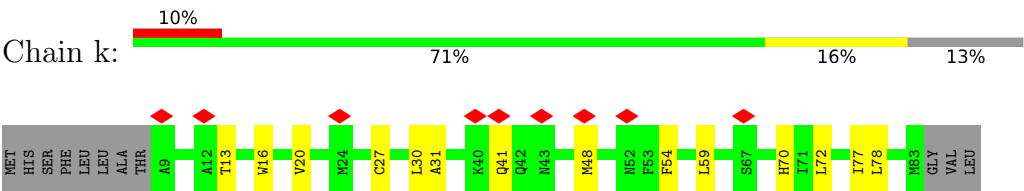


- Molecule 14: Photosystem I reaction center subunit IX

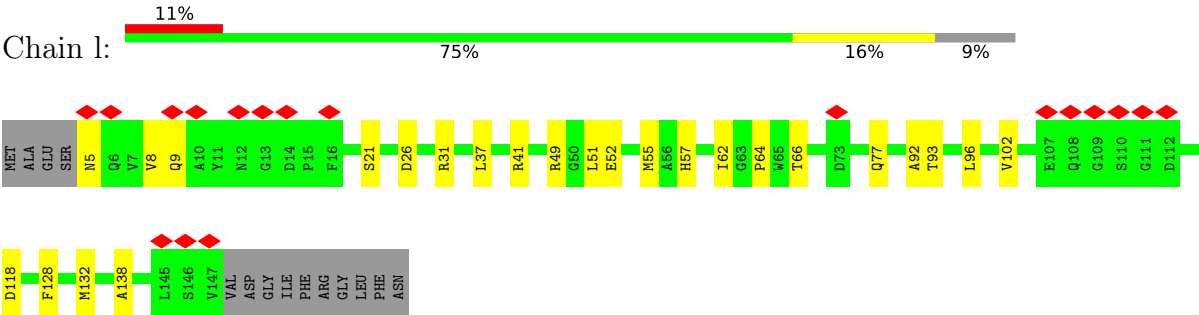
Chain j: 68% 32%



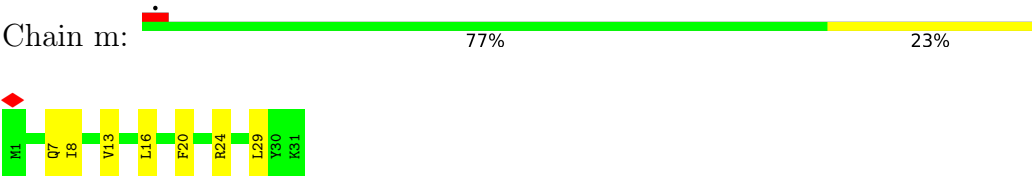
- Molecule 15: Photosystem I reaction center subunit PsaK 1



• Molecule 16: Photosystem I reaction center subunit XI



• Molecule 17: Photosystem I reaction center subunit XII



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 178513                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS GLACIOS                             | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 90.9                                    | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 120000                                  | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.510                                   | Depositor |
| Minimum map value                    | -0.104                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.011                                   | Depositor |
| Recommended contour level            | 0.0845                                  | Depositor |
| Map size (Å)                         | 488.0, 488.0, 488.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.22, 1.22, 1.22                        | 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: LMT, LHG, CLA, PQN, PHO, 45D, FE2, ZEX, CL0, BCR, ECH, LMG, HEM, EQ3, SF4

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     | 0.11         | 0/2330  | 0.25        | 0/3180         |
| 2   | D     | 0.12         | 0/2266  | 0.29        | 0/3086         |
| 3   | E     | 0.12         | 0/314   | 0.25        | 0/431          |
| 4   | F     | 0.14         | 0/228   | 0.35        | 0/309          |
| 5   | I     | 0.22         | 0/234   | 0.58        | 1/317 (0.3%)   |
| 6   | S     | 0.11         | 0/2390  | 0.28        | 0/3258         |
| 7   | a     | 0.16         | 0/5993  | 0.26        | 0/8169         |
| 8   | b     | 0.16         | 0/5981  | 0.27        | 0/8178         |
| 9   | c     | 0.15         | 0/610   | 0.31        | 0/826          |
| 10  | d     | 0.14         | 0/1111  | 0.29        | 0/1497         |
| 11  | e     | 0.14         | 0/547   | 0.34        | 0/741          |
| 12  | f     | 0.12         | 0/1138  | 0.28        | 0/1546         |
| 13  | i     | 0.16         | 0/322   | 0.35        | 0/438          |
| 14  | j     | 0.15         | 0/328   | 0.34        | 0/443          |
| 15  | k     | 0.15         | 0/535   | 0.35        | 0/726          |
| 16  | l     | 0.12         | 0/1097  | 0.29        | 0/1493         |
| 17  | m     | 0.14         | 0/241   | 0.22        | 0/326          |
| All | All   | 0.14         | 0/25665 | 0.28        | 1/34964 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | I     | 28  | PRO  | CA-N-CD | -6.99 | 102.22      | 112.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2256  | 0        | 2181     | 59      | 0            |
| 2   | D     | 2188  | 0        | 2129     | 54      | 0            |
| 3   | E     | 301   | 0        | 287      | 8       | 0            |
| 4   | F     | 222   | 0        | 230      | 8       | 0            |
| 5   | I     | 229   | 0        | 247      | 7       | 0            |
| 6   | S     | 2328  | 0        | 2227     | 64      | 0            |
| 7   | a     | 5795  | 0        | 5653     | 163     | 0            |
| 8   | b     | 5770  | 0        | 5547     | 136     | 0            |
| 9   | c     | 600   | 0        | 581      | 16      | 0            |
| 10  | d     | 1087  | 0        | 1082     | 26      | 0            |
| 11  | e     | 538   | 0        | 514      | 10      | 0            |
| 12  | f     | 1108  | 0        | 1100     | 21      | 0            |
| 13  | i     | 311   | 0        | 304      | 8       | 0            |
| 14  | j     | 319   | 0        | 328      | 12      | 0            |
| 15  | k     | 524   | 0        | 547      | 13      | 0            |
| 16  | l     | 1069  | 0        | 1044     | 21      | 0            |
| 17  | m     | 238   | 0        | 260      | 5       | 0            |
| 18  | A     | 1     | 0        | 0        | 0       | 0            |
| 19  | A     | 226   | 0        | 216      | 18      | 0            |
| 19  | D     | 101   | 0        | 82       | 10      | 0            |
| 19  | a     | 2811  | 0        | 2986     | 200     | 0            |
| 19  | b     | 2410  | 0        | 2456     | 160     | 0            |
| 19  | f     | 165   | 0        | 150      | 5       | 0            |
| 19  | j     | 101   | 0        | 82       | 7       | 0            |
| 19  | k     | 91    | 0        | 66       | 5       | 0            |
| 19  | l     | 167   | 0        | 154      | 8       | 0            |
| 20  | A     | 64    | 0        | 74       | 4       | 0            |
| 20  | D     | 64    | 0        | 74       | 3       | 0            |
| 21  | A     | 40    | 0        | 56       | 6       | 0            |
| 21  | a     | 265   | 0        | 369      | 23      | 0            |
| 21  | b     | 200   | 0        | 280      | 21      | 0            |
| 21  | f     | 40    | 0        | 56       | 7       | 0            |
| 21  | i     | 80    | 0        | 112      | 6       | 0            |
| 21  | j     | 40    | 0        | 56       | 3       | 0            |
| 21  | k     | 40    | 0        | 56       | 2       | 0            |
| 21  | l     | 40    | 0        | 56       | 4       | 0            |
| 22  | E     | 43    | 0        | 30       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | a     | 65    | 0        | 72       | 4       | 0            |
| 24  | a     | 33    | 0        | 46       | 2       | 0            |
| 24  | b     | 33    | 0        | 46       | 3       | 0            |
| 25  | a     | 8     | 0        | 0        | 0       | 0            |
| 25  | c     | 16    | 0        | 0        | 2       | 0            |
| 26  | a     | 147   | 0        | 222      | 10      | 0            |
| 26  | b     | 38    | 0        | 49       | 1       | 0            |
| 26  | f     | 49    | 0        | 74       | 4       | 0            |
| 27  | a     | 40    | 0        | 50       | 1       | 0            |
| 27  | b     | 110   | 0        | 172      | 9       | 0            |
| 27  | l     | 50    | 0        | 73       | 3       | 0            |
| 28  | a     | 42    | 0        | 52       | 3       | 0            |
| 29  | b     | 41    | 0        | 54       | 4       | 0            |
| 29  | m     | 41    | 0        | 54       | 4       | 0            |
| 30  | b     | 42    | 0        | 0        | 1       | 0            |
| 31  | b     | 42    | 0        | 56       | 4       | 0            |
| 31  | f     | 42    | 0        | 56       | 1       | 0            |
| 32  | j     | 35    | 0        | 45       | 0       | 0            |
| All | All   | 32746 | 0        | 32793    | 857     | 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 13.

All (857) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:a:392:HIS:HE1   | 19:a:829:CLA:ND   | 1.64                     | 0.94              |
| 7:a:93:HIS:HE1    | 19:a:808:CLA:NA   | 1.73                     | 0.87              |
| 8:b:275:HIS:HE1   | 19:b:815:CLA:ND   | 1.74                     | 0.84              |
| 2:D:186:GLN:HB2   | 19:D:402:CLA:HBC1 | 1.59                     | 0.83              |
| 7:a:407:HIS:HE1   | 19:a:831:CLA:NA   | 1.76                     | 0.82              |
| 8:b:387:HIS:HE1   | 19:b:828:CLA:NA   | 1.77                     | 0.81              |
| 8:b:193:HIS:HE1   | 19:b:813:CLA:NA   | 1.80                     | 0.80              |
| 19:b:805:CLA:H162 | 19:b:827:CLA:HBB2 | 1.64                     | 0.79              |
| 19:b:819:CLA:HBB1 | 21:b:842:BCR:H14C | 1.63                     | 0.79              |
| 19:b:821:CLA:HHC  | 19:b:821:CLA:HBB1 | 1.66                     | 0.78              |
| 6:S:322:VAL:HB    | 6:S:330:LEU:HB2   | 1.67                     | 0.76              |
| 19:a:835:CLA:H2   | 16:l:64:PRO:HB2   | 1.69                     | 0.75              |
| 7:a:374:PRO:HG3   | 7:a:380:ALA:HB2   | 1.69                     | 0.74              |
| 7:a:197:MET:HE2   | 19:a:822:CLA:HMA2 | 1.69                     | 0.74              |
| 1:A:211:PHE:HB3   | 1:A:275:LEU:HD13  | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:a:823:CLA:HMD2 | 21:a:846:BCR:H24C | 1.70                     | 0.71              |
| 7:a:457:HIS:HE1   | 19:a:835:CLA:NA   | 1.84                     | 0.71              |
| 7:a:684:MET:HG3   | 19:a:803:CLA:NC   | 2.04                     | 0.71              |
| 7:a:684:MET:HB2   | 19:a:803:CLA:C1C  | 2.21                     | 0.71              |
| 19:a:804:CLA:HBB1 | 21:a:859:BCR:H292 | 1.72                     | 0.70              |
| 7:a:52:HIS:HE1    | 19:a:804:CLA:ND   | 1.89                     | 0.70              |
| 7:a:450:HIS:HE1   | 19:a:834:CLA:NA   | 1.88                     | 0.70              |
| 8:b:709:HIS:HE1   | 19:b:839:CLA:ND   | 1.90                     | 0.69              |
| 19:b:828:CLA:H91  | 27:b:848:LMG:H262 | 1.74                     | 0.69              |
| 2:D:68:LEU:HA     | 4:F:39:MET:HE1    | 1.75                     | 0.69              |
| 7:a:429:MET:HE2   | 7:a:429:MET:HA    | 1.75                     | 0.68              |
| 10:d:42:MET:HE1   | 10:d:57:LEU:HD21  | 1.75                     | 0.68              |
| 6:S:113:SER:HB3   | 6:S:130:LEU:HD12  | 1.75                     | 0.68              |
| 20:D:401:PHO:HAB  | 19:D:402:CLA:H11  | 1.76                     | 0.68              |
| 4:F:29:SER:O      | 4:F:33:VAL:HG23   | 1.93                     | 0.68              |
| 19:a:831:CLA:HBA1 | 19:a:831:CLA:HBD  | 1.76                     | 0.68              |
| 7:a:684:MET:HG3   | 19:a:803:CLA:C4C  | 2.23                     | 0.67              |
| 8:b:195:VAL:HG21  | 19:b:814:CLA:HBC2 | 1.74                     | 0.67              |
| 2:D:161:PRO:HB3   | 2:D:170:ALA:HB2   | 1.76                     | 0.67              |
| 19:b:826:CLA:HBC3 | 27:b:848:LMG:H442 | 1.76                     | 0.66              |
| 19:b:816:CLA:HBC1 | 19:b:823:CLA:H191 | 1.78                     | 0.66              |
| 7:a:118:TRP:HE1   | 21:a:851:BCR:H332 | 1.60                     | 0.66              |
| 8:b:456:VAL:HG11  | 12:f:78:ASP:HB3   | 1.77                     | 0.66              |
| 8:b:409:MET:HG3   | 21:b:847:BCR:H402 | 1.78                     | 0.66              |
| 10:d:61:ARG:NH2   | 10:d:63:GLU:OE1   | 2.28                     | 0.65              |
| 8:b:441:VAL:HG11  | 8:b:449:LYS:HB2   | 1.79                     | 0.65              |
| 19:b:806:CLA:H2   | 19:b:806:CLA:C4D  | 2.27                     | 0.65              |
| 7:a:362:LEU:HD11  | 19:a:820:CLA:H71  | 1.78                     | 0.64              |
| 19:b:818:CLA:HBB1 | 19:b:823:CLA:H62  | 1.77                     | 0.64              |
| 21:b:845:BCR:H23C | 21:b:847:BCR:H393 | 1.78                     | 0.64              |
| 2:D:78:VAL:HB     | 2:D:173:PHE:HB2   | 1.78                     | 0.64              |
| 12:f:97:ILE:HG23  | 19:f:203:CLA:HAA1 | 1.79                     | 0.64              |
| 8:b:89:HIS:CD2    | 19:b:807:CLA:NA   | 2.66                     | 0.64              |
| 19:b:832:CLA:H62  | 21:f:202:BCR:HC22 | 1.79                     | 0.64              |
| 1:A:334:ARG:HG3   | 1:A:335:ASN:H     | 1.63                     | 0.63              |
| 19:a:841:CLA:HAB  | 19:a:841:CLA:H122 | 1.80                     | 0.63              |
| 9:c:5:VAL:HG22    | 9:c:67:VAL:HG22   | 1.79                     | 0.63              |
| 19:A:403:CLA:HAB  | 19:D:402:CLA:H72  | 1.80                     | 0.63              |
| 1:A:39:PRO:HB2    | 19:A:405:CLA:HAB  | 1.81                     | 0.63              |
| 13:i:22:PHE:O     | 13:i:26:THR:HG22  | 1.99                     | 0.63              |
| 8:b:44:GLN:OE1    | 8:b:162:ARG:NH1   | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:E:101:HEM:HBC2 | 22:E:101:HEM:HHD  | 1.81                     | 0.63              |
| 7:a:586:SER:OG    | 7:a:589:ASP:OD1   | 2.17                     | 0.63              |
| 19:A:405:CLA:HAC1 | 21:A:406:BCR:H14C | 1.81                     | 0.62              |
| 7:a:234:LYS:NZ    | 7:a:235:ASP:OD1   | 2.32                     | 0.62              |
| 7:a:673:LEU:HB3   | 19:a:802:CLA:H11  | 1.80                     | 0.62              |
| 19:a:813:CLA:H43  | 19:a:821:CLA:H41  | 1.81                     | 0.62              |
| 6:S:40:TRP:HB3    | 6:S:330:LEU:HD22  | 1.80                     | 0.62              |
| 2:D:246:MET:HE1   | 2:D:250:ASN:HD22  | 1.64                     | 0.62              |
| 7:a:497:THR:HG21  | 19:a:836:CLA:HMD1 | 1.81                     | 0.62              |
| 7:a:730:HIS:HE1   | 19:a:842:CLA:ND   | 1.98                     | 0.62              |
| 8:b:38:THR:OG1    | 8:b:41:ASN:ND2    | 2.32                     | 0.62              |
| 7:a:337:HIS:CD2   | 19:a:825:CLA:ND   | 2.67                     | 0.62              |
| 6:S:291:ASP:OD2   | 6:S:295:THR:OG1   | 2.17                     | 0.62              |
| 19:b:829:CLA:HAC1 | 21:b:847:BCR:H383 | 1.82                     | 0.62              |
| 16:l:26:ASP:O     | 16:l:31:ARG:NH1   | 2.33                     | 0.62              |
| 19:a:856:CLA:H11  | 8:b:648:LEU:HB3   | 1.82                     | 0.62              |
| 9:c:19:ARG:NH1    | 10:d:106:GLU:OE1  | 2.32                     | 0.61              |
| 7:a:457:HIS:HE1   | 19:a:835:CLA:C1A  | 2.11                     | 0.61              |
| 7:a:692:TYR:OH    | 19:a:803:CLA:OBD  | 2.16                     | 0.61              |
| 11:e:68:LEU:HD11  | 11:e:70:GLN:HG3   | 1.82                     | 0.61              |
| 7:a:27:LYS:HD2    | 19:a:812:CLA:HAA2 | 1.82                     | 0.61              |
| 12:f:33:SER:OG    | 12:f:34:GLU:OE1   | 2.18                     | 0.61              |
| 8:b:684:LEU:HD12  | 19:l:203:CLA:H42  | 1.83                     | 0.61              |
| 16:l:55:MET:HE1   | 21:l:205:BCR:H383 | 1.82                     | 0.61              |
| 2:D:125:PHE:O     | 2:D:129:GLN:NE2   | 2.33                     | 0.60              |
| 7:a:392:HIS:HE1   | 19:a:829:CLA:C1D  | 2.13                     | 0.60              |
| 19:j:104:CLA:H2A  | 19:j:104:CLA:HED3 | 1.81                     | 0.60              |
| 8:b:286:ILE:HD13  | 21:b:842:BCR:H17C | 1.83                     | 0.60              |
| 7:a:59:ASP:OD2    | 7:a:349:HIS:NE2   | 2.34                     | 0.60              |
| 7:a:179:HIS:HE1   | 19:a:811:CLA:NA   | 1.96                     | 0.60              |
| 10:d:10:LYS:NZ    | 10:d:37:GLU:OE1   | 2.35                     | 0.60              |
| 7:a:295:HIS:HE1   | 19:a:818:CLA:C4D  | 2.14                     | 0.60              |
| 5:I:8:VAL:O       | 5:I:12:VAL:HG22   | 2.01                     | 0.60              |
| 19:b:840:CLA:HBB2 | 21:b:847:BCR:H14C | 1.84                     | 0.60              |
| 16:l:52:GLU:HG3   | 19:l:202:CLA:HMA3 | 1.84                     | 0.60              |
| 8:b:403:ASP:OD1   | 8:b:408:ARG:NH2   | 2.34                     | 0.59              |
| 7:a:117:VAL:O     | 7:a:127:ASN:ND2   | 2.35                     | 0.59              |
| 19:a:824:CLA:HBA1 | 19:a:824:CLA:HBD  | 1.83                     | 0.59              |
| 16:l:41:ARG:O     | 16:l:49:ARG:NH2   | 2.29                     | 0.59              |
| 6:S:51:PHE:HB3    | 6:S:323:LEU:HD23  | 1.84                     | 0.59              |
| 8:b:694:PRO:O     | 9:c:81:TYR:OH     | 2.18                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:343:LEU:HD13  | 6:S:131:SER:HB3   | 1.84                     | 0.59              |
| 6:S:97:SER:OG     | 6:S:111:LYS:NZ    | 2.32                     | 0.59              |
| 21:a:859:BCR:H312 | 14:j:31:ARG:HD3   | 1.83                     | 0.59              |
| 19:a:820:CLA:H203 | 19:a:828:CLA:H3A  | 1.84                     | 0.59              |
| 1:A:317:TRP:HZ3   | 2:D:180:ARG:HD2   | 1.68                     | 0.58              |
| 19:a:807:CLA:H151 | 19:a:830:CLA:HBB2 | 1.85                     | 0.58              |
| 19:b:827:CLA:H8   | 21:b:843:BCR:H21C | 1.84                     | 0.58              |
| 6:S:207:GLN:HG2   | 6:S:209:GLU:H     | 1.68                     | 0.58              |
| 7:a:56:HIS:HE1    | 19:a:805:CLA:C1C  | 2.16                     | 0.58              |
| 6:S:272:ARG:HE    | 6:S:332:TYR:HE2   | 1.51                     | 0.58              |
| 1:A:343:LEU:HD21  | 6:S:133:LYS:HB2   | 1.83                     | 0.58              |
| 2:D:61:HIS:HE2    | 2:D:80:SER:HG     | 1.49                     | 0.58              |
| 5:I:4:LEU:O       | 5:I:8:VAL:HG23    | 2.03                     | 0.58              |
| 7:a:704:HIS:HE1   | 19:a:841:CLA:ND   | 2.02                     | 0.58              |
| 8:b:516:VAL:HG21  | 8:b:590:TYR:HB2   | 1.85                     | 0.58              |
| 8:b:667:TYR:OH    | 19:b:802:CLA:OBD  | 2.15                     | 0.58              |
| 19:b:822:CLA:HMC2 | 21:b:847:BCR:H24C | 1.85                     | 0.58              |
| 1:A:87:ASN:ND2    | 6:S:222:GLN:OE1   | 2.37                     | 0.58              |
| 1:A:308:ASP:OD1   | 1:A:312:ARG:N     | 2.36                     | 0.58              |
| 8:b:542:LYS:NZ    | 11:e:17:TYR:O     | 2.35                     | 0.58              |
| 15:k:16:TRP:NE1   | 19:k:101:CLA:OBD  | 2.34                     | 0.58              |
| 16:l:51:LEU:HG    | 16:l:55:MET:HE2   | 1.84                     | 0.58              |
| 1:A:50:ILE:HG21   | 21:A:406:BCR:H23C | 1.85                     | 0.58              |
| 22:E:101:HEM:HBB2 | 22:E:101:HEM:HMB2 | 1.86                     | 0.57              |
| 7:a:215:HIS:HB2   | 19:a:815:CLA:CHC  | 2.34                     | 0.57              |
| 8:b:275:HIS:HE1   | 19:b:815:CLA:C4D  | 2.16                     | 0.57              |
| 7:a:450:HIS:HE1   | 19:a:834:CLA:C1A  | 2.18                     | 0.57              |
| 26:a:853:LHG:H192 | 26:a:853:LHG:H332 | 1.86                     | 0.57              |
| 7:a:295:HIS:HE1   | 19:a:818:CLA:ND   | 2.02                     | 0.57              |
| 19:a:805:CLA:H11  | 19:a:812:CLA:H52  | 1.85                     | 0.57              |
| 19:a:811:CLA:H41  | 19:a:813:CLA:H91  | 1.87                     | 0.57              |
| 19:a:828:CLA:H171 | 19:a:860:CLA:H171 | 1.85                     | 0.57              |
| 3:E:53:ASP:OD1    | 3:E:54:GLU:N      | 2.37                     | 0.57              |
| 19:a:837:CLA:H191 | 19:a:860:CLA:H111 | 1.86                     | 0.57              |
| 19:a:841:CLA:HED3 | 19:a:841:CLA:H2A  | 1.86                     | 0.57              |
| 15:k:70:HIS:CD2   | 19:k:101:CLA:NC   | 2.71                     | 0.57              |
| 19:a:834:CLA:H122 | 24:b:841:PQN:H191 | 1.87                     | 0.57              |
| 21:i:102:BCR:H403 | 21:i:102:BCR:H23C | 1.87                     | 0.57              |
| 6:S:139:TYR:HE2   | 6:S:182:ILE:H     | 1.52                     | 0.57              |
| 16:l:66:THR:O     | 16:l:77:GLN:NE2   | 2.38                     | 0.57              |
| 31:b:852:ZEX:H221 | 19:j:104:CLA:HMD2 | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:131:TRP:HH2   | 19:b:814:CLA:HED1 | 1.70                     | 0.57              |
| 19:a:818:CLA:H61  | 15:k:78:LEU:HD13  | 1.87                     | 0.57              |
| 3:E:30:LEU:HD23   | 4:F:30:VAL:HG23   | 1.87                     | 0.56              |
| 8:b:193:HIS:HE1   | 19:b:813:CLA:C1A  | 2.18                     | 0.56              |
| 8:b:462:GLN:HE21  | 8:b:506:PHE:HB3   | 1.70                     | 0.56              |
| 19:b:822:CLA:H51  | 19:b:823:CLA:H142 | 1.86                     | 0.56              |
| 7:a:17:ASP:OD2    | 7:a:70:ARG:NH2    | 2.34                     | 0.56              |
| 8:b:210:ASP:N     | 8:b:210:ASP:OD1   | 2.39                     | 0.56              |
| 8:b:276:HIS:HB2   | 19:b:816:CLA:C1B  | 2.36                     | 0.56              |
| 2:D:83:ASP:N      | 2:D:83:ASP:OD1    | 2.36                     | 0.56              |
| 6:S:200:TYR:CG    | 6:S:224:MET:HE1   | 2.41                     | 0.56              |
| 7:a:199:HIS:HE1   | 19:a:813:CLA:NA   | 2.04                     | 0.56              |
| 19:a:806:CLA:HED3 | 19:a:806:CLA:H2A  | 1.88                     | 0.56              |
| 19:a:822:CLA:H101 | 21:a:850:BCR:H10C | 1.89                     | 0.55              |
| 7:a:355:ASN:ND2   | 19:a:806:CLA:OBD  | 2.28                     | 0.55              |
| 21:i:102:BCR:H383 | 16:l:96:LEU:HD21  | 1.88                     | 0.55              |
| 7:a:219:VAL:HG13  | 7:a:239:PRO:HB3   | 1.89                     | 0.55              |
| 21:a:846:BCR:HC8  | 21:a:847:BCR:H392 | 1.87                     | 0.55              |
| 1:A:59:ASP:OD2    | 6:S:310:TYR:OH    | 2.22                     | 0.55              |
| 8:b:90:ALA:HA     | 8:b:113:VAL:HG23  | 1.87                     | 0.55              |
| 8:b:387:HIS:HA    | 8:b:390:ILE:HD12  | 1.88                     | 0.55              |
| 8:b:518:HIS:HE1   | 19:b:836:CLA:ND   | 2.05                     | 0.55              |
| 16:l:57:HIS:HE1   | 19:l:203:CLA:C4D  | 2.08                     | 0.55              |
| 19:a:832:CLA:HAA2 | 16:l:8:VAL:HG11   | 1.87                     | 0.55              |
| 11:e:8:LYS:HD2    | 11:e:24:THR:HG22  | 1.88                     | 0.55              |
| 2:D:98:GLN:OE1    | 2:D:103:ARG:NH1   | 2.40                     | 0.55              |
| 8:b:120:VAL:HG21  | 19:b:807:CLA:HED1 | 1.88                     | 0.55              |
| 8:b:356:TYR:OH    | 19:b:827:CLA:OBD  | 2.25                     | 0.55              |
| 1:A:216:GLY:HA3   | 2:D:272:LEU:HB2   | 1.89                     | 0.55              |
| 20:A:404:PHO:H172 | 19:A:407:CLA:H143 | 1.89                     | 0.55              |
| 5:I:12:VAL:O      | 5:I:16:ILE:HG23   | 2.06                     | 0.55              |
| 7:a:304:PHE:HE1   | 19:a:822:CLA:HAB  | 1.71                     | 0.55              |
| 8:b:437:HIS:HE1   | 19:b:832:CLA:C1A  | 2.10                     | 0.55              |
| 19:b:824:CLA:HBA2 | 19:b:837:CLA:HAA1 | 1.88                     | 0.55              |
| 7:a:168:MET:O     | 7:a:172:MET:HG2   | 2.07                     | 0.55              |
| 7:a:437:ILE:HG13  | 7:a:555:TYR:HE2   | 1.72                     | 0.55              |
| 8:b:277:HIS:HE1   | 19:b:817:CLA:NA   | 2.04                     | 0.55              |
| 8:b:317:HIS:CD2   | 19:b:822:CLA:ND   | 2.75                     | 0.55              |
| 1:A:189:GLU:OE2   | 6:S:220:ARG:NE    | 2.40                     | 0.54              |
| 2:D:61:HIS:NE2    | 2:D:80:SER:OG     | 2.36                     | 0.54              |
| 19:a:834:CLA:H91  | 19:b:839:CLA:H71  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:b:301:ILE:HG21  | 19:b:823:CLA:HAC1 | 1.89                     | 0.54              |
| 7:a:557:ARG:NH2   | 10:d:41:GLU:OE1   | 2.40                     | 0.54              |
| 7:a:583:CYS:HB2   | 8:b:664:TRP:HB3   | 1.87                     | 0.54              |
| 7:a:708:ASN:OD1   | 12:f:113:ARG:NH1  | 2.40                     | 0.54              |
| 19:a:831:CLA:H2A  | 19:a:831:CLA:O2D  | 2.06                     | 0.54              |
| 7:a:704:HIS:HE1   | 19:a:841:CLA:C4D  | 2.20                     | 0.54              |
| 19:a:834:CLA:H161 | 21:i:102:BCR:H11C | 1.88                     | 0.54              |
| 13:i:13:ILE:O     | 13:i:17:MET:HG3   | 2.06                     | 0.54              |
| 7:a:56:HIS:HE1    | 19:a:805:CLA:NC   | 1.99                     | 0.54              |
| 6:S:85:LYS:NZ     | 6:S:86:LEU:O      | 2.37                     | 0.54              |
| 19:a:825:CLA:HAB  | 19:a:832:CLA:HMD1 | 1.90                     | 0.54              |
| 8:b:32:GLU:OE1    | 8:b:394:ARG:NH1   | 2.41                     | 0.54              |
| 8:b:196:HIS:HE1   | 19:b:814:CLA:NA   | 1.99                     | 0.54              |
| 9:c:61:ASP:HB2    | 11:e:59:ASN:CG    | 2.33                     | 0.54              |
| 2:D:69:GLU:OE2    | 3:E:55:TYR:OH     | 2.26                     | 0.54              |
| 7:a:398:GLY:HA3   | 7:a:602:LEU:HD11  | 1.89                     | 0.54              |
| 6:S:139:TYR:HD2   | 6:S:182:ILE:HD12  | 1.73                     | 0.54              |
| 7:a:706:LYS:NZ    | 12:f:157:ASP:OD1  | 2.38                     | 0.54              |
| 8:b:349:HIS:CD2   | 19:b:825:CLA:NC   | 2.75                     | 0.54              |
| 8:b:98:GLU:OE2    | 8:b:102:ASN:ND2   | 2.41                     | 0.53              |
| 19:b:802:CLA:CGA  | 19:b:802:CLA:H3A  | 2.38                     | 0.53              |
| 2:D:55:VAL:HG21   | 2:D:110:LEU:HD22  | 1.90                     | 0.53              |
| 6:S:128:ILE:HD13  | 6:S:165:GLY:HA3   | 1.90                     | 0.53              |
| 7:a:245:GLU:OE2   | 7:a:247:SER:OG    | 2.24                     | 0.53              |
| 7:a:326:GLU:HG2   | 7:a:338:LYS:HG3   | 1.90                     | 0.53              |
| 8:b:323:THR:OG1   | 8:b:401:ASN:OD1   | 2.24                     | 0.53              |
| 8:b:343:THR:HB    | 8:b:377:ALA:HB2   | 1.91                     | 0.53              |
| 2:D:192:THR:HG23  | 19:D:402:CLA:HBC2 | 1.90                     | 0.53              |
| 8:b:335:ALA:HB1   | 19:b:804:CLA:HED2 | 1.90                     | 0.53              |
| 6:S:138:PRO:HB3   | 6:S:151:MET:SD    | 2.48                     | 0.53              |
| 7:a:429:MET:HE1   | 19:a:832:CLA:CHD  | 2.39                     | 0.53              |
| 7:a:369:HIS:CD2   | 19:a:828:CLA:NC   | 2.77                     | 0.53              |
| 8:b:342:ILE:HD12  | 19:b:817:CLA:H102 | 1.91                     | 0.53              |
| 4:F:32:PHE:O      | 4:F:36:ILE:HG12   | 2.09                     | 0.53              |
| 10:d:51:ASN:O     | 10:d:55:ASN:ND2   | 2.42                     | 0.53              |
| 7:a:74:SER:OG     | 7:a:180:TYR:HB2   | 2.09                     | 0.53              |
| 7:a:223:ILE:HD11  | 7:a:239:PRO:HG3   | 1.90                     | 0.53              |
| 7:a:621:VAL:HG22  | 7:a:627:VAL:HG22  | 1.90                     | 0.53              |
| 7:a:19:ASN:N      | 7:a:182:VAL:O     | 2.31                     | 0.53              |
| 7:a:531:ASP:OD2   | 7:a:612:LYS:NZ    | 2.32                     | 0.53              |
| 7:a:93:HIS:HE1    | 19:a:808:CLA:C1A  | 2.23                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:a:804:CLA:H193 | 24:a:844:PQN:H302 | 1.91                     | 0.52              |
| 8:b:448:GLU:OE2   | 12:f:58:ARG:NE    | 2.40                     | 0.52              |
| 8:b:605:GLN:O     | 8:b:609:ASN:ND2   | 2.41                     | 0.52              |
| 10:d:4:LEU:HB3    | 10:d:56:LEU:HD11  | 1.90                     | 0.52              |
| 19:a:806:CLA:H151 | 21:a:847:BCR:H323 | 1.90                     | 0.52              |
| 19:b:828:CLA:H142 | 27:b:848:LMG:H212 | 1.90                     | 0.52              |
| 19:a:856:CLA:H122 | 21:b:846:BCR:H12C | 1.91                     | 0.52              |
| 8:b:95:HIS:HE1    | 19:b:809:CLA:C4B  | 2.22                     | 0.52              |
| 8:b:646:MET:HG2   | 8:b:720:ALA:HB2   | 1.92                     | 0.52              |
| 2:D:100:ASN:HB3   | 2:D:103:ARG:HB2   | 1.91                     | 0.52              |
| 6:S:282:ALA:O     | 6:S:285:ASN:ND2   | 2.36                     | 0.52              |
| 7:a:179:HIS:HE1   | 19:a:811:CLA:C1A  | 2.21                     | 0.52              |
| 7:a:417:ASP:O     | 7:a:421:ASN:ND2   | 2.42                     | 0.52              |
| 1:A:42:LEU:HB3    | 21:A:406:BCR:H353 | 1.91                     | 0.52              |
| 1:A:302:PHE:HE2   | 2:D:74:LEU:HD12   | 1.74                     | 0.52              |
| 19:a:818:CLA:H202 | 19:a:860:CLA:HBC1 | 1.90                     | 0.52              |
| 19:a:829:CLA:H203 | 21:j:101:BCR:H12C | 1.92                     | 0.52              |
| 10:d:42:MET:HE3   | 10:d:43:PRO:HD2   | 1.90                     | 0.52              |
| 4:F:25:LEU:HD23   | 4:F:25:LEU:H      | 1.75                     | 0.52              |
| 6:S:307:ALA:HB2   | 6:S:328:ILE:HD12  | 1.92                     | 0.52              |
| 15:k:54:PHE:HZ    | 21:k:103:BCR:H393 | 1.75                     | 0.52              |
| 7:a:307:ALA:HB2   | 19:a:822:CLA:HBC2 | 1.92                     | 0.51              |
| 7:a:500:ASN:HB2   | 19:a:837:CLA:HED2 | 1.91                     | 0.51              |
| 19:a:827:CLA:HAA2 | 19:a:828:CLA:OBD  | 2.09                     | 0.51              |
| 8:b:136:TYR:OH    | 17:m:7:GLN:O      | 2.23                     | 0.51              |
| 28:a:858:45D:H231 | 28:a:858:45D:H122 | 1.91                     | 0.51              |
| 8:b:371:THR:HG23  | 8:b:588:THR:HG21  | 1.91                     | 0.51              |
| 16:l:62:ILE:HG21  | 16:l:138:ALA:HB1  | 1.93                     | 0.51              |
| 19:a:822:CLA:H102 | 19:a:825:CLA:H93  | 1.92                     | 0.51              |
| 19:a:831:CLA:H102 | 26:a:852:LHG:H182 | 1.91                     | 0.51              |
| 26:a:855:LHG:H191 | 26:a:855:LHG:H122 | 1.92                     | 0.51              |
| 19:b:825:CLA:H13  | 21:b:845:BCR:H15C | 1.90                     | 0.51              |
| 1:A:310:GLN:HE21  | 1:A:312:ARG:HH21  | 1.58                     | 0.51              |
| 7:a:181:HIS:HE1   | 19:a:812:CLA:NA   | 2.07                     | 0.51              |
| 19:a:828:CLA:HBB1 | 19:a:836:CLA:HAA2 | 1.91                     | 0.51              |
| 1:A:74:GLY:HA3    | 2:D:304:ARG:HH12  | 1.76                     | 0.51              |
| 19:a:803:CLA:H12  | 8:b:425:LEU:HD23  | 1.92                     | 0.51              |
| 21:a:859:BCR:H17C | 14:j:20:THR:HG22  | 1.93                     | 0.51              |
| 11:e:3:LEU:HD13   | 11:e:9:VAL:HG11   | 1.91                     | 0.51              |
| 6:S:66:VAL:HG12   | 6:S:72:ILE:HG22   | 1.93                     | 0.51              |
| 7:a:490:HIS:CD2   | 19:a:836:CLA:ND   | 2.78                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:a:827:CLA:H91  | 21:a:850:BCR:H23C | 1.93                     | 0.51              |
| 8:b:177:HIS:HE1   | 19:b:811:CLA:NA   | 2.07                     | 0.51              |
| 8:b:346:VAL:O     | 8:b:350:MET:HB2   | 2.10                     | 0.51              |
| 1:A:142:TRP:HB2   | 2:D:220:ASN:OD1   | 2.10                     | 0.51              |
| 19:a:807:CLA:H52  | 26:a:852:LHG:H272 | 1.92                     | 0.51              |
| 8:b:95:HIS:HE1    | 19:b:809:CLA:NB   | 2.02                     | 0.51              |
| 27:l:201:LMG:H322 | 27:l:201:LMG:HC91 | 1.92                     | 0.51              |
| 8:b:196:HIS:HE1   | 19:b:814:CLA:C1A  | 2.23                     | 0.51              |
| 19:b:821:CLA:HMC2 | 21:b:847:BCR:HC8  | 1.91                     | 0.51              |
| 14:j:9:SER:HA     | 14:j:14:MET:HE3   | 1.93                     | 0.51              |
| 6:S:62:HIS:HA     | 6:S:76:THR:HA     | 1.92                     | 0.51              |
| 6:S:105:GLU:HG3   | 6:S:119:THR:HG22  | 1.93                     | 0.51              |
| 8:b:180:ALA:HB2   | 8:b:288:GLY:HA3   | 1.92                     | 0.51              |
| 8:b:337:ALA:HB2   | 21:b:845:BCR:H372 | 1.92                     | 0.51              |
| 10:d:27:LYS:HG3   | 10:d:88:VAL:HB    | 1.93                     | 0.50              |
| 2:D:263:ASN:HB3   | 2:D:265:ARG:HG3   | 1.93                     | 0.50              |
| 7:a:297:HIS:HE1   | 19:a:820:CLA:NA   | 2.09                     | 0.50              |
| 1:A:219:VAL:HG21  | 2:D:268:HIS:CD2   | 2.47                     | 0.50              |
| 19:A:407:CLA:H2A  | 19:A:407:CLA:HED3 | 1.92                     | 0.50              |
| 2:D:88:SER:OG     | 2:D:96:GLU:OE2    | 2.28                     | 0.50              |
| 2:D:111:TRP:HB3   | 2:D:112:PRO:HD3   | 1.94                     | 0.50              |
| 1:A:309:SER:OG    | 1:A:310:GLN:OE1   | 2.29                     | 0.50              |
| 7:a:730:HIS:HE1   | 19:a:842:CLA:C4D  | 2.24                     | 0.50              |
| 8:b:472:PHE:HE2   | 19:f:204:CLA:HBC1 | 1.77                     | 0.50              |
| 10:d:36:SER:HA    | 10:d:52:GLU:HG3   | 1.93                     | 0.50              |
| 19:a:825:CLA:H141 | 26:a:853:LHG:H171 | 1.93                     | 0.50              |
| 1:A:133:LEU:HD23  | 2:D:256:ILE:HG12  | 1.94                     | 0.50              |
| 7:a:200:HIS:CD2   | 19:a:814:CLA:NB   | 2.80                     | 0.50              |
| 19:b:813:CLA:H202 | 29:b:844:ECH:H36B | 1.94                     | 0.50              |
| 19:b:816:CLA:H161 | 19:b:834:CLA:HBA1 | 1.92                     | 0.50              |
| 10:d:31:THR:O     | 10:d:83:TYR:HA    | 2.12                     | 0.50              |
| 3:E:30:LEU:HG     | 4:F:31:PHE:HA     | 1.94                     | 0.50              |
| 7:a:312:ARG:NH1   | 15:k:41:GLN:OE1   | 2.45                     | 0.50              |
| 19:a:821:CLA:HBB1 | 21:a:846:BCR:H16C | 1.93                     | 0.50              |
| 19:a:835:CLA:O2D  | 19:a:835:CLA:H2A  | 2.12                     | 0.50              |
| 8:b:412:HIS:CD2   | 19:b:829:CLA:C4A  | 2.95                     | 0.50              |
| 6:S:57:THR:OG1    | 6:S:61:ASN:ND2    | 2.45                     | 0.49              |
| 8:b:223:MET:HB3   | 8:b:224:PRO:HD3   | 1.93                     | 0.49              |
| 8:b:566:ASP:HA    | 8:b:571:ASP:OD2   | 2.11                     | 0.49              |
| 19:b:824:CLA:H51  | 19:b:835:CLA:H11  | 1.93                     | 0.49              |
| 8:b:313:THR:OG1   | 26:b:849:LHG:O1   | 2.26                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:S:259:GLN:OE1   | 6:S:264:TRP:HB2   | 2.13                     | 0.49              |
| 9:c:22:PRO:HG2    | 9:c:23:LEU:HD12   | 1.94                     | 0.49              |
| 26:f:206:LHG:H252 | 26:f:206:LHG:HC42 | 1.95                     | 0.49              |
| 8:b:412:HIS:CE1   | 19:b:829:CLA:ND   | 2.81                     | 0.49              |
| 10:d:40:PHE:CE1   | 10:d:50:MET:HB3   | 2.48                     | 0.49              |
| 19:f:201:CLA:H71  | 14:j:14:MET:HB3   | 1.94                     | 0.49              |
| 2:D:281:MET:HE2   | 2:D:281:MET:N     | 2.27                     | 0.49              |
| 7:a:473:ASP:HA    | 7:a:477:GLN:HG2   | 1.95                     | 0.49              |
| 8:b:614:MET:HE3   | 8:b:617:PHE:HB3   | 1.94                     | 0.49              |
| 7:a:55:ALA:O      | 7:a:61:GLN:NE2    | 2.45                     | 0.49              |
| 8:b:17:THR:HG21   | 9:c:77:MET:HE2    | 1.93                     | 0.49              |
| 8:b:372:HIS:HE1   | 19:b:826:CLA:C1D  | 2.15                     | 0.49              |
| 19:b:803:CLA:H192 | 29:m:101:ECH:H35  | 1.95                     | 0.49              |
| 19:a:833:CLA:HAB  | 19:a:839:CLA:H191 | 1.95                     | 0.48              |
| 8:b:413:LYS:HB2   | 8:b:536:LEU:HD13  | 1.94                     | 0.48              |
| 19:b:829:CLA:HBB2 | 19:b:837:CLA:HMC2 | 1.95                     | 0.48              |
| 2:D:149:PRO:HB3   | 19:D:402:CLA:H62  | 1.95                     | 0.48              |
| 6:S:70:GLU:OE2    | 6:S:94:ALA:N      | 2.45                     | 0.48              |
| 8:b:525:HIS:CD2   | 19:b:837:CLA:NB   | 2.79                     | 0.48              |
| 7:a:362:LEU:HD21  | 19:a:820:CLA:H93  | 1.95                     | 0.48              |
| 19:a:804:CLA:H92  | 24:a:844:PQN:H201 | 1.95                     | 0.48              |
| 19:b:809:CLA:HHC  | 19:b:809:CLA:HBB1 | 1.94                     | 0.48              |
| 7:a:94:GLY:O      | 7:a:98:SER:OG     | 2.19                     | 0.48              |
| 7:a:676:HIS:CD2   | 23:a:801:CL0:NB   | 2.80                     | 0.48              |
| 21:i:102:BCR:H401 | 16:l:92:ALA:HB1   | 1.95                     | 0.48              |
| 7:a:317:ILE:HG22  | 19:a:823:CLA:HMD1 | 1.96                     | 0.48              |
| 8:b:308:HIS:HE1   | 19:b:821:CLA:ND   | 2.11                     | 0.48              |
| 19:b:831:CLA:HBB1 | 21:f:202:BCR:H323 | 1.94                     | 0.48              |
| 9:c:27:GLU:OE2    | 10:d:112:ARG:NE   | 2.46                     | 0.48              |
| 1:A:149:ALA:HB1   | 1:A:283:ILE:HB    | 1.96                     | 0.48              |
| 6:S:53:ASP:HB3    | 6:S:99:VAL:HG12   | 1.95                     | 0.48              |
| 7:a:202:ALA:HB2   | 7:a:308:GLY:HA3   | 1.96                     | 0.48              |
| 19:a:806:CLA:HBA1 | 19:a:806:CLA:H3A  | 1.38                     | 0.48              |
| 8:b:308:HIS:HE1   | 19:b:821:CLA:C4D  | 2.27                     | 0.48              |
| 26:f:206:LHG:H282 | 26:f:206:LHG:H182 | 1.94                     | 0.48              |
| 7:a:447:LEU:HB3   | 7:a:540:PHE:HB2   | 1.96                     | 0.48              |
| 19:a:821:CLA:HBB1 | 21:a:846:BCR:H14C | 1.95                     | 0.48              |
| 8:b:669:GLN:O     | 8:b:673:GLU:HG2   | 2.13                     | 0.48              |
| 12:f:77:VAL:HG12  | 12:f:77:VAL:O     | 2.14                     | 0.48              |
| 16:l:118:ASP:OD2  | 16:l:118:ASP:N    | 2.47                     | 0.48              |
| 7:a:118:TRP:CD2   | 19:a:810:CLA:HED3 | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:a:801:CL0:H41  | 23:a:801:CL0:H49  | 1.66                     | 0.48              |
| 19:a:837:CLA:H12  | 19:a:860:CLA:H51  | 1.96                     | 0.48              |
| 19:b:811:CLA:HHC  | 19:b:811:CLA:HBB1 | 1.96                     | 0.48              |
| 6:S:302:VAL:HB    | 6:S:305:ILE:HD12  | 1.95                     | 0.48              |
| 7:a:551:LYS:NZ    | 8:b:670:GLU:OE1   | 2.46                     | 0.48              |
| 19:a:822:CLA:H143 | 19:a:825:CLA:H112 | 1.95                     | 0.48              |
| 8:b:427:LEU:HB3   | 8:b:522:LEU:HB2   | 1.95                     | 0.48              |
| 19:b:828:CLA:HBA1 | 19:b:828:CLA:HBD  | 1.96                     | 0.48              |
| 9:c:55:GLU:OE2    | 9:c:67:VAL:N      | 2.46                     | 0.48              |
| 9:c:61:ASP:OD2    | 11:e:16:SER:HB2   | 2.14                     | 0.48              |
| 2:D:323:GLU:OE1   | 2:D:323:GLU:N     | 2.47                     | 0.47              |
| 6:S:293:GLY:HA2   | 6:S:296:TRP:CZ2   | 2.49                     | 0.47              |
| 7:a:589:ASP:OD2   | 7:a:724:ARG:NH1   | 2.47                     | 0.47              |
| 8:b:367:ALA:HB1   | 8:b:722:LEU:HD11  | 1.95                     | 0.47              |
| 19:b:840:CLA:CBB  | 21:b:847:BCR:H14C | 2.44                     | 0.47              |
| 1:A:308:ASP:HB3   | 1:A:314:ILE:HD11  | 1.96                     | 0.47              |
| 6:S:278:TRP:CE2   | 6:S:288:MET:HG3   | 2.48                     | 0.47              |
| 7:a:120:ILE:HD13  | 21:a:859:BCR:H313 | 1.96                     | 0.47              |
| 19:a:832:CLA:H3A  | 19:a:832:CLA:HBA2 | 1.45                     | 0.47              |
| 19:a:843:CLA:HMA1 | 26:a:853:LHG:HC62 | 1.96                     | 0.47              |
| 19:b:806:CLA:HHB  | 19:b:807:CLA:HMB3 | 1.96                     | 0.47              |
| 19:b:821:CLA:HBC2 | 19:b:822:CLA:HAA2 | 1.95                     | 0.47              |
| 19:k:101:CLA:H3A  | 19:k:101:CLA:HBA2 | 1.57                     | 0.47              |
| 1:A:334:ARG:HH12  | 6:S:212:PRO:HG3   | 1.79                     | 0.47              |
| 8:b:112:PRO:HG2   | 13:i:1:MET:HE1    | 1.95                     | 0.47              |
| 8:b:642:VAL:HG21  | 19:b:807:CLA:HAC1 | 1.96                     | 0.47              |
| 19:b:807:CLA:O1A  | 19:b:826:CLA:HBD  | 2.13                     | 0.47              |
| 19:b:828:CLA:H102 | 19:b:839:CLA:HED1 | 1.96                     | 0.47              |
| 16:l:55:MET:HB3   | 21:l:205:BCR:H19C | 1.95                     | 0.47              |
| 1:A:195:HIS:CG    | 1:A:293:MET:HE1   | 2.49                     | 0.47              |
| 8:b:701:GLN:HG3   | 27:b:848:LMG:H131 | 1.96                     | 0.47              |
| 9:c:32:ASP:OD1    | 9:c:32:ASP:N      | 2.47                     | 0.47              |
| 14:j:11:ALA:O     | 14:j:15:ILE:HG22  | 2.14                     | 0.47              |
| 1:A:140:ARG:HH12  | 2:D:222:LEU:HB2   | 1.79                     | 0.47              |
| 1:A:162:PRO:HB3   | 1:A:168:PHE:HA    | 1.97                     | 0.47              |
| 1:A:339:PHE:CZ    | 6:S:175:ALA:HB2   | 2.50                     | 0.47              |
| 20:A:404:PHO:H18  | 19:A:407:CLA:HBB1 | 1.96                     | 0.47              |
| 2:D:44:ALA:HB2    | 2:D:117:HIS:HB3   | 1.96                     | 0.47              |
| 5:I:27:ASP:HB2    | 5:I:28:PRO:HD2    | 1.97                     | 0.47              |
| 6:S:107:TRP:HE3   | 6:S:115:LEU:HD21  | 1.80                     | 0.47              |
| 6:S:160:LYS:N     | 6:S:169:LYS:O     | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:a:833:CLA:H3A  | 19:a:833:CLA:HBA2 | 1.56                     | 0.47              |
| 19:a:836:CLA:H62  | 19:a:836:CLA:H41  | 1.65                     | 0.47              |
| 19:b:806:CLA:H41  | 19:b:806:CLA:H62  | 1.57                     | 0.47              |
| 19:b:822:CLA:H2A  | 19:b:822:CLA:HED3 | 1.96                     | 0.47              |
| 19:b:838:CLA:HAA2 | 13:i:31:PHE:CE1   | 2.49                     | 0.47              |
| 19:b:838:CLA:HBA2 | 19:b:838:CLA:H3A  | 1.55                     | 0.47              |
| 9:c:24:ASP:OD1    | 10:d:105:PRO:HG3  | 2.14                     | 0.47              |
| 11:e:10:ARG:HB3   | 11:e:67:GLU:HG2   | 1.97                     | 0.47              |
| 19:l:202:CLA:H3A  | 19:l:202:CLA:HBA2 | 1.41                     | 0.47              |
| 2:D:120:PHE:N     | 2:D:120:PHE:CD1   | 2.82                     | 0.47              |
| 6:S:160:LYS:HB2   | 6:S:171:LEU:HD11  | 1.97                     | 0.47              |
| 7:a:484:GLN:HB3   | 27:a:854:LMG:HC5  | 1.97                     | 0.47              |
| 19:b:804:CLA:H8   | 19:b:823:CLA:HBA1 | 1.97                     | 0.47              |
| 19:b:815:CLA:C4D  | 19:b:815:CLA:H2   | 2.44                     | 0.47              |
| 1:A:187:GLN:HB2   | 19:A:402:CLA:HAC2 | 1.95                     | 0.47              |
| 19:a:821:CLA:H101 | 19:a:821:CLA:H61  | 1.50                     | 0.47              |
| 19:a:826:CLA:HBA1 | 19:a:830:CLA:H191 | 1.96                     | 0.47              |
| 8:b:230:TRP:HZ3   | 19:b:815:CLA:H92  | 1.80                     | 0.47              |
| 19:b:813:CLA:HBA1 | 29:b:844:ECH:H38B | 1.97                     | 0.47              |
| 20:A:404:PHO:H13  | 20:A:404:PHO:H102 | 1.61                     | 0.47              |
| 7:a:340:LEU:HD21  | 19:a:825:CLA:HBC3 | 1.97                     | 0.47              |
| 7:a:534:VAL:HG11  | 7:a:608:HIS:CG    | 2.49                     | 0.47              |
| 16:l:9:GLN:O      | 16:l:21:SER:N     | 2.47                     | 0.47              |
| 7:a:52:HIS:HE1    | 19:a:804:CLA:C4D  | 2.28                     | 0.46              |
| 7:a:432:HIS:CE1   | 7:a:436:ILE:HD11  | 2.50                     | 0.46              |
| 7:a:536:HIS:HE1   | 19:a:839:CLA:ND   | 2.12                     | 0.46              |
| 19:a:806:CLA:H202 | 19:a:814:CLA:H102 | 1.96                     | 0.46              |
| 12:f:116:LYS:HB2  | 12:f:116:LYS:HE2  | 1.59                     | 0.46              |
| 26:f:206:LHG:H151 | 26:f:206:LHG:H262 | 1.96                     | 0.46              |
| 2:D:201:VAL:HG22  | 19:D:402:CLA:C1B  | 2.46                     | 0.46              |
| 2:D:277:THR:O     | 2:D:281:MET:HG2   | 2.15                     | 0.46              |
| 8:b:193:HIS:HB2   | 19:b:813:CLA:CHC  | 2.46                     | 0.46              |
| 8:b:287:ALA:HB2   | 19:b:818:CLA:HBC2 | 1.97                     | 0.46              |
| 10:d:77:LYS:HB3   | 10:d:78:PRO:HD3   | 1.96                     | 0.46              |
| 13:i:17:MET:HA    | 13:i:21:LEU:HB3   | 1.97                     | 0.46              |
| 1:A:212:SER:OG    | 2:D:271:MET:HB2   | 2.16                     | 0.46              |
| 2:D:39:PRO:O      | 2:D:42:PHE:HB3    | 2.15                     | 0.46              |
| 7:a:458:ASN:HA    | 7:a:470:MET:HG2   | 1.98                     | 0.46              |
| 8:b:160:LYS:HA    | 8:b:160:LYS:HD3   | 1.72                     | 0.46              |
| 8:b:194:LEU:HA    | 8:b:198:ALA:HB3   | 1.96                     | 0.46              |
| 8:b:513:ASP:HA    | 8:b:516:VAL:HG12  | 1.95                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:b:814:CLA:H41  | 19:b:814:CLA:H62  | 1.53                     | 0.46              |
| 1:A:91:LEU:HD13   | 1:A:168:PHE:CE2   | 2.50                     | 0.46              |
| 23:a:801:CL0:H23  | 8:b:617:PHE:HE1   | 1.81                     | 0.46              |
| 19:l:203:CLA:H3A  | 19:l:203:CLA:HBA2 | 1.61                     | 0.46              |
| 6:S:151:MET:HE2   | 6:S:151:MET:HA    | 1.97                     | 0.46              |
| 19:a:803:CLA:H2   | 19:a:803:CLA:H3A  | 1.97                     | 0.46              |
| 8:b:571:ASP:OD2   | 8:b:703:ARG:NH1   | 2.49                     | 0.46              |
| 1:A:339:PHE:HZ    | 6:S:175:ALA:HB2   | 1.81                     | 0.46              |
| 7:a:407:HIS:HE1   | 19:a:831:CLA:C4A  | 2.27                     | 0.46              |
| 7:a:740:TRP:NE1   | 19:a:829:CLA:O1A  | 2.49                     | 0.46              |
| 19:a:803:CLA:H3A  | 19:a:803:CLA:C2   | 2.46                     | 0.46              |
| 19:b:824:CLA:HAA2 | 19:b:825:CLA:OBD  | 2.14                     | 0.46              |
| 19:D:403:CLA:HBA1 | 19:D:403:CLA:H3A  | 1.50                     | 0.46              |
| 7:a:217:ILE:HA    | 7:a:221:MET:HG3   | 1.96                     | 0.46              |
| 7:a:658:ILE:HD12  | 8:b:618:ARG:HG3   | 1.98                     | 0.46              |
| 7:a:684:MET:CG    | 19:a:803:CLA:NC   | 2.73                     | 0.46              |
| 8:b:3:THR:OG1     | 8:b:13:ALA:O      | 2.34                     | 0.46              |
| 8:b:29:HIS:HE1    | 19:b:803:CLA:C1C  | 2.28                     | 0.46              |
| 19:b:815:CLA:HBA2 | 19:b:815:CLA:H3A  | 1.72                     | 0.46              |
| 1:A:198:HIS:HE1   | 19:A:402:CLA:NB   | 2.13                     | 0.46              |
| 2:D:111:TRP:NE1   | 2:D:171:PRO:O     | 2.44                     | 0.46              |
| 6:S:115:LEU:HD22  | 6:S:128:ILE:HD12  | 1.98                     | 0.46              |
| 7:a:16:VAL:HG12   | 7:a:185:PRO:HA    | 1.98                     | 0.46              |
| 1:A:88:ALA:HB1    | 6:S:282:ALA:HB2   | 1.98                     | 0.46              |
| 7:a:543:HIS:CD2   | 19:a:840:CLA:NB   | 2.83                     | 0.46              |
| 7:a:711:PRO:HA    | 12:f:109:LEU:HD21 | 1.98                     | 0.46              |
| 19:a:802:CLA:H13  | 19:a:829:CLA:H18  | 1.97                     | 0.46              |
| 8:b:633:ASN:OD1   | 8:b:634:PRO:HD2   | 2.15                     | 0.46              |
| 19:b:814:CLA:HBB1 | 21:b:842:BCR:H323 | 1.96                     | 0.46              |
| 19:k:101:CLA:H3A  | 19:k:101:CLA:O2A  | 2.15                     | 0.46              |
| 6:S:187:ASP:OD1   | 6:S:187:ASP:N     | 2.35                     | 0.45              |
| 1:A:186:PHE:O     | 1:A:190:HIS:HB2   | 2.17                     | 0.45              |
| 1:A:283:ILE:HA    | 1:A:286:THR:HG22  | 1.98                     | 0.45              |
| 6:S:244:SER:HB2   | 6:S:249:ALA:HB1   | 1.98                     | 0.45              |
| 7:a:152:PHE:CE1   | 19:a:815:CLA:HED1 | 2.51                     | 0.45              |
| 7:a:177:TRP:HB2   | 19:a:812:CLA:HMC3 | 1.98                     | 0.45              |
| 8:b:568:SER:OG    | 8:b:571:ASP:OD1   | 2.31                     | 0.45              |
| 7:a:304:PHE:CE1   | 19:a:822:CLA:HAB  | 2.51                     | 0.45              |
| 19:a:808:CLA:H3A  | 19:a:808:CLA:HBA2 | 1.36                     | 0.45              |
| 19:b:837:CLA:CHA  | 19:b:837:CLA:HBA1 | 2.46                     | 0.45              |
| 2:D:196:PHE:HB3   | 2:D:281:MET:O     | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:a:366:VAL:HG13  | 7:a:370:MET:HE3   | 1.97                     | 0.45              |
| 7:a:389:LEU:HD11  | 19:a:830:CLA:HED3 | 1.98                     | 0.45              |
| 7:a:406:ALA:O     | 7:a:410:ILE:HG13  | 2.17                     | 0.45              |
| 8:b:708:ALA:HA    | 27:b:848:LMG:H392 | 1.99                     | 0.45              |
| 19:b:823:CLA:H162 | 19:b:823:CLA:H141 | 1.73                     | 0.45              |
| 15:k:48:MET:CE    | 15:k:59:LEU:HA    | 2.46                     | 0.45              |
| 1:A:20:TRP:O      | 1:A:26:ASN:ND2    | 2.44                     | 0.45              |
| 1:A:153:ALA:HB1   | 19:A:402:CLA:HED1 | 1.98                     | 0.45              |
| 20:A:404:PHO:H152 | 19:A:407:CLA:H151 | 1.99                     | 0.45              |
| 7:a:216:GLN:HA    | 7:a:220:SER:HB2   | 1.97                     | 0.45              |
| 7:a:456:ILE:HG22  | 19:a:835:CLA:HBC2 | 1.98                     | 0.45              |
| 19:a:818:CLA:C4D  | 19:a:818:CLA:H12  | 2.47                     | 0.45              |
| 19:a:824:CLA:H93  | 19:a:824:CLA:H112 | 1.76                     | 0.45              |
| 8:b:299:HIS:HB3   | 8:b:304:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:334:ARG:NH1   | 6:S:212:PRO:HG3   | 2.32                     | 0.45              |
| 7:a:100:TYR:OH    | 7:a:152:PHE:O     | 2.34                     | 0.45              |
| 7:a:113:SER:HB2   | 7:a:130:VAL:HG11  | 1.98                     | 0.45              |
| 19:a:839:CLA:HBA2 | 19:a:839:CLA:H3A  | 1.66                     | 0.45              |
| 8:b:440:VAL:HG21  | 19:b:832:CLA:HAC2 | 1.98                     | 0.45              |
| 19:b:837:CLA:H2   | 21:b:845:BCR:H352 | 1.99                     | 0.45              |
| 10:d:118:LYS:NZ   | 10:d:139:TYR:O    | 2.39                     | 0.45              |
| 10:d:121:ARG:N    | 10:d:124:GLN:OE1  | 2.46                     | 0.45              |
| 15:k:48:MET:HG3   | 15:k:54:PHE:CD2   | 2.51                     | 0.45              |
| 17:m:20:PHE:CZ    | 17:m:24:ARG:HD2   | 2.51                     | 0.45              |
| 7:a:159:TYR:O     | 7:a:163:ILE:HG12  | 2.16                     | 0.45              |
| 7:a:535:HIS:CD2   | 19:a:838:CLA:NB   | 2.85                     | 0.45              |
| 19:a:813:CLA:H71  | 19:a:813:CLA:H112 | 1.50                     | 0.45              |
| 1:A:210:LEU:HD12  | 20:D:401:PHO:NC   | 2.32                     | 0.45              |
| 21:A:406:BCR:H15C | 21:A:406:BCR:H351 | 1.87                     | 0.45              |
| 2:D:49:LEU:H      | 2:D:49:LEU:HD12   | 1.82                     | 0.45              |
| 19:b:818:CLA:H11  | 19:b:822:CLA:H11  | 1.97                     | 0.45              |
| 19:b:829:CLA:HED3 | 19:b:829:CLA:HBD  | 1.85                     | 0.45              |
| 21:b:842:BCR:H15C | 21:b:842:BCR:H351 | 1.86                     | 0.45              |
| 22:E:101:HEM:HBC2 | 22:E:101:HEM:CHD  | 2.47                     | 0.45              |
| 7:a:168:MET:HE3   | 7:a:168:MET:HB2   | 1.87                     | 0.45              |
| 7:a:429:MET:HG3   | 19:a:822:CLA:H192 | 1.99                     | 0.45              |
| 19:a:807:CLA:H42  | 19:a:831:CLA:H51  | 1.99                     | 0.45              |
| 19:a:829:CLA:H61  | 28:a:858:45D:H221 | 1.99                     | 0.45              |
| 28:a:858:45D:O01  | 21:f:202:BCR:H14C | 2.17                     | 0.45              |
| 8:b:48:ALA:HB3    | 17:m:29:LEU:HD21  | 1.99                     | 0.45              |
| 8:b:459:GLN:HG2   | 8:b:470:TYR:CZ    | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:b:828:CLA:H143 | 27:b:848:LMG:H272 | 1.98                     | 0.45              |
| 1:A:156:ALA:HA    | 1:A:160:ILE:HB    | 1.98                     | 0.45              |
| 7:a:348:TRP:HB3   | 19:a:806:CLA:HAC1 | 1.99                     | 0.45              |
| 7:a:434:ASP:OD1   | 7:a:555:TYR:OH    | 2.35                     | 0.45              |
| 19:a:839:CLA:HBB2 | 19:a:840:CLA:HBC3 | 1.99                     | 0.45              |
| 19:b:806:CLA:H93  | 19:b:806:CLA:H61  | 1.80                     | 0.45              |
| 21:i:101:BCR:H20C | 21:i:101:BCR:H361 | 1.85                     | 0.45              |
| 2:D:54:PHE:O      | 3:E:49:THR:OG1    | 2.32                     | 0.44              |
| 2:D:55:VAL:O      | 2:D:66:SER:HB2    | 2.17                     | 0.44              |
| 8:b:571:ASP:OD1   | 8:b:571:ASP:N     | 2.50                     | 0.44              |
| 15:k:30:LEU:HD12  | 15:k:31:ALA:N     | 2.33                     | 0.44              |
| 19:a:837:CLA:H193 | 19:a:837:CLA:H161 | 1.81                     | 0.44              |
| 19:a:857:CLA:H41  | 19:a:857:CLA:H62  | 1.41                     | 0.44              |
| 29:b:844:ECH:H36  | 29:b:844:ECH:H20  | 1.77                     | 0.44              |
| 19:j:103:CLA:H11  | 19:j:103:CLA:HBD  | 1.98                     | 0.44              |
| 4:F:42:ILE:HD12   | 4:F:43:GLN:HG3    | 1.99                     | 0.44              |
| 19:b:808:CLA:H142 | 27:b:848:LMG:H242 | 2.00                     | 0.44              |
| 1:A:331:MET:HB3   | 2:D:324:GLY:HA3   | 1.99                     | 0.44              |
| 5:I:6:ILE:O       | 5:I:10:ILE:HG23   | 2.18                     | 0.44              |
| 7:a:15:SER:HB2    | 7:a:186:LYS:HD2   | 1.99                     | 0.44              |
| 7:a:265:THR:HB    | 15:k:16:TRP:HB2   | 1.99                     | 0.44              |
| 19:b:831:CLA:H62  | 19:b:831:CLA:H2   | 1.74                     | 0.44              |
| 19:b:831:CLA:H202 | 19:b:831:CLA:H161 | 1.83                     | 0.44              |
| 19:b:832:CLA:HBA2 | 19:b:832:CLA:H3A  | 1.39                     | 0.44              |
| 1:A:85:SER:HB3    | 1:A:89:ILE:HD12   | 2.00                     | 0.44              |
| 19:a:827:CLA:CHB  | 19:a:840:CLA:HAA2 | 2.48                     | 0.44              |
| 19:a:840:CLA:H192 | 19:a:840:CLA:H161 | 1.77                     | 0.44              |
| 8:b:684:LEU:HD11  | 16:l:37:LEU:HD13  | 1.98                     | 0.44              |
| 19:b:806:CLA:HHB  | 19:b:807:CLA:HHB  | 1.99                     | 0.44              |
| 19:b:816:CLA:HBA2 | 19:b:825:CLA:HBB2 | 2.00                     | 0.44              |
| 19:b:839:CLA:H2   | 24:b:841:PQN:H243 | 1.98                     | 0.44              |
| 19:f:201:CLA:H141 | 19:f:201:CLA:H161 | 1.80                     | 0.44              |
| 7:a:342:GLU:O     | 7:a:346:THR:OG1   | 2.27                     | 0.44              |
| 19:a:834:CLA:HAA1 | 30:b:851:EQ3:C14  | 2.48                     | 0.44              |
| 19:a:836:CLA:H141 | 19:a:836:CLA:H161 | 1.85                     | 0.44              |
| 21:a:848:BCR:H15C | 21:a:848:BCR:H351 | 1.89                     | 0.44              |
| 8:b:714:TYR:CZ    | 19:b:801:CLA:HED1 | 2.53                     | 0.44              |
| 12:f:129:LEU:O    | 12:f:133:LYS:HG2  | 2.17                     | 0.44              |
| 12:f:130:ALA:O    | 12:f:134:MET:HG2  | 2.17                     | 0.44              |
| 14:j:28:GLU:HG3   | 19:j:103:CLA:C4C  | 2.47                     | 0.44              |
| 7:a:557:ARG:HE    | 7:a:557:ARG:HB3   | 1.66                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:a:809:CLA:H193 | 19:a:809:CLA:H161 | 1.83                     | 0.44              |
| 19:a:841:CLA:CHA  | 19:a:841:CLA:H11  | 2.47                     | 0.44              |
| 19:b:808:CLA:H162 | 19:b:808:CLA:H141 | 1.75                     | 0.44              |
| 19:b:820:CLA:H3A  | 19:b:820:CLA:HBA2 | 1.44                     | 0.44              |
| 10:d:87:ARG:HB2   | 10:d:97:LEU:HD11  | 2.00                     | 0.44              |
| 12:f:93:LEU:HG    | 21:f:202:BCR:H313 | 1.99                     | 0.44              |
| 4:F:36:ILE:O      | 4:F:39:MET:HB2    | 2.17                     | 0.44              |
| 6:S:72:ILE:HG13   | 6:S:85:LYS:HB3    | 1.99                     | 0.44              |
| 7:a:267:ASN:OD1   | 15:k:13:THR:OG1   | 2.35                     | 0.44              |
| 7:a:382:ASP:OD2   | 7:a:385:THR:OG1   | 2.34                     | 0.44              |
| 19:a:837:CLA:H122 | 19:a:837:CLA:H52  | 2.00                     | 0.44              |
| 8:b:22:TRP:CD1    | 8:b:701:GLN:HE22  | 2.36                     | 0.44              |
| 10:d:82:ASP:C     | 10:d:82:ASP:OD2   | 2.61                     | 0.44              |
| 1:A:206:PHE:CD2   | 20:D:401:PHO:HBB2 | 2.53                     | 0.44              |
| 6:S:152:ILE:HG12  | 6:S:158:ILE:HD12  | 2.00                     | 0.44              |
| 7:a:679:PHE:O     | 7:a:682:SER:OG    | 2.34                     | 0.44              |
| 19:a:810:CLA:HBB1 | 19:a:810:CLA:HMB3 | 1.99                     | 0.44              |
| 19:a:827:CLA:HBA2 | 19:a:827:CLA:H3A  | 1.78                     | 0.44              |
| 19:a:835:CLA:CHA  | 19:a:835:CLA:HBA1 | 2.47                     | 0.44              |
| 19:a:856:CLA:H193 | 21:b:846:BCR:H321 | 2.00                     | 0.44              |
| 8:b:66:PHE:HZ     | 17:m:8:ILE:HG23   | 1.82                     | 0.44              |
| 8:b:363:HIS:HB3   | 8:b:599:TRP:CZ3   | 2.53                     | 0.44              |
| 19:b:816:CLA:H62  | 19:b:816:CLA:H101 | 1.64                     | 0.44              |
| 16:l:37:LEU:HD22  | 19:l:203:CLA:HBD  | 1.99                     | 0.44              |
| 16:l:128:PHE:O    | 16:l:132:MET:HG2  | 2.17                     | 0.44              |
| 1:A:334:ARG:CG    | 1:A:335:ASN:H     | 2.31                     | 0.43              |
| 7:a:431:ARG:HD2   | 10:d:13:GLY:O     | 2.18                     | 0.43              |
| 19:a:813:CLA:H3A  | 19:a:813:CLA:HBA2 | 1.46                     | 0.43              |
| 21:a:847:BCR:H24C | 21:a:847:BCR:H371 | 1.81                     | 0.43              |
| 21:a:859:BCR:H331 | 19:j:103:CLA:O1D  | 2.18                     | 0.43              |
| 8:b:188:LEU:HG    | 19:b:814:CLA:HBB2 | 2.00                     | 0.43              |
| 1:A:118:HIS:HE1   | 19:A:405:CLA:C4D  | 2.31                     | 0.43              |
| 6:S:219:ARG:HD2   | 6:S:240:GLN:HG3   | 2.00                     | 0.43              |
| 7:a:296:HIS:HB2   | 19:a:819:CLA:C1B  | 2.48                     | 0.43              |
| 19:b:816:CLA:H62  | 19:b:816:CLA:H41  | 1.84                     | 0.43              |
| 15:k:48:MET:HE2   | 15:k:59:LEU:HA    | 1.99                     | 0.43              |
| 1:A:196:PRO:HA    | 1:A:199:MET:HE3   | 2.01                     | 0.43              |
| 2:D:81:PRO:HG3    | 2:D:112:PRO:HD3   | 2.00                     | 0.43              |
| 2:D:120:PHE:N     | 2:D:120:PHE:HD1   | 2.15                     | 0.43              |
| 6:S:242:GLN:NE2   | 6:S:253:SER:O     | 2.39                     | 0.43              |
| 7:a:239:PRO:HG2   | 19:a:815:CLA:O1D  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:a:269:GLY:O     | 7:a:272:SER:HB3   | 2.19                     | 0.43              |
| 19:a:819:CLA:H3A  | 19:a:819:CLA:HBA2 | 1.45                     | 0.43              |
| 19:b:823:CLA:H111 | 19:b:823:CLA:H72  | 1.84                     | 0.43              |
| 9:c:17:CYS:HB3    | 25:c:102:SF4:S4   | 2.59                     | 0.43              |
| 9:c:62:PHE:CE2    | 10:d:122:ILE:HD13 | 2.53                     | 0.43              |
| 12:f:85:GLY:HA2   | 12:f:89:ILE:HD12  | 2.00                     | 0.43              |
| 17:m:13:VAL:O     | 17:m:16:LEU:HB2   | 2.19                     | 0.43              |
| 7:a:475:ALA:O     | 7:a:477:GLN:HG3   | 2.18                     | 0.43              |
| 7:a:587:GLY:O     | 7:a:591:VAL:HG23  | 2.18                     | 0.43              |
| 19:a:815:CLA:H3A  | 19:a:815:CLA:HBA2 | 1.52                     | 0.43              |
| 19:a:837:CLA:H12  | 19:a:860:CLA:H11  | 2.01                     | 0.43              |
| 6:S:160:LYS:O     | 6:S:169:LYS:N     | 2.50                     | 0.43              |
| 7:a:440:LEU:HG    | 7:a:547:LEU:HB2   | 2.01                     | 0.43              |
| 8:b:4:LYS:NZ      | 13:i:39:GLU:OE2   | 2.35                     | 0.43              |
| 8:b:518:HIS:CD2   | 19:b:836:CLA:NB   | 2.87                     | 0.43              |
| 19:D:402:CLA:H62  | 19:D:402:CLA:H41  | 1.75                     | 0.43              |
| 7:a:200:HIS:O     | 7:a:204:LEU:HB3   | 2.18                     | 0.43              |
| 19:a:815:CLA:H52  | 19:a:815:CLA:H13  | 2.00                     | 0.43              |
| 8:b:339:LEU:HD12  | 8:b:339:LEU:HA    | 1.89                     | 0.43              |
| 16:l:93:THR:HG21  | 16:l:128:PHE:HB2  | 2.01                     | 0.43              |
| 19:A:405:CLA:H2   | 5:I:12:VAL:HG21   | 2.00                     | 0.43              |
| 7:a:120:ILE:HG23  | 7:a:121:VAL:HG22  | 2.00                     | 0.43              |
| 19:a:830:CLA:H41  | 19:a:830:CLA:H61  | 1.73                     | 0.43              |
| 19:b:814:CLA:CHA  | 19:b:814:CLA:HBA1 | 2.49                     | 0.43              |
| 21:b:845:BCR:H20C | 21:b:845:BCR:H361 | 1.86                     | 0.43              |
| 21:b:846:BCR:H20C | 21:b:846:BCR:H361 | 1.81                     | 0.43              |
| 12:f:99:GLY:HA3   | 12:f:140:TRP:CE2  | 2.54                     | 0.43              |
| 14:j:39:HIS:CD2   | 19:j:104:CLA:NB   | 2.86                     | 0.43              |
| 7:a:14:VAL:HG21   | 19:a:811:CLA:HAA2 | 2.00                     | 0.43              |
| 7:a:90:MET:SD     | 19:a:809:CLA:HAA2 | 2.59                     | 0.43              |
| 19:a:809:CLA:H143 | 19:a:809:CLA:H112 | 1.77                     | 0.43              |
| 19:a:824:CLA:H11  | 26:a:855:LHG:H211 | 2.00                     | 0.43              |
| 19:a:835:CLA:H93  | 19:a:835:CLA:H61  | 1.82                     | 0.43              |
| 19:b:807:CLA:H51  | 19:b:807:CLA:H8   | 1.82                     | 0.43              |
| 19:b:829:CLA:H3A  | 19:b:830:CLA:OBD  | 2.19                     | 0.43              |
| 29:b:844:ECH:H21  | 29:b:844:ECH:H24  | 1.76                     | 0.43              |
| 19:k:102:CLA:HAB  | 21:k:103:BCR:H381 | 2.01                     | 0.43              |
| 2:D:72:ASN:N      | 2:D:75:THR:OG1    | 2.52                     | 0.43              |
| 3:E:35:TRP:O      | 3:E:39:SER:OG     | 2.27                     | 0.43              |
| 7:a:497:THR:HG21  | 19:a:836:CLA:CMD  | 2.49                     | 0.43              |
| 7:a:646:LEU:HD22  | 8:b:648:LEU:HD21  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:a:830:CLA:O1A  | 19:a:830:CLA:H2   | 2.19                     | 0.43              |
| 19:a:857:CLA:H3A  | 19:a:857:CLA:HBA2 | 1.64                     | 0.43              |
| 11:e:68:LEU:HD12  | 11:e:69:VAL:N     | 2.34                     | 0.43              |
| 12:f:70:GLU:OE1   | 12:f:70:GLU:N     | 2.48                     | 0.43              |
| 19:a:842:CLA:H152 | 14:j:19:LEU:HB3   | 2.01                     | 0.43              |
| 19:b:819:CLA:H141 | 19:b:819:CLA:H161 | 1.77                     | 0.43              |
| 19:b:819:CLA:CBB  | 21:b:842:BCR:H14C | 2.41                     | 0.43              |
| 11:e:12:LYS:HD3   | 11:e:67:GLU:OE1   | 2.19                     | 0.43              |
| 7:a:426:LEU:O     | 7:a:429:MET:HB2   | 2.18                     | 0.42              |
| 7:a:536:HIS:CD2   | 19:a:839:CLA:NB   | 2.86                     | 0.42              |
| 19:a:806:CLA:HBC2 | 19:a:831:CLA:HMA1 | 2.01                     | 0.42              |
| 19:a:829:CLA:H141 | 19:a:829:CLA:H162 | 1.85                     | 0.42              |
| 19:a:841:CLA:HBA2 | 19:a:841:CLA:H3A  | 1.82                     | 0.42              |
| 8:b:701:GLN:HB2   | 27:b:848:LMG:H111 | 2.01                     | 0.42              |
| 31:b:852:ZEX:H182 | 31:b:852:ZEX:H8   | 2.01                     | 0.42              |
| 7:a:115:GLN:HB3   | 7:a:137:ILE:HB    | 2.01                     | 0.42              |
| 21:a:849:BCR:H20C | 21:a:849:BCR:H361 | 1.83                     | 0.42              |
| 8:b:178:HIS:CD2   | 19:b:812:CLA:NB   | 2.87                     | 0.42              |
| 19:b:831:CLA:H112 | 19:b:831:CLA:H143 | 1.81                     | 0.42              |
| 19:b:836:CLA:H62  | 19:b:836:CLA:H41  | 1.61                     | 0.42              |
| 21:b:845:BCR:H11C | 21:b:845:BCR:H341 | 1.90                     | 0.42              |
| 1:A:89:ILE:HG12   | 6:S:264:TRP:HZ3   | 1.84                     | 0.42              |
| 7:a:457:HIS:HE1   | 19:a:835:CLA:CHA  | 2.33                     | 0.42              |
| 19:a:808:CLA:H91  | 19:a:808:CLA:H112 | 1.65                     | 0.42              |
| 19:a:836:CLA:H42  | 21:a:850:BCR:H392 | 2.02                     | 0.42              |
| 19:a:841:CLA:H162 | 19:a:841:CLA:H141 | 1.78                     | 0.42              |
| 21:a:850:BCR:H15C | 21:a:850:BCR:H351 | 1.84                     | 0.42              |
| 8:b:30:ASP:HB2    | 19:b:828:CLA:HAA1 | 2.02                     | 0.42              |
| 19:b:826:CLA:H3A  | 19:b:826:CLA:HBA2 | 1.39                     | 0.42              |
| 19:b:827:CLA:H141 | 19:b:827:CLA:H162 | 1.79                     | 0.42              |
| 19:b:838:CLA:HBB2 | 24:b:841:PQN:H141 | 2.02                     | 0.42              |
| 19:f:201:CLA:H61  | 19:f:201:CLA:H41  | 1.53                     | 0.42              |
| 1:A:87:ASN:HD21   | 6:S:237:ARG:NE    | 2.17                     | 0.42              |
| 19:a:820:CLA:HBA2 | 19:a:820:CLA:H3A  | 1.46                     | 0.42              |
| 8:b:525:HIS:HE1   | 19:b:837:CLA:C4D  | 2.32                     | 0.42              |
| 7:a:432:HIS:CD2   | 19:a:832:CLA:C4A  | 3.03                     | 0.42              |
| 19:a:805:CLA:HHC  | 19:a:807:CLA:OBD  | 2.20                     | 0.42              |
| 19:a:821:CLA:H3A  | 19:a:821:CLA:HBA2 | 1.71                     | 0.42              |
| 19:a:843:CLA:H71  | 26:a:855:LHG:H311 | 2.01                     | 0.42              |
| 8:b:183:PHE:HE1   | 19:b:812:CLA:H52  | 1.84                     | 0.42              |
| 19:b:814:CLA:HBD  | 19:b:814:CLA:HED2 | 1.73                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:b:828:CLA:H8   | 27:b:848:LMG:H211 | 2.01                     | 0.42              |
| 19:b:828:CLA:H141 | 19:b:828:CLA:H162 | 1.82                     | 0.42              |
| 19:b:835:CLA:H12  | 19:b:835:CLA:H51  | 1.70                     | 0.42              |
| 9:c:62:PHE:HD2    | 10:d:122:ILE:HG21 | 1.84                     | 0.42              |
| 10:d:22:ALA:HA    | 10:d:26:GLU:O     | 2.19                     | 0.42              |
| 10:d:139:TYR:CE1  | 10:d:140:GLU:HG3  | 2.54                     | 0.42              |
| 11:e:18:TRP:HB3   | 11:e:21:ASP:HB2   | 2.01                     | 0.42              |
| 14:j:26:LEU:HD13  | 21:j:101:BCR:HC7  | 2.02                     | 0.42              |
| 19:l:203:CLA:H192 | 19:l:203:CLA:H162 | 1.86                     | 0.42              |
| 2:D:286:ILE:HD13  | 2:D:289:LEU:HD12  | 2.00                     | 0.42              |
| 6:S:65:LEU:HD23   | 6:S:82:TRP:CH2    | 2.54                     | 0.42              |
| 7:a:656:ASN:OD1   | 7:a:746:ARG:NH1   | 2.45                     | 0.42              |
| 19:a:813:CLA:H93  | 19:a:813:CLA:H61  | 1.73                     | 0.42              |
| 19:a:837:CLA:H61  | 19:a:837:CLA:H41  | 1.90                     | 0.42              |
| 8:b:293:THR:H     | 19:b:819:CLA:HED2 | 1.84                     | 0.42              |
| 8:b:544:MET:HE3   | 8:b:544:MET:HB2   | 1.91                     | 0.42              |
| 19:b:805:CLA:H41  | 19:b:805:CLA:H61  | 1.76                     | 0.42              |
| 19:b:812:CLA:H62  | 19:b:812:CLA:H2   | 1.64                     | 0.42              |
| 1:A:32:TRP:CD2    | 5:I:22:GLY:HA3    | 2.54                     | 0.42              |
| 7:a:331:PRO:HB3   | 16:l:5:ASN:HB3    | 2.02                     | 0.42              |
| 7:a:543:HIS:HE1   | 19:a:840:CLA:C4D  | 2.32                     | 0.42              |
| 7:a:583:CYS:HB3   | 8:b:664:TRP:HE3   | 1.85                     | 0.42              |
| 8:b:490:TRP:CG    | 19:b:816:CLA:H42  | 2.54                     | 0.42              |
| 19:b:821:CLA:CHA  | 19:b:821:CLA:HBA1 | 2.50                     | 0.42              |
| 12:f:94:PHE:HB2   | 21:f:202:BCR:H321 | 2.01                     | 0.42              |
| 1:A:172:MET:HG3   | 1:A:182:PHE:CD2   | 2.55                     | 0.42              |
| 21:A:406:BCR:H11C | 21:A:406:BCR:H341 | 1.93                     | 0.42              |
| 7:a:692:TYR:CE1   | 8:b:533:LYS:HD2   | 2.55                     | 0.42              |
| 8:b:59:LEU:HD12   | 29:m:101:ECH:H37A | 2.02                     | 0.42              |
| 31:b:852:ZEX:H25  | 14:j:40:PRO:HD2   | 2.02                     | 0.42              |
| 19:j:103:CLA:H3A  | 19:j:103:CLA:HBA2 | 1.57                     | 0.42              |
| 1:A:72:LEU:HD23   | 1:A:72:LEU:HA     | 1.90                     | 0.42              |
| 6:S:216:ASN:OD1   | 6:S:252:TRP:NE1   | 2.52                     | 0.42              |
| 7:a:384:ALA:HA    | 7:a:747:SER:HB2   | 2.02                     | 0.42              |
| 19:b:806:CLA:HBA2 | 19:b:806:CLA:H3A  | 1.76                     | 0.42              |
| 19:b:807:CLA:H142 | 19:b:807:CLA:H111 | 1.93                     | 0.42              |
| 1:A:267:ASN:HB3   | 1:A:270:SER:HB3   | 2.02                     | 0.42              |
| 19:A:403:CLA:HBA2 | 19:A:403:CLA:H3A  | 1.45                     | 0.42              |
| 19:A:403:CLA:CHC  | 19:D:402:CLA:H2   | 2.50                     | 0.42              |
| 6:S:312:VAL:HG22  | 6:S:322:VAL:HG22  | 2.01                     | 0.42              |
| 7:a:42:PRO:HB3    | 7:a:47:TRP:CD2    | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:a:509:PHE:CE1   | 19:a:828:CLA:HBC2 | 2.55                     | 0.42              |
| 19:a:814:CLA:H122 | 19:a:814:CLA:H161 | 1.76                     | 0.42              |
| 19:a:824:CLA:H92  | 19:a:824:CLA:H61  | 1.82                     | 0.42              |
| 19:a:832:CLA:H62  | 19:a:832:CLA:H41  | 1.81                     | 0.42              |
| 8:b:69:ALA:HB2    | 8:b:135:LEU:HB3   | 2.01                     | 0.42              |
| 8:b:182:LEU:HD13  | 19:b:812:CLA:HBB  | 2.01                     | 0.42              |
| 19:b:801:CLA:H143 | 19:b:801:CLA:H111 | 1.85                     | 0.42              |
| 19:b:804:CLA:H2   | 19:b:804:CLA:H61  | 1.87                     | 0.42              |
| 10:d:136:LYS:HA   | 10:d:136:LYS:HD3  | 1.78                     | 0.42              |
| 12:f:38:TYR:O     | 12:f:42:SER:HB2   | 2.19                     | 0.42              |
| 1:A:186:PHE:CE1   | 1:A:293:MET:HG2   | 2.55                     | 0.41              |
| 2:D:189:HIS:ND1   | 2:D:289:LEU:HD22  | 2.35                     | 0.41              |
| 3:E:43:ALA:O      | 3:E:47:PHE:HD1    | 2.03                     | 0.41              |
| 7:a:215:HIS:HE1   | 19:a:815:CLA:C1A  | 2.18                     | 0.41              |
| 7:a:412:MET:HE2   | 7:a:412:MET:HB2   | 1.90                     | 0.41              |
| 19:a:809:CLA:H62  | 19:a:809:CLA:H102 | 1.83                     | 0.41              |
| 19:a:821:CLA:H91  | 19:a:821:CLA:H111 | 1.82                     | 0.41              |
| 31:b:852:ZEX:H11  | 31:b:852:ZEX:H191 | 1.88                     | 0.41              |
| 26:f:206:LHG:H122 | 26:f:206:LHG:HC92 | 1.78                     | 0.41              |
| 3:E:51:ARG:HB2    | 3:E:53:ASP:OD1    | 2.20                     | 0.41              |
| 6:S:269:LEU:HD21  | 6:S:271:PHE:HE1   | 1.85                     | 0.41              |
| 19:a:822:CLA:C4A  | 19:a:822:CLA:HBA2 | 2.50                     | 0.41              |
| 19:a:831:CLA:H122 | 19:a:831:CLA:H161 | 1.92                     | 0.41              |
| 8:b:420:LEU:HD13  | 19:b:837:CLA:HBB1 | 2.01                     | 0.41              |
| 8:b:590:TYR:HA    | 8:b:616:TRP:HH2   | 1.85                     | 0.41              |
| 19:b:819:CLA:HBA2 | 19:b:819:CLA:H3A  | 1.41                     | 0.41              |
| 19:b:838:CLA:H41  | 19:b:838:CLA:H61  | 1.84                     | 0.41              |
| 27:l:201:LMG:H322 | 27:l:201:LMG:H291 | 1.82                     | 0.41              |
| 1:A:170:ASP:OD1   | 6:S:220:ARG:NH2   | 2.53                     | 0.41              |
| 7:a:429:MET:SD    | 19:a:832:CLA:HBC3 | 2.60                     | 0.41              |
| 19:a:807:CLA:H161 | 19:a:807:CLA:H193 | 1.82                     | 0.41              |
| 8:b:225:PHE:HB2   | 8:b:233:TYR:HE2   | 1.85                     | 0.41              |
| 19:b:833:CLA:H3A  | 19:b:833:CLA:HBA2 | 1.45                     | 0.41              |
| 6:S:73:PHE:CZ     | 6:S:84:GLN:HB2    | 2.55                     | 0.41              |
| 19:a:809:CLA:H152 | 21:j:101:BCR:H402 | 2.01                     | 0.41              |
| 19:a:827:CLA:HMB1 | 19:a:840:CLA:HBA1 | 2.02                     | 0.41              |
| 19:a:840:CLA:H2A  | 19:a:840:CLA:O2D  | 2.20                     | 0.41              |
| 21:a:859:BCR:H15C | 21:a:859:BCR:H351 | 1.87                     | 0.41              |
| 8:b:270:LEU:HD23  | 8:b:270:LEU:HA    | 1.92                     | 0.41              |
| 8:b:320:LEU:HD23  | 8:b:320:LEU:HA    | 1.90                     | 0.41              |
| 8:b:628:LEU:HD22  | 8:b:721:PHE:HA    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:f:202:BCR:H20C | 21:f:202:BCR:H361 | 1.89                     | 0.41              |
| 21:i:101:BCR:H15C | 21:i:101:BCR:H351 | 1.96                     | 0.41              |
| 14:j:16:MET:HE3   | 14:j:16:MET:HB3   | 1.96                     | 0.41              |
| 2:D:128:ARG:O     | 2:D:131:GLU:HG3   | 2.20                     | 0.41              |
| 7:a:120:ILE:HG12  | 14:j:27:ILE:HG23  | 2.02                     | 0.41              |
| 8:b:637:VAL:HG13  | 8:b:641:SER:HB2   | 2.03                     | 0.41              |
| 19:b:807:CLA:CGA  | 19:b:807:CLA:C1A  | 2.99                     | 0.41              |
| 19:b:813:CLA:H72  | 19:b:813:CLA:H112 | 1.47                     | 0.41              |
| 10:d:120:ARG:NH2  | 10:d:141:VAL:O    | 2.48                     | 0.41              |
| 29:m:101:ECH:H11  | 29:m:101:ECH:H34  | 1.91                     | 0.41              |
| 2:D:329:MET:SD    | 2:D:329:MET:N     | 2.93                     | 0.41              |
| 6:S:105:GLU:CD    | 6:S:147:GLN:H     | 2.29                     | 0.41              |
| 7:a:31:PRO:HB2    | 7:a:51:LEU:HD11   | 2.03                     | 0.41              |
| 7:a:49:TRP:CG     | 7:a:722:GLN:HE22  | 2.38                     | 0.41              |
| 7:a:296:HIS:HB2   | 19:a:819:CLA:CHB  | 2.50                     | 0.41              |
| 7:a:337:HIS:HE1   | 26:a:853:LHG:HC12 | 1.86                     | 0.41              |
| 19:a:826:CLA:H141 | 19:a:826:CLA:H161 | 1.74                     | 0.41              |
| 21:a:848:BCR:H361 | 21:a:848:BCR:H20C | 1.82                     | 0.41              |
| 8:b:193:HIS:HB2   | 19:b:813:CLA:C1C  | 2.51                     | 0.41              |
| 8:b:338:SER:O     | 8:b:342:ILE:HG12  | 2.21                     | 0.41              |
| 19:b:807:CLA:H11  | 19:b:807:CLA:C4D  | 2.50                     | 0.41              |
| 19:b:822:CLA:HMD3 | 19:b:823:CLA:HHC  | 2.03                     | 0.41              |
| 31:f:205:ZEX:H11  | 31:f:205:ZEX:H191 | 1.87                     | 0.41              |
| 1:A:335:ASN:ND2   | 6:S:210:TRP:H     | 2.18                     | 0.41              |
| 6:S:57:THR:OG1    | 6:S:58:GLU:N      | 2.53                     | 0.41              |
| 7:a:576:GLY:HA2   | 8:b:559:PRO:HD3   | 2.02                     | 0.41              |
| 8:b:14:GLN:NE2    | 9:c:71:ALA:HB1    | 2.35                     | 0.41              |
| 8:b:230:TRP:CZ3   | 19:b:815:CLA:H92  | 2.55                     | 0.41              |
| 19:b:803:CLA:H62  | 19:b:803:CLA:H2   | 1.69                     | 0.41              |
| 19:b:809:CLA:HBA1 | 19:b:809:CLA:H3A  | 1.79                     | 0.41              |
| 19:a:809:CLA:HBB2 | 19:a:829:CLA:H142 | 2.03                     | 0.41              |
| 19:a:833:CLA:H61  | 19:a:833:CLA:H41  | 1.84                     | 0.41              |
| 19:b:837:CLA:HBA2 | 19:b:837:CLA:H11  | 1.63                     | 0.41              |
| 1:A:212:SER:OG    | 2:D:271:MET:O     | 2.36                     | 0.41              |
| 19:A:407:CLA:H92  | 19:A:407:CLA:H62  | 1.78                     | 0.41              |
| 2:D:201:VAL:HG22  | 19:D:402:CLA:C2B  | 2.50                     | 0.41              |
| 7:a:175:ALA:HB2   | 19:a:811:CLA:HBC2 | 2.03                     | 0.41              |
| 19:a:807:CLA:H62  | 19:a:807:CLA:H41  | 1.56                     | 0.41              |
| 19:a:823:CLA:H141 | 19:a:837:CLA:H91  | 2.03                     | 0.41              |
| 21:a:846:BCR:H15C | 21:a:846:BCR:H351 | 1.88                     | 0.41              |
| 21:a:849:BCR:H351 | 21:a:849:BCR:H15C | 1.83                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:b:174:ARG:HB2   | 19:b:812:CLA:HBC2 | 2.02                     | 0.41              |
| 12:f:140:TRP:CD1  | 12:f:141:PRO:HD3  | 2.55                     | 0.41              |
| 12:f:156:LYS:HB2  | 12:f:159:GLU:HG2  | 2.03                     | 0.41              |
| 15:k:20:VAL:HG13  | 15:k:77:ILE:HD13  | 2.01                     | 0.41              |
| 21:l:205:BCR:H20C | 21:l:205:BCR:H361 | 1.93                     | 0.41              |
| 19:A:402:CLA:H203 | 19:A:402:CLA:H161 | 1.83                     | 0.41              |
| 2:D:56:THR:OG1    | 2:D:57:SER:N      | 2.54                     | 0.41              |
| 2:D:95:PRO:O      | 2:D:98:GLN:NE2    | 2.54                     | 0.41              |
| 6:S:141:ILE:HB    | 6:S:151:MET:HE1   | 2.03                     | 0.41              |
| 7:a:84:PHE:HB3    | 7:a:169:ALA:HB2   | 2.03                     | 0.41              |
| 7:a:141:SER:HA    | 19:a:829:CLA:HMA2 | 2.02                     | 0.41              |
| 8:b:387:HIS:HE1   | 19:b:828:CLA:C4A  | 2.32                     | 0.41              |
| 19:b:801:CLA:H62  | 19:b:801:CLA:H41  | 1.92                     | 0.41              |
| 12:f:78:ASP:OD2   | 12:f:80:ARG:NE    | 2.40                     | 0.41              |
| 12:f:140:TRP:CG   | 12:f:141:PRO:HD3  | 2.56                     | 0.41              |
| 21:l:205:BCR:H371 | 21:l:205:BCR:H24C | 1.88                     | 0.41              |
| 19:A:405:CLA:HBA2 | 19:A:405:CLA:H3A  | 1.27                     | 0.40              |
| 6:S:77:ASP:OD1    | 6:S:77:ASP:N      | 2.42                     | 0.40              |
| 7:a:439:HIS:HE1   | 19:a:833:CLA:NA   | 2.18                     | 0.40              |
| 19:a:805:CLA:H142 | 19:a:805:CLA:H112 | 1.91                     | 0.40              |
| 19:a:832:CLA:H92  | 26:a:853:LHG:H121 | 2.04                     | 0.40              |
| 19:a:832:CLA:HMC3 | 19:a:840:CLA:HAB  | 2.03                     | 0.40              |
| 9:c:21:CYS:HA     | 25:c:101:SF4:S4   | 2.61                     | 0.40              |
| 15:k:27:CYS:HA    | 15:k:30:LEU:HG    | 2.03                     | 0.40              |
| 29:m:101:ECH:H36  | 29:m:101:ECH:H20  | 1.84                     | 0.40              |
| 6:S:45:LEU:N      | 6:S:327:GLY:O     | 2.54                     | 0.40              |
| 6:S:234:LEU:HG    | 6:S:242:GLN:HB3   | 2.02                     | 0.40              |
| 23:a:801:CL0:NA   | 19:b:801:CLA:HAB  | 2.36                     | 0.40              |
| 19:a:820:CLA:H92  | 19:a:830:CLA:H91  | 2.02                     | 0.40              |
| 8:b:348:GLN:HG3   | 19:b:824:CLA:HED1 | 2.03                     | 0.40              |
| 19:b:836:CLA:HBA2 | 19:b:836:CLA:H3A  | 1.75                     | 0.40              |
| 1:A:331:MET:SD    | 1:A:331:MET:N     | 2.94                     | 0.40              |
| 2:D:50:THR:HA     | 2:D:53:THR:HG22   | 2.04                     | 0.40              |
| 7:a:312:ARG:HD3   | 7:a:316:GLY:HA2   | 2.03                     | 0.40              |
| 7:a:530:ALA:O     | 7:a:534:VAL:HG23  | 2.21                     | 0.40              |
| 7:a:689:GLY:HA3   | 8:b:566:ASP:HB2   | 2.04                     | 0.40              |
| 19:a:805:CLA:H43  | 19:a:812:CLA:CHC  | 2.51                     | 0.40              |
| 19:b:828:CLA:H142 | 19:b:828:CLA:H111 | 1.79                     | 0.40              |
| 19:b:834:CLA:H3A  | 19:b:834:CLA:HBA2 | 1.48                     | 0.40              |
| 19:A:403:CLA:HBC3 | 2:D:178:ILE:HG23  | 2.02                     | 0.40              |
| 2:D:283:SER:O     | 2:D:287:VAL:HG23  | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:S:58:GLU:HB2    | 6:S:61:ASN:HB2    | 2.03                     | 0.40              |
| 19:a:822:CLA:HBA1 | 19:a:826:CLA:C3B  | 2.52                     | 0.40              |
| 19:a:839:CLA:H141 | 19:a:839:CLA:H161 | 1.72                     | 0.40              |
| 21:a:846:BCR:H11C | 21:a:846:BCR:H341 | 1.95                     | 0.40              |
| 8:b:694:PRO:HB3   | 19:b:838:CLA:C1C  | 2.51                     | 0.40              |
| 21:f:202:BCR:H11C | 21:f:202:BCR:H341 | 1.96                     | 0.40              |
| 19:l:203:CLA:H61  | 19:l:203:CLA:H41  | 1.95                     | 0.40              |
| 1:A:43:THR:HG23   | 21:A:406:BCR:H362 | 2.04                     | 0.40              |
| 7:a:106:ASP:HB3   | 7:a:110:ILE:HD12  | 2.04                     | 0.40              |
| 7:a:425:LEU:HD23  | 7:a:425:LEU:HA    | 1.88                     | 0.40              |
| 7:a:514:ILE:HD13  | 7:a:514:ILE:HA    | 1.91                     | 0.40              |
| 7:a:733:LEU:HD22  | 19:a:842:CLA:HMA3 | 2.03                     | 0.40              |
| 8:b:178:HIS:O     | 8:b:182:LEU:HB3   | 2.21                     | 0.40              |
| 8:b:257:PHE:CD2   | 8:b:490:TRP:HB3   | 2.56                     | 0.40              |
| 19:b:816:CLA:H111 | 19:b:816:CLA:H91  | 1.87                     | 0.40              |
| 19:b:816:CLA:H162 | 19:b:816:CLA:H141 | 1.89                     | 0.40              |
| 19:b:818:CLA:H41  | 19:b:818:CLA:H61  | 1.83                     | 0.40              |
| 19:b:832:CLA:H12  | 19:b:832:CLA:HBA1 | 1.70                     | 0.40              |
| 19:b:836:CLA:H162 | 19:b:836:CLA:H141 | 1.72                     | 0.40              |
| 13:i:15:ILE:O     | 13:i:19:GLY:N     | 2.54                     | 0.40              |
| 13:i:31:PHE:CZ    | 16:l:102:VAL:HG21 | 2.56                     | 0.40              |
| 27:l:201:LMG:H291 | 27:l:201:LMG:H341 | 2.03                     | 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     | 286/344 (83%) | 278 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 2   | D     | 274/336 (82%) | 264 (96%) | 10 (4%) | 0        | 100         | 100 |
| 3   | E     | 35/81 (43%)   | 33 (94%)  | 2 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 4   | F     | 26/44 (59%)     | 26 (100%)  | 0       | 0        | 100         | 100 |
| 5   | I     | 27/38 (71%)     | 26 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 6   | S     | 301/342 (88%)   | 292 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 7   | a     | 739/751 (98%)   | 715 (97%)  | 24 (3%) | 0        | 100         | 100 |
| 8   | b     | 727/731 (100%)  | 707 (97%)  | 20 (3%) | 0        | 100         | 100 |
| 9   | c     | 78/81 (96%)     | 74 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 10  | d     | 137/141 (97%)   | 134 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 11  | e     | 67/74 (90%)     | 63 (94%)   | 4 (6%)  | 0        | 100         | 100 |
| 12  | f     | 140/165 (85%)   | 135 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 13  | i     | 38/40 (95%)     | 37 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 14  | j     | 38/40 (95%)     | 38 (100%)  | 0       | 0        | 100         | 100 |
| 15  | k     | 73/86 (85%)     | 72 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 16  | l     | 141/157 (90%)   | 137 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 17  | m     | 29/31 (94%)     | 29 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 3156/3482 (91%) | 3060 (97%) | 96 (3%) | 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     | 236/283 (83%) | 235 (100%) | 1 (0%)   | 84          | 86  |
| 2   | D     | 220/271 (81%) | 220 (100%) | 0        | 100         | 100 |
| 3   | E     | 31/73 (42%)   | 31 (100%)  | 0        | 100         | 100 |
| 4   | F     | 22/37 (60%)   | 22 (100%)  | 0        | 100         | 100 |
| 5   | I     | 26/34 (76%)   | 26 (100%)  | 0        | 100         | 100 |
| 6   | S     | 239/279 (86%) | 239 (100%) | 0        | 100         | 100 |
| 7   | a     | 593/603 (98%) | 592 (100%) | 1 (0%)   | 87          | 89  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 8   | b     | 582/583 (100%)  | 581 (100%)  | 1 (0%)   | 87          | 89  |
| 9   | c     | 68/69 (99%)     | 68 (100%)   | 0        | 100         | 100 |
| 10  | d     | 114/116 (98%)   | 114 (100%)  | 0        | 100         | 100 |
| 11  | e     | 57/60 (95%)     | 57 (100%)   | 0        | 100         | 100 |
| 12  | f     | 119/137 (87%)   | 119 (100%)  | 0        | 100         | 100 |
| 13  | i     | 32/32 (100%)    | 32 (100%)   | 0        | 100         | 100 |
| 14  | j     | 35/35 (100%)    | 35 (100%)   | 0        | 100         | 100 |
| 15  | k     | 53/62 (86%)     | 52 (98%)    | 1 (2%)   | 50          | 73  |
| 16  | l     | 107/118 (91%)   | 107 (100%)  | 0        | 100         | 100 |
| 17  | m     | 25/25 (100%)    | 25 (100%)   | 0        | 100         | 100 |
| All | All   | 2559/2817 (91%) | 2555 (100%) | 4 (0%)   | 85          | 89  |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 91  | LEU  |
| 7   | a     | 90  | MET  |
| 8   | b     | 129 | MET  |
| 15  | k     | 72  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | ASN  |
| 2   | D     | 129 | GLN  |
| 6   | S     | 123 | GLN  |
| 6   | S     | 213 | HIS  |
| 7   | a     | 19  | ASN  |
| 7   | a     | 54  | ASN  |
| 7   | a     | 216 | GLN  |
| 7   | a     | 224 | ASN  |
| 7   | a     | 379 | GLN  |
| 7   | a     | 386 | GLN  |
| 8   | b     | 41  | ASN  |
| 8   | b     | 366 | GLN  |
| 8   | b     | 478 | ASN  |
| 9   | c     | 16  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | k     | 82  | ASN  |
| 16  | l     | 6   | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 1 is monoatomic - leaving 145 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | CLA  | l     | 204 | -    | 56,60,73     | 1.29 | 9 (16%)  | 65,97,113   | 1.37 | 5 (7%)   |
| 21  | BCR  | a     | 849 | -    | 41,41,41     | 1.19 | 3 (7%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 19  | CLA  | a     | 812 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 19  | CLA  | a     | 834 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 21  | BCR  | k     | 103 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.28 | 5 (8%)   |
| 21  | BCR  | b     | 842 | -    | 41,41,41     | 1.21 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 31  | ZEX  | b     | 852 | -    | 43,43,43     | 1.33 | 8 (18%)  | 51,60,60    | 1.44 | 10 (19%) |
| 19  | CLA  | a     | 815 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 19  | CLA  | a     | 843 | 26   | 60,64,73     | 1.24 | 9 (15%)  | 71,102,113  | 1.35 | 7 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | CLA  | b     | 819 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 21  | BCR  | b     | 845 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.31 | 6 (10%)  |
| 19  | CLA  | a     | 805 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 26  | LHG  | b     | 849 | 19   | 37,37,48     | 0.72 | 1 (2%)   | 40,43,54    | 1.25 | 4 (10%)  |
| 19  | CLA  | a     | 804 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 4 (4%)   |
| 19  | CLA  | b     | 824 | -    | 59,63,73     | 1.25 | 9 (15%)  | 70,101,113  | 1.36 | 6 (8%)   |
| 19  | CLA  | b     | 838 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 19  | CLA  | b     | 804 | -    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.32 | 7 (8%)   |
| 19  | CLA  | b     | 829 | -    | 55,59,73     | 1.30 | 8 (14%)  | 64,96,113   | 1.38 | 6 (9%)   |
| 21  | BCR  | a     | 848 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 19  | CLA  | b     | 805 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 21  | BCR  | f     | 202 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 21  | BCR  | i     | 101 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 22  | HEM  | E     | 101 | 3,4  | 50,50,50     | 1.52 | 7 (14%)  | 67,82,82    | 1.09 | 2 (2%)   |
| 21  | BCR  | a     | 850 | -    | 41,41,41     | 1.21 | 3 (7%)   | 56,56,56    | 1.27 | 6 (10%)  |
| 19  | CLA  | a     | 829 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 19  | CLA  | b     | 835 | -    | 56,60,73     | 1.28 | 9 (16%)  | 65,97,113   | 1.41 | 9 (13%)  |
| 19  | CLA  | a     | 817 | -    | 50,54,73     | 1.35 | 8 (16%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 21  | BCR  | a     | 846 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.24 | 7 (12%)  |
| 19  | CLA  | f     | 203 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.37 | 6 (9%)   |
| 27  | LMG  | b     | 850 | -    | 55,55,55     | 0.78 | 1 (1%)   | 63,63,63    | 1.34 | 9 (14%)  |
| 19  | CLA  | a     | 810 | 7    | 55,59,73     | 1.29 | 8 (14%)  | 64,96,113   | 1.43 | 8 (12%)  |
| 19  | CLA  | b     | 821 | -    | 50,54,73     | 1.34 | 9 (18%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 19  | CLA  | a     | 833 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.29 | 6 (7%)   |
| 19  | CLA  | b     | 813 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 19  | CLA  | l     | 203 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 19  | CLA  | b     | 832 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 19  | CLA  | b     | 839 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 25  | SF4  | c     | 101 | 9    | 0,12,12      | -    | -        | -           | -    | -        |
| 19  | CLA  | a     | 808 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 19  | CLA  | b     | 812 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 19  | CLA  | a     | 826 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 19  | CLA  | b     | 820 | -    | 64,68,73     | 1.20 | 9 (14%)  | 76,107,113  | 1.30 | 5 (6%)   |
| 24  | PQN  | a     | 844 | -    | 34,34,34     | 0.39 | 0        | 43,45,45    | 0.58 | 1 (2%)   |
| 26  | LHG  | a     | 853 | 19   | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.29 | 6 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | CLA  | b     | 802 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 19  | CLA  | a     | 860 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 19  | CLA  | a     | 814 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.32 | 8 (9%)   |
| 21  | BCR  | a     | 847 | -    | 41,41,41     | 1.19 | 2 (4%)   | 56,56,56    | 1.23 | 5 (8%)   |
| 19  | CLA  | f     | 204 | 12   | 54,58,73     | 1.32 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 19  | CLA  | b     | 801 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.21 | 5 (6%)   |
| 21  | BCR  | b     | 846 | -    | 41,41,41     | 1.17 | 2 (4%)   | 56,56,56    | 1.17 | 5 (8%)   |
| 23  | CL0  | a     | 801 | -    | 58,73,73     | 2.21 | 11 (18%) | 60,113,113  | 1.65 | 14 (23%) |
| 19  | CLA  | A     | 407 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 4 (4%)   |
| 19  | CLA  | D     | 403 | -    | 50,54,73     | 1.36 | 8 (16%)  | 59,90,113   | 1.41 | 4 (6%)   |
| 19  | CLA  | a     | 830 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.20 | 5 (6%)   |
| 19  | CLA  | a     | 831 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.39 | 8 (9%)   |
| 19  | CLA  | A     | 402 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 4 (4%)   |
| 25  | SF4  | c     | 102 | 9    | 0,12,12      | -    | -        | -           | -    | -        |
| 19  | CLA  | A     | 403 | -    | 50,54,73     | 1.36 | 8 (16%)  | 59,90,113   | 1.39 | 4 (6%)   |
| 21  | BCR  | b     | 847 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.15 | 6 (10%)  |
| 19  | CLA  | a     | 823 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 19  | CLA  | b     | 811 | -    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 26  | LHG  | a     | 852 | -    | 48,48,48     | 0.64 | 1 (2%)   | 51,54,54    | 1.31 | 6 (11%)  |
| 19  | CLA  | a     | 836 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 27  | LMG  | a     | 854 | -    | 40,40,55     | 0.81 | 0        | 48,48,63    | 1.30 | 5 (10%)  |
| 19  | CLA  | a     | 842 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 19  | CLA  | a     | 856 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.20 | 7 (8%)   |
| 30  | EQ3  | b     | 851 | -    | 43,43,43     | 1.40 | 7 (16%)  | 55,60,60    | 1.49 | 11 (20%) |
| 19  | CLA  | b     | 830 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.39 | 7 (10%)  |
| 19  | CLA  | f     | 201 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 19  | CLA  | A     | 405 | -    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 21  | BCR  | A     | 406 | -    | 41,41,41     | 1.16 | 2 (4%)   | 56,56,56    | 1.25 | 7 (12%)  |
| 20  | PHO  | A     | 404 | -    | 58,69,69     | 2.14 | 9 (15%)  | 55,99,99    | 1.44 | 7 (12%)  |
| 28  | 45D  | a     | 858 | -    | 43,43,43     | 1.43 | 9 (20%)  | 54,60,60    | 1.56 | 11 (20%) |
| 19  | CLA  | a     | 840 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 26  | LHG  | a     | 855 | -    | 48,48,48     | 0.61 | 1 (2%)   | 51,54,54    | 1.29 | 6 (11%)  |
| 19  | CLA  | D     | 402 | -    | 59,63,73     | 1.26 | 9 (15%)  | 70,101,113  | 1.34 | 5 (7%)   |
| 19  | CLA  | a     | 809 | 7    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 19  | CLA  | b     | 817 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.24 | 4 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | CLA  | a     | 816 | -    | 50,54,73     | 1.35 | 9 (18%)  | 59,90,113   | 1.41 | 5 (8%)   |
| 19  | CLA  | a     | 821 | -    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 19  | CLA  | b     | 807 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 19  | CLA  | b     | 836 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 25  | SF4  | a     | 845 | 8,7  | 0,12,12      | -    | -        | -           | -    | -        |
| 19  | CLA  | b     | 825 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 19  | CLA  | k     | 101 | -    | 50,54,73     | 1.36 | 9 (18%)  | 59,90,113   | 1.31 | 4 (6%)   |
| 21  | BCR  | j     | 101 | -    | 41,41,41     | 1.17 | 3 (7%)   | 56,56,56    | 1.24 | 6 (10%)  |
| 19  | CLA  | b     | 818 | -    | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 19  | CLA  | b     | 834 | -    | 54,58,73     | 1.30 | 9 (16%)  | 64,95,113   | 1.41 | 7 (10%)  |
| 31  | ZEX  | f     | 205 | -    | 43,43,43     | 1.34 | 8 (18%)  | 51,60,60    | 1.44 | 10 (19%) |
| 19  | CLA  | j     | 104 | -    | 50,54,73     | 1.37 | 7 (14%)  | 59,90,113   | 1.37 | 4 (6%)   |
| 19  | CLA  | b     | 822 | -    | 61,65,73     | 1.24 | 9 (14%)  | 72,103,113  | 1.35 | 6 (8%)   |
| 19  | CLA  | a     | 837 | 7    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 4 (4%)   |
| 19  | CLA  | k     | 102 | 15   | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 19  | CLA  | b     | 809 | -    | 60,64,73     | 1.26 | 8 (13%)  | 71,102,113  | 1.30 | 6 (8%)   |
| 19  | CLA  | b     | 833 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 19  | CLA  | b     | 814 | -    | 59,63,73     | 1.24 | 9 (15%)  | 70,101,113  | 1.35 | 5 (7%)   |
| 19  | CLA  | b     | 808 | 8    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 19  | CLA  | b     | 826 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 19  | CLA  | a     | 811 | -    | 54,58,73     | 1.29 | 8 (14%)  | 64,95,113   | 1.38 | 7 (10%)  |
| 19  | CLA  | a     | 819 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 4 (4%)   |
| 19  | CLA  | b     | 840 | 26   | 50,54,73     | 1.35 | 9 (18%)  | 59,90,113   | 1.40 | 4 (6%)   |
| 19  | CLA  | a     | 824 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.33 | 7 (8%)   |
| 19  | CLA  | b     | 828 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.32 | 5 (6%)   |
| 21  | BCR  | l     | 205 | -    | 41,41,41     | 1.13 | 2 (4%)   | 56,56,56    | 1.22 | 5 (8%)   |
| 19  | CLA  | a     | 838 | -    | 55,59,73     | 1.29 | 9 (16%)  | 64,96,113   | 1.39 | 6 (9%)   |
| 19  | CLA  | a     | 841 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 24  | PQN  | b     | 841 | -    | 34,34,34     | 0.40 | 0        | 43,45,45    | 0.55 | 1 (2%)   |
| 19  | CLA  | b     | 803 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 19  | CLA  | a     | 827 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 21  | BCR  | b     | 843 | -    | 41,41,41     | 1.18 | 2 (4%)   | 56,56,56    | 1.22 | 7 (12%)  |
| 19  | CLA  | a     | 822 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 19  | CLA  | b     | 806 | -    | 69,73,73     | 1.14 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 19  | CLA  | a     | 835 | -    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.34 | 6 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 29  | ECH  | m     | 101 | -    | 42,42,42     | 1.45 | 9 (21%)  | 55,58,58    | 1.77 | 13 (23%) |
| 19  | CLA  | a     | 807 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 19  | CLA  | b     | 810 | -    | 60,64,73     | 1.24 | 8 (13%)  | 71,102,113  | 1.33 | 4 (5%)   |
| 19  | CLA  | a     | 825 | -    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.31 | 5 (6%)   |
| 19  | CLA  | a     | 802 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 7 (8%)   |
| 19  | CLA  | a     | 813 | -    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 19  | CLA  | a     | 818 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 26  | LHG  | f     | 206 | -    | 48,48,48     | 0.59 | 0        | 51,54,54    | 1.27 | 6 (11%)  |
| 19  | CLA  | b     | 837 | -    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.39 | 6 (9%)   |
| 19  | CLA  | j     | 103 | 14   | 59,63,73     | 1.26 | 8 (13%)  | 70,101,113  | 1.33 | 5 (7%)   |
| 27  | LMG  | l     | 201 | -    | 50,50,55     | 0.73 | 1 (2%)   | 58,58,63    | 1.35 | 7 (12%)  |
| 19  | CLA  | a     | 832 | -    | 60,64,73     | 1.24 | 8 (13%)  | 71,102,113  | 1.34 | 6 (8%)   |
| 19  | CLA  | a     | 828 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 29  | ECH  | b     | 844 | -    | 42,42,42     | 1.41 | 8 (19%)  | 55,58,58    | 2.32 | 16 (29%) |
| 19  | CLA  | l     | 202 | -    | 54,58,73     | 1.32 | 6 (11%)  | 64,95,113   | 1.35 | 6 (9%)   |
| 19  | CLA  | a     | 806 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.33 | 6 (7%)   |
| 19  | CLA  | a     | 803 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 19  | CLA  | a     | 839 | -    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.23 | 5 (6%)   |
| 20  | PHO  | D     | 401 | -    | 58,69,69     | 2.16 | 10 (17%) | 55,99,99    | 1.48 | 8 (14%)  |
| 19  | CLA  | b     | 831 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 4 (4%)   |
| 21  | BCR  | i     | 102 | -    | 41,41,41     | 1.12 | 2 (4%)   | 56,56,56    | 1.26 | 7 (12%)  |
| 27  | LMG  | b     | 848 | -    | 55,55,55     | 0.70 | 1 (1%)   | 63,63,63    | 1.40 | 9 (14%)  |
| 21  | BCR  | a     | 851 | -    | 25,25,41     | 1.19 | 1 (4%)   | 33,33,56    | 1.31 | 4 (12%)  |
| 19  | CLA  | b     | 827 | -    | 69,73,73     | 1.14 | 9 (13%)  | 82,113,113  | 1.23 | 5 (6%)   |
| 19  | CLA  | a     | 820 | -    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 32  | LMT  | j     | 102 | -    | 36,36,36     | 1.16 | 5 (13%)  | 47,47,47    | 0.96 | 2 (4%)   |
| 19  | CLA  | a     | 857 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 4 (4%)   |
| 19  | CLA  | b     | 823 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 19  | CLA  | b     | 815 | -    | 60,64,73     | 1.23 | 9 (15%)  | 71,102,113  | 1.35 | 7 (9%)   |
| 21  | BCR  | a     | 859 | -    | 41,41,41     | 1.20 | 3 (7%)   | 56,56,56    | 1.22 | 6 (10%)  |
| 19  | CLA  | b     | 816 | -    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.31 | 6 (7%)   |

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

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 19  | CLA  | l     | 204 | -    | 1/1/12/20 | 6/24/100/115  | -       |
| 21  | BCR  | a     | 849 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 19  | CLA  | a     | 812 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 19  | CLA  | a     | 834 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 21  | BCR  | k     | 103 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 21  | BCR  | b     | 842 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 31  | ZEX  | b     | 852 | -    | -         | 3/29/67/67    | 0/2/2/2 |
| 19  | CLA  | a     | 815 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 19  | CLA  | a     | 843 | 26   | 1/1/13/20 | 10/29/105/115 | -       |
| 19  | CLA  | b     | 819 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 21  | BCR  | b     | 845 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 19  | CLA  | a     | 805 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 26  | LHG  | b     | 849 | 19   | -         | 19/42/42/53   | -       |
| 19  | CLA  | a     | 804 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 19  | CLA  | b     | 824 | -    | 1/1/13/20 | 5/27/103/115  | -       |
| 19  | CLA  | b     | 838 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | b     | 804 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 19  | CLA  | b     | 829 | -    | 1/1/12/20 | 5/23/99/115   | -       |
| 21  | BCR  | a     | 848 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 19  | CLA  | b     | 805 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 21  | BCR  | f     | 202 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 21  | BCR  | i     | 101 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 22  | HEM  | E     | 101 | 3,4  | -         | 2/14/54/54    | -       |
| 21  | BCR  | a     | 850 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 19  | CLA  | a     | 829 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 19  | CLA  | b     | 835 | -    | 1/1/12/20 | 6/24/100/115  | -       |
| 19  | CLA  | a     | 817 | -    | 1/1/11/20 | 5/17/93/115   | -       |
| 21  | BCR  | a     | 846 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 19  | CLA  | f     | 203 | -    | 1/1/12/20 | 2/21/97/115   | -       |
| 27  | LMG  | b     | 850 | -    | -         | 24/50/70/70   | 0/1/1/1 |
| 19  | CLA  | a     | 810 | 7    | 1/1/12/20 | 2/23/99/115   | -       |
| 19  | CLA  | b     | 821 | -    | 1/1/11/20 | 4/17/93/115   | -       |
| 19  | CLA  | a     | 833 | -    | 1/1/14/20 | 13/33/109/115 | -       |
| 19  | CLA  | b     | 813 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 19  | CLA  | l     | 203 | -    | 1/1/15/20 | 10/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 19  | CLA  | b     | 832 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 19  | CLA  | b     | 839 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | SF4  | c     | 101 | 9    | -         | -             | 0/6/5/5 |
| 19  | CLA  | a     | 808 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 19  | CLA  | b     | 812 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 19  | CLA  | a     | 826 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 19  | CLA  | b     | 820 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 24  | PQN  | a     | 844 | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 26  | LHG  | a     | 853 | 19   | -         | 21/53/53/53   | -       |
| 19  | CLA  | b     | 802 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | a     | 860 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 19  | CLA  | a     | 814 | -    | -         | 11/39/115/115 | -       |
| 21  | BCR  | a     | 847 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 19  | CLA  | f     | 204 | 12   | 1/1/12/20 | 5/21/97/115   | -       |
| 19  | CLA  | b     | 801 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 21  | BCR  | b     | 846 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 23  | CL0  | a     | 801 | -    | 3/3/20/25 | 12/37/135/135 | -       |
| 19  | CLA  | A     | 407 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 19  | CLA  | D     | 403 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 19  | CLA  | a     | 830 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 19  | CLA  | a     | 831 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 19  | CLA  | A     | 402 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 25  | SF4  | c     | 102 | 9    | -         | -             | 0/6/5/5 |
| 19  | CLA  | A     | 403 | -    | 1/1/11/20 | 10/17/93/115  | -       |
| 21  | BCR  | b     | 847 | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 19  | CLA  | a     | 823 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | b     | 811 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 26  | LHG  | a     | 852 | -    | -         | 25/53/53/53   | -       |
| 19  | CLA  | a     | 836 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 27  | LMG  | a     | 854 | -    | -         | 18/35/55/70   | 0/1/1/1 |
| 19  | CLA  | a     | 842 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | a     | 856 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 30  | EQ3  | b     | 851 | -    | -         | 3/29/68/68    | 0/2/2/2 |
| 19  | CLA  | b     | 830 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 19  | CLA  | f     | 201 | -    | 1/1/15/20 | 14/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 19  | CLA  | A     | 405 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 21  | BCR  | A     | 406 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 20  | PHO  | A     | 404 | -    | -         | 9/37/103/103  | 0/5/6/6 |
| 28  | 45D  | a     | 858 | -    | -         | 4/29/69/69    | 0/2/2/2 |
| 19  | CLA  | a     | 840 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 26  | LHG  | a     | 855 | -    | -         | 19/53/53/53   | -       |
| 19  | CLA  | D     | 402 | -    | 1/1/13/20 | 12/27/103/115 | -       |
| 19  | CLA  | a     | 809 | 7    | 1/1/15/20 | 14/39/115/115 | -       |
| 19  | CLA  | b     | 817 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | a     | 816 | -    | 1/1/11/20 | 7/17/93/115   | -       |
| 19  | CLA  | a     | 821 | -    | 1/1/15/20 | 21/39/115/115 | -       |
| 19  | CLA  | b     | 807 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 19  | CLA  | b     | 836 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 25  | SF4  | a     | 845 | 8,7  | -         | -             | 0/6/5/5 |
| 19  | CLA  | b     | 825 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 19  | CLA  | k     | 101 | -    | 1/1/11/20 | 10/17/93/115  | -       |
| 21  | BCR  | j     | 101 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 19  | CLA  | b     | 818 | -    | 1/1/14/20 | 5/33/109/115  | -       |
| 19  | CLA  | b     | 834 | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 31  | ZEX  | f     | 205 | -    | -         | 4/29/67/67    | 0/2/2/2 |
| 19  | CLA  | j     | 104 | -    | 1/1/11/20 | 5/17/93/115   | -       |
| 19  | CLA  | b     | 822 | -    | 1/1/13/20 | 11/30/106/115 | -       |
| 19  | CLA  | a     | 837 | 7    | 1/1/15/20 | 11/39/115/115 | -       |
| 19  | CLA  | k     | 102 | 15   | 1/1/11/20 | 5/15/91/115   | -       |
| 19  | CLA  | b     | 809 | -    | 1/1/13/20 | 8/29/105/115  | -       |
| 19  | CLA  | b     | 833 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 19  | CLA  | b     | 814 | -    | 1/1/13/20 | 14/27/103/115 | -       |
| 19  | CLA  | b     | 808 | 8    | 1/1/15/20 | 9/39/115/115  | -       |
| 19  | CLA  | b     | 826 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | a     | 811 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 19  | CLA  | a     | 819 | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 19  | CLA  | b     | 840 | 26   | 1/1/11/20 | 7/17/93/115   | -       |
| 19  | CLA  | a     | 824 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 19  | CLA  | b     | 828 | -    | 1/1/15/20 | 14/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 21  | BCR  | l     | 205 | -    | -         | 10/29/63/63   | 0/2/2/2 |
| 19  | CLA  | a     | 838 | -    | 1/1/12/20 | 5/23/99/115   | -       |
| 19  | CLA  | a     | 841 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 24  | PQN  | b     | 841 | -    | -         | 0/23/43/43    | 0/2/2/2 |
| 19  | CLA  | b     | 803 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | a     | 827 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 21  | BCR  | b     | 843 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 19  | CLA  | a     | 822 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 19  | CLA  | b     | 806 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 19  | CLA  | a     | 835 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 29  | ECH  | m     | 101 | -    | -         | 6/29/66/66    | 0/2/2/2 |
| 19  | CLA  | a     | 807 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 19  | CLA  | b     | 810 | -    | 1/1/13/20 | 7/29/105/115  | -       |
| 19  | CLA  | a     | 825 | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 19  | CLA  | a     | 802 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | a     | 813 | -    | 1/1/14/20 | 12/33/109/115 | -       |
| 19  | CLA  | a     | 818 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 26  | LHG  | f     | 206 | -    | -         | 30/53/53/53   | -       |
| 19  | CLA  | b     | 837 | -    | 1/1/12/20 | 6/21/97/115   | -       |
| 19  | CLA  | j     | 103 | 14   | 1/1/13/20 | 10/27/103/115 | -       |
| 27  | LMG  | l     | 201 | -    | -         | 25/45/65/70   | 0/1/1/1 |
| 19  | CLA  | a     | 832 | -    | 1/1/13/20 | 12/29/105/115 | -       |
| 19  | CLA  | a     | 828 | -    | 1/1/15/20 | 17/39/115/115 | -       |
| 29  | ECH  | b     | 844 | -    | -         | 10/29/66/66   | 0/2/2/2 |
| 19  | CLA  | l     | 202 | -    | 1/1/12/20 | 8/21/97/115   | -       |
| 19  | CLA  | a     | 806 | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 19  | CLA  | a     | 803 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 19  | CLA  | a     | 839 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 20  | PHO  | D     | 401 | -    | -         | 10/37/103/103 | 0/5/6/6 |
| 19  | CLA  | b     | 831 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 21  | BCR  | i     | 102 | -    | -         | 13/29/63/63   | 0/2/2/2 |
| 27  | LMG  | b     | 848 | -    | -         | 22/50/70/70   | 0/1/1/1 |
| 21  | BCR  | a     | 851 | -    | -         | 7/18/35/63    | 0/1/1/2 |
| 19  | CLA  | b     | 827 | -    | 1/1/15/20 | 11/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 19  | CLA  | a     | 820 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 32  | LMT  | j     | 102 | -    | -         | 5/21/61/61    | 0/2/2/2 |
| 19  | CLA  | a     | 857 | -    | 1/1/15/20 | 19/39/115/115 | -       |
| 19  | CLA  | b     | 823 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CLA  | b     | 815 | -    | 1/1/13/20 | 5/29/105/115  | -       |
| 21  | BCR  | a     | 859 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 19  | CLA  | b     | 816 | -    | 1/1/15/20 | 9/39/115/115  | -       |

All (1012) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | D     | 401 | PHO  | C1B-C2B | 9.55  | 1.50        | 1.39     |
| 20  | A     | 404 | PHO  | C1B-C2B | 9.47  | 1.49        | 1.39     |
| 23  | a     | 801 | CL0  | C1B-C2B | 8.70  | 1.49        | 1.39     |
| 20  | A     | 404 | PHO  | C3B-C4B | 8.37  | 1.50        | 1.41     |
| 20  | D     | 401 | PHO  | C3B-C4B | 8.34  | 1.49        | 1.41     |
| 23  | a     | 801 | CL0  | C3B-C4B | 7.77  | 1.49        | 1.41     |
| 23  | a     | 801 | CL0  | C1D-C2D | 7.45  | 1.48        | 1.39     |
| 20  | D     | 401 | PHO  | C1D-C2D | 4.25  | 1.44        | 1.39     |
| 20  | A     | 404 | PHO  | C1D-C2D | 4.14  | 1.44        | 1.39     |
| 23  | a     | 801 | CL0  | C3D-C4D | 4.11  | 1.47        | 1.41     |
| 21  | a     | 850 | BCR  | C1-C6   | -4.01 | 1.48        | 1.53     |
| 21  | b     | 842 | BCR  | C1-C6   | -3.99 | 1.48        | 1.53     |
| 22  | E     | 101 | HEM  | FE-NB   | 3.92  | 2.07        | 1.94     |
| 21  | a     | 859 | BCR  | C1-C6   | -3.89 | 1.48        | 1.53     |
| 21  | a     | 846 | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |
| 21  | f     | 202 | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |
| 21  | a     | 849 | BCR  | C1-C6   | -3.88 | 1.48        | 1.53     |
| 20  | D     | 401 | PHO  | C4D-CHA | 3.86  | 1.45        | 1.39     |
| 21  | j     | 101 | BCR  | C1-C6   | -3.84 | 1.48        | 1.53     |
| 21  | a     | 847 | BCR  | C1-C6   | -3.83 | 1.48        | 1.53     |
| 21  | a     | 848 | BCR  | C1-C6   | -3.82 | 1.48        | 1.53     |
| 22  | E     | 101 | HEM  | FE-ND   | 3.77  | 2.06        | 1.94     |
| 21  | A     | 406 | BCR  | C1-C6   | -3.75 | 1.49        | 1.53     |
| 21  | l     | 205 | BCR  | C1-C6   | -3.73 | 1.49        | 1.53     |
| 21  | a     | 851 | BCR  | C1-C6   | -3.71 | 1.49        | 1.53     |
| 20  | A     | 404 | PHO  | C4D-CHA | 3.70  | 1.45        | 1.39     |
| 22  | E     | 101 | HEM  | FE-NA   | 3.70  | 2.07        | 1.95     |
| 21  | b     | 843 | BCR  | C1-C6   | -3.64 | 1.49        | 1.53     |
| 21  | a     | 847 | BCR  | C30-C25 | -3.62 | 1.49        | 1.53     |
| 19  | j     | 104 | CLA  | C1D-ND  | 3.59  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 21  | b     | 846 | BCR  | C30-C25 | -3.58 | 1.49        | 1.53     |
| 21  | a     | 859 | BCR  | C30-C25 | -3.57 | 1.49        | 1.53     |
| 19  | a     | 814 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 21  | b     | 842 | BCR  | C30-C25 | -3.56 | 1.49        | 1.53     |
| 19  | b     | 816 | CLA  | C1D-ND  | 3.56  | 1.42        | 1.37     |
| 19  | k     | 101 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 19  | l     | 202 | CLA  | C1D-ND  | 3.55  | 1.42        | 1.37     |
| 21  | A     | 406 | BCR  | C30-C25 | -3.53 | 1.49        | 1.53     |
| 19  | j     | 103 | CLA  | C1D-ND  | 3.53  | 1.42        | 1.37     |
| 21  | i     | 101 | BCR  | C30-C25 | -3.52 | 1.49        | 1.53     |
| 19  | D     | 403 | CLA  | C1D-ND  | 3.52  | 1.42        | 1.37     |
| 21  | k     | 103 | BCR  | C1-C6   | -3.51 | 1.49        | 1.53     |
| 19  | a     | 829 | CLA  | C1D-ND  | 3.51  | 1.42        | 1.37     |
| 19  | A     | 403 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 19  | a     | 840 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 19  | b     | 809 | CLA  | C1D-ND  | 3.49  | 1.42        | 1.37     |
| 19  | A     | 405 | CLA  | C1D-ND  | 3.47  | 1.42        | 1.37     |
| 21  | b     | 843 | BCR  | C30-C25 | -3.47 | 1.49        | 1.53     |
| 21  | b     | 845 | BCR  | C1-C6   | -3.47 | 1.49        | 1.53     |
| 21  | i     | 102 | BCR  | C1-C6   | -3.46 | 1.49        | 1.53     |
| 19  | k     | 102 | CLA  | C1D-ND  | 3.46  | 1.42        | 1.37     |
| 19  | b     | 829 | CLA  | C1D-ND  | 3.45  | 1.42        | 1.37     |
| 21  | b     | 847 | BCR  | C30-C25 | -3.45 | 1.49        | 1.53     |
| 21  | b     | 846 | BCR  | C1-C6   | -3.44 | 1.49        | 1.53     |
| 19  | A     | 407 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 19  | a     | 819 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 19  | a     | 841 | CLA  | C1D-ND  | 3.44  | 1.42        | 1.37     |
| 19  | b     | 812 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 19  | f     | 203 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 19  | a     | 837 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 21  | i     | 101 | BCR  | C1-C6   | -3.43 | 1.49        | 1.53     |
| 19  | a     | 817 | CLA  | C1D-ND  | 3.43  | 1.42        | 1.37     |
| 19  | a     | 824 | CLA  | C1D-ND  | 3.42  | 1.42        | 1.37     |
| 21  | k     | 103 | BCR  | C30-C25 | -3.41 | 1.49        | 1.53     |
| 19  | a     | 825 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 19  | a     | 802 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 19  | a     | 842 | CLA  | C1D-ND  | 3.41  | 1.42        | 1.37     |
| 21  | a     | 849 | BCR  | C30-C25 | -3.40 | 1.49        | 1.53     |
| 19  | l     | 204 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 19  | b     | 826 | CLA  | C1D-ND  | 3.40  | 1.42        | 1.37     |
| 19  | a     | 860 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 19  | f     | 204 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 813 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 19  | a     | 821 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 19  | a     | 812 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 21  | b     | 847 | BCR  | C1-C6   | -3.39 | 1.49        | 1.53     |
| 19  | a     | 822 | CLA  | C1D-ND  | 3.39  | 1.42        | 1.37     |
| 19  | b     | 808 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 19  | a     | 823 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 19  | f     | 201 | CLA  | C1D-ND  | 3.38  | 1.42        | 1.37     |
| 19  | b     | 815 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 19  | b     | 832 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 19  | a     | 818 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 19  | b     | 801 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 19  | b     | 837 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 19  | a     | 803 | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 19  | b     | 820 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 21  | a     | 850 | BCR  | C30-C25 | -3.36 | 1.49        | 1.53     |
| 19  | a     | 838 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 19  | b     | 840 | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 19  | b     | 835 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 19  | a     | 804 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 21  | f     | 202 | BCR  | C30-C25 | -3.35 | 1.49        | 1.53     |
| 29  | m     | 101 | ECH  | C25-C26 | 3.35  | 1.40        | 1.35     |
| 19  | a     | 839 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 19  | b     | 813 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 19  | b     | 831 | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 19  | b     | 811 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 19  | b     | 825 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 19  | b     | 839 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 19  | b     | 806 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 19  | b     | 803 | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 19  | a     | 828 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 19  | b     | 807 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 19  | b     | 836 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 19  | A     | 402 | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 19  | b     | 823 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 19  | a     | 835 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 19  | a     | 833 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 19  | b     | 804 | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 19  | a     | 857 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 19  | b     | 821 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 19  | a     | 806 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 19  | a     | 815 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 817 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 19  | b     | 833 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 19  | D     | 402 | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 19  | b     | 834 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 19  | a     | 831 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 19  | a     | 811 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 19  | a     | 807 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 19  | b     | 818 | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 21  | b     | 845 | BCR  | C30-C25 | -3.29 | 1.49        | 1.53     |
| 19  | a     | 809 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 19  | a     | 826 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 19  | b     | 830 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 19  | a     | 843 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 21  | a     | 846 | BCR  | C30-C25 | -3.28 | 1.49        | 1.53     |
| 19  | b     | 819 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 19  | a     | 808 | CLA  | C1D-ND  | 3.28  | 1.42        | 1.37     |
| 19  | b     | 810 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 19  | a     | 816 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 19  | a     | 820 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 19  | a     | 827 | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 19  | b     | 822 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 19  | b     | 824 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 19  | a     | 834 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 19  | l     | 203 | CLA  | C1D-ND  | 3.26  | 1.42        | 1.37     |
| 21  | j     | 101 | BCR  | C30-C25 | -3.25 | 1.49        | 1.53     |
| 19  | b     | 838 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 19  | a     | 856 | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 19  | b     | 809 | CLA  | C4B-NB  | 3.24  | 1.42        | 1.37     |
| 19  | b     | 814 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 19  | b     | 821 | CLA  | C4B-NB  | 3.23  | 1.42        | 1.37     |
| 19  | b     | 828 | CLA  | C1D-ND  | 3.23  | 1.42        | 1.37     |
| 19  | a     | 810 | CLA  | C1D-ND  | 3.22  | 1.42        | 1.37     |
| 21  | a     | 848 | BCR  | C30-C25 | -3.21 | 1.49        | 1.53     |
| 19  | j     | 103 | CLA  | C4B-NB  | 3.21  | 1.42        | 1.37     |
| 19  | a     | 805 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 19  | b     | 805 | CLA  | C1D-ND  | 3.19  | 1.42        | 1.37     |
| 19  | a     | 836 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 19  | a     | 830 | CLA  | C1D-ND  | 3.17  | 1.42        | 1.37     |
| 19  | b     | 802 | CLA  | C1D-ND  | 3.16  | 1.42        | 1.37     |
| 19  | a     | 832 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |
| 19  | b     | 839 | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 19  | b     | 827 | CLA  | C1D-ND  | 3.15  | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22  | E     | 101 | HEM  | FE-NC   | 3.15  | 2.05        | 1.95     |
| 29  | b     | 844 | ECH  | C23-C22 | -3.13 | 1.39        | 1.46     |
| 19  | b     | 837 | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 28  | a     | 858 | 45D  | C24-C26 | -3.12 | 1.39        | 1.46     |
| 19  | f     | 204 | CLA  | C4B-NB  | 3.09  | 1.41        | 1.37     |
| 22  | E     | 101 | HEM  | CAB-C3B | 3.09  | 1.55        | 1.47     |
| 21  | l     | 205 | BCR  | C30-C25 | -3.09 | 1.49        | 1.53     |
| 19  | l     | 202 | CLA  | C4B-NB  | 3.08  | 1.41        | 1.37     |
| 19  | a     | 840 | CLA  | C4B-NB  | 3.07  | 1.41        | 1.37     |
| 19  | D     | 402 | CLA  | C4B-NB  | 3.06  | 1.41        | 1.37     |
| 19  | A     | 405 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 19  | a     | 803 | CLA  | C4B-NB  | 3.05  | 1.41        | 1.37     |
| 19  | k     | 102 | CLA  | C4B-NB  | 3.04  | 1.41        | 1.37     |
| 19  | j     | 104 | CLA  | C4B-NB  | 3.04  | 1.41        | 1.37     |
| 30  | b     | 851 | EQ3  | C23-C22 | -3.04 | 1.39        | 1.46     |
| 19  | a     | 821 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 19  | f     | 203 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 19  | a     | 802 | CLA  | C4B-NB  | 3.03  | 1.41        | 1.37     |
| 28  | a     | 858 | 45D  | C23-C25 | -3.03 | 1.39        | 1.46     |
| 19  | k     | 101 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 19  | b     | 831 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 19  | a     | 824 | CLA  | C4B-NB  | 3.02  | 1.41        | 1.37     |
| 31  | f     | 205 | ZEX  | C8-C9   | -3.01 | 1.39        | 1.46     |
| 22  | E     | 101 | HEM  | CAC-C3C | 3.01  | 1.55        | 1.47     |
| 19  | b     | 811 | CLA  | C4B-NB  | 2.99  | 1.41        | 1.37     |
| 31  | b     | 852 | ZEX  | C8-C9   | -2.98 | 1.39        | 1.46     |
| 19  | D     | 403 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 19  | A     | 403 | CLA  | C4B-NB  | 2.98  | 1.41        | 1.37     |
| 19  | a     | 804 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 19  | a     | 813 | CLA  | C4B-NB  | 2.97  | 1.41        | 1.37     |
| 19  | f     | 201 | CLA  | C4B-NB  | 2.96  | 1.41        | 1.37     |
| 19  | a     | 841 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 31  | f     | 205 | ZEX  | C28-C29 | -2.95 | 1.39        | 1.46     |
| 19  | a     | 822 | CLA  | C4B-NB  | 2.95  | 1.41        | 1.37     |
| 19  | l     | 203 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 30  | b     | 851 | EQ3  | C25-C26 | 2.94  | 1.39        | 1.35     |
| 19  | b     | 801 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 19  | a     | 805 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 19  | a     | 816 | CLA  | C4B-NB  | 2.94  | 1.41        | 1.37     |
| 19  | a     | 837 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |
| 30  | b     | 851 | EQ3  | C8-C9   | -2.93 | 1.39        | 1.46     |
| 19  | b     | 828 | CLA  | C4B-NB  | 2.93  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 808 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 19  | b     | 819 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 19  | a     | 832 | CLA  | C4B-NB  | 2.92  | 1.41        | 1.37     |
| 19  | a     | 836 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 19  | a     | 857 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 19  | a     | 827 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 19  | b     | 810 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 19  | a     | 860 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 19  | a     | 815 | CLA  | C4B-NB  | 2.91  | 1.41        | 1.37     |
| 19  | a     | 819 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 19  | A     | 402 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 19  | a     | 808 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 29  | m     | 101 | ECH  | C23-C22 | -2.90 | 1.39        | 1.46     |
| 19  | a     | 810 | CLA  | C4B-NB  | 2.90  | 1.41        | 1.37     |
| 19  | a     | 812 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 19  | A     | 407 | CLA  | C4B-NB  | 2.89  | 1.41        | 1.37     |
| 19  | b     | 803 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 19  | a     | 842 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 19  | b     | 829 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 19  | b     | 840 | CLA  | C4B-NB  | 2.88  | 1.41        | 1.37     |
| 19  | a     | 835 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 19  | a     | 811 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 19  | a     | 829 | CLA  | C4B-NB  | 2.87  | 1.41        | 1.37     |
| 19  | l     | 204 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 19  | b     | 834 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 19  | a     | 806 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 19  | a     | 818 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 19  | a     | 833 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 19  | b     | 802 | CLA  | C4B-NB  | 2.86  | 1.41        | 1.37     |
| 19  | b     | 807 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 21  | i     | 102 | BCR  | C30-C25 | -2.85 | 1.50        | 1.53     |
| 19  | b     | 826 | CLA  | C4B-NB  | 2.85  | 1.41        | 1.37     |
| 19  | a     | 830 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 31  | b     | 852 | ZEX  | C28-C29 | -2.84 | 1.39        | 1.46     |
| 19  | b     | 813 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 19  | a     | 820 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 19  | b     | 833 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 19  | a     | 831 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 19  | a     | 823 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 19  | a     | 843 | CLA  | C4B-NB  | 2.84  | 1.41        | 1.37     |
| 19  | b     | 812 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |
| 19  | b     | 823 | CLA  | C4B-NB  | 2.83  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 839 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 19  | b     | 822 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 19  | b     | 814 | CLA  | C4B-NB  | 2.82  | 1.41        | 1.37     |
| 29  | m     | 101 | ECH  | C8-C9   | -2.81 | 1.39        | 1.46     |
| 29  | b     | 844 | ECH  | C8-C9   | -2.81 | 1.39        | 1.46     |
| 19  | b     | 820 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 19  | b     | 832 | CLA  | C4B-NB  | 2.81  | 1.41        | 1.37     |
| 19  | a     | 856 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 19  | a     | 834 | CLA  | C4B-NB  | 2.80  | 1.41        | 1.37     |
| 19  | b     | 838 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 19  | a     | 807 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 19  | b     | 830 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 19  | b     | 825 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 19  | b     | 815 | CLA  | C4B-NB  | 2.79  | 1.41        | 1.37     |
| 19  | a     | 826 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 19  | b     | 817 | CLA  | C4B-NB  | 2.78  | 1.41        | 1.37     |
| 19  | a     | 817 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 19  | b     | 816 | CLA  | C4B-NB  | 2.77  | 1.41        | 1.37     |
| 19  | b     | 805 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 19  | b     | 836 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 19  | a     | 825 | CLA  | C4B-NB  | 2.76  | 1.41        | 1.37     |
| 19  | D     | 402 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 19  | D     | 403 | CLA  | C1B-C2B | 2.75  | 1.49        | 1.43     |
| 19  | b     | 827 | CLA  | C4B-NB  | 2.74  | 1.41        | 1.37     |
| 19  | a     | 817 | CLA  | C1B-C2B | 2.74  | 1.49        | 1.43     |
| 19  | A     | 405 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 19  | b     | 824 | CLA  | C4B-NB  | 2.72  | 1.41        | 1.37     |
| 19  | l     | 204 | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 19  | b     | 804 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 28  | a     | 858 | 45D  | C08-C16 | 2.71  | 1.39        | 1.35     |
| 19  | a     | 838 | CLA  | C4B-NB  | 2.71  | 1.41        | 1.37     |
| 19  | a     | 841 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 19  | k     | 102 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 19  | a     | 809 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 19  | A     | 403 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 19  | a     | 814 | CLA  | C4B-NB  | 2.70  | 1.41        | 1.37     |
| 19  | A     | 407 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 19  | l     | 202 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 19  | A     | 402 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 19  | b     | 835 | CLA  | C4B-NB  | 2.69  | 1.41        | 1.37     |
| 19  | j     | 104 | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 19  | b     | 818 | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | a     | 801 | CL0  | CMB-C2B | -2.68 | 1.46        | 1.51     |
| 19  | a     | 818 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 19  | a     | 842 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 19  | a     | 806 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 19  | a     | 815 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | b     | 806 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 19  | a     | 860 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | a     | 832 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | a     | 823 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | a     | 828 | CLA  | C4B-NB  | 2.67  | 1.41        | 1.37     |
| 19  | a     | 808 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | b     | 840 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | b     | 824 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 19  | b     | 836 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 19  | a     | 834 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 19  | l     | 203 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 19  | f     | 203 | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 19  | a     | 814 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 19  | a     | 824 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 19  | a     | 838 | CLA  | C1B-C2B | 2.65  | 1.49        | 1.43     |
| 19  | a     | 816 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 19  | b     | 829 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 19  | a     | 835 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 19  | b     | 820 | CLA  | C1B-C2B | 2.64  | 1.49        | 1.43     |
| 19  | a     | 857 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 19  | b     | 826 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 19  | b     | 832 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 19  | b     | 810 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 19  | a     | 810 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 19  | b     | 806 | CLA  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 19  | a     | 833 | CLA  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 19  | b     | 816 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | b     | 805 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | a     | 825 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | b     | 815 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | a     | 827 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | j     | 103 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | b     | 804 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | b     | 818 | CLA  | C1B-C2B | 2.61  | 1.49        | 1.43     |
| 19  | b     | 821 | CLA  | C3B-C4B | 2.60  | 1.50        | 1.42     |
| 19  | a     | 807 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 19  | a     | 812 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 833 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 19  | b     | 828 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 19  | b     | 822 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 19  | b     | 812 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 19  | k     | 101 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 19  | a     | 830 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 19  | b     | 808 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 19  | f     | 201 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 20  | D     | 401 | PHO  | CMC-C2C | -2.59 | 1.46        | 1.50     |
| 20  | A     | 404 | PHO  | CMC-C2C | -2.59 | 1.46        | 1.50     |
| 19  | a     | 829 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 19  | b     | 834 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 26  | a     | 852 | LHG  | O7-C5   | -2.58 | 1.40        | 1.46     |
| 19  | a     | 821 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 19  | f     | 204 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 23  | a     | 801 | CL0  | CMD-C2D | -2.58 | 1.46        | 1.51     |
| 19  | b     | 813 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 19  | a     | 805 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 19  | b     | 817 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 19  | a     | 809 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 19  | a     | 843 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 19  | a     | 828 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 19  | b     | 803 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 19  | a     | 856 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 19  | b     | 819 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 19  | a     | 837 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 30  | b     | 851 | EQ3  | C19-C18 | -2.56 | 1.40        | 1.46     |
| 19  | b     | 825 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 19  | a     | 811 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 19  | b     | 801 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 23  | a     | 801 | CL0  | CMC-C2C | -2.55 | 1.46        | 1.50     |
| 19  | b     | 837 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 19  | a     | 803 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 19  | b     | 811 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 19  | b     | 831 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 19  | b     | 838 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 19  | a     | 804 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 19  | a     | 822 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 19  | b     | 830 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 19  | a     | 831 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 20  | A     | 404 | PHO  | CMD-C2D | -2.54 | 1.46        | 1.51     |
| 19  | a     | 839 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | j     | 102 | LMT  | O3'-C3' | -2.54 | 1.36        | 1.43     |
| 19  | a     | 826 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 19  | a     | 802 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 19  | a     | 813 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 19  | b     | 809 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 19  | a     | 836 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 29  | b     | 844 | ECH  | C19-C18 | -2.51 | 1.40        | 1.46     |
| 19  | a     | 820 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 19  | b     | 839 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 19  | b     | 821 | CLA  | C1B-C2B | 2.51  | 1.49        | 1.43     |
| 29  | b     | 844 | ECH  | C12-C13 | -2.50 | 1.40        | 1.46     |
| 19  | b     | 807 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 30  | b     | 851 | EQ3  | C12-C13 | -2.50 | 1.40        | 1.46     |
| 31  | b     | 852 | ZEX  | C12-C13 | -2.49 | 1.40        | 1.46     |
| 19  | b     | 835 | CLA  | C1B-C2B | 2.49  | 1.49        | 1.43     |
| 19  | b     | 814 | CLA  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 19  | b     | 809 | CLA  | C3B-C4B | 2.48  | 1.50        | 1.42     |
| 20  | D     | 401 | PHO  | C3D-C4D | 2.47  | 1.44        | 1.41     |
| 19  | a     | 819 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 28  | a     | 858 | 45D  | C34-C36 | -2.47 | 1.40        | 1.46     |
| 31  | f     | 205 | ZEX  | C12-C13 | -2.47 | 1.40        | 1.46     |
| 19  | b     | 823 | CLA  | C1B-C2B | 2.46  | 1.48        | 1.43     |
| 20  | A     | 404 | PHO  | CMB-C2B | -2.46 | 1.46        | 1.51     |
| 26  | b     | 849 | LHG  | O7-C5   | -2.45 | 1.40        | 1.46     |
| 19  | a     | 840 | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 20  | D     | 401 | PHO  | CMB-C2B | -2.44 | 1.46        | 1.51     |
| 19  | b     | 827 | CLA  | C1B-C2B | 2.44  | 1.48        | 1.43     |
| 19  | b     | 811 | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 20  | D     | 401 | PHO  | CMD-C2D | -2.44 | 1.46        | 1.51     |
| 19  | b     | 802 | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 28  | a     | 858 | 45D  | C33-C35 | -2.43 | 1.40        | 1.46     |
| 19  | b     | 831 | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 20  | D     | 401 | PHO  | CAC-C3C | -2.41 | 1.47        | 1.51     |
| 19  | b     | 839 | CLA  | CMB-C2B | -2.41 | 1.45        | 1.50     |
| 19  | j     | 103 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 31  | b     | 852 | ZEX  | C32-C33 | -2.41 | 1.40        | 1.46     |
| 19  | l     | 202 | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 19  | a     | 805 | CLA  | CHC-C1C | 2.39  | 1.43        | 1.38     |
| 20  | A     | 404 | PHO  | CAC-C3C | -2.39 | 1.47        | 1.51     |
| 19  | j     | 104 | CLA  | CHC-C1C | 2.39  | 1.43        | 1.38     |
| 31  | f     | 205 | ZEX  | C32-C33 | -2.38 | 1.40        | 1.46     |
| 19  | j     | 104 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 32  | j     | 102 | LMT  | O2'-C2' | -2.38 | 1.37        | 1.43     |
| 19  | k     | 101 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 19  | a     | 803 | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 23  | a     | 801 | CL0  | CAC-C3C | -2.37 | 1.47        | 1.51     |
| 19  | a     | 813 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 19  | f     | 204 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 19  | a     | 836 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 19  | a     | 804 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 20  | A     | 404 | PHO  | C3D-C4D | 2.36  | 1.44        | 1.41     |
| 19  | b     | 828 | CLA  | CMD-C2D | -2.35 | 1.45        | 1.50     |
| 19  | a     | 822 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 19  | b     | 814 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 27  | b     | 850 | LMG  | O7-C8   | -2.35 | 1.41        | 1.46     |
| 19  | a     | 840 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 23  | a     | 801 | CL0  | C1A-CHA | -2.34 | 1.37        | 1.40     |
| 19  | A     | 403 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 19  | a     | 805 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 29  | b     | 844 | ECH  | C21-C22 | 2.34  | 1.41        | 1.35     |
| 29  | m     | 101 | ECH  | C14-C13 | 2.34  | 1.41        | 1.35     |
| 32  | j     | 102 | LMT  | O2B-C2B | -2.33 | 1.37        | 1.43     |
| 19  | f     | 201 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 19  | b     | 819 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 19  | b     | 836 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 19  | D     | 403 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 19  | a     | 839 | CLA  | MG-NB   | -2.33 | 2.01        | 2.05     |
| 19  | b     | 802 | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 19  | b     | 822 | CLA  | CMD-C2D | -2.32 | 1.46        | 1.50     |
| 19  | b     | 830 | CLA  | MG-NB   | -2.31 | 2.01        | 2.05     |
| 29  | m     | 101 | ECH  | C12-C13 | -2.31 | 1.41        | 1.46     |
| 29  | m     | 101 | ECH  | C21-C22 | 2.31  | 1.41        | 1.35     |
| 19  | a     | 810 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |
| 19  | a     | 843 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 19  | a     | 803 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 19  | a     | 824 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 19  | b     | 812 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 19  | b     | 802 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 19  | b     | 823 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 19  | k     | 102 | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 19  | b     | 835 | CLA  | MG-NB   | -2.29 | 2.01        | 2.05     |
| 29  | m     | 101 | ECH  | C17-C18 | 2.29  | 1.41        | 1.35     |
| 19  | a     | 833 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 19  | b     | 807 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | m     | 101 | ECH  | C10-C9  | 2.28  | 1.41        | 1.35     |
| 19  | a     | 820 | CLA  | MG-NB   | -2.28 | 2.01        | 2.05     |
| 19  | b     | 840 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 19  | D     | 403 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 19  | a     | 809 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 19  | b     | 801 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 19  | b     | 822 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 19  | b     | 801 | CLA  | CMD-C2D | -2.27 | 1.46        | 1.50     |
| 19  | b     | 838 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 19  | a     | 842 | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 19  | a     | 815 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 19  | b     | 817 | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 19  | b     | 824 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | b     | 834 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 19  | a     | 828 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | b     | 837 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | b     | 831 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 19  | a     | 821 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | b     | 828 | CLA  | CMB-C2B | -2.26 | 1.46        | 1.50     |
| 19  | a     | 860 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | a     | 834 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | b     | 803 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 19  | a     | 838 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | b     | 823 | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 19  | a     | 808 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | b     | 803 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | a     | 822 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | a     | 839 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | a     | 823 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | a     | 837 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | a     | 827 | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 19  | b     | 825 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | a     | 857 | CLA  | MG-NB   | -2.26 | 2.01        | 2.05     |
| 19  | a     | 831 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 19  | a     | 837 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 19  | b     | 808 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 29  | b     | 844 | ECH  | C17-C18 | 2.25  | 1.41        | 1.35     |
| 19  | a     | 836 | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 19  | b     | 830 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 19  | a     | 808 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 19  | l     | 202 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 19  | a     | 832 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 857 | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 19  | b     | 812 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 19  | a     | 811 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 19  | a     | 816 | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 19  | b     | 813 | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 19  | b     | 840 | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 19  | b     | 806 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 19  | a     | 811 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 19  | b     | 830 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 19  | b     | 815 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 19  | b     | 834 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 19  | b     | 816 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 19  | k     | 102 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 19  | b     | 802 | CLA  | CMC-C2C | -2.24 | 1.46        | 1.50     |
| 19  | A     | 407 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 19  | b     | 820 | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 19  | a     | 815 | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 19  | b     | 827 | CLA  | CMD-C2D | -2.24 | 1.46        | 1.50     |
| 19  | a     | 843 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 19  | a     | 828 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 19  | a     | 826 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 29  | b     | 844 | ECH  | C10-C9  | 2.23  | 1.41        | 1.35     |
| 19  | a     | 842 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 19  | b     | 828 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 19  | l     | 203 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 19  | b     | 815 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 19  | b     | 823 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 19  | b     | 825 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 19  | b     | 806 | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 19  | f     | 203 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 19  | b     | 823 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 19  | a     | 812 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 19  | a     | 836 | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 19  | f     | 204 | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 19  | a     | 802 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 19  | a     | 828 | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 19  | b     | 810 | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 19  | b     | 835 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 19  | b     | 804 | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 19  | f     | 201 | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 19  | b     | 827 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 19  | a     | 802 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 830 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 19  | b     | 802 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 19  | A     | 405 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 19  | a     | 809 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 19  | a     | 810 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 19  | a     | 819 | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 19  | b     | 813 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 19  | l     | 203 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 19  | a     | 827 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 19  | b     | 805 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 19  | b     | 838 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 19  | a     | 819 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 19  | b     | 807 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 19  | b     | 827 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 19  | a     | 826 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 19  | a     | 806 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 19  | a     | 830 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 19  | a     | 820 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 19  | b     | 829 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 19  | a     | 836 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 19  | b     | 817 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 19  | a     | 818 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 19  | a     | 809 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 26  | a     | 855 | LHG  | O7-C5   | -2.21 | 1.41        | 1.46     |
| 23  | a     | 801 | CL0  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 19  | b     | 832 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 19  | l     | 204 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 19  | b     | 833 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 19  | b     | 837 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 19  | a     | 816 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 19  | b     | 822 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 19  | b     | 808 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 27  | b     | 848 | LMG  | O7-C8   | -2.21 | 1.41        | 1.46     |
| 19  | b     | 825 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 19  | A     | 405 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 19  | a     | 806 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 19  | a     | 826 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |
| 19  | b     | 805 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | b     | 839 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 26  | a     | 853 | LHG  | O7-C5   | -2.20 | 1.41        | 1.46     |
| 19  | a     | 814 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | a     | 817 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | A     | 402 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | a     | 822 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 19  | f     | 203 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 19  | a     | 828 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | b     | 819 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | b     | 801 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 19  | a     | 809 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 19  | b     | 801 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | a     | 829 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | b     | 827 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 19  | a     | 804 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | b     | 808 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | b     | 820 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | a     | 822 | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 19  | a     | 815 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | a     | 830 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | a     | 805 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 19  | b     | 828 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 19  | b     | 833 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | a     | 825 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | b     | 813 | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 19  | a     | 826 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 31  | f     | 205 | ZEX  | C30-C29 | 2.19  | 1.40        | 1.35     |
| 19  | D     | 402 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | b     | 824 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 32  | j     | 102 | LMT  | O3B-C3B | -2.19 | 1.37        | 1.43     |
| 19  | a     | 830 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | b     | 814 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 19  | a     | 856 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 19  | a     | 831 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 19  | b     | 822 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 19  | b     | 838 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 19  | a     | 833 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | b     | 826 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | a     | 831 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 19  | b     | 813 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 19  | j     | 103 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 19  | l     | 204 | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 19  | a     | 816 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 19  | b     | 818 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 19  | l     | 204 | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 19  | a     | 827 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 818 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 19  | b     | 809 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 19  | A     | 402 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | a     | 804 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | a     | 823 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | a     | 832 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 19  | a     | 813 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | b     | 824 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 19  | b     | 838 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 19  | a     | 840 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | b     | 834 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 19  | a     | 821 | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 19  | A     | 402 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 19  | b     | 824 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | a     | 841 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 19  | b     | 826 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | b     | 840 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | a     | 825 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | A     | 403 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | a     | 821 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | b     | 839 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 19  | a     | 812 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | a     | 842 | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 19  | a     | 819 | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 19  | a     | 825 | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 19  | a     | 807 | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 19  | b     | 821 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | a     | 824 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | b     | 818 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | b     | 812 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 29  | b     | 844 | ECH  | C14-C13 | 2.17  | 1.40        | 1.35     |
| 19  | f     | 201 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 19  | A     | 405 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | a     | 834 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 19  | a     | 810 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 19  | A     | 407 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | a     | 820 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 19  | b     | 835 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 19  | b     | 828 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | b     | 804 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 19  | a     | 835 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 19  | b     | 811 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 821 | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 19  | a     | 831 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 19  | a     | 834 | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 19  | b     | 820 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 19  | b     | 837 | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 29  | m     | 101 | ECH  | C19-C18 | -2.17 | 1.41        | 1.46     |
| 19  | a     | 804 | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 19  | a     | 819 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 19  | b     | 815 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 19  | b     | 835 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 19  | f     | 201 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 19  | k     | 102 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 19  | a     | 819 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 19  | a     | 860 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 19  | b     | 832 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 19  | b     | 819 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 19  | b     | 807 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 19  | a     | 842 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 19  | a     | 829 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 19  | a     | 832 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 19  | a     | 805 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 19  | b     | 825 | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 19  | f     | 201 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 19  | b     | 833 | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 31  | b     | 852 | ZEX  | C14-C13 | 2.16  | 1.40        | 1.35     |
| 19  | a     | 804 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 19  | a     | 820 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 19  | a     | 807 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 19  | a     | 835 | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 19  | b     | 837 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 19  | a     | 802 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 19  | a     | 815 | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 19  | a     | 818 | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 19  | a     | 839 | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 19  | a     | 810 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 19  | b     | 803 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 19  | A     | 407 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 19  | a     | 857 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 19  | l     | 203 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 19  | b     | 826 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 19  | b     | 829 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 19  | l     | 203 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 833 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 19  | b     | 837 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 19  | a     | 808 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 19  | b     | 808 | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 19  | a     | 841 | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 19  | b     | 807 | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 19  | a     | 818 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 19  | b     | 810 | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 19  | a     | 816 | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 19  | b     | 809 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 19  | b     | 808 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 827 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 840 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 19  | b     | 826 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 833 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 19  | k     | 101 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 19  | a     | 838 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | b     | 829 | CLA  | C3B-C4B | 2.14  | 1.49        | 1.42     |
| 19  | b     | 801 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 19  | b     | 822 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 19  | b     | 831 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 19  | a     | 839 | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 19  | a     | 840 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 814 | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 19  | a     | 835 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | b     | 817 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | b     | 811 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 19  | b     | 803 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | b     | 820 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | b     | 811 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 19  | b     | 818 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 833 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | b     | 814 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 19  | D     | 402 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 835 | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 19  | b     | 819 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 19  | a     | 814 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 19  | k     | 101 | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 19  | b     | 818 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | b     | 832 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 19  | b     | 802 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 19  | a     | 828 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 814 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 19  | a     | 829 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 19  | a     | 843 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 19  | a     | 813 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | a     | 824 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 19  | b     | 836 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 19  | f     | 204 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 19  | a     | 834 | CLA  | C3B-C4B | 2.13  | 1.48        | 1.42     |
| 19  | a     | 818 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 19  | f     | 203 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 19  | a     | 841 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | b     | 830 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 19  | a     | 820 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 19  | a     | 832 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 19  | b     | 836 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | b     | 817 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | b     | 829 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | a     | 824 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | a     | 833 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 19  | a     | 856 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 31  | b     | 852 | ZEX  | C34-C33 | 2.12  | 1.40        | 1.35     |
| 19  | a     | 857 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 19  | a     | 841 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 19  | b     | 816 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 31  | f     | 205 | ZEX  | C34-C33 | 2.12  | 1.40        | 1.35     |
| 19  | a     | 857 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 19  | l     | 203 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 19  | a     | 811 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 19  | a     | 824 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 19  | a     | 812 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 19  | a     | 860 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 19  | a     | 823 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 19  | b     | 836 | CLA  | C3B-C4B | 2.12  | 1.48        | 1.42     |
| 19  | b     | 804 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 19  | b     | 832 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 19  | a     | 807 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 19  | a     | 806 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 19  | a     | 829 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 19  | b     | 804 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 19  | b     | 815 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 19  | b     | 823 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 19  | a     | 808 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 31  | b     | 852 | ZEX  | C30-C29 | 2.12  | 1.40        | 1.35     |
| 19  | b     | 807 | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 19  | a     | 803 | CLA  | CMC-C2C | -2.12 | 1.46        | 1.50     |
| 19  | b     | 806 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 19  | D     | 402 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 19  | a     | 838 | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 19  | a     | 805 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 19  | a     | 837 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 19  | a     | 817 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 19  | f     | 203 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 31  | f     | 205 | ZEX  | C10-C9  | 2.11  | 1.40        | 1.35     |
| 19  | b     | 831 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 19  | D     | 402 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 19  | a     | 828 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 19  | b     | 838 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 19  | b     | 805 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 19  | a     | 806 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 19  | b     | 816 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 31  | f     | 205 | ZEX  | C14-C13 | 2.11  | 1.40        | 1.35     |
| 19  | a     | 812 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 19  | b     | 819 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 22  | E     | 101 | HEM  | CMB-C2B | 2.11  | 1.55        | 1.50     |
| 19  | b     | 832 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 19  | b     | 821 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 19  | b     | 805 | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 19  | a     | 856 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 19  | a     | 809 | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 20  | D     | 401 | PHO  | C3B-C2B | -2.11 | 1.37        | 1.40     |
| 19  | a     | 836 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 19  | a     | 841 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | b     | 825 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | f     | 204 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | b     | 829 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | a     | 807 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 19  | a     | 839 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | b     | 834 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | a     | 814 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 21  | a     | 859 | BCR  | C33-C5  | -2.10 | 1.47        | 1.50     |
| 19  | a     | 817 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | a     | 843 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 19  | a     | 819 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 19  | a     | 831 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 838 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 19  | b     | 807 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | b     | 821 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | b     | 823 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | a     | 806 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 19  | b     | 813 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | b     | 832 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | b     | 839 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | k     | 101 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | a     | 817 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 19  | a     | 825 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 19  | b     | 833 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | a     | 825 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 19  | a     | 842 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | a     | 821 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 19  | b     | 824 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 28  | a     | 858 | 45D  | C37-C35 | 2.10  | 1.40        | 1.35     |
| 19  | a     | 817 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 32  | j     | 102 | LMT  | O1'-C1' | -2.09 | 1.36        | 1.40     |
| 19  | a     | 856 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 19  | b     | 812 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 19  | a     | 813 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 19  | D     | 402 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 19  | a     | 813 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 19  | a     | 838 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 19  | a     | 856 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 19  | b     | 806 | CLA  | C3B-C4B | 2.09  | 1.48        | 1.42     |
| 19  | a     | 837 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 19  | a     | 807 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 19  | a     | 806 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 19  | A     | 402 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 19  | j     | 103 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 19  | b     | 834 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 19  | a     | 803 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 19  | b     | 827 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 19  | a     | 829 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 19  | l     | 203 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 19  | b     | 814 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 19  | b     | 831 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 19  | b     | 810 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 19  | b     | 805 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 19  | a     | 826 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 805 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 19  | a     | 843 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 19  | b     | 815 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 19  | a     | 818 | CLA  | CHC-C1C | 2.08  | 1.42        | 1.38     |
| 19  | a     | 811 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 19  | k     | 102 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 19  | a     | 803 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 19  | a     | 843 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 19  | a     | 804 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 19  | A     | 403 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 19  | A     | 407 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 19  | a     | 860 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 19  | A     | 403 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 19  | b     | 812 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 19  | D     | 403 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 19  | a     | 841 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 19  | a     | 812 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 19  | a     | 835 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 19  | a     | 816 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 19  | a     | 832 | CLA  | C3B-C4B | 2.07  | 1.48        | 1.42     |
| 19  | A     | 402 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 19  | a     | 856 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 19  | a     | 840 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 19  | a     | 818 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 19  | j     | 104 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 19  | b     | 835 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 28  | a     | 858 | 45D  | C38-C36 | 2.07  | 1.40        | 1.35     |
| 19  | a     | 826 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 19  | a     | 813 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 19  | a     | 815 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 28  | a     | 858 | 45D  | C29-C25 | 2.07  | 1.40        | 1.35     |
| 19  | b     | 816 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 19  | b     | 821 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | b     | 827 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | b     | 836 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 31  | b     | 852 | ZEX  | C10-C9  | 2.06  | 1.40        | 1.35     |
| 19  | a     | 821 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | A     | 405 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 19  | a     | 827 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 19  | b     | 810 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 19  | a     | 822 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 19  | l     | 202 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | l     | 204 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 19  | A     | 407 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 19  | b     | 803 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 19  | b     | 809 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 19  | a     | 805 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | b     | 801 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | a     | 831 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | b     | 814 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 19  | a     | 834 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 19  | k     | 102 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 19  | b     | 817 | CLA  | CHC-C1C | 2.06  | 1.42        | 1.38     |
| 19  | l     | 204 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 19  | b     | 828 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 19  | b     | 840 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 19  | b     | 811 | CLA  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 19  | a     | 823 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 19  | f     | 203 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 19  | a     | 802 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 19  | a     | 812 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 19  | a     | 836 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 19  | b     | 825 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 19  | b     | 804 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 19  | b     | 810 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 19  | b     | 821 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 19  | a     | 815 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 19  | j     | 104 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 30  | b     | 851 | EQ3  | C21-C22 | 2.05  | 1.40        | 1.35     |
| 19  | a     | 839 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 23  | a     | 801 | CL0  | CHC-C4B | -2.05 | 1.36        | 1.39     |
| 19  | b     | 809 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 19  | a     | 830 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 19  | a     | 860 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 19  | b     | 836 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 21  | j     | 101 | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 19  | b     | 830 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 19  | a     | 827 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 19  | k     | 101 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 19  | k     | 101 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 19  | D     | 402 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 19  | b     | 838 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 19  | b     | 811 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 19  | b     | 822 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | b     | 826 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 21  | a     | 849 | BCR  | C33-C5  | -2.04 | 1.47        | 1.50     |
| 19  | A     | 403 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | j     | 103 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 19  | A     | 402 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | b     | 817 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | b     | 840 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | a     | 808 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | a     | 857 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | b     | 802 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | f     | 204 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 19  | b     | 804 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | b     | 819 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | b     | 806 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 830 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 838 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | b     | 831 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 807 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 820 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 834 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 808 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 810 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 19  | b     | 840 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | a     | 814 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 19  | b     | 813 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 19  | b     | 824 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 19  | a     | 837 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 19  | a     | 802 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 19  | A     | 405 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 19  | D     | 403 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 30  | b     | 851 | EQ3  | C17-C18 | 2.02  | 1.40        | 1.35     |
| 19  | a     | 816 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 19  | a     | 814 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 19  | b     | 820 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 19  | b     | 826 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 19  | b     | 815 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 19  | a     | 833 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | l     | 204 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | a     | 803 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 19  | b     | 834 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | a     | 825 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | b     | 835 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 19  | a     | 822 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 21  | a     | 850 | BCR  | C33-C5  | -2.01 | 1.47        | 1.50     |
| 19  | D     | 403 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 19  | a     | 809 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | b     | 820 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | f     | 204 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 19  | j     | 103 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 27  | l     | 201 | LMG  | O7-C8   | -2.01 | 1.41        | 1.46     |
| 19  | a     | 840 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 28  | a     | 858 | 45D  | C30-C26 | 2.01  | 1.40        | 1.35     |
| 19  | a     | 811 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 19  | b     | 839 | CLA  | CHC-C1C | 2.00  | 1.42        | 1.38     |
| 19  | a     | 823 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 19  | b     | 803 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 19  | b     | 839 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 19  | b     | 808 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |

All (849) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 29  | b     | 844 | ECH  | C15-C16-C17 | 8.38 | 140.66      | 123.52   |
| 19  | a     | 806 | CLA  | C4A-NA-C1A  | 7.16 | 109.94      | 106.68   |
| 19  | a     | 842 | CLA  | C4A-NA-C1A  | 7.05 | 109.89      | 106.68   |
| 19  | a     | 841 | CLA  | C4A-NA-C1A  | 7.01 | 109.88      | 106.68   |
| 19  | a     | 818 | CLA  | C4A-NA-C1A  | 6.99 | 109.87      | 106.68   |
| 19  | b     | 836 | CLA  | C4A-NA-C1A  | 6.99 | 109.87      | 106.68   |
| 19  | a     | 835 | CLA  | C4A-NA-C1A  | 6.96 | 109.86      | 106.68   |
| 19  | b     | 815 | CLA  | C4A-NA-C1A  | 6.94 | 109.84      | 106.68   |
| 19  | j     | 103 | CLA  | C4A-NA-C1A  | 6.87 | 109.81      | 106.68   |
| 19  | b     | 828 | CLA  | C4A-NA-C1A  | 6.85 | 109.80      | 106.68   |
| 19  | b     | 839 | CLA  | C4A-NA-C1A  | 6.84 | 109.80      | 106.68   |
| 19  | a     | 810 | CLA  | C4A-NA-C1A  | 6.83 | 109.79      | 106.68   |
| 19  | a     | 823 | CLA  | C4A-NA-C1A  | 6.82 | 109.79      | 106.68   |
| 19  | a     | 840 | CLA  | C4A-NA-C1A  | 6.82 | 109.79      | 106.68   |
| 19  | D     | 402 | CLA  | C4A-NA-C1A  | 6.79 | 109.78      | 106.68   |
| 19  | l     | 203 | CLA  | C4A-NA-C1A  | 6.77 | 109.77      | 106.68   |
| 19  | a     | 832 | CLA  | C4A-NA-C1A  | 6.76 | 109.76      | 106.68   |
| 19  | b     | 806 | CLA  | C4A-NA-C1A  | 6.76 | 109.76      | 106.68   |
| 19  | a     | 817 | CLA  | C4A-NA-C1A  | 6.75 | 109.76      | 106.68   |
| 19  | b     | 816 | CLA  | C4A-NA-C1A  | 6.74 | 109.75      | 106.68   |
| 19  | D     | 403 | CLA  | C4A-NA-C1A  | 6.72 | 109.75      | 106.68   |
| 19  | b     | 826 | CLA  | C4A-NA-C1A  | 6.71 | 109.74      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | b     | 834 | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 19  | b     | 837 | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 19  | b     | 821 | CLA  | C4A-NA-C1A  | 6.65  | 109.72      | 106.68   |
| 19  | b     | 832 | CLA  | C4A-NA-C1A  | 6.65  | 109.72      | 106.68   |
| 19  | l     | 204 | CLA  | C4A-NA-C1A  | 6.65  | 109.71      | 106.68   |
| 19  | a     | 824 | CLA  | C4A-NA-C1A  | 6.64  | 109.71      | 106.68   |
| 19  | a     | 814 | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 19  | a     | 834 | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 19  | b     | 824 | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 19  | a     | 826 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 19  | b     | 805 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 19  | b     | 838 | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 19  | a     | 808 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 19  | b     | 833 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 19  | a     | 831 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 19  | b     | 811 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 19  | b     | 804 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 19  | a     | 837 | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 19  | A     | 407 | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 19  | a     | 819 | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 19  | b     | 802 | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 19  | f     | 201 | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 19  | a     | 857 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 19  | A     | 403 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 19  | a     | 816 | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 19  | a     | 804 | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 19  | a     | 821 | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 19  | a     | 807 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 19  | a     | 860 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 19  | b     | 810 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 19  | a     | 829 | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 19  | b     | 813 | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 19  | b     | 803 | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 19  | b     | 808 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 19  | a     | 838 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 19  | b     | 840 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 19  | b     | 817 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 19  | a     | 809 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 19  | b     | 820 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 19  | a     | 839 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 19  | f     | 203 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |
| 20  | D     | 401 | PHO  | C4D-CHA-CBD | -6.41 | 105.38      | 108.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 813 | CLA  | C4A-NA-C1A  | 6.39  | 109.60      | 106.68   |
| 19  | A     | 405 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 19  | a     | 828 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 19  | b     | 822 | CLA  | C4A-NA-C1A  | 6.39  | 109.59      | 106.68   |
| 19  | a     | 827 | CLA  | C4A-NA-C1A  | 6.37  | 109.59      | 106.68   |
| 19  | a     | 815 | CLA  | C4A-NA-C1A  | 6.37  | 109.58      | 106.68   |
| 19  | b     | 818 | CLA  | C4A-NA-C1A  | 6.35  | 109.58      | 106.68   |
| 19  | b     | 807 | CLA  | C4A-NA-C1A  | 6.35  | 109.58      | 106.68   |
| 19  | a     | 836 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 19  | a     | 825 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 19  | b     | 831 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 19  | b     | 823 | CLA  | C4A-NA-C1A  | 6.30  | 109.56      | 106.68   |
| 19  | b     | 819 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 19  | f     | 204 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 19  | A     | 402 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 19  | b     | 825 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 19  | a     | 811 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 19  | a     | 843 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 19  | a     | 802 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 19  | a     | 805 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 19  | k     | 102 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 19  | b     | 829 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 23  | a     | 801 | CL0  | C1B-CHB-C4A | 6.22  | 125.32      | 121.32   |
| 19  | l     | 202 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 19  | b     | 812 | CLA  | C4A-NA-C1A  | 6.20  | 109.51      | 106.68   |
| 19  | a     | 812 | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 19  | a     | 833 | CLA  | C4A-NA-C1A  | 6.15  | 109.48      | 106.68   |
| 19  | b     | 809 | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 19  | a     | 830 | CLA  | C4A-NA-C1A  | 6.10  | 109.46      | 106.68   |
| 19  | b     | 814 | CLA  | C4A-NA-C1A  | 6.10  | 109.46      | 106.68   |
| 19  | a     | 820 | CLA  | C4A-NA-C1A  | 6.08  | 109.45      | 106.68   |
| 19  | j     | 104 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 19  | b     | 830 | CLA  | C4A-NA-C1A  | 6.00  | 109.42      | 106.68   |
| 19  | a     | 822 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 20  | A     | 404 | PHO  | C4D-CHA-CBD | -5.95 | 105.60      | 108.45   |
| 19  | a     | 803 | CLA  | C4A-NA-C1A  | 5.91  | 109.38      | 106.68   |
| 19  | b     | 827 | CLA  | C4A-NA-C1A  | 5.85  | 109.35      | 106.68   |
| 19  | k     | 101 | CLA  | C4A-NA-C1A  | 5.80  | 109.32      | 106.68   |
| 19  | a     | 856 | CLA  | C4A-NA-C1A  | 5.76  | 109.31      | 106.68   |
| 19  | b     | 835 | CLA  | C4A-NA-C1A  | 5.68  | 109.27      | 106.68   |
| 19  | b     | 801 | CLA  | C4A-NA-C1A  | 5.49  | 109.18      | 106.68   |
| 28  | a     | 858 | 45D  | C42-C41-C37 | 5.26  | 134.28      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | b     | 844 | ECH  | C12-C13-C14 | 4.81  | 126.57      | 119.01   |
| 29  | b     | 844 | ECH  | C19-C18-C17 | 4.68  | 126.37      | 119.01   |
| 29  | b     | 844 | ECH  | C24-C23-C22 | -4.55 | 119.51      | 126.23   |
| 26  | a     | 853 | LHG  | O4-P-O5     | 4.47  | 133.24      | 112.44   |
| 26  | a     | 852 | LHG  | O4-P-O5     | 4.45  | 133.14      | 112.44   |
| 26  | a     | 855 | LHG  | O4-P-O5     | 4.43  | 133.04      | 112.44   |
| 26  | f     | 206 | LHG  | O4-P-O5     | 4.41  | 132.96      | 112.44   |
| 29  | b     | 844 | ECH  | C1-C6-C5    | -4.39 | 116.64      | 122.64   |
| 26  | b     | 849 | LHG  | O4-P-O5     | 4.38  | 132.84      | 112.44   |
| 29  | m     | 101 | ECH  | C15-C16-C17 | 4.20  | 132.12      | 123.52   |
| 31  | f     | 205 | ZEX  | C35-C15-C14 | 4.16  | 132.04      | 123.52   |
| 29  | m     | 101 | ECH  | C1-C6-C5    | -4.11 | 117.02      | 122.64   |
| 29  | b     | 844 | ECH  | C10-C11-C12 | 4.07  | 135.00      | 123.20   |
| 20  | A     | 404 | PHO  | C2B-C1B-NB  | -3.82 | 106.67      | 109.43   |
| 29  | m     | 101 | ECH  | C23-C22-C21 | 3.80  | 124.98      | 119.01   |
| 29  | b     | 844 | ECH  | C35-C13-C14 | -3.77 | 116.71      | 122.82   |
| 29  | b     | 844 | ECH  | C36-C18-C17 | -3.73 | 116.77      | 122.82   |
| 29  | m     | 101 | ECH  | C37-C22-C21 | -3.69 | 116.84      | 122.82   |
| 19  | a     | 831 | CLA  | CAA-C2A-C3A | -3.65 | 103.13      | 113.00   |
| 31  | b     | 852 | ZEX  | C39-C29-C30 | -3.57 | 117.04      | 122.82   |
| 21  | b     | 845 | BCR  | C15-C16-C17 | -3.53 | 116.29      | 123.52   |
| 19  | b     | 812 | CLA  | O2D-CGD-O1D | -3.53 | 116.98      | 123.85   |
| 28  | a     | 858 | 45D  | C28-C26-C30 | -3.52 | 117.11      | 122.82   |
| 31  | b     | 852 | ZEX  | C35-C15-C14 | 3.48  | 130.63      | 123.52   |
| 31  | f     | 205 | ZEX  | C19-C9-C10  | -3.47 | 117.20      | 122.82   |
| 31  | b     | 852 | ZEX  | C19-C9-C10  | -3.46 | 117.21      | 122.82   |
| 19  | a     | 815 | CLA  | O2D-CGD-O1D | -3.46 | 117.12      | 123.85   |
| 29  | m     | 101 | ECH  | C34-C9-C10  | -3.44 | 117.24      | 122.82   |
| 28  | a     | 858 | 45D  | C27-C25-C29 | -3.43 | 117.26      | 122.82   |
| 29  | b     | 844 | ECH  | C15-C14-C13 | 3.42  | 132.07      | 127.28   |
| 29  | m     | 101 | ECH  | C19-C18-C17 | 3.42  | 124.38      | 119.01   |
| 19  | a     | 814 | CLA  | O2D-CGD-O1D | -3.41 | 117.22      | 123.85   |
| 31  | f     | 205 | ZEX  | C39-C29-C30 | -3.40 | 117.31      | 122.82   |
| 19  | a     | 831 | CLA  | O2D-CGD-O1D | -3.39 | 117.26      | 123.85   |
| 30  | b     | 851 | EQ3  | C34-C9-C10  | -3.36 | 117.37      | 122.82   |
| 30  | b     | 851 | EQ3  | C24-C23-C22 | 3.34  | 131.17      | 126.23   |
| 21  | k     | 103 | BCR  | C2-C1-C6    | 3.31  | 115.25      | 110.44   |
| 20  | D     | 401 | PHO  | C2B-C1B-NB  | -3.30 | 107.04      | 109.43   |
| 19  | b     | 835 | CLA  | O2D-CGD-O1D | -3.29 | 117.45      | 123.85   |
| 23  | a     | 801 | CL0  | O2D-CGD-CBD | 3.29  | 114.56      | 110.95   |
| 29  | b     | 844 | ECH  | C30-C25-C24 | 3.28  | 124.56      | 115.65   |
| 19  | b     | 804 | CLA  | O2D-CGD-O1D | -3.26 | 117.50      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | b     | 851 | EQ3  | C16-C15-C14 | 3.22  | 130.10      | 123.52   |
| 19  | a     | 805 | CLA  | O2D-CGD-O1D | -3.19 | 117.63      | 123.85   |
| 19  | b     | 828 | CLA  | O2D-CGD-O1D | -3.17 | 117.67      | 123.85   |
| 19  | a     | 804 | CLA  | C3B-C4B-NB  | -3.15 | 107.72      | 110.53   |
| 29  | m     | 101 | ECH  | C16-C15-C14 | 3.15  | 129.97      | 123.52   |
| 19  | b     | 806 | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 19  | a     | 834 | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 30  | b     | 851 | EQ3  | C37-C22-C21 | -3.14 | 117.73      | 122.82   |
| 31  | b     | 852 | ZEX  | C15-C35-C34 | 3.14  | 129.94      | 123.52   |
| 21  | b     | 845 | BCR  | C15-C14-C13 | -3.13 | 122.89      | 127.28   |
| 29  | b     | 844 | ECH  | C34-C9-C10  | -3.13 | 117.75      | 122.82   |
| 30  | b     | 851 | EQ3  | C15-C16-C17 | 3.13  | 129.91      | 123.52   |
| 19  | b     | 836 | CLA  | O2D-CGD-O1D | -3.12 | 117.78      | 123.85   |
| 19  | a     | 805 | CLA  | C3B-C4B-NB  | -3.12 | 107.75      | 110.53   |
| 19  | a     | 835 | CLA  | O2D-CGD-O1D | -3.12 | 117.78      | 123.85   |
| 19  | b     | 801 | CLA  | CAA-CBA-CGA | -3.12 | 104.36      | 113.21   |
| 19  | a     | 836 | CLA  | C3B-C4B-NB  | -3.11 | 107.75      | 110.53   |
| 19  | b     | 802 | CLA  | C3B-C4B-NB  | -3.11 | 107.76      | 110.53   |
| 19  | b     | 832 | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 19  | a     | 860 | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 29  | m     | 101 | ECH  | C36-C18-C17 | -3.09 | 117.80      | 122.82   |
| 19  | b     | 831 | CLA  | C3B-C4B-NB  | -3.09 | 107.77      | 110.53   |
| 19  | b     | 823 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 19  | a     | 809 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 19  | b     | 837 | CLA  | O2D-CGD-O1D | -3.08 | 117.85      | 123.85   |
| 19  | A     | 405 | CLA  | O2D-CGD-O1D | -3.08 | 117.85      | 123.85   |
| 19  | a     | 828 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 19  | a     | 808 | CLA  | C3B-C4B-NB  | -3.07 | 107.78      | 110.53   |
| 20  | A     | 404 | PHO  | O1D-CGD-CBD | 3.07  | 129.39      | 124.72   |
| 19  | a     | 840 | CLA  | O2D-CGD-O1D | -3.07 | 117.88      | 123.85   |
| 29  | b     | 844 | ECH  | C37-C22-C21 | -3.06 | 117.85      | 122.82   |
| 19  | b     | 809 | CLA  | C3B-C4B-NB  | -3.06 | 107.80      | 110.53   |
| 23  | a     | 801 | CL0  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 30  | b     | 851 | EQ3  | C37-C22-C23 | 3.06  | 122.76      | 118.09   |
| 19  | a     | 813 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 19  | a     | 832 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 19  | b     | 802 | CLA  | O2D-CGD-O1D | -3.05 | 117.92      | 123.85   |
| 19  | j     | 104 | CLA  | C3B-C4B-NB  | -3.03 | 107.82      | 110.53   |
| 19  | a     | 821 | CLA  | O2D-CGD-O1D | -3.03 | 117.94      | 123.85   |
| 31  | f     | 205 | ZEX  | C15-C35-C34 | 3.03  | 129.72      | 123.52   |
| 19  | b     | 838 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 19  | b     | 824 | CLA  | O2D-CGD-O1D | -3.02 | 117.98      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 836 | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 19  | a     | 838 | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 19  | a     | 826 | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 19  | a     | 818 | CLA  | O2D-CGD-O1D | -3.00 | 118.00      | 123.85   |
| 19  | a     | 804 | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 19  | b     | 813 | CLA  | O2D-CGD-O1D | -2.99 | 118.02      | 123.85   |
| 19  | b     | 823 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 19  | b     | 803 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 19  | b     | 839 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 19  | b     | 821 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 19  | b     | 827 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 19  | a     | 829 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 19  | b     | 803 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 19  | a     | 839 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 19  | f     | 204 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 19  | a     | 833 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 19  | b     | 801 | CLA  | O2D-CGD-O1D | -2.98 | 118.06      | 123.85   |
| 23  | a     | 801 | CL0  | C4D-CHA-CBD | -2.97 | 105.97      | 108.97   |
| 19  | b     | 815 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 19  | a     | 811 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 20  | D     | 401 | PHO  | O1D-CGD-CBD | 2.97  | 129.23      | 124.72   |
| 19  | a     | 842 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 19  | a     | 841 | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 21  | b     | 845 | BCR  | C2-C1-C6    | 2.96  | 114.73      | 110.44   |
| 19  | f     | 201 | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 19  | a     | 812 | CLA  | O2D-CGD-O1D | -2.96 | 118.10      | 123.85   |
| 19  | b     | 818 | CLA  | C3B-C4B-NB  | -2.95 | 107.89      | 110.53   |
| 19  | a     | 808 | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 19  | a     | 806 | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 23  | a     | 801 | CL0  | CHA-C1A-C2A | -2.95 | 126.38      | 133.31   |
| 19  | a     | 820 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 19  | D     | 403 | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 19  | b     | 809 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 19  | a     | 843 | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 21  | a     | 851 | BCR  | C15-C16-C17 | -2.94 | 117.50      | 123.52   |
| 19  | l     | 203 | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 19  | a     | 839 | CLA  | O2D-CGD-O1D | -2.94 | 118.14      | 123.85   |
| 19  | a     | 828 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 19  | a     | 833 | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 19  | b     | 840 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 19  | a     | 827 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 21  | a     | 849 | BCR  | C15-C16-C17 | -2.92 | 117.54      | 123.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | a     | 855 | LHG  | O8-C23-C24  | 2.92  | 120.74      | 111.83   |
| 19  | b     | 831 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 19  | f     | 201 | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 19  | A     | 402 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 19  | b     | 814 | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 19  | b     | 822 | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 19  | b     | 825 | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 19  | b     | 819 | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 19  | l     | 204 | CLA  | O2D-CGD-O1D | -2.90 | 118.19      | 123.85   |
| 19  | b     | 807 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 19  | b     | 820 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 21  | j     | 101 | BCR  | C15-C16-C17 | -2.90 | 117.58      | 123.52   |
| 19  | a     | 816 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 19  | f     | 204 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 19  | b     | 816 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 19  | a     | 822 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 26  | f     | 206 | LHG  | O8-C23-C24  | 2.89  | 120.65      | 111.83   |
| 20  | D     | 401 | PHO  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 19  | a     | 824 | CLA  | CAA-C2A-C3A | -2.89 | 105.19      | 113.00   |
| 19  | a     | 827 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 26  | b     | 849 | LHG  | O8-C23-C24  | 2.89  | 120.64      | 111.83   |
| 19  | b     | 810 | CLA  | O2D-CGD-O1D | -2.88 | 118.23      | 123.85   |
| 19  | a     | 802 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 19  | b     | 822 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 19  | A     | 403 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 19  | b     | 807 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 27  | l     | 201 | LMG  | O6-C1-O1    | -2.88 | 103.24      | 110.04   |
| 19  | a     | 819 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |
| 19  | b     | 829 | CLA  | O2D-CGD-O1D | -2.87 | 118.25      | 123.85   |
| 19  | b     | 834 | CLA  | O2D-CGD-O1D | -2.87 | 118.25      | 123.85   |
| 19  | a     | 842 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 19  | a     | 821 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 19  | k     | 102 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 21  | i     | 102 | BCR  | C2-C1-C6    | 2.86  | 114.60      | 110.44   |
| 27  | b     | 848 | LMG  | O6-C1-O1    | -2.86 | 103.28      | 110.04   |
| 21  | b     | 842 | BCR  | C33-C5-C6   | -2.86 | 121.36      | 124.48   |
| 19  | b     | 833 | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 19  | a     | 860 | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 19  | A     | 407 | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 19  | b     | 805 | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 19  | b     | 811 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 19  | a     | 857 | CLA  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | b     | 814 | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 19  | a     | 817 | CLA  | O2D-CGD-O1D | -2.85 | 118.31      | 123.85   |
| 19  | b     | 801 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 19  | a     | 813 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 19  | l     | 202 | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 19  | a     | 819 | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 19  | a     | 857 | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 19  | b     | 812 | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 19  | b     | 811 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 19  | b     | 821 | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 19  | b     | 808 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 19  | a     | 823 | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 19  | b     | 817 | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 19  | a     | 824 | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 19  | b     | 820 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 19  | a     | 812 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 19  | j     | 104 | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 19  | A     | 403 | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 19  | b     | 840 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 19  | b     | 830 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 31  | f     | 205 | ZEX  | C40-C33-C34 | -2.79 | 118.30      | 122.82   |
| 19  | b     | 828 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 19  | a     | 825 | CLA  | O2D-CGD-O1D | -2.79 | 118.43      | 123.85   |
| 19  | b     | 819 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 27  | a     | 854 | LMG  | O6-C1-O1    | -2.78 | 103.47      | 110.04   |
| 19  | b     | 838 | CLA  | C1-C2-C3    | -2.78 | 121.65      | 126.20   |
| 19  | b     | 826 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 19  | b     | 808 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 19  | b     | 827 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 19  | a     | 810 | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 21  | a     | 847 | BCR  | C24-C23-C22 | -2.77 | 122.14      | 126.23   |
| 30  | b     | 851 | EQ3  | C35-C13-C14 | -2.77 | 118.33      | 122.82   |
| 19  | k     | 102 | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 19  | a     | 825 | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 19  | b     | 838 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 26  | a     | 853 | LHG  | O8-C23-C24  | 2.76  | 120.26      | 111.83   |
| 19  | b     | 835 | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 19  | a     | 856 | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 19  | a     | 832 | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 29  | m     | 101 | ECH  | C21-C20-C19 | 2.76  | 131.19      | 123.20   |
| 24  | a     | 844 | PQN  | C11-C3-C2   | -2.75 | 120.17      | 124.89   |
| 19  | a     | 822 | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | m     | 101 | ECH  | C12-C13-C14 | 2.75  | 123.34      | 119.01   |
| 21  | a     | 851 | BCR  | C15-C14-C13 | -2.75 | 123.42      | 127.28   |
| 28  | a     | 858 | 45D  | C03-C07-C19 | 2.75  | 123.10      | 115.65   |
| 19  | A     | 405 | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 21  | l     | 205 | BCR  | C33-C5-C6   | -2.75 | 121.49      | 124.48   |
| 19  | b     | 822 | CLA  | C1-C2-C3    | -2.74 | 121.70      | 126.20   |
| 19  | a     | 809 | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 19  | D     | 402 | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 21  | A     | 406 | BCR  | C27-C26-C25 | 2.74  | 126.40      | 122.70   |
| 19  | a     | 806 | CLA  | CHB-C4A-NA  | 2.73  | 128.35      | 124.40   |
| 19  | a     | 837 | CLA  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 19  | a     | 815 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 19  | b     | 825 | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 19  | D     | 403 | CLA  | C3B-C4B-NB  | -2.73 | 108.10      | 110.53   |
| 19  | f     | 203 | CLA  | O2D-CGD-O1D | -2.73 | 118.54      | 123.85   |
| 21  | l     | 205 | BCR  | C27-C26-C25 | 2.72  | 126.39      | 122.70   |
| 19  | a     | 818 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 29  | m     | 101 | ECH  | C35-C13-C14 | -2.72 | 118.41      | 122.82   |
| 19  | b     | 833 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 21  | b     | 847 | BCR  | C27-C26-C25 | 2.72  | 126.38      | 122.70   |
| 19  | l     | 203 | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 19  | a     | 824 | CLA  | CHB-C4A-NA  | 2.72  | 128.32      | 124.40   |
| 21  | j     | 101 | BCR  | C15-C14-C13 | -2.72 | 123.47      | 127.28   |
| 19  | k     | 101 | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 19  | a     | 807 | CLA  | C3B-C4B-NB  | -2.72 | 108.11      | 110.53   |
| 19  | a     | 824 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 19  | a     | 803 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 19  | a     | 843 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 19  | b     | 805 | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 19  | j     | 103 | CLA  | O2D-CGD-O1D | -2.71 | 118.57      | 123.85   |
| 19  | b     | 805 | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 23  | a     | 801 | CL0  | C1C-CHC-C4B | 2.71  | 125.76      | 116.07   |
| 19  | b     | 812 | CLA  | O2D-CGD-CBD | 2.71  | 115.97      | 111.23   |
| 19  | b     | 818 | CLA  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 31  | f     | 205 | ZEX  | C32-C33-C34 | 2.71  | 123.26      | 119.01   |
| 21  | a     | 859 | BCR  | C33-C5-C6   | -2.70 | 121.53      | 124.48   |
| 19  | b     | 816 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 19  | a     | 830 | CLA  | O2D-CGD-O1D | -2.70 | 118.59      | 123.85   |
| 21  | A     | 406 | BCR  | C24-C23-C22 | -2.70 | 122.24      | 126.23   |
| 19  | j     | 103 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 31  | b     | 852 | ZEX  | C40-C33-C34 | -2.70 | 118.45      | 122.82   |
| 21  | b     | 842 | BCR  | C24-C23-C22 | -2.69 | 122.25      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | a     | 850 | BCR  | C15-C16-C17 | -2.69 | 118.02      | 123.52   |
| 21  | a     | 849 | BCR  | C15-C14-C13 | -2.68 | 123.51      | 127.28   |
| 31  | b     | 852 | ZEX  | C20-C13-C14 | -2.68 | 118.47      | 122.82   |
| 19  | a     | 826 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 23  | a     | 801 | CL0  | C3D-C4D-CHA | 2.68  | 112.61      | 108.54   |
| 19  | a     | 803 | CLA  | O2D-CGD-O1D | -2.68 | 118.64      | 123.85   |
| 19  | b     | 815 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 19  | b     | 804 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 19  | k     | 101 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 32  | j     | 102 | LMT  | C1'-O5'-C5' | -2.67 | 108.50      | 113.72   |
| 19  | a     | 807 | CLA  | O2D-CGD-O1D | -2.67 | 118.65      | 123.85   |
| 21  | l     | 205 | BCR  | C15-C16-C17 | -2.67 | 118.06      | 123.52   |
| 19  | a     | 831 | CLA  | O2D-CGD-CBD | 2.66  | 115.89      | 111.23   |
| 21  | a     | 859 | BCR  | C27-C26-C25 | 2.66  | 126.30      | 122.70   |
| 29  | b     | 844 | ECH  | C37-C22-C23 | 2.66  | 122.14      | 118.09   |
| 21  | a     | 850 | BCR  | C33-C5-C6   | -2.65 | 121.59      | 124.48   |
| 19  | a     | 837 | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 19  | a     | 836 | CLA  | C1-C2-C3    | -2.65 | 121.86      | 126.20   |
| 21  | b     | 846 | BCR  | C27-C26-C25 | 2.65  | 126.28      | 122.70   |
| 21  | a     | 846 | BCR  | C24-C23-C22 | -2.65 | 122.32      | 126.23   |
| 31  | f     | 205 | ZEX  | C20-C13-C14 | -2.65 | 118.53      | 122.82   |
| 20  | A     | 404 | PHO  | O2D-CGD-O1D | -2.64 | 118.71      | 123.85   |
| 19  | A     | 407 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 19  | b     | 829 | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 19  | b     | 816 | CLA  | C1-C2-C3    | -2.64 | 121.88      | 126.20   |
| 19  | a     | 835 | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 19  | a     | 816 | CLA  | C3B-C4B-NB  | -2.64 | 108.18      | 110.53   |
| 21  | b     | 842 | BCR  | C27-C26-C25 | 2.64  | 126.27      | 122.70   |
| 19  | b     | 813 | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 21  | k     | 103 | BCR  | C15-C14-C13 | -2.63 | 123.58      | 127.28   |
| 19  | a     | 831 | CLA  | CHB-C4A-NA  | 2.63  | 128.20      | 124.40   |
| 21  | b     | 845 | BCR  | C27-C26-C25 | 2.63  | 126.25      | 122.70   |
| 19  | a     | 838 | CLA  | C3B-C4B-NB  | -2.63 | 108.19      | 110.53   |
| 19  | b     | 823 | CLA  | CHB-C4A-NA  | 2.62  | 128.18      | 124.40   |
| 19  | a     | 841 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 19  | a     | 811 | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 21  | a     | 850 | BCR  | C15-C14-C13 | -2.61 | 123.62      | 127.28   |
| 30  | b     | 851 | EQ3  | C12-C13-C14 | 2.61  | 123.12      | 119.01   |
| 21  | a     | 849 | BCR  | C24-C23-C22 | -2.61 | 122.38      | 126.23   |
| 19  | b     | 811 | CLA  | C1-C2-C3    | -2.61 | 122.54      | 126.76   |
| 19  | a     | 814 | CLA  | O2D-CGD-CBD | 2.61  | 115.79      | 111.23   |
| 24  | b     | 841 | PQN  | C11-C3-C2   | -2.61 | 120.42      | 124.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 818 | CLA  | CHB-C4A-NA  | 2.60  | 128.16      | 124.40   |
| 19  | a     | 803 | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 19  | b     | 830 | CLA  | CMB-C2B-C1B | -2.60 | 121.46      | 125.42   |
| 19  | a     | 837 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 19  | f     | 204 | CLA  | C1-C2-C3    | -2.60 | 122.56      | 126.76   |
| 19  | D     | 403 | CLA  | CHB-C4A-NA  | 2.60  | 128.15      | 124.40   |
| 19  | a     | 821 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 19  | j     | 103 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 19  | b     | 816 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 19  | b     | 832 | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 19  | a     | 826 | CLA  | CHB-C4A-NA  | 2.59  | 128.14      | 124.40   |
| 21  | a     | 850 | BCR  | C27-C26-C25 | 2.59  | 126.20      | 122.70   |
| 21  | k     | 103 | BCR  | C15-C16-C17 | -2.59 | 118.23      | 123.52   |
| 19  | b     | 830 | CLA  | C3B-C4B-NB  | -2.58 | 108.22      | 110.53   |
| 21  | i     | 101 | BCR  | C27-C26-C25 | 2.58  | 126.20      | 122.70   |
| 29  | b     | 844 | ECH  | C34-C9-C8   | 2.58  | 122.03      | 118.09   |
| 31  | b     | 852 | ZEX  | C12-C13-C14 | 2.58  | 123.07      | 119.01   |
| 31  | b     | 852 | ZEX  | C32-C33-C34 | 2.58  | 123.07      | 119.01   |
| 19  | a     | 831 | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 21  | a     | 847 | BCR  | C27-C26-C25 | 2.58  | 126.19      | 122.70   |
| 19  | b     | 838 | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 19  | b     | 834 | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 30  | b     | 851 | EQ3  | C36-C18-C17 | -2.57 | 118.66      | 122.82   |
| 19  | a     | 818 | CLA  | O2A-CGA-O1A | -2.56 | 117.21      | 123.63   |
| 19  | a     | 806 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 21  | a     | 848 | BCR  | C33-C5-C6   | -2.56 | 121.69      | 124.48   |
| 21  | b     | 843 | BCR  | C33-C5-C6   | -2.56 | 121.69      | 124.48   |
| 19  | b     | 835 | CLA  | CMB-C2B-C1B | -2.56 | 121.52      | 125.42   |
| 21  | i     | 102 | BCR  | C28-C27-C26 | -2.56 | 109.49      | 114.06   |
| 21  | b     | 846 | BCR  | C2-C1-C6    | 2.56  | 114.16      | 110.44   |
| 19  | a     | 834 | CLA  | C3B-C4B-NB  | -2.56 | 108.25      | 110.53   |
| 31  | f     | 205 | ZEX  | C12-C13-C14 | 2.56  | 123.03      | 119.01   |
| 21  | a     | 859 | BCR  | C15-C16-C17 | -2.56 | 118.29      | 123.52   |
| 21  | A     | 406 | BCR  | C33-C5-C6   | -2.55 | 121.70      | 124.48   |
| 19  | a     | 817 | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 21  | j     | 101 | BCR  | C33-C5-C6   | -2.55 | 121.70      | 124.48   |
| 21  | a     | 849 | BCR  | C27-C26-C25 | 2.55  | 126.15      | 122.70   |
| 21  | k     | 103 | BCR  | C27-C26-C25 | 2.54  | 126.14      | 122.70   |
| 21  | a     | 846 | BCR  | C33-C5-C6   | -2.54 | 121.71      | 124.48   |
| 19  | b     | 810 | CLA  | C3B-C4B-NB  | -2.54 | 108.26      | 110.53   |
| 21  | a     | 848 | BCR  | C27-C26-C25 | 2.54  | 126.14      | 122.70   |
| 28  | a     | 858 | 45D  | C24-C26-C30 | 2.54  | 123.00      | 119.01   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | b     | 818 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 19  | a     | 815 | CLA  | C1-C2-C3    | -2.53 | 122.05      | 126.20   |
| 19  | b     | 804 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 26  | a     | 852 | LHG  | O8-C23-C24  | 2.53  | 119.55      | 111.83   |
| 19  | a     | 835 | CLA  | C1-C2-C3    | -2.53 | 122.05      | 126.20   |
| 23  | a     | 801 | CL0  | C4C-CHD-C1D | 2.53  | 125.12      | 116.07   |
| 21  | b     | 845 | BCR  | C11-C10-C9  | -2.52 | 123.74      | 127.28   |
| 26  | a     | 853 | LHG  | C11-C10-C9  | -2.52 | 101.61      | 114.37   |
| 19  | l     | 204 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 19  | a     | 860 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 19  | a     | 836 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 21  | f     | 202 | BCR  | C27-C26-C25 | 2.52  | 126.11      | 122.70   |
| 19  | a     | 820 | CLA  | C1-C2-C3    | -2.52 | 122.07      | 126.20   |
| 19  | b     | 831 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 26  | a     | 855 | LHG  | C11-C10-C9  | -2.52 | 101.64      | 114.37   |
| 19  | a     | 823 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 19  | l     | 203 | CLA  | CHB-C4A-NA  | 2.52  | 128.03      | 124.40   |
| 21  | a     | 851 | BCR  | C33-C5-C6   | -2.51 | 121.74      | 124.48   |
| 19  | a     | 840 | CLA  | CHB-C4A-NA  | 2.51  | 128.03      | 124.40   |
| 19  | a     | 804 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 21  | i     | 102 | BCR  | C15-C16-C17 | -2.51 | 118.38      | 123.52   |
| 19  | f     | 203 | CLA  | C1-C2-C3    | -2.51 | 122.70      | 126.76   |
| 19  | b     | 821 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 21  | b     | 842 | BCR  | C15-C16-C17 | -2.51 | 118.39      | 123.52   |
| 19  | f     | 201 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 21  | a     | 859 | BCR  | C24-C23-C22 | -2.51 | 122.53      | 126.23   |
| 19  | b     | 815 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 19  | b     | 836 | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 19  | a     | 814 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 19  | b     | 828 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 19  | b     | 832 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 21  | i     | 102 | BCR  | C7-C8-C9    | -2.50 | 122.54      | 126.23   |
| 19  | a     | 840 | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 19  | A     | 407 | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 19  | b     | 837 | CLA  | C1-C2-C3    | -2.49 | 122.73      | 126.76   |
| 19  | b     | 814 | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 19  | a     | 828 | CLA  | C1-C2-C3    | -2.49 | 122.11      | 126.20   |
| 19  | a     | 819 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 23  | a     | 801 | CL0  | CMD-C2D-C3D | 2.49  | 129.65      | 124.68   |
| 19  | a     | 803 | CLA  | O2A-CGA-O1A | -2.49 | 117.41      | 123.63   |
| 21  | b     | 843 | BCR  | C27-C26-C25 | 2.48  | 126.06      | 122.70   |
| 19  | l     | 202 | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 810 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 19  | a     | 842 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 19  | A     | 402 | CLA  | C3B-C4B-NB  | -2.48 | 108.32      | 110.53   |
| 29  | m     | 101 | ECH  | C24-C23-C22 | 2.48  | 129.90      | 126.23   |
| 19  | f     | 204 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 19  | b     | 817 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 19  | a     | 809 | CLA  | CMB-C2B-C1B | -2.47 | 121.66      | 125.42   |
| 19  | l     | 204 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 27  | l     | 201 | LMG  | C38-C37-C36 | -2.46 | 101.92      | 114.37   |
| 21  | b     | 842 | BCR  | C11-C10-C9  | -2.46 | 123.83      | 127.28   |
| 19  | b     | 810 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 19  | a     | 843 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 20  | A     | 404 | PHO  | CMB-C2B-C3B | 2.46  | 129.60      | 124.68   |
| 19  | D     | 402 | CLA  | C3B-C4B-NB  | -2.46 | 108.34      | 110.53   |
| 19  | b     | 834 | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 19  | a     | 813 | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 19  | b     | 802 | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 19  | l     | 202 | CLA  | C1-C2-C3    | -2.46 | 122.79      | 126.76   |
| 21  | a     | 849 | BCR  | C33-C5-C6   | -2.45 | 121.81      | 124.48   |
| 19  | a     | 807 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 19  | a     | 830 | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 19  | a     | 838 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 19  | b     | 830 | CLA  | C1-C2-C3    | -2.44 | 122.81      | 126.76   |
| 19  | b     | 827 | CLA  | CHB-C4A-NA  | 2.44  | 127.93      | 124.40   |
| 19  | b     | 805 | CLA  | C1-C2-C3    | -2.44 | 122.19      | 126.20   |
| 19  | b     | 813 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 19  | a     | 829 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 19  | b     | 840 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 19  | a     | 806 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 19  | b     | 822 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 19  | a     | 815 | CLA  | O2D-CGD-CBD | 2.44  | 115.49      | 111.23   |
| 28  | a     | 858 | 45D  | C39-C35-C37 | -2.44 | 118.87      | 122.82   |
| 19  | A     | 405 | CLA  | CHB-C4A-NA  | 2.44  | 127.91      | 124.40   |
| 19  | a     | 817 | CLA  | CHB-C4A-NA  | 2.44  | 127.91      | 124.40   |
| 26  | a     | 852 | LHG  | C11-C10-C9  | -2.43 | 102.08      | 114.37   |
| 19  | a     | 834 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 19  | a     | 816 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 19  | b     | 812 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 27  | b     | 850 | LMG  | C1-O6-C5    | -2.43 | 108.98      | 113.72   |
| 19  | a     | 809 | CLA  | C1-C2-C3    | -2.43 | 122.22      | 126.20   |
| 19  | A     | 403 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 19  | a     | 814 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | a     | 858 | 45D  | C40-C36-C38 | -2.42 | 118.89      | 122.82   |
| 19  | b     | 807 | CLA  | O2A-CGA-O1A | -2.42 | 117.58      | 123.63   |
| 19  | a     | 857 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 26  | f     | 206 | LHG  | C11-C10-C9  | -2.42 | 102.14      | 114.37   |
| 19  | a     | 825 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 19  | a     | 828 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 19  | a     | 812 | CLA  | CHB-C4A-NA  | 2.41  | 127.89      | 124.40   |
| 19  | k     | 102 | CLA  | CHB-C4A-NA  | 2.41  | 127.89      | 124.40   |
| 21  | i     | 102 | BCR  | C29-C30-C25 | 2.41  | 113.95      | 110.44   |
| 26  | a     | 852 | LHG  | C20-C19-C18 | -2.41 | 102.17      | 114.37   |
| 27  | b     | 850 | LMG  | C40-C39-C38 | -2.41 | 102.18      | 114.37   |
| 19  | b     | 811 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 19  | a     | 811 | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 21  | i     | 101 | BCR  | C15-C16-C17 | -2.41 | 118.60      | 123.52   |
| 21  | j     | 101 | BCR  | C27-C26-C25 | 2.41  | 125.95      | 122.70   |
| 19  | a     | 833 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 19  | a     | 841 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 27  | b     | 848 | LMG  | C40-C39-C38 | -2.40 | 102.23      | 114.37   |
| 19  | a     | 802 | CLA  | O2A-CGA-O1A | -2.40 | 117.62      | 123.63   |
| 19  | A     | 402 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 27  | a     | 854 | LMG  | O1-C7-C8    | -2.40 | 104.98      | 110.82   |
| 20  | D     | 401 | PHO  | CMB-C2B-C3B | 2.40  | 129.48      | 124.68   |
| 19  | b     | 803 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 19  | b     | 820 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 19  | a     | 810 | CLA  | C3B-C4B-NB  | -2.40 | 108.39      | 110.53   |
| 19  | b     | 819 | CLA  | O2A-CGA-O1A | -2.40 | 117.63      | 123.63   |
| 19  | a     | 809 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 19  | a     | 823 | CLA  | C3B-C4B-NB  | -2.39 | 108.39      | 110.53   |
| 19  | b     | 819 | CLA  | CHB-C4A-NA  | 2.39  | 127.86      | 124.40   |
| 27  | b     | 850 | LMG  | O6-C1-O1    | -2.39 | 104.39      | 110.04   |
| 19  | b     | 835 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 21  | a     | 846 | BCR  | C27-C26-C25 | 2.39  | 125.94      | 122.70   |
| 19  | a     | 802 | CLA  | C1-C2-C3    | -2.39 | 122.28      | 126.20   |
| 19  | b     | 806 | CLA  | O2A-CGA-O1A | -2.39 | 117.65      | 123.63   |
| 19  | b     | 808 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 19  | b     | 833 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 21  | f     | 202 | BCR  | C33-C5-C6   | -2.39 | 121.88      | 124.48   |
| 27  | b     | 848 | LMG  | C38-C37-C36 | -2.39 | 102.30      | 114.37   |
| 19  | b     | 835 | CLA  | O2A-CGA-O1A | -2.39 | 117.66      | 123.63   |
| 27  | b     | 850 | LMG  | C38-C37-C36 | -2.39 | 102.31      | 114.37   |
| 19  | b     | 824 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 21  | a     | 846 | BCR  | C15-C14-C13 | -2.38 | 123.94      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 831 | CLA  | CMB-C2B-C1B | -2.38 | 121.80      | 125.42   |
| 19  | b     | 801 | CLA  | C1-C2-C3    | -2.38 | 122.30      | 126.20   |
| 19  | a     | 808 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 26  | a     | 855 | LHG  | C20-C19-C18 | -2.38 | 102.35      | 114.37   |
| 21  | b     | 843 | BCR  | C15-C16-C17 | -2.38 | 118.66      | 123.52   |
| 19  | b     | 824 | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 26  | f     | 206 | LHG  | C20-C19-C18 | -2.37 | 102.39      | 114.37   |
| 21  | a     | 847 | BCR  | C33-C5-C6   | -2.37 | 121.90      | 124.48   |
| 23  | a     | 801 | CL0  | CAA-CBA-CGA | -2.37 | 106.49      | 113.21   |
| 19  | a     | 805 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 19  | a     | 835 | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |
| 19  | j     | 104 | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 19  | a     | 833 | CLA  | C1-C2-C3    | -2.36 | 122.34      | 126.20   |
| 19  | a     | 803 | CLA  | CMB-C2B-C1B | -2.36 | 121.83      | 125.42   |
| 19  | a     | 827 | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 19  | b     | 830 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 19  | f     | 203 | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 19  | b     | 815 | CLA  | O2A-CGA-O1A | -2.35 | 117.75      | 123.63   |
| 30  | b     | 851 | EQ3  | C34-C9-C8   | 2.35  | 121.67      | 118.09   |
| 21  | a     | 846 | BCR  | C15-C16-C17 | -2.35 | 118.72      | 123.52   |
| 19  | b     | 806 | CLA  | C3B-C4B-NB  | -2.35 | 108.44      | 110.53   |
| 32  | j     | 102 | LMT  | C3'-C4'-C5' | -2.34 | 105.74      | 110.93   |
| 21  | b     | 847 | BCR  | C33-C5-C6   | -2.34 | 121.93      | 124.48   |
| 26  | a     | 853 | LHG  | C20-C19-C18 | -2.34 | 102.55      | 114.37   |
| 19  | a     | 820 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 19  | a     | 810 | CLA  | CMB-C2B-C1B | -2.34 | 121.86      | 125.42   |
| 19  | b     | 836 | CLA  | O2A-CGA-O1A | -2.34 | 117.78      | 123.63   |
| 19  | a     | 839 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 19  | a     | 820 | CLA  | C3B-C4B-NB  | -2.33 | 108.45      | 110.53   |
| 19  | a     | 835 | CLA  | O2D-CGD-CBD | 2.33  | 115.31      | 111.23   |
| 29  | b     | 844 | ECH  | C7-C8-C9    | 2.32  | 129.67      | 126.23   |
| 19  | b     | 825 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 19  | k     | 101 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 19  | l     | 202 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 21  | f     | 202 | BCR  | C24-C23-C22 | -2.32 | 122.81      | 126.23   |
| 19  | a     | 811 | CLA  | C1-C2-C3    | -2.32 | 123.01      | 126.76   |
| 19  | D     | 402 | CLA  | CHB-C4A-NA  | 2.32  | 127.74      | 124.40   |
| 21  | i     | 102 | BCR  | C33-C5-C6   | -2.31 | 121.96      | 124.48   |
| 19  | b     | 826 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 19  | b     | 835 | CLA  | O2D-CGD-CBD | 2.31  | 115.27      | 111.23   |
| 19  | b     | 839 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 19  | a     | 815 | CLA  | CMB-C2B-C1B | -2.31 | 121.91      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | a     | 854 | LMG  | O2-C2-C1    | -2.31 | 104.58      | 110.08   |
| 19  | b     | 806 | CLA  | CHB-C4A-NA  | 2.30  | 127.73      | 124.40   |
| 27  | b     | 850 | LMG  | C42-C41-C40 | -2.30 | 102.75      | 114.37   |
| 19  | a     | 815 | CLA  | CHB-C4A-NA  | 2.30  | 127.71      | 124.40   |
| 23  | a     | 801 | CL0  | CMB-C2B-C3B | 2.30  | 129.27      | 124.68   |
| 26  | f     | 206 | LHG  | C27-C26-C25 | -2.30 | 102.76      | 114.37   |
| 19  | b     | 834 | CLA  | C1-C2-C3    | -2.30 | 123.05      | 126.76   |
| 26  | a     | 853 | LHG  | C27-C26-C25 | -2.29 | 102.79      | 114.37   |
| 27  | b     | 848 | LMG  | O3-C3-C2    | -2.29 | 104.98      | 110.38   |
| 21  | b     | 843 | BCR  | C15-C14-C13 | -2.29 | 124.07      | 127.28   |
| 19  | a     | 822 | CLA  | CMB-C2B-C1B | -2.28 | 121.94      | 125.42   |
| 19  | A     | 405 | CLA  | C1-C2-C3    | -2.28 | 123.07      | 126.76   |
| 21  | a     | 847 | BCR  | C15-C16-C17 | -2.28 | 118.85      | 123.52   |
| 21  | b     | 843 | BCR  | C24-C23-C22 | -2.28 | 122.86      | 126.23   |
| 19  | b     | 807 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 27  | b     | 848 | LMG  | O2-C2-C1    | -2.28 | 104.64      | 110.08   |
| 19  | b     | 808 | CLA  | C1-C2-C3    | -2.28 | 122.47      | 126.20   |
| 21  | A     | 406 | BCR  | C15-C14-C13 | -2.28 | 124.08      | 127.28   |
| 19  | a     | 826 | CLA  | O2D-CGD-CBD | 2.28  | 115.21      | 111.23   |
| 19  | f     | 203 | CLA  | CHB-C4A-NA  | 2.28  | 127.68      | 124.40   |
| 27  | l     | 201 | LMG  | O3-C3-C2    | -2.28 | 105.01      | 110.38   |
| 19  | b     | 839 | CLA  | C3B-C4B-NB  | -2.27 | 108.50      | 110.53   |
| 19  | b     | 824 | CLA  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 19  | a     | 811 | CLA  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 19  | a     | 810 | CLA  | C1-C2-C3    | -2.27 | 122.47      | 126.20   |
| 19  | b     | 835 | CLA  | CMB-C2B-C3B | 2.27  | 131.89      | 126.55   |
| 19  | b     | 832 | CLA  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |
| 30  | b     | 851 | EQ3  | C19-C18-C17 | 2.27  | 122.58      | 119.01   |
| 19  | D     | 402 | CLA  | O2A-CGA-O1A | -2.26 | 117.97      | 123.63   |
| 19  | b     | 822 | CLA  | O2A-CGA-O1A | -2.26 | 117.97      | 123.63   |
| 21  | b     | 842 | BCR  | C15-C14-C13 | -2.26 | 124.11      | 127.28   |
| 19  | b     | 835 | CLA  | C1-C2-C3    | -2.26 | 122.50      | 126.20   |
| 21  | l     | 205 | BCR  | C15-C14-C13 | -2.26 | 124.11      | 127.28   |
| 19  | b     | 836 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 21  | A     | 406 | BCR  | C15-C16-C17 | -2.26 | 118.90      | 123.52   |
| 22  | E     | 101 | HEM  | C4D-ND-C1D  | 2.25  | 107.88      | 105.21   |
| 19  | b     | 830 | CLA  | CMB-C2B-C3B | 2.25  | 131.85      | 126.55   |
| 28  | a     | 858 | 45D  | C10-C06-C04 | -2.25 | 109.91      | 113.21   |
| 19  | b     | 817 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 19  | a     | 820 | CLA  | O2A-CGA-O1A | -2.25 | 118.00      | 123.63   |
| 19  | a     | 814 | CLA  | O2A-CGA-O1A | -2.25 | 118.00      | 123.63   |
| 19  | a     | 816 | CLA  | CMB-C2B-C1B | -2.25 | 121.99      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 814 | CLA  | CMB-C2B-C1B | -2.25 | 122.00      | 125.42   |
| 19  | b     | 804 | CLA  | CMB-C2B-C1B | -2.25 | 122.00      | 125.42   |
| 19  | b     | 809 | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 19  | a     | 824 | CLA  | C1-C2-C3    | -2.25 | 122.52      | 126.20   |
| 21  | f     | 202 | BCR  | C15-C16-C17 | -2.24 | 118.93      | 123.52   |
| 21  | a     | 848 | BCR  | C16-C15-C14 | -2.24 | 118.93      | 123.52   |
| 27  | b     | 848 | LMG  | O1-C1-C2    | -2.24 | 104.87      | 108.27   |
| 27  | a     | 854 | LMG  | O3-C3-C2    | -2.24 | 105.10      | 110.38   |
| 19  | b     | 804 | CLA  | O2D-CGD-CBD | 2.24  | 115.14      | 111.23   |
| 19  | a     | 823 | CLA  | CMB-C2B-C1B | -2.23 | 122.02      | 125.42   |
| 19  | b     | 825 | CLA  | O2A-CGA-O1A | -2.23 | 118.05      | 123.63   |
| 27  | l     | 201 | LMG  | C40-C39-C38 | -2.23 | 103.10      | 114.37   |
| 19  | a     | 820 | CLA  | CMB-C2B-C1B | -2.23 | 122.03      | 125.42   |
| 19  | b     | 815 | CLA  | CMB-C2B-C1B | -2.23 | 122.03      | 125.42   |
| 19  | a     | 839 | CLA  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 19  | a     | 826 | CLA  | CMB-C2B-C1B | -2.23 | 122.03      | 125.42   |
| 19  | a     | 824 | CLA  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 21  | b     | 842 | BCR  | C7-C8-C9    | -2.23 | 122.94      | 126.23   |
| 27  | b     | 848 | LMG  | C42-C41-C40 | -2.22 | 103.12      | 114.37   |
| 21  | a     | 849 | BCR  | C11-C10-C9  | -2.22 | 124.16      | 127.28   |
| 19  | b     | 813 | CLA  | CMB-C2B-C1B | -2.22 | 122.03      | 125.42   |
| 27  | b     | 850 | LMG  | O2-C2-C1    | -2.22 | 104.79      | 110.08   |
| 29  | b     | 844 | ECH  | C21-C20-C19 | 2.22  | 129.63      | 123.20   |
| 19  | b     | 837 | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 28  | a     | 858 | 45D  | C33-C35-C37 | 2.22  | 122.50      | 119.01   |
| 21  | a     | 846 | BCR  | C11-C10-C9  | -2.22 | 124.17      | 127.28   |
| 19  | b     | 813 | CLA  | C1-C2-C3    | -2.21 | 122.57      | 126.20   |
| 19  | b     | 824 | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 23  | a     | 801 | CL0  | C3C-C4C-NC  | -2.21 | 109.25      | 114.65   |
| 19  | b     | 814 | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 21  | b     | 847 | BCR  | C2-C1-C6    | 2.21  | 113.65      | 110.44   |
| 19  | b     | 803 | CLA  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 19  | a     | 856 | CLA  | O2A-CGA-O1A | -2.20 | 118.11      | 123.63   |
| 19  | a     | 832 | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 19  | a     | 825 | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 27  | a     | 854 | LMG  | O1-C1-C2    | -2.20 | 104.93      | 108.27   |
| 21  | i     | 101 | BCR  | C2-C1-C6    | 2.19  | 113.62      | 110.44   |
| 31  | b     | 852 | ZEX  | C39-C29-C28 | 2.19  | 121.44      | 118.09   |
| 21  | b     | 843 | BCR  | C11-C10-C9  | -2.19 | 124.20      | 127.28   |
| 26  | a     | 852 | LHG  | C18-C17-C16 | -2.19 | 103.29      | 114.37   |
| 27  | b     | 848 | LMG  | O1-C7-C8    | -2.19 | 105.49      | 110.82   |
| 19  | a     | 843 | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | b     | 838 | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 26  | f     | 206 | LHG  | C18-C17-C16 | -2.19 | 103.30      | 114.37   |
| 19  | a     | 802 | CLA  | CMB-C2B-C1B | -2.19 | 122.09      | 125.42   |
| 26  | a     | 855 | LHG  | C27-C26-C25 | -2.19 | 103.31      | 114.37   |
| 21  | a     | 859 | BCR  | C15-C14-C13 | -2.19 | 124.21      | 127.28   |
| 19  | a     | 830 | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 21  | a     | 849 | BCR  | C7-C8-C9    | -2.19 | 123.00      | 126.23   |
| 19  | a     | 842 | CLA  | C1-C2-C3    | -2.19 | 122.61      | 126.20   |
| 26  | a     | 852 | LHG  | C27-C26-C25 | -2.19 | 103.32      | 114.37   |
| 19  | b     | 837 | CLA  | C3B-C4B-NB  | -2.18 | 108.58      | 110.53   |
| 21  | f     | 202 | BCR  | C8-C7-C6    | -2.18 | 121.17      | 127.00   |
| 27  | l     | 201 | LMG  | O1-C7-C8    | -2.18 | 105.52      | 110.82   |
| 21  | a     | 850 | BCR  | C24-C23-C22 | -2.18 | 123.02      | 126.23   |
| 19  | a     | 806 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 19  | b     | 812 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 26  | b     | 849 | LHG  | C27-C26-C25 | -2.17 | 103.39      | 114.37   |
| 19  | b     | 829 | CLA  | CHB-C4A-NA  | 2.17  | 127.53      | 124.40   |
| 19  | b     | 809 | CLA  | C1-C2-C3    | -2.17 | 122.65      | 126.20   |
| 31  | b     | 852 | ZEX  | C8-C9-C10   | 2.17  | 122.42      | 119.01   |
| 19  | b     | 826 | CLA  | C3B-C4B-NB  | -2.17 | 108.60      | 110.53   |
| 19  | a     | 836 | CLA  | O2A-CGA-O1A | -2.16 | 118.21      | 123.63   |
| 21  | b     | 847 | BCR  | C24-C23-C22 | -2.16 | 123.03      | 126.23   |
| 19  | j     | 103 | CLA  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |
| 19  | a     | 843 | CLA  | C1-C2-C3    | -2.16 | 122.65      | 126.20   |
| 19  | a     | 827 | CLA  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |
| 19  | a     | 826 | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 19  | a     | 802 | CLA  | CHB-C4A-NA  | 2.15  | 127.50      | 124.40   |
| 19  | b     | 803 | CLA  | C1-C2-C3    | -2.15 | 122.68      | 126.20   |
| 19  | a     | 812 | CLA  | C1-C2-C3    | -2.15 | 122.68      | 126.20   |
| 19  | a     | 810 | CLA  | O2A-CGA-O1A | -2.15 | 118.26      | 123.63   |
| 21  | b     | 846 | BCR  | C16-C15-C14 | -2.15 | 119.13      | 123.52   |
| 19  | a     | 809 | CLA  | CMB-C2B-C3B | 2.14  | 131.59      | 126.55   |
| 26  | a     | 855 | LHG  | C18-C17-C16 | -2.14 | 103.53      | 114.37   |
| 19  | a     | 821 | CLA  | CAA-CBA-CGA | -2.14 | 107.12      | 113.21   |
| 21  | a     | 847 | BCR  | C15-C14-C13 | -2.14 | 124.28      | 127.28   |
| 21  | A     | 406 | BCR  | C11-C10-C9  | -2.14 | 124.28      | 127.28   |
| 19  | a     | 841 | CLA  | O2A-CGA-O1A | -2.13 | 118.29      | 123.63   |
| 19  | a     | 838 | CLA  | C1-C2-C3    | -2.13 | 122.70      | 126.20   |
| 21  | k     | 103 | BCR  | C24-C23-C22 | -2.13 | 123.08      | 126.23   |
| 21  | b     | 847 | BCR  | C15-C14-C13 | -2.13 | 124.29      | 127.28   |
| 21  | i     | 102 | BCR  | C15-C14-C13 | -2.13 | 124.29      | 127.28   |
| 19  | a     | 860 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21  | i     | 101 | BCR  | C33-C5-C6   | -2.13 | 122.16      | 124.48   |
| 26  | a     | 853 | LHG  | C18-C17-C16 | -2.13 | 103.60      | 114.37   |
| 19  | b     | 820 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |
| 19  | a     | 829 | CLA  | C3B-C4B-NB  | -2.13 | 108.63      | 110.53   |
| 21  | a     | 846 | BCR  | C7-C8-C9    | -2.12 | 123.09      | 126.23   |
| 19  | l     | 204 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 19  | b     | 839 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 19  | a     | 809 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 21  | b     | 847 | BCR  | C15-C16-C17 | -2.12 | 119.18      | 123.52   |
| 21  | b     | 846 | BCR  | C33-C5-C6   | -2.12 | 122.17      | 124.48   |
| 19  | a     | 830 | CLA  | CMB-C2B-C1B | -2.12 | 122.20      | 125.42   |
| 19  | a     | 838 | CLA  | O2A-CGA-O1A | -2.12 | 118.34      | 123.63   |
| 19  | f     | 201 | CLA  | C1-C2-C3    | -2.11 | 122.73      | 126.20   |
| 19  | a     | 807 | CLA  | CMB-C2B-C1B | -2.11 | 122.20      | 125.42   |
| 27  | l     | 201 | LMG  | C42-C41-C40 | -2.11 | 103.69      | 114.37   |
| 19  | a     | 811 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 19  | a     | 856 | CLA  | C3B-C4B-NB  | -2.11 | 108.64      | 110.53   |
| 19  | f     | 203 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 19  | f     | 204 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 19  | b     | 825 | CLA  | C1-C2-C3    | -2.11 | 122.75      | 126.20   |
| 27  | b     | 850 | LMG  | O1-C7-C8    | -2.11 | 105.70      | 110.82   |
| 19  | a     | 827 | CLA  | C1-C2-C3    | -2.10 | 122.75      | 126.20   |
| 21  | j     | 101 | BCR  | C11-C10-C9  | -2.10 | 124.34      | 127.28   |
| 19  | l     | 203 | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 19  | b     | 827 | CLA  | CMB-C2B-C1B | -2.10 | 122.23      | 125.42   |
| 19  | b     | 805 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 19  | a     | 832 | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 19  | b     | 826 | CLA  | CMB-C2B-C1B | -2.09 | 122.23      | 125.42   |
| 19  | a     | 834 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 19  | b     | 802 | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 19  | a     | 856 | CLA  | CMB-C2B-C1B | -2.09 | 122.24      | 125.42   |
| 19  | b     | 829 | CLA  | C1-C2-C3    | -2.09 | 122.78      | 126.20   |
| 19  | a     | 810 | CLA  | CMB-C2B-C3B | 2.09  | 131.46      | 126.55   |
| 21  | a     | 859 | BCR  | C38-C26-C25 | -2.08 | 122.21      | 124.48   |
| 19  | b     | 834 | CLA  | CMB-C2B-C1B | -2.08 | 122.25      | 125.42   |
| 31  | f     | 205 | ZEX  | C28-C29-C30 | 2.08  | 122.29      | 119.01   |
| 19  | b     | 826 | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 28  | a     | 858 | 45D  | C23-C25-C29 | 2.08  | 122.28      | 119.01   |
| 27  | l     | 201 | LMG  | O2-C2-C1    | -2.08 | 105.12      | 110.08   |
| 19  | b     | 829 | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 27  | b     | 850 | LMG  | O7-C10-O9   | -2.08 | 118.84      | 123.70   |
| 21  | b     | 846 | BCR  | C10-C11-C12 | -2.08 | 117.17      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | b     | 816 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 19  | b     | 813 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 19  | b     | 832 | CLA  | CMB-C2B-C1B | -2.08 | 122.26      | 125.42   |
| 19  | a     | 856 | CLA  | O1D-CGD-CBD | 2.08  | 128.61      | 124.52   |
| 19  | a     | 843 | CLA  | CMB-C2B-C1B | -2.08 | 122.26      | 125.42   |
| 27  | b     | 850 | LMG  | O3-C3-C2    | -2.07 | 105.48      | 110.38   |
| 19  | a     | 823 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 19  | a     | 833 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 19  | A     | 405 | CLA  | O2D-CGD-CBD | 2.07  | 114.86      | 111.23   |
| 19  | a     | 831 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 19  | a     | 808 | CLA  | C1-C2-C3    | -2.07 | 122.80      | 126.20   |
| 19  | b     | 823 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 19  | a     | 803 | CLA  | O1D-CGD-CBD | 2.07  | 128.59      | 124.52   |
| 19  | a     | 822 | CLA  | CHB-C4A-NA  | 2.06  | 127.38      | 124.40   |
| 19  | b     | 804 | CLA  | CMB-C2B-C3B | 2.06  | 131.40      | 126.55   |
| 21  | i     | 101 | BCR  | C16-C15-C14 | -2.06 | 119.30      | 123.52   |
| 31  | f     | 205 | ZEX  | C8-C9-C10   | 2.06  | 122.25      | 119.01   |
| 21  | j     | 101 | BCR  | C24-C23-C22 | -2.06 | 123.19      | 126.23   |
| 19  | b     | 812 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 20  | A     | 404 | PHO  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 19  | a     | 856 | CLA  | CMB-C2B-C3B | 2.06  | 131.39      | 126.55   |
| 21  | b     | 843 | BCR  | C2-C1-C6    | 2.06  | 113.43      | 110.44   |
| 19  | a     | 808 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 19  | b     | 802 | CLA  | CMB-C2B-C1B | -2.05 | 122.29      | 125.42   |
| 19  | l     | 202 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 28  | a     | 858 | 45D  | C34-C36-C38 | 2.05  | 122.24      | 119.01   |
| 26  | b     | 849 | LHG  | C5-O7-C7    | -2.05 | 112.89      | 117.80   |
| 21  | a     | 848 | BCR  | C8-C7-C6    | -2.05 | 121.52      | 127.00   |
| 29  | m     | 101 | ECH  | C8-C9-C10   | 2.05  | 122.23      | 119.01   |
| 20  | D     | 401 | PHO  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 19  | a     | 807 | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 19  | a     | 814 | CLA  | CMB-C2B-C3B | 2.05  | 131.37      | 126.55   |
| 19  | a     | 832 | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 19  | a     | 818 | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 19  | b     | 809 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 19  | b     | 833 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 19  | a     | 802 | CLA  | CMB-C2B-C3B | 2.04  | 131.35      | 126.55   |
| 20  | D     | 401 | PHO  | C2D-C1D-ND  | -2.04 | 107.95      | 109.43   |
| 23  | a     | 801 | CL0  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 19  | a     | 829 | CLA  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 19  | b     | 828 | CLA  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 19  | a     | 812 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | D     | 401 | PHO  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 21  | a     | 850 | BCR  | C8-C7-C6    | -2.03 | 121.56      | 127.00   |
| 19  | a     | 813 | CLA  | O2A-CGA-O1A | -2.03 | 118.54      | 123.63   |
| 21  | a     | 848 | BCR  | C15-C16-C17 | -2.03 | 119.36      | 123.52   |
| 19  | b     | 834 | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 19  | b     | 823 | CLA  | O2D-CGD-CBD | 2.03  | 114.78      | 111.23   |
| 21  | a     | 848 | BCR  | C15-C14-C13 | -2.03 | 124.43      | 127.28   |
| 19  | a     | 805 | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 19  | b     | 832 | CLA  | O2D-CGD-CBD | 2.03  | 114.78      | 111.23   |
| 27  | b     | 848 | LMG  | O7-C10-O9   | -2.03 | 118.97      | 123.70   |
| 19  | a     | 822 | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 19  | b     | 808 | CLA  | O2A-CGA-O1A | -2.02 | 118.59      | 123.63   |
| 19  | b     | 806 | CLA  | O2D-CGD-CBD | 2.01  | 114.75      | 111.23   |
| 19  | b     | 815 | CLA  | CMB-C2B-C3B | 2.01  | 131.29      | 126.55   |
| 20  | A     | 404 | PHO  | C3B-C4B-NB  | -2.01 | 106.15      | 107.46   |
| 19  | b     | 818 | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 21  | A     | 406 | BCR  | C7-C8-C9    | -2.01 | 123.26      | 126.23   |
| 19  | b     | 811 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 19  | a     | 840 | CLA  | O2D-CGD-CBD | 2.01  | 114.75      | 111.23   |
| 21  | a     | 851 | BCR  | C8-C7-C6    | -2.01 | 121.63      | 127.00   |
| 21  | l     | 205 | BCR  | C8-C7-C6    | -2.01 | 121.63      | 127.00   |
| 21  | b     | 845 | BCR  | C33-C5-C6   | -2.01 | 122.29      | 124.48   |
| 22  | E     | 101 | HEM  | C2A-C1A-NA  | -2.01 | 107.93      | 110.15   |
| 19  | b     | 832 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 19  | a     | 828 | CLA  | O2A-CGA-O1A | -2.00 | 118.61      | 123.63   |
| 19  | a     | 815 | CLA  | CMB-C2B-C3B | 2.00  | 131.26      | 126.55   |
| 21  | f     | 202 | BCR  | C15-C14-C13 | -2.00 | 124.47      | 127.28   |
| 23  | a     | 801 | CL0  | CMA-C3A-C4A | -2.00 | 110.30      | 114.61   |
| 19  | b     | 837 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |

All (103) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 19  | A     | 402 | CLA  | ND   |
| 19  | A     | 403 | CLA  | ND   |
| 19  | A     | 405 | CLA  | ND   |
| 19  | A     | 407 | CLA  | ND   |
| 19  | D     | 402 | CLA  | ND   |
| 19  | D     | 403 | CLA  | ND   |
| 19  | a     | 802 | CLA  | ND   |
| 19  | a     | 803 | CLA  | ND   |
| 19  | a     | 804 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 19  | a     | 805 | CLA  | ND   |
| 19  | a     | 806 | CLA  | ND   |
| 19  | a     | 807 | CLA  | ND   |
| 19  | a     | 808 | CLA  | ND   |
| 19  | a     | 809 | CLA  | ND   |
| 19  | a     | 810 | CLA  | ND   |
| 19  | a     | 811 | CLA  | ND   |
| 19  | a     | 812 | CLA  | ND   |
| 19  | a     | 813 | CLA  | ND   |
| 19  | a     | 815 | CLA  | ND   |
| 19  | a     | 816 | CLA  | ND   |
| 19  | a     | 817 | CLA  | ND   |
| 19  | a     | 818 | CLA  | ND   |
| 19  | a     | 819 | CLA  | ND   |
| 19  | a     | 820 | CLA  | ND   |
| 19  | a     | 821 | CLA  | ND   |
| 19  | a     | 822 | CLA  | ND   |
| 19  | a     | 823 | CLA  | ND   |
| 19  | a     | 824 | CLA  | ND   |
| 19  | a     | 825 | CLA  | ND   |
| 19  | a     | 826 | CLA  | ND   |
| 19  | a     | 827 | CLA  | ND   |
| 19  | a     | 828 | CLA  | ND   |
| 19  | a     | 829 | CLA  | ND   |
| 19  | a     | 830 | CLA  | ND   |
| 19  | a     | 831 | CLA  | ND   |
| 19  | a     | 832 | CLA  | ND   |
| 19  | a     | 833 | CLA  | ND   |
| 19  | a     | 834 | CLA  | ND   |
| 19  | a     | 835 | CLA  | ND   |
| 19  | a     | 836 | CLA  | ND   |
| 19  | a     | 837 | CLA  | ND   |
| 19  | a     | 838 | CLA  | ND   |
| 19  | a     | 839 | CLA  | ND   |
| 19  | a     | 840 | CLA  | ND   |
| 19  | a     | 841 | CLA  | ND   |
| 19  | a     | 842 | CLA  | ND   |
| 19  | a     | 843 | CLA  | ND   |
| 19  | a     | 856 | CLA  | ND   |
| 19  | a     | 857 | CLA  | ND   |
| 19  | a     | 860 | CLA  | ND   |
| 19  | b     | 801 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 19  | b     | 802 | CLA  | ND   |
| 19  | b     | 803 | CLA  | ND   |
| 19  | b     | 804 | CLA  | ND   |
| 19  | b     | 805 | CLA  | ND   |
| 19  | b     | 806 | CLA  | ND   |
| 19  | b     | 807 | CLA  | ND   |
| 19  | b     | 808 | CLA  | ND   |
| 19  | b     | 809 | CLA  | ND   |
| 19  | b     | 810 | CLA  | ND   |
| 19  | b     | 811 | CLA  | ND   |
| 19  | b     | 812 | CLA  | ND   |
| 19  | b     | 813 | CLA  | ND   |
| 19  | b     | 814 | CLA  | ND   |
| 19  | b     | 815 | CLA  | ND   |
| 19  | b     | 816 | CLA  | ND   |
| 19  | b     | 817 | CLA  | ND   |
| 19  | b     | 818 | CLA  | ND   |
| 19  | b     | 819 | CLA  | ND   |
| 19  | b     | 820 | CLA  | ND   |
| 19  | b     | 821 | CLA  | ND   |
| 19  | b     | 822 | CLA  | ND   |
| 19  | b     | 823 | CLA  | ND   |
| 19  | b     | 824 | CLA  | ND   |
| 19  | b     | 825 | CLA  | ND   |
| 19  | b     | 826 | CLA  | ND   |
| 19  | b     | 827 | CLA  | ND   |
| 19  | b     | 828 | CLA  | ND   |
| 19  | b     | 829 | CLA  | ND   |
| 19  | b     | 830 | CLA  | ND   |
| 19  | b     | 831 | CLA  | ND   |
| 19  | b     | 832 | CLA  | ND   |
| 19  | b     | 833 | CLA  | ND   |
| 19  | b     | 834 | CLA  | ND   |
| 19  | b     | 835 | CLA  | ND   |
| 19  | b     | 836 | CLA  | ND   |
| 19  | b     | 837 | CLA  | ND   |
| 19  | b     | 838 | CLA  | ND   |
| 19  | b     | 839 | CLA  | ND   |
| 19  | b     | 840 | CLA  | ND   |
| 19  | f     | 201 | CLA  | ND   |
| 19  | f     | 203 | CLA  | ND   |
| 19  | f     | 204 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 19  | j     | 103 | CLA  | ND   |
| 19  | j     | 104 | CLA  | ND   |
| 19  | k     | 101 | CLA  | ND   |
| 19  | k     | 102 | CLA  | ND   |
| 19  | l     | 202 | CLA  | ND   |
| 19  | l     | 203 | CLA  | ND   |
| 19  | l     | 204 | CLA  | ND   |
| 23  | a     | 801 | CL0  | NA   |
| 23  | a     | 801 | CL0  | ND   |
| 23  | a     | 801 | CL0  | NC   |

All (1482) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 19  | A     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 19  | A     | 405 | CLA  | C1A-C2A-CAA-CBA |
| 19  | A     | 405 | CLA  | C3A-C2A-CAA-CBA |
| 19  | D     | 402 | CLA  | C1A-C2A-CAA-CBA |
| 19  | D     | 402 | CLA  | C3A-C2A-CAA-CBA |
| 19  | D     | 402 | CLA  | CBD-CGD-O2D-CED |
| 19  | D     | 403 | CLA  | C1A-C2A-CAA-CBA |
| 19  | D     | 403 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 802 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 803 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 805 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 809 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 809 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 809 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 811 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 811 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 813 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 815 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 816 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 19  | a     | 817 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 819 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 821 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 821 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 821 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 823 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 823 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 835 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 835 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 837 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 839 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 841 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 841 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 857 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 857 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 802 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 810 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 811 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 814 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 815 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 815 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 817 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 823 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 823 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 828 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 829 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 832 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 832 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 19  | b     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 19  | b     | 836 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 836 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 837 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 838 | CLA  | C4B-C3B-CAB-CBB |
| 19  | b     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 840 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 840 | CLA  | CAD-CBD-CGD-O1D |
| 19  | b     | 840 | CLA  | CAD-CBD-CGD-O2D |
| 19  | f     | 201 | CLA  | CBD-CGD-O2D-CED |
| 19  | j     | 103 | CLA  | C1A-C2A-CAA-CBA |
| 19  | j     | 103 | CLA  | CBD-CGD-O2D-CED |
| 19  | j     | 104 | CLA  | CBA-CGA-O2A-C1  |
| 19  | k     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 19  | k     | 101 | CLA  | CBA-CGA-O2A-C1  |
| 19  | k     | 101 | CLA  | CBD-CGD-O2D-CED |
| 19  | l     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 19  | l     | 202 | CLA  | C3A-C2A-CAA-CBA |
| 19  | l     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 20  | D     | 401 | PHO  | CBD-CGD-O2D-CED |
| 21  | A     | 406 | BCR  | C6-C7-C8-C9     |
| 21  | A     | 406 | BCR  | C22-C23-C24-C25 |
| 21  | a     | 846 | BCR  | C7-C8-C9-C10    |
| 21  | a     | 846 | BCR  | C7-C8-C9-C34    |
| 21  | a     | 847 | BCR  | C7-C8-C9-C34    |
| 21  | a     | 849 | BCR  | C21-C22-C23-C24 |
| 21  | a     | 850 | BCR  | C21-C22-C23-C24 |
| 21  | a     | 859 | BCR  | C6-C7-C8-C9     |
| 21  | b     | 842 | BCR  | C6-C7-C8-C9     |
| 21  | b     | 842 | BCR  | C7-C8-C9-C10    |
| 21  | b     | 842 | BCR  | C18-C19-C20-C21 |
| 21  | b     | 842 | BCR  | C21-C22-C23-C24 |
| 21  | b     | 842 | BCR  | C22-C23-C24-C25 |
| 21  | b     | 843 | BCR  | C21-C22-C23-C24 |
| 21  | b     | 845 | BCR  | C22-C23-C24-C25 |
| 21  | b     | 846 | BCR  | C20-C21-C22-C37 |
| 21  | b     | 846 | BCR  | C21-C22-C23-C24 |
| 21  | b     | 847 | BCR  | C11-C10-C9-C8   |
| 21  | b     | 847 | BCR  | C10-C11-C12-C13 |
| 21  | b     | 847 | BCR  | C11-C12-C13-C14 |
| 21  | b     | 847 | BCR  | C16-C17-C18-C36 |
| 21  | b     | 847 | BCR  | C21-C22-C23-C24 |
| 21  | b     | 847 | BCR  | C37-C22-C23-C24 |
| 21  | f     | 202 | BCR  | C7-C8-C9-C10    |
| 21  | i     | 101 | BCR  | C20-C21-C22-C37 |
| 21  | i     | 101 | BCR  | C21-C22-C23-C24 |
| 21  | i     | 102 | BCR  | C7-C8-C9-C34    |
| 21  | i     | 102 | BCR  | C21-C22-C23-C24 |
| 21  | i     | 102 | BCR  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | i     | 102 | BCR  | C23-C24-C25-C30 |
| 21  | j     | 101 | BCR  | C21-C22-C23-C24 |
| 21  | l     | 205 | BCR  | C7-C8-C9-C10    |
| 26  | a     | 852 | LHG  | O1-C1-C2-C3     |
| 26  | a     | 852 | LHG  | C3-O3-P-O4      |
| 26  | a     | 852 | LHG  | C3-O3-P-O6      |
| 26  | a     | 853 | LHG  | C3-O3-P-O5      |
| 26  | a     | 855 | LHG  | C4-O6-P-O5      |
| 26  | a     | 855 | LHG  | O9-C7-O7-C5     |
| 26  | b     | 849 | LHG  | O1-C1-C2-C3     |
| 26  | b     | 849 | LHG  | C3-O3-P-O5      |
| 26  | b     | 849 | LHG  | C4-O6-P-O5      |
| 26  | f     | 206 | LHG  | O2-C2-C3-O3     |
| 26  | f     | 206 | LHG  | C2-C3-O3-P      |
| 26  | f     | 206 | LHG  | C3-O3-P-O4      |
| 26  | f     | 206 | LHG  | C3-O3-P-O6      |
| 26  | f     | 206 | LHG  | C4-O6-P-O3      |
| 26  | f     | 206 | LHG  | C4-O6-P-O5      |
| 27  | l     | 201 | LMG  | O6-C1-O1-C7     |
| 27  | l     | 201 | LMG  | O9-C10-O7-C8    |
| 27  | l     | 201 | LMG  | C11-C10-O7-C8   |
| 19  | a     | 821 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 801 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 808 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 829 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 834 | CLA  | O1D-CGD-O2D-CED |
| 19  | k     | 101 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 802 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 802 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 806 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 814 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 819 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 841 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 801 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 808 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 813 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 819 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 820 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 826 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 827 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 834 | CLA  | CBD-CGD-O2D-CED |
| 19  | j     | 104 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | k     | 102 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 843 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 820 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 826 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 832 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 26  | a     | 852 | LHG  | O10-C23-O8-C6   |
| 19  | a     | 816 | CLA  | O1A-CGA-O2A-C1  |
| 19  | j     | 104 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 827 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 814 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 843 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 832 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 19  | l     | 203 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 829 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 820 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 832 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 856 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 804 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 810 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 828 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 833 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 838 | CLA  | O1A-CGA-O2A-C1  |
| 19  | f     | 203 | CLA  | O1A-CGA-O2A-C1  |
| 19  | l     | 202 | CLA  | O1A-CGA-O2A-C1  |
| 19  | l     | 203 | CLA  | O1A-CGA-O2A-C1  |
| 26  | f     | 206 | LHG  | O10-C23-O8-C6   |
| 27  | a     | 854 | LMG  | O10-C28-O8-C9   |
| 27  | b     | 850 | LMG  | O10-C28-O8-C9   |
| 27  | l     | 201 | LMG  | O10-C28-O8-C9   |
| 19  | a     | 817 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | k     | 101 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 841 | CLA  | O1D-CGD-O2D-CED |
| 19  | f     | 201 | CLA  | O1D-CGD-O2D-CED |
| 19  | k     | 102 | CLA  | O1D-CGD-O2D-CED |
| 19  | j     | 103 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 26  | f     | 206 | LHG  | O9-C7-O7-C5     |
| 19  | D     | 402 | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 403 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 803 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 818 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 824 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 836 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 840 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 841 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 843 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 812 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 836 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 819 | CLA  | O1D-CGD-O2D-CED |
| 19  | A     | 402 | CLA  | CBA-CGA-O2A-C1  |
| 19  | A     | 405 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 832 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 835 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 839 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 857 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 860 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 826 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 828 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 835 | CLA  | CBA-CGA-O2A-C1  |
| 19  | j     | 103 | CLA  | CBA-CGA-O2A-C1  |
| 19  | l     | 202 | CLA  | CBA-CGA-O2A-C1  |
| 26  | a     | 852 | LHG  | C24-C23-O8-C6   |
| 26  | f     | 206 | LHG  | C24-C23-O8-C6   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 402 | CLA  | CBD-CGD-O2D-CED |
| 19  | A     | 403 | CLA  | CBD-CGD-O2D-CED |
| 19  | A     | 407 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 805 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 812 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 835 | CLA  | CBD-CGD-O2D-CED |
| 26  | a     | 855 | LHG  | C8-C7-O7-C5     |
| 20  | D     | 401 | PHO  | O1D-CGD-O2D-CED |
| 19  | a     | 802 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 807 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 836 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 857 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 806 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 808 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 814 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 836 | CLA  | C4-C3-C5-C6     |
| 19  | f     | 201 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 802 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 807 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 836 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 837 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 806 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 814 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 828 | CLA  | C2-C3-C5-C6     |
| 19  | f     | 201 | CLA  | C2-C3-C5-C6     |
| 19  | A     | 403 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 840 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 813 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 826 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 801 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 802 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 831 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 832 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 857 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 860 | CLA  | C3-C5-C6-C7     |
| 20  | D     | 401 | PHO  | C3-C5-C6-C7     |
| 19  | a     | 808 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 842 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 856 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 801 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 804 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 810 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 833 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 834 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 838 | CLA  | CBA-CGA-O2A-C1  |
| 19  | f     | 203 | CLA  | CBA-CGA-O2A-C1  |
| 20  | A     | 404 | PHO  | CBA-CGA-O2A-C1  |
| 27  | a     | 854 | LMG  | C29-C28-O8-C9   |
| 27  | b     | 850 | LMG  | C29-C28-O8-C9   |
| 27  | l     | 201 | LMG  | C29-C28-O8-C9   |
| 27  | b     | 850 | LMG  | O6-C5-C6-O5     |
| 19  | A     | 402 | CLA  | O1A-CGA-O2A-C1  |
| 19  | A     | 405 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 808 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 821 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 828 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 839 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 860 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 806 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 816 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 19  | f     | 201 | CLA  | O1A-CGA-O2A-C1  |
| 19  | j     | 103 | CLA  | O1A-CGA-O2A-C1  |
| 20  | A     | 404 | PHO  | O1A-CGA-O2A-C1  |
| 23  | a     | 801 | CL0  | O1A-CGA-O2A-C1  |
| 19  | a     | 819 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 813 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 803 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 816 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 822 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 833 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 806 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 820 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 804 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 809 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 828 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 833 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 808 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 23  | a     | 801 | CL0  | CBA-CGA-O2A-C1  |
| 19  | a     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 857 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 815 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 19  | j     | 104 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 828 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 826 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 828 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 832 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 825 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 19  | f     | 201 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 857 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 836 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 804 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 833 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 842 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 32  | j     | 102 | LMT  | O5'-C5'-C6'-O6' |
| 27  | b     | 850 | LMG  | C4-C5-C6-O5     |
| 19  | b     | 804 | CLA  | CBD-CGD-O2D-CED |
| 19  | l     | 204 | CLA  | CBD-CGD-O2D-CED |
| 27  | a     | 854 | LMG  | C4-C5-C6-O5     |
| 19  | a     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 837 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | A     | 404 | PHO  | C2A-CAA-CBA-CGA |
| 19  | a     | 809 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 841 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 808 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 819 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 841 | CLA  | CBA-CGA-O2A-C1  |
| 19  | f     | 204 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 805 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 815 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 831 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 840 | CLA  | CBD-CGD-O2D-CED |
| 27  | b     | 848 | LMG  | O6-C5-C6-O5     |
| 19  | a     | 814 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 823 | CLA  | CBD-CGD-O2D-CED |
| 26  | a     | 853 | LHG  | C29-C30-C31-C32 |
| 19  | a     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 827 | CLA  | O1A-CGA-O2A-C1  |
| 19  | f     | 204 | CLA  | O1A-CGA-O2A-C1  |
| 26  | f     | 206 | LHG  | C1-C2-C3-O3     |
| 19  | a     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 822 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 826 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 827 | CLA  | CBA-CGA-O2A-C1  |
| 27  | a     | 854 | LMG  | O6-C5-C6-O5     |
| 19  | a     | 829 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 808 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 807 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 808 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 809 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 836 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 836 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 839 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 842 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 801 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 803 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 806 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 816 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 817 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 818 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 828 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 832 | CLA  | C14-C13-C15-C16 |
| 27  | b     | 848 | LMG  | C4-C5-C6-O5     |
| 19  | A     | 407 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 835 | CLA  | O1D-CGD-O2D-CED |
| 26  | a     | 853 | LHG  | O2-C2-C3-O3     |
| 19  | A     | 402 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 831 | CLA  | O1A-CGA-O2A-C1  |
| 26  | b     | 849 | LHG  | C32-C33-C34-C35 |
| 21  | a     | 847 | BCR  | C11-C12-C13-C35 |
| 21  | a     | 848 | BCR  | C37-C22-C23-C24 |
| 21  | a     | 850 | BCR  | C7-C8-C9-C34    |
| 21  | b     | 842 | BCR  | C7-C8-C9-C34    |
| 21  | b     | 842 | BCR  | C37-C22-C23-C24 |
| 21  | b     | 847 | BCR  | C11-C12-C13-C35 |
| 21  | f     | 202 | BCR  | C7-C8-C9-C34    |
| 21  | f     | 202 | BCR  | C37-C22-C23-C24 |
| 21  | i     | 102 | BCR  | C37-C22-C23-C24 |
| 29  | b     | 844 | ECH  | C37-C22-C23-C24 |
| 29  | m     | 101 | ECH  | C37-C22-C23-C24 |
| 21  | i     | 102 | BCR  | C7-C8-C9-C10    |
| 29  | b     | 844 | ECH  | C21-C22-C23-C24 |
| 29  | m     | 101 | ECH  | C21-C22-C23-C24 |
| 19  | a     | 826 | CLA  | O1A-CGA-O2A-C1  |
| 26  | a     | 852 | LHG  | O7-C5-C6-O8     |
| 26  | a     | 853 | LHG  | O7-C5-C6-O8     |
| 19  | b     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 804 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 824 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 856 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 820 | CLA  | C2-C1-O2A-CGA   |
| 19  | A     | 403 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 803 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 836 | CLA  | CBD-CGD-O2D-CED |
| 21  | f     | 202 | BCR  | C14-C15-C16-C17 |
| 19  | a     | 819 | CLA  | C8-C10-C11-C12  |
| 19  | a     | 835 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 840 | CLA  | C8-C10-C11-C12  |
| 19  | a     | 842 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 857 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 813 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 814 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 821 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 834 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 813 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 823 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 815 | CLA  | C8-C10-C11-C12  |
| 26  | b     | 849 | LHG  | C23-C24-C25-C26 |
| 21  | a     | 851 | BCR  | C9-C10-C11-C12  |
| 21  | b     | 847 | BCR  | C13-C14-C15-C16 |
| 20  | D     | 401 | PHO  | C15-C16-C17-C18 |
| 32  | j     | 102 | LMT  | C4'-C5'-C6'-O6' |
| 26  | a     | 853 | LHG  | C7-C8-C9-C10    |
| 26  | a     | 853 | LHG  | C23-C24-C25-C26 |
| 26  | f     | 206 | LHG  | C7-C8-C9-C10    |
| 19  | b     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 805 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 814 | CLA  | C15-C16-C17-C18 |
| 19  | b     | 802 | CLA  | C15-C16-C17-C18 |
| 19  | b     | 805 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 826 | CLA  | C8-C10-C11-C12  |
| 24  | a     | 844 | PQN  | C18-C20-C21-C22 |
| 19  | A     | 405 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 842 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 827 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 830 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 831 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 19  | l     | 202 | CLA  | C2A-CAA-CBA-CGA |
| 21  | b     | 843 | BCR  | C18-C19-C20-C21 |
| 19  | a     | 815 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 829 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 840 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 841 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 860 | CLA  | C13-C15-C16-C17 |
| 26  | a     | 855 | LHG  | C23-C24-C25-C26 |
| 27  | b     | 848 | LMG  | C28-C29-C30-C31 |
| 19  | a     | 822 | CLA  | O1A-CGA-O2A-C1  |
| 20  | A     | 404 | PHO  | C3-C5-C6-C7     |
| 19  | a     | 814 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 822 | CLA  | C8-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 834 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 802 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 803 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 804 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 806 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 809 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 825 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 828 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 832 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 26  | a     | 852 | LHG  | C23-C24-C25-C26 |
| 19  | a     | 802 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 805 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 832 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 812 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 823 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 825 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 816 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 823 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 827 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 407 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 822 | CLA  | CBA-CGA-O2A-C1  |
| 19  | D     | 403 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 809 | CLA  | CBD-CGD-O2D-CED |
| 19  | b     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 808 | CLA  | C13-C15-C16-C17 |
| 20  | A     | 404 | PHO  | C8-C10-C11-C12  |
| 31  | b     | 852 | ZEX  | C25-C26-C27-C28 |
| 31  | f     | 205 | ZEX  | C25-C26-C27-C28 |
| 26  | a     | 853 | LHG  | C1-C2-C3-O3     |
| 19  | a     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 19  | j     | 104 | CLA  | C2A-CAA-CBA-CGA |
| 19  | l     | 204 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 828 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 837 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 808 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 831 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 822 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 833 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 860 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 838 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 821 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 813 | CLA  | C15-C16-C17-C18 |
| 19  | b     | 819 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 838 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 828 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 828 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 805 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 805 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 839 | CLA  | C16-C17-C18-C20 |
| 21  | a     | 847 | BCR  | C20-C21-C22-C37 |
| 21  | a     | 850 | BCR  | C20-C21-C22-C37 |
| 21  | b     | 847 | BCR  | C11-C10-C9-C34  |
| 21  | i     | 102 | BCR  | C20-C21-C22-C37 |
| 21  | k     | 103 | BCR  | C16-C17-C18-C36 |
| 21  | l     | 205 | BCR  | C35-C13-C14-C15 |
| 21  | A     | 406 | BCR  | C7-C8-C9-C34    |
| 21  | k     | 103 | BCR  | C11-C12-C13-C35 |
| 21  | l     | 205 | BCR  | C11-C12-C13-C35 |
| 19  | A     | 407 | CLA  | O1A-CGA-O2A-C1  |
| 19  | D     | 403 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 802 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 804 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 815 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 825 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 803 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 812 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 820 | CLA  | C15-C16-C17-C18 |
| 26  | a     | 853 | LHG  | O1-C1-C2-C3     |
| 26  | f     | 206 | LHG  | O1-C1-C2-C3     |
| 23  | a     | 801 | CL0  | C16-C17-C18-C19 |
| 19  | a     | 830 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 817 | CLA  | C3-C5-C6-C7     |
| 21  | b     | 847 | BCR  | C16-C17-C18-C19 |
| 19  | l     | 204 | CLA  | O1D-CGD-O2D-CED |
| 19  | l     | 204 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 804 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 832 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 811 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 830 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 801 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 802 | CLA  | C2-C1-O2A-CGA   |
| 19  | l     | 203 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 804 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 830 | CLA  | C16-C17-C18-C20 |
| 19  | f     | 201 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 822 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 826 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 831 | CLA  | O1D-CGD-O2D-CED |
| 27  | b     | 848 | LMG  | C37-C38-C39-C40 |
| 27  | l     | 201 | LMG  | C32-C33-C34-C35 |
| 21  | a     | 851 | BCR  | C14-C15-C16-C17 |
| 21  | i     | 101 | BCR  | C14-C15-C16-C17 |
| 27  | a     | 854 | LMG  | C32-C33-C34-C35 |
| 19  | a     | 808 | CLA  | C8-C10-C11-C12  |
| 26  | a     | 852 | LHG  | C24-C25-C26-C27 |
| 26  | a     | 853 | LHG  | C28-C29-C30-C31 |
| 26  | f     | 206 | LHG  | C27-C28-C29-C30 |
| 27  | b     | 848 | LMG  | C33-C34-C35-C36 |
| 27  | b     | 850 | LMG  | C18-C19-C20-C21 |
| 26  | a     | 852 | LHG  | O1-C1-C2-O2     |
| 26  | b     | 849 | LHG  | O1-C1-C2-O2     |
| 26  | a     | 853 | LHG  | C27-C28-C29-C30 |
| 26  | b     | 849 | LHG  | C27-C28-C29-C30 |
| 27  | b     | 848 | LMG  | C16-C17-C18-C19 |
| 19  | a     | 805 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 804 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 819 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 834 | CLA  | C4B-C3B-CAB-CBB |
| 26  | a     | 855 | LHG  | C7-C8-C9-C10    |
| 19  | a     | 825 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 825 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 830 | CLA  | C16-C17-C18-C19 |
| 19  | b     | 839 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 803 | CLA  | C10-C11-C12-C13 |
| 27  | b     | 850 | LMG  | C17-C18-C19-C20 |
| 19  | a     | 836 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 816 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 828 | CLA  | C8-C10-C11-C12  |
| 27  | b     | 850 | LMG  | C13-C14-C15-C16 |
| 19  | a     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 818 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 830 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 835 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 843 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 823 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 838 | CLA  | C3A-C2A-CAA-CBA |
| 19  | j     | 103 | CLA  | C3A-C2A-CAA-CBA |
| 19  | l     | 203 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 803 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 822 | CLA  | O1A-CGA-O2A-C1  |
| 26  | a     | 853 | LHG  | C32-C33-C34-C35 |
| 26  | b     | 849 | LHG  | C30-C31-C32-C33 |
| 19  | b     | 809 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 813 | CLA  | C3-C5-C6-C7     |
| 23  | a     | 801 | CL0  | C3-C5-C6-C7     |
| 19  | a     | 833 | CLA  | C10-C11-C12-C13 |
| 26  | f     | 206 | LHG  | C31-C32-C33-C34 |
| 27  | b     | 848 | LMG  | C30-C31-C32-C33 |
| 27  | b     | 848 | LMG  | C34-C35-C36-C37 |
| 19  | a     | 838 | CLA  | O1A-CGA-O2A-C1  |
| 31  | b     | 852 | ZEX  | C21-C26-C27-C28 |
| 31  | f     | 205 | ZEX  | C21-C26-C27-C28 |
| 27  | b     | 850 | LMG  | C30-C31-C32-C33 |
| 19  | a     | 840 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 833 | CLA  | C11-C12-C13-C15 |
| 19  | f     | 201 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 821 | CLA  | C2B-C3B-CAB-CBB |
| 19  | b     | 838 | CLA  | C2B-C3B-CAB-CBB |
| 21  | a     | 859 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 859 | BCR  | C5-C6-C7-C8     |
| 29  | b     | 844 | ECH  | C1-C6-C7-C8     |
| 29  | b     | 844 | ECH  | C5-C6-C7-C8     |
| 29  | m     | 101 | ECH  | C5-C6-C7-C8     |
| 27  | l     | 201 | LMG  | C18-C19-C20-C21 |
| 19  | b     | 809 | CLA  | C3-C5-C6-C7     |
| 22  | E     | 101 | HEM  | C2A-CAA-CBA-CGA |
| 19  | a     | 805 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 811 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 829 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | l     | 204 | CLA  | O1A-CGA-O2A-C1  |
| 26  | b     | 849 | LHG  | C24-C25-C26-C27 |
| 21  | i     | 102 | BCR  | C10-C11-C12-C13 |
| 21  | i     | 102 | BCR  | C18-C19-C20-C21 |
| 19  | b     | 812 | CLA  | C13-C15-C16-C17 |
| 27  | b     | 848 | LMG  | C32-C33-C34-C35 |
| 27  | b     | 850 | LMG  | C16-C17-C18-C19 |
| 19  | a     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 818 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 826 | CLA  | C14-C13-C15-C16 |
| 26  | f     | 206 | LHG  | C24-C25-C26-C27 |
| 27  | l     | 201 | LMG  | C17-C18-C19-C20 |
| 26  | a     | 855 | LHG  | C32-C33-C34-C35 |
| 26  | a     | 855 | LHG  | C16-C17-C18-C19 |
| 19  | b     | 805 | CLA  | C16-C17-C18-C19 |
| 23  | a     | 801 | CL0  | C16-C17-C18-C20 |
| 26  | f     | 206 | LHG  | C8-C7-O7-C5     |
| 19  | a     | 833 | CLA  | C11-C12-C13-C14 |
| 27  | b     | 850 | LMG  | C14-C15-C16-C17 |
| 19  | a     | 824 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 804 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 809 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 856 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 817 | CLA  | C10-C11-C12-C13 |
| 26  | a     | 852 | LHG  | C15-C16-C17-C18 |
| 26  | a     | 852 | LHG  | C8-C7-O7-C5     |
| 26  | b     | 849 | LHG  | C8-C7-O7-C5     |
| 27  | a     | 854 | LMG  | C11-C10-O7-C8   |
| 22  | E     | 101 | HEM  | C4C-C3C-CAC-CBC |
| 19  | a     | 804 | CLA  | C16-C17-C18-C20 |
| 27  | l     | 201 | LMG  | C31-C32-C33-C34 |
| 19  | a     | 824 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 842 | CLA  | C8-C10-C11-C12  |
| 19  | f     | 201 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 815 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 814 | CLA  | C3-C5-C6-C7     |
| 19  | f     | 201 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 823 | CLA  | O1D-CGD-O2D-CED |
| 26  | a     | 852 | LHG  | C29-C30-C31-C32 |
| 19  | a     | 857 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 823 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 836 | CLA  | C2-C1-O2A-CGA   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | a     | 852 | LHG  | C11-C10-C9-C8   |
| 26  | a     | 852 | LHG  | C26-C27-C28-C29 |
| 27  | a     | 854 | LMG  | C15-C16-C17-C18 |
| 19  | b     | 804 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 803 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 831 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 826 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 834 | CLA  | CBD-CGD-O2D-CED |
| 27  | l     | 201 | LMG  | O6-C5-C6-O5     |
| 19  | a     | 824 | CLA  | C8-C10-C11-C12  |
| 26  | f     | 206 | LHG  | C23-C24-C25-C26 |
| 19  | A     | 407 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 824 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 842 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 843 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 19  | k     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 802 | CLA  | C8-C10-C11-C12  |
| 19  | a     | 814 | CLA  | O1A-CGA-O2A-C1  |
| 26  | f     | 206 | LHG  | C34-C35-C36-C37 |
| 19  | a     | 841 | CLA  | C5-C6-C7-C8     |
| 26  | b     | 849 | LHG  | O6-C4-C5-C6     |
| 19  | b     | 806 | CLA  | C3-C5-C6-C7     |
| 19  | A     | 402 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 808 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 809 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 814 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 820 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 822 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 825 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 830 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 830 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 837 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 842 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 801 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 804 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 806 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 813 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 817 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 831 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 833 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 836 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 838 | CLA  | C6-C7-C8-C10    |
| 19  | l     | 203 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 813 | CLA  | C8-C10-C11-C12  |
| 27  | l     | 201 | LMG  | C15-C16-C17-C18 |
| 19  | a     | 830 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 811 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 804 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 807 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 808 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 814 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 821 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 828 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 831 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 837 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 840 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 842 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 813 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 817 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 823 | CLA  | C6-C7-C8-C9     |
| 27  | b     | 850 | LMG  | C34-C35-C36-C37 |
| 19  | a     | 840 | CLA  | CBA-CGA-O2A-C1  |
| 27  | b     | 850 | LMG  | C2-C1-O1-C7     |
| 26  | a     | 855 | LHG  | C4-C5-C6-O8     |
| 27  | a     | 854 | LMG  | O1-C7-C8-C9     |
| 27  | l     | 201 | LMG  | O1-C7-C8-C9     |
| 19  | b     | 803 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 836 | CLA  | O1D-CGD-O2D-CED |
| 21  | k     | 103 | BCR  | C20-C21-C22-C37 |
| 20  | A     | 404 | PHO  | C5-C6-C7-C8     |
| 19  | a     | 820 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 19  | b     | 805 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 817 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 815 | CLA  | C13-C15-C16-C17 |
| 26  | f     | 206 | LHG  | C6-C5-O7-C7     |
| 26  | a     | 852 | LHG  | C18-C19-C20-C21 |
| 21  | a     | 846 | BCR  | C18-C19-C20-C21 |
| 21  | a     | 850 | BCR  | C18-C19-C20-C21 |
| 19  | a     | 821 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | b     | 846 | BCR  | C20-C21-C22-C23 |
| 26  | b     | 849 | LHG  | C33-C34-C35-C36 |
| 19  | b     | 801 | CLA  | C4-C3-C5-C6     |
| 27  | b     | 850 | LMG  | C41-C42-C43-C44 |
| 26  | f     | 206 | LHG  | C11-C12-C13-C14 |
| 27  | b     | 848 | LMG  | C31-C32-C33-C34 |
| 19  | l     | 203 | CLA  | C10-C11-C12-C13 |
| 27  | a     | 854 | LMG  | C30-C31-C32-C33 |
| 27  | b     | 848 | LMG  | O7-C8-C9-O8     |
| 27  | l     | 201 | LMG  | O1-C7-C8-O7     |
| 27  | l     | 201 | LMG  | C42-C43-C44-C45 |
| 19  | a     | 842 | CLA  | C5-C6-C7-C8     |
| 27  | a     | 854 | LMG  | C16-C17-C18-C19 |
| 26  | a     | 853 | LHG  | C24-C25-C26-C27 |
| 26  | f     | 206 | LHG  | C35-C36-C37-C38 |
| 19  | D     | 403 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 841 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 806 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 820 | CLA  | C16-C17-C18-C19 |
| 26  | a     | 853 | LHG  | C19-C20-C21-C22 |
| 19  | b     | 809 | CLA  | O1D-CGD-O2D-CED |
| 19  | b     | 833 | CLA  | C4-C3-C5-C6     |
| 27  | b     | 848 | LMG  | C29-C28-O8-C9   |
| 32  | j     | 102 | LMT  | C2-C1-O1'-C1'   |
| 19  | A     | 402 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 802 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 815 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 820 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 824 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 825 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 828 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 830 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 830 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 833 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 836 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 843 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 801 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 802 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 804 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 813 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 826 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 831 | CLA  | C11-C10-C8-C9   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 833 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 833 | CLA  | C14-C13-C15-C16 |
| 19  | l     | 203 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 820 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 832 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 806 | CLA  | C10-C11-C12-C13 |
| 26  | a     | 855 | LHG  | C11-C10-C9-C8   |
| 19  | k     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 27  | l     | 201 | LMG  | C2-C1-O1-C7     |
| 19  | b     | 801 | CLA  | C5-C6-C7-C8     |
| 27  | l     | 201 | LMG  | C37-C38-C39-C40 |
| 19  | b     | 805 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 802 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 804 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 807 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 807 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 815 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 819 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 821 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 822 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 823 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 828 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 828 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 831 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 833 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 835 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 836 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 840 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 843 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 857 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 802 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 812 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 823 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 826 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 827 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 831 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 833 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 816 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 803 | CLA  | C3A-C2A-CAA-CBA |
| 23  | a     | 801 | CL0  | C3A-C2A-CAA-CBA |
| 19  | a     | 839 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 857 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | D     | 402 | CLA  | CBA-CGA-O2A-C1  |
| 21  | l     | 205 | BCR  | C9-C10-C11-C12  |
| 20  | A     | 404 | PHO  | C10-C11-C12-C13 |
| 21  | b     | 843 | BCR  | C37-C22-C23-C24 |
| 26  | a     | 852 | LHG  | C32-C33-C34-C35 |
| 19  | b     | 805 | CLA  | C15-C16-C17-C18 |
| 26  | a     | 852 | LHG  | C4-C5-C6-O8     |
| 26  | a     | 853 | LHG  | C4-C5-C6-O8     |
| 27  | b     | 848 | LMG  | C17-C18-C19-C20 |
| 19  | a     | 829 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 828 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 812 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 828 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 812 | CLA  | C2-C3-C5-C6     |
| 19  | b     | 833 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 819 | CLA  | C2B-C3B-CAB-CBB |
| 19  | f     | 201 | CLA  | C2B-C3B-CAB-CBB |
| 21  | a     | 848 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 850 | BCR  | C23-C24-C25-C30 |
| 21  | a     | 859 | BCR  | C23-C24-C25-C30 |
| 21  | b     | 842 | BCR  | C1-C6-C7-C8     |
| 21  | b     | 842 | BCR  | C23-C24-C25-C30 |
| 21  | b     | 843 | BCR  | C1-C6-C7-C8     |
| 21  | j     | 101 | BCR  | C1-C6-C7-C8     |
| 21  | l     | 205 | BCR  | C1-C6-C7-C8     |
| 29  | m     | 101 | ECH  | C1-C6-C7-C8     |
| 29  | m     | 101 | ECH  | C23-C24-C25-C26 |
| 30  | b     | 851 | EQ3  | C23-C24-C25-C26 |
| 19  | b     | 819 | CLA  | C15-C16-C17-C18 |
| 27  | b     | 850 | LMG  | C32-C33-C34-C35 |
| 19  | b     | 823 | CLA  | C5-C6-C7-C8     |
| 27  | a     | 854 | LMG  | C33-C34-C35-C36 |
| 27  | b     | 848 | LMG  | C36-C37-C38-C39 |
| 19  | A     | 407 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 807 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 823 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 823 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 836 | CLA  | C6-C7-C8-C9     |
| 21  | b     | 847 | BCR  | C6-C7-C8-C9     |
| 21  | b     | 847 | BCR  | C22-C23-C24-C25 |
| 19  | a     | 857 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 807 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 832 | CLA  | C3-C5-C6-C7     |
| 23  | a     | 801 | CL0  | C2A-CAA-CBA-CGA |
| 19  | b     | 813 | CLA  | C8-C10-C11-C12  |
| 19  | a     | 834 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 830 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 812 | CLA  | C5-C6-C7-C8     |
| 21  | A     | 406 | BCR  | C20-C21-C22-C37 |
| 21  | b     | 847 | BCR  | C20-C21-C22-C37 |
| 21  | f     | 202 | BCR  | C35-C13-C14-C15 |
| 21  | f     | 202 | BCR  | C20-C21-C22-C37 |
| 27  | l     | 201 | LMG  | C19-C20-C21-C22 |
| 19  | a     | 806 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 819 | CLA  | C5-C6-C7-C8     |
| 21  | a     | 851 | BCR  | C11-C12-C13-C35 |
| 19  | A     | 407 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 826 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 836 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 839 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 860 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 813 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 828 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 831 | CLA  | C12-C13-C15-C16 |
| 26  | a     | 852 | LHG  | C30-C31-C32-C33 |
| 27  | b     | 848 | LMG  | C42-C43-C44-C45 |
| 21  | a     | 846 | BCR  | C21-C22-C23-C24 |
| 21  | a     | 851 | BCR  | C16-C17-C18-C36 |
| 26  | a     | 855 | LHG  | C14-C15-C16-C17 |
| 26  | f     | 206 | LHG  | C30-C31-C32-C33 |
| 19  | a     | 826 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 830 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 837 | CLA  | C5-C6-C7-C8     |
| 26  | b     | 849 | LHG  | C26-C27-C28-C29 |
| 27  | l     | 201 | LMG  | C30-C31-C32-C33 |
| 27  | b     | 848 | LMG  | C18-C19-C20-C21 |
| 19  | D     | 402 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 831 | CLA  | C4-C3-C5-C6     |
| 26  | a     | 855 | LHG  | C31-C32-C33-C34 |
| 27  | b     | 848 | LMG  | C38-C39-C40-C41 |
| 19  | a     | 857 | CLA  | O2A-C1-C2-C3    |
| 19  | b     | 802 | CLA  | O2A-C1-C2-C3    |
| 19  | D     | 402 | CLA  | O1A-CGA-O2A-C1  |
| 19  | A     | 407 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | a     | 852 | LHG  | C11-C12-C13-C14 |
| 27  | b     | 848 | LMG  | C21-C22-C23-C24 |
| 27  | l     | 201 | LMG  | C14-C15-C16-C17 |
| 27  | b     | 850 | LMG  | O1-C7-C8-C9     |
| 26  | a     | 853 | LHG  | C24-C23-O8-C6   |
| 19  | A     | 402 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 817 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 834 | CLA  | O1D-CGD-O2D-CED |
| 26  | a     | 855 | LHG  | O7-C5-C6-O8     |
| 26  | f     | 206 | LHG  | O7-C5-C6-O8     |
| 27  | a     | 854 | LMG  | O1-C7-C8-O7     |
| 19  | a     | 824 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 860 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 812 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 827 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 833 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 834 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 819 | CLA  | C13-C15-C16-C17 |
| 19  | b     | 839 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 839 | CLA  | C2-C1-O2A-CGA   |
| 23  | a     | 801 | CL0  | C2-C1-O2A-CGA   |
| 20  | D     | 401 | PHO  | CBA-CGA-O2A-C1  |
| 19  | a     | 813 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 813 | CLA  | C5-C6-C7-C8     |
| 27  | l     | 201 | LMG  | C40-C41-C42-C43 |
| 26  | f     | 206 | LHG  | C29-C30-C31-C32 |
| 19  | b     | 826 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 824 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 818 | CLA  | C15-C16-C17-C18 |
| 19  | b     | 839 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 808 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 817 | CLA  | C5-C6-C7-C8     |
| 19  | l     | 203 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 808 | CLA  | C3-C5-C6-C7     |
| 26  | f     | 206 | LHG  | O1-C1-C2-O2     |
| 19  | A     | 403 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 804 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 824 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 836 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 839 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 842 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 801 | CLA  | C4B-C3B-CAB-CBB |
| 19  | b     | 807 | CLA  | C4B-C3B-CAB-CBB |
| 19  | b     | 814 | CLA  | C4B-C3B-CAB-CBB |
| 19  | b     | 837 | CLA  | C4B-C3B-CAB-CBB |
| 19  | b     | 839 | CLA  | C4B-C3B-CAB-CBB |
| 19  | f     | 201 | CLA  | C4B-C3B-CAB-CBB |
| 19  | f     | 204 | CLA  | C4B-C3B-CAB-CBB |
| 27  | b     | 850 | LMG  | C42-C43-C44-C45 |
| 19  | b     | 838 | CLA  | C8-C10-C11-C12  |
| 21  | a     | 848 | BCR  | C6-C7-C8-C9     |
| 21  | a     | 849 | BCR  | C22-C23-C24-C25 |
| 21  | l     | 205 | BCR  | C22-C23-C24-C25 |
| 29  | b     | 844 | ECH  | C22-C23-C24-C25 |
| 21  | b     | 845 | BCR  | C21-C22-C23-C24 |
| 27  | l     | 201 | LMG  | C12-C13-C14-C15 |
| 26  | a     | 853 | LHG  | C34-C35-C36-C37 |
| 19  | a     | 815 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 819 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 839 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 841 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 857 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 860 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 816 | CLA  | C11-C10-C8-C7   |
| 26  | a     | 852 | LHG  | C28-C29-C30-C31 |
| 19  | b     | 825 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 860 | CLA  | C15-C16-C17-C18 |
| 20  | D     | 401 | PHO  | O1A-CGA-O2A-C1  |
| 19  | b     | 833 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 824 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 857 | CLA  | C16-C17-C18-C19 |
| 26  | b     | 849 | LHG  | O6-C4-C5-O7     |
| 19  | b     | 802 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 814 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 826 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 831 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 831 | CLA  | C14-C13-C15-C16 |
| 32  | j     | 102 | LMT  | C4-C5-C6-C7     |
| 19  | a     | 841 | CLA  | C13-C15-C16-C17 |
| 26  | a     | 855 | LHG  | C33-C34-C35-C36 |
| 26  | f     | 206 | LHG  | C33-C34-C35-C36 |
| 21  | i     | 102 | BCR  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 836 | CLA  | C5-C6-C7-C8     |
| 27  | b     | 848 | LMG  | C39-C40-C41-C42 |
| 19  | a     | 807 | CLA  | C3-C5-C6-C7     |
| 26  | f     | 206 | LHG  | C4-C5-C6-O8     |
| 19  | a     | 840 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 826 | CLA  | C2-C3-C5-C6     |
| 19  | D     | 403 | CLA  | CAD-CBD-CGD-O2D |
| 19  | a     | 823 | CLA  | CAD-CBD-CGD-O2D |
| 19  | a     | 834 | CLA  | CAD-CBD-CGD-O2D |
| 19  | b     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 19  | b     | 828 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 19  | D     | 403 | CLA  | CAD-CBD-CGD-O1D |
| 19  | a     | 823 | CLA  | CAD-CBD-CGD-O1D |
| 19  | a     | 834 | CLA  | CAD-CBD-CGD-O1D |
| 20  | D     | 401 | PHO  | CHA-CBD-CGD-O1D |
| 20  | D     | 401 | PHO  | CHA-CBD-CGD-O2D |
| 21  | A     | 406 | BCR  | C19-C20-C21-C22 |
| 21  | b     | 843 | BCR  | C19-C20-C21-C22 |
| 23  | a     | 801 | CL0  | CHA-CBD-CGD-O1D |
| 23  | a     | 801 | CL0  | CHA-CBD-CGD-O2D |
| 26  | b     | 849 | LHG  | C3-O3-P-O4      |
| 26  | b     | 849 | LHG  | C3-O3-P-O6      |
| 26  | f     | 206 | LHG  | C4-O6-P-O4      |
| 19  | b     | 814 | CLA  | C2C-C3C-CAC-CBC |
| 19  | a     | 832 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 824 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 834 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 839 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 842 | CLA  | C2B-C3B-CAB-CBB |
| 19  | b     | 801 | CLA  | C2B-C3B-CAB-CBB |
| 21  | A     | 406 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 850 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 851 | BCR  | C1-C6-C7-C8     |
| 21  | l     | 205 | BCR  | C23-C24-C25-C30 |
| 26  | a     | 852 | LHG  | C12-C13-C14-C15 |
| 19  | b     | 806 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 808 | CLA  | C16-C17-C18-C19 |
| 19  | f     | 201 | CLA  | C13-C15-C16-C17 |
| 19  | A     | 407 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 812 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 813 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 821 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 822 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 823 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 841 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 857 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 803 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 832 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 833 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 839 | CLA  | O1D-CGD-O2D-CED |
| 19  | a     | 812 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 805 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 833 | CLA  | C11-C12-C13-C15 |
| 27  | b     | 850 | LMG  | C19-C20-C21-C22 |
| 27  | b     | 850 | LMG  | C39-C40-C41-C42 |
| 26  | a     | 853 | LHG  | C30-C31-C32-C33 |
| 19  | b     | 801 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 809 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 802 | CLA  | C2C-C3C-CAC-CBC |
| 27  | b     | 850 | LMG  | O1-C7-C8-O7     |
| 27  | b     | 850 | LMG  | C28-C29-C30-C31 |
| 19  | b     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 819 | CLA  | C2-C1-O2A-CGA   |
| 19  | l     | 202 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 828 | CLA  | C10-C11-C12-C13 |
| 21  | j     | 101 | BCR  | C37-C22-C23-C24 |
| 26  | a     | 852 | LHG  | C34-C35-C36-C37 |
| 26  | a     | 853 | LHG  | C11-C10-C9-C8   |
| 19  | a     | 802 | CLA  | C5-C6-C7-C8     |
| 21  | a     | 851 | BCR  | C11-C12-C13-C14 |
| 27  | l     | 201 | LMG  | C8-C7-O1-C1     |
| 19  | A     | 402 | CLA  | C2A-CAA-CBA-CGA |
| 19  | k     | 102 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 833 | CLA  | C8-C10-C11-C12  |
| 26  | a     | 855 | LHG  | C28-C29-C30-C31 |
| 19  | a     | 803 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 815 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 839 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 819 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 818 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 835 | CLA  | C16-C17-C18-C19 |
| 19  | b     | 820 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 838 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | A     | 407 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 812 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 834 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 837 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 816 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 838 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 808 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 809 | CLA  | C15-C16-C17-C18 |
| 19  | b     | 807 | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 830 | CLA  | C3A-C2A-CAA-CBA |
| 20  | A     | 404 | PHO  | C3A-C2A-CAA-CBA |
| 21  | a     | 849 | BCR  | C20-C21-C22-C37 |
| 28  | a     | 858 | 45D  | C28-C26-C30-C32 |
| 28  | a     | 858 | 45D  | C39-C35-C37-C41 |
| 29  | b     | 844 | ECH  | C11-C10-C9-C34  |
| 29  | b     | 844 | ECH  | C35-C13-C14-C15 |
| 31  | f     | 205 | ZEX  | C20-C13-C14-C15 |
| 19  | b     | 827 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 843 | CLA  | C2-C1-O2A-CGA   |
| 21  | a     | 859 | BCR  | C19-C20-C21-C22 |
| 19  | a     | 830 | CLA  | C13-C15-C16-C17 |
| 23  | a     | 801 | CL0  | C5-C6-C7-C8     |
| 21  | k     | 103 | BCR  | C7-C8-C9-C34    |
| 26  | a     | 853 | LHG  | C12-C13-C14-C15 |
| 27  | b     | 848 | LMG  | C35-C36-C37-C38 |
| 19  | b     | 833 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 826 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 802 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 809 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 812 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 827 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 837 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 804 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 812 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 825 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 838 | CLA  | C11-C12-C13-C14 |
| 20  | A     | 404 | PHO  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 804 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 28  | a     | 858 | 45D  | C24-C26-C30-C32 |
| 28  | a     | 858 | 45D  | C33-C35-C37-C41 |
| 29  | b     | 844 | ECH  | C11-C10-C9-C8   |
| 29  | b     | 844 | ECH  | C12-C13-C14-C15 |
| 31  | f     | 205 | ZEX  | C12-C13-C14-C15 |
| 19  | A     | 403 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 804 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 836 | CLA  | C2B-C3B-CAB-CBB |
| 19  | a     | 857 | CLA  | C2B-C3B-CAB-CBB |
| 19  | b     | 807 | CLA  | C2B-C3B-CAB-CBB |
| 19  | b     | 814 | CLA  | C2B-C3B-CAB-CBB |
| 19  | b     | 837 | CLA  | C2B-C3B-CAB-CBB |
| 19  | b     | 839 | CLA  | C2B-C3B-CAB-CBB |
| 19  | f     | 204 | CLA  | C2B-C3B-CAB-CBB |
| 21  | A     | 406 | BCR  | C23-C24-C25-C30 |
| 21  | a     | 846 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 847 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 848 | BCR  | C5-C6-C7-C8     |
| 21  | a     | 848 | BCR  | C23-C24-C25-C30 |
| 21  | a     | 849 | BCR  | C1-C6-C7-C8     |
| 21  | a     | 850 | BCR  | C5-C6-C7-C8     |
| 21  | a     | 850 | BCR  | C23-C24-C25-C26 |
| 21  | a     | 859 | BCR  | C23-C24-C25-C26 |
| 21  | b     | 842 | BCR  | C5-C6-C7-C8     |
| 21  | b     | 842 | BCR  | C23-C24-C25-C26 |
| 21  | b     | 843 | BCR  | C5-C6-C7-C8     |
| 21  | b     | 845 | BCR  | C23-C24-C25-C30 |
| 21  | f     | 202 | BCR  | C1-C6-C7-C8     |
| 21  | j     | 101 | BCR  | C5-C6-C7-C8     |
| 21  | k     | 103 | BCR  | C23-C24-C25-C30 |
| 21  | l     | 205 | BCR  | C5-C6-C7-C8     |
| 21  | l     | 205 | BCR  | C23-C24-C25-C26 |
| 29  | b     | 844 | ECH  | C23-C24-C25-C26 |
| 19  | a     | 834 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 819 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 810 | CLA  | CBD-CGD-O2D-CED |
| 19  | a     | 827 | CLA  | C11-C10-C8-C7   |
| 19  | a     | 842 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 803 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 805 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 818 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 832 | CLA  | C12-C13-C15-C16 |
| 19  | a     | 819 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 809 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 831 | CLA  | C15-C16-C17-C18 |
| 19  | b     | 827 | CLA  | C16-C17-C18-C19 |
| 21  | a     | 850 | BCR  | C37-C22-C23-C24 |
| 19  | b     | 805 | CLA  | C4-C3-C5-C6     |
| 19  | D     | 402 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 831 | CLA  | C2-C3-C5-C6     |
| 27  | a     | 854 | LMG  | C11-C12-C13-C14 |
| 26  | b     | 849 | LHG  | C28-C29-C30-C31 |
| 19  | b     | 819 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 806 | CLA  | C11-C12-C13-C14 |
| 26  | f     | 206 | LHG  | C32-C33-C34-C35 |
| 21  | i     | 101 | BCR  | C13-C14-C15-C16 |
| 19  | b     | 803 | CLA  | C8-C10-C11-C12  |
| 19  | a     | 835 | CLA  | C8-C10-C11-C12  |
| 21  | a     | 850 | BCR  | C14-C15-C16-C17 |
| 19  | a     | 832 | CLA  | C2-C3-C5-C6     |
| 26  | a     | 855 | LHG  | C26-C27-C28-C29 |
| 20  | D     | 401 | PHO  | C10-C11-C12-C13 |
| 20  | D     | 401 | PHO  | C13-C15-C16-C17 |
| 19  | a     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 27  | a     | 854 | LMG  | C7-C8-C9-O8     |
| 27  | l     | 201 | LMG  | C28-C29-C30-C31 |
| 19  | D     | 402 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 856 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 832 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 810 | CLA  | C4-C3-C5-C6     |
| 19  | b     | 822 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 818 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 857 | CLA  | C4B-C3B-CAB-CBB |
| 19  | k     | 102 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 821 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 835 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 810 | CLA  | O1D-CGD-O2D-CED |
| 21  | j     | 101 | BCR  | C20-C21-C22-C37 |
| 21  | l     | 205 | BCR  | C16-C17-C18-C36 |
| 30  | b     | 851 | EQ3  | C11-C10-C9-C34  |
| 19  | a     | 860 | CLA  | C16-C17-C18-C19 |
| 19  | b     | 831 | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | a     | 855 | LHG  | C24-C25-C26-C27 |
| 19  | l     | 204 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 817 | CLA  | C14-C13-C15-C16 |
| 19  | b     | 823 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 819 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 838 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 818 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 809 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 836 | CLA  | C10-C11-C12-C13 |
| 19  | a     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 19  | b     | 801 | CLA  | C3A-C2A-CAA-CBA |
| 19  | a     | 840 | CLA  | C2-C3-C5-C6     |
| 26  | a     | 855 | LHG  | C13-C14-C15-C16 |
| 27  | b     | 850 | LMG  | C40-C41-C42-C43 |
| 19  | a     | 805 | CLA  | C13-C15-C16-C17 |
| 26  | a     | 853 | LHG  | C17-C18-C19-C20 |
| 19  | b     | 807 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 807 | CLA  | C16-C17-C18-C20 |
| 30  | b     | 851 | EQ3  | C11-C10-C9-C8   |
| 26  | a     | 853 | LHG  | C9-C10-C11-C12  |
| 19  | l     | 202 | CLA  | O1D-CGD-O2D-CED |
| 26  | a     | 852 | LHG  | C33-C34-C35-C36 |
| 27  | b     | 848 | LMG  | C7-C8-C9-O8     |
| 19  | a     | 819 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 825 | CLA  | C5-C6-C7-C8     |
| 26  | a     | 852 | LHG  | O8-C23-C24-C25  |
| 19  | a     | 840 | CLA  | C10-C11-C12-C13 |
| 26  | a     | 855 | LHG  | O2-C2-C3-O3     |
| 19  | a     | 819 | CLA  | C14-C13-C15-C16 |
| 19  | a     | 821 | CLA  | C11-C10-C8-C9   |
| 19  | a     | 857 | CLA  | C11-C12-C13-C14 |
| 19  | a     | 860 | CLA  | C11-C12-C13-C14 |
| 19  | b     | 818 | CLA  | C6-C7-C8-C9     |
| 19  | a     | 813 | CLA  | C11-C12-C13-C14 |
| 19  | D     | 402 | CLA  | CAA-CBA-CGA-O2A |
| 26  | f     | 206 | LHG  | O7-C7-C8-C9     |
| 19  | l     | 202 | CLA  | CBD-CGD-O2D-CED |
| 27  | a     | 854 | LMG  | O7-C10-C11-C12  |
| 19  | a     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 19  | f     | 204 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 806 | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 826 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 827 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 801 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 804 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 817 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 819 | CLA  | C6-C7-C8-C10    |
| 19  | a     | 832 | CLA  | C2B-C3B-CAB-CBB |
| 21  | A     | 406 | BCR  | C5-C6-C7-C8     |
| 21  | a     | 847 | BCR  | C5-C6-C7-C8     |
| 21  | a     | 849 | BCR  | C5-C6-C7-C8     |
| 21  | a     | 851 | BCR  | C5-C6-C7-C8     |
| 21  | b     | 845 | BCR  | C23-C24-C25-C26 |
| 21  | f     | 202 | BCR  | C5-C6-C7-C8     |
| 21  | i     | 101 | BCR  | C1-C6-C7-C8     |
| 21  | i     | 102 | BCR  | C1-C6-C7-C8     |
| 21  | i     | 102 | BCR  | C5-C6-C7-C8     |
| 21  | j     | 101 | BCR  | C23-C24-C25-C30 |
| 21  | k     | 103 | BCR  | C23-C24-C25-C26 |
| 29  | m     | 101 | ECH  | C23-C24-C25-C30 |
| 31  | b     | 852 | ZEX  | C1-C6-C7-C8     |
| 19  | a     | 826 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 833 | CLA  | C2-C1-O2A-CGA   |
| 19  | b     | 839 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 824 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 832 | CLA  | CAA-CBA-CGA-O2A |
| 26  | a     | 852 | LHG  | O7-C7-C8-C9     |
| 19  | b     | 822 | CLA  | C2-C3-C5-C6     |
| 27  | a     | 854 | LMG  | O9-C10-O7-C8    |
| 32  | j     | 102 | LMT  | C5-C6-C7-C8     |
| 19  | a     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 832 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 843 | CLA  | C2A-CAA-CBA-CGA |
| 26  | b     | 849 | LHG  | C35-C36-C37-C38 |
| 19  | a     | 812 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 840 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 834 | CLA  | CAA-CBA-CGA-O2A |
| 26  | a     | 855 | LHG  | C29-C30-C31-C32 |
| 19  | b     | 832 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 831 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 810 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 828 | CLA  | C15-C16-C17-C18 |
| 19  | a     | 834 | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | b     | 849 | LHG  | C29-C30-C31-C32 |
| 19  | b     | 832 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 833 | CLA  | CAA-CBA-CGA-O2A |
| 19  | A     | 407 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 830 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 27  | b     | 850 | LMG  | C38-C39-C40-C41 |
| 19  | a     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 813 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 825 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 827 | CLA  | C4B-C3B-CAB-CBB |
| 19  | a     | 828 | CLA  | C4B-C3B-CAB-CBB |
| 19  | b     | 801 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 19  | b     | 831 | CLA  | C4B-C3B-CAB-CBB |
| 19  | k     | 101 | CLA  | C4B-C3B-CAB-CBB |
| 19  | k     | 102 | CLA  | C1A-C2A-CAA-CBA |
| 19  | a     | 809 | CLA  | C8-C10-C11-C12  |
| 19  | A     | 403 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 21  | b     | 847 | BCR  | C15-C16-C17-C18 |
| 21  | k     | 103 | BCR  | C15-C16-C17-C18 |
| 19  | a     | 821 | CLA  | C16-C17-C18-C19 |
| 27  | b     | 850 | LMG  | C37-C38-C39-C40 |
| 19  | a     | 829 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 804 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 816 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 807 | CLA  | CAA-CBA-CGA-O2A |
| 19  | j     | 103 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 829 | CLA  | C11-C12-C13-C15 |
| 19  | a     | 834 | CLA  | C11-C10-C8-C7   |
| 19  | b     | 803 | CLA  | C11-C12-C13-C15 |
| 19  | b     | 805 | CLA  | C12-C13-C15-C16 |
| 19  | b     | 817 | CLA  | C6-C7-C8-C10    |
| 19  | f     | 201 | CLA  | C6-C7-C8-C10    |
| 19  | b     | 807 | CLA  | C16-C17-C18-C19 |
| 19  | A     | 402 | CLA  | O2A-C1-C2-C3    |
| 19  | a     | 819 | CLA  | O2A-C1-C2-C3    |
| 19  | l     | 203 | CLA  | CAA-CBA-CGA-O2A |
| 27  | l     | 201 | LMG  | C38-C39-C40-C41 |
| 19  | b     | 832 | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 806 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 821 | CLA  | CAA-CBA-CGA-O2A |
| 27  | l     | 201 | LMG  | C39-C40-C41-C42 |
| 19  | b     | 817 | CLA  | C8-C10-C11-C12  |
| 19  | a     | 808 | CLA  | C5-C6-C7-C8     |
| 27  | b     | 848 | LMG  | O7-C10-C11-C12  |
| 19  | a     | 812 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 840 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 822 | CLA  | C13-C15-C16-C17 |
| 19  | a     | 831 | CLA  | C10-C11-C12-C13 |
| 19  | k     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 27  | a     | 854 | LMG  | O8-C28-C29-C30  |
| 19  | a     | 834 | CLA  | C11-C10-C8-C9   |
| 19  | b     | 803 | CLA  | C6-C7-C8-C9     |
| 19  | b     | 838 | CLA  | C6-C7-C8-C9     |
| 19  | D     | 402 | CLA  | CAA-CBA-CGA-O1A |
| 19  | b     | 834 | CLA  | CAA-CBA-CGA-O1A |
| 21  | i     | 102 | BCR  | C15-C16-C17-C18 |
| 19  | j     | 103 | CLA  | C4-C3-C5-C6     |
| 19  | a     | 824 | CLA  | CAA-CBA-CGA-O1A |
| 19  | b     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 19  | j     | 103 | CLA  | C2-C3-C5-C6     |
| 27  | a     | 854 | LMG  | O10-C28-C29-C30 |
| 19  | a     | 821 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 812 | CLA  | C8-C10-C11-C12  |
| 19  | b     | 813 | CLA  | C13-C15-C16-C17 |
| 19  | D     | 402 | CLA  | C3-C5-C6-C7     |
| 19  | b     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 815 | CLA  | C15-C16-C17-C18 |
| 19  | A     | 407 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 835 | CLA  | CAA-CBA-CGA-O1A |
| 27  | b     | 850 | LMG  | O10-C28-C29-C30 |
| 19  | a     | 826 | CLA  | C5-C6-C7-C8     |
| 19  | a     | 839 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 833 | CLA  | C2A-CAA-CBA-CGA |
| 19  | b     | 833 | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 841 | CLA  | C16-C17-C18-C19 |
| 19  | a     | 860 | CLA  | C16-C17-C18-C20 |
| 19  | A     | 403 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 831 | CLA  | CAA-CBA-CGA-O1A |
| 19  | j     | 103 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 806 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | b     | 805 | CLA  | C2-C3-C5-C6     |
| 19  | A     | 405 | CLA  | CAD-CBD-CGD-O2D |
| 19  | a     | 809 | CLA  | CAD-CBD-CGD-O2D |
| 19  | a     | 826 | CLA  | CAD-CBD-CGD-O2D |
| 19  | a     | 825 | CLA  | C10-C11-C12-C13 |
| 19  | b     | 822 | CLA  | C3-C5-C6-C7     |
| 19  | a     | 807 | CLA  | CAA-CBA-CGA-O1A |
| 19  | b     | 810 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 823 | CLA  | C2-C1-O2A-CGA   |
| 19  | a     | 832 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 833 | CLA  | CAA-CBA-CGA-O1A |
| 19  | b     | 804 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 822 | CLA  | CAA-CBA-CGA-O2A |
| 23  | a     | 801 | CL0  | C1A-C2A-CAA-CBA |
| 19  | a     | 841 | CLA  | C16-C17-C18-C20 |
| 19  | b     | 827 | CLA  | C16-C17-C18-C20 |
| 19  | a     | 830 | CLA  | CAA-CBA-CGA-O1A |
| 19  | b     | 806 | CLA  | CAA-CBA-CGA-O1A |
| 19  | k     | 101 | CLA  | CAA-CBA-CGA-O1A |
| 19  | a     | 843 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 811 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 19  | b     | 828 | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 820 | CLA  | C2-C3-C5-C6     |
| 19  | a     | 834 | CLA  | C5-C6-C7-C8     |
| 19  | b     | 824 | CLA  | CAA-CBA-CGA-O2A |

There are no ring outliers.

138 monomers are involved in 489 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | a     | 849 | BCR  | 2       | 0            |
| 19  | a     | 812 | CLA  | 5       | 0            |
| 19  | a     | 834 | CLA  | 6       | 0            |
| 21  | k     | 103 | BCR  | 2       | 0            |
| 21  | b     | 842 | BCR  | 5       | 0            |
| 31  | b     | 852 | ZEX  | 4       | 0            |
| 19  | a     | 815 | CLA  | 6       | 0            |
| 19  | a     | 843 | CLA  | 2       | 0            |
| 19  | b     | 819 | CLA  | 5       | 0            |
| 21  | b     | 845 | BCR  | 6       | 0            |
| 19  | a     | 805 | CLA  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 26  | b     | 849 | LHG  | 1       | 0            |
| 19  | a     | 804 | CLA  | 5       | 0            |
| 19  | b     | 824 | CLA  | 4       | 0            |
| 19  | b     | 838 | CLA  | 5       | 0            |
| 19  | b     | 804 | CLA  | 3       | 0            |
| 19  | b     | 829 | CLA  | 6       | 0            |
| 21  | a     | 848 | BCR  | 2       | 0            |
| 19  | b     | 805 | CLA  | 2       | 0            |
| 21  | f     | 202 | BCR  | 7       | 0            |
| 21  | i     | 101 | BCR  | 2       | 0            |
| 22  | E     | 101 | HEM  | 3       | 0            |
| 21  | a     | 850 | BCR  | 4       | 0            |
| 19  | a     | 829 | CLA  | 9       | 0            |
| 19  | b     | 835 | CLA  | 2       | 0            |
| 21  | a     | 846 | BCR  | 6       | 0            |
| 19  | f     | 203 | CLA  | 1       | 0            |
| 19  | a     | 810 | CLA  | 2       | 0            |
| 19  | b     | 821 | CLA  | 6       | 0            |
| 19  | a     | 833 | CLA  | 4       | 0            |
| 19  | b     | 813 | CLA  | 7       | 0            |
| 19  | l     | 203 | CLA  | 6       | 0            |
| 19  | b     | 832 | CLA  | 5       | 0            |
| 19  | b     | 839 | CLA  | 4       | 0            |
| 25  | c     | 101 | SF4  | 1       | 0            |
| 19  | a     | 808 | CLA  | 4       | 0            |
| 19  | b     | 812 | CLA  | 5       | 0            |
| 19  | a     | 826 | CLA  | 3       | 0            |
| 19  | b     | 820 | CLA  | 1       | 0            |
| 24  | a     | 844 | PQN  | 2       | 0            |
| 26  | a     | 853 | LHG  | 5       | 0            |
| 19  | b     | 802 | CLA  | 2       | 0            |
| 19  | a     | 860 | CLA  | 5       | 0            |
| 19  | a     | 814 | CLA  | 3       | 0            |
| 21  | a     | 847 | BCR  | 3       | 0            |
| 19  | f     | 204 | CLA  | 1       | 0            |
| 19  | b     | 801 | CLA  | 4       | 0            |
| 21  | b     | 846 | BCR  | 3       | 0            |
| 23  | a     | 801 | CL0  | 4       | 0            |
| 19  | A     | 407 | CLA  | 5       | 0            |
| 19  | D     | 403 | CLA  | 1       | 0            |
| 19  | a     | 830 | CLA  | 6       | 0            |
| 19  | a     | 831 | CLA  | 8       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 19  | A     | 402 | CLA  | 4       | 0            |
| 25  | c     | 102 | SF4  | 1       | 0            |
| 19  | A     | 403 | CLA  | 4       | 0            |
| 21  | b     | 847 | BCR  | 7       | 0            |
| 19  | a     | 823 | CLA  | 3       | 0            |
| 19  | b     | 811 | CLA  | 2       | 0            |
| 26  | a     | 852 | LHG  | 2       | 0            |
| 19  | a     | 836 | CLA  | 7       | 0            |
| 27  | a     | 854 | LMG  | 1       | 0            |
| 19  | a     | 842 | CLA  | 4       | 0            |
| 19  | a     | 856 | CLA  | 3       | 0            |
| 30  | b     | 851 | EQ3  | 1       | 0            |
| 19  | b     | 830 | CLA  | 1       | 0            |
| 19  | f     | 201 | CLA  | 3       | 0            |
| 19  | A     | 405 | CLA  | 5       | 0            |
| 21  | A     | 406 | BCR  | 6       | 0            |
| 20  | A     | 404 | PHO  | 4       | 0            |
| 28  | a     | 858 | 45D  | 3       | 0            |
| 19  | a     | 840 | CLA  | 8       | 0            |
| 26  | a     | 855 | LHG  | 3       | 0            |
| 19  | D     | 402 | CLA  | 9       | 0            |
| 19  | a     | 809 | CLA  | 6       | 0            |
| 19  | b     | 817 | CLA  | 2       | 0            |
| 19  | a     | 821 | CLA  | 6       | 0            |
| 19  | b     | 807 | CLA  | 10      | 0            |
| 19  | b     | 836 | CLA  | 5       | 0            |
| 19  | b     | 825 | CLA  | 4       | 0            |
| 19  | k     | 101 | CLA  | 4       | 0            |
| 21  | j     | 101 | BCR  | 3       | 0            |
| 19  | b     | 818 | CLA  | 4       | 0            |
| 19  | b     | 834 | CLA  | 2       | 0            |
| 31  | f     | 205 | ZEX  | 1       | 0            |
| 19  | j     | 104 | CLA  | 3       | 0            |
| 19  | b     | 822 | CLA  | 7       | 0            |
| 19  | a     | 837 | CLA  | 8       | 0            |
| 19  | k     | 102 | CLA  | 1       | 0            |
| 19  | b     | 809 | CLA  | 4       | 0            |
| 19  | b     | 833 | CLA  | 1       | 0            |
| 19  | b     | 814 | CLA  | 9       | 0            |
| 19  | b     | 808 | CLA  | 2       | 0            |
| 19  | b     | 826 | CLA  | 4       | 0            |
| 19  | a     | 811 | CLA  | 5       | 0            |

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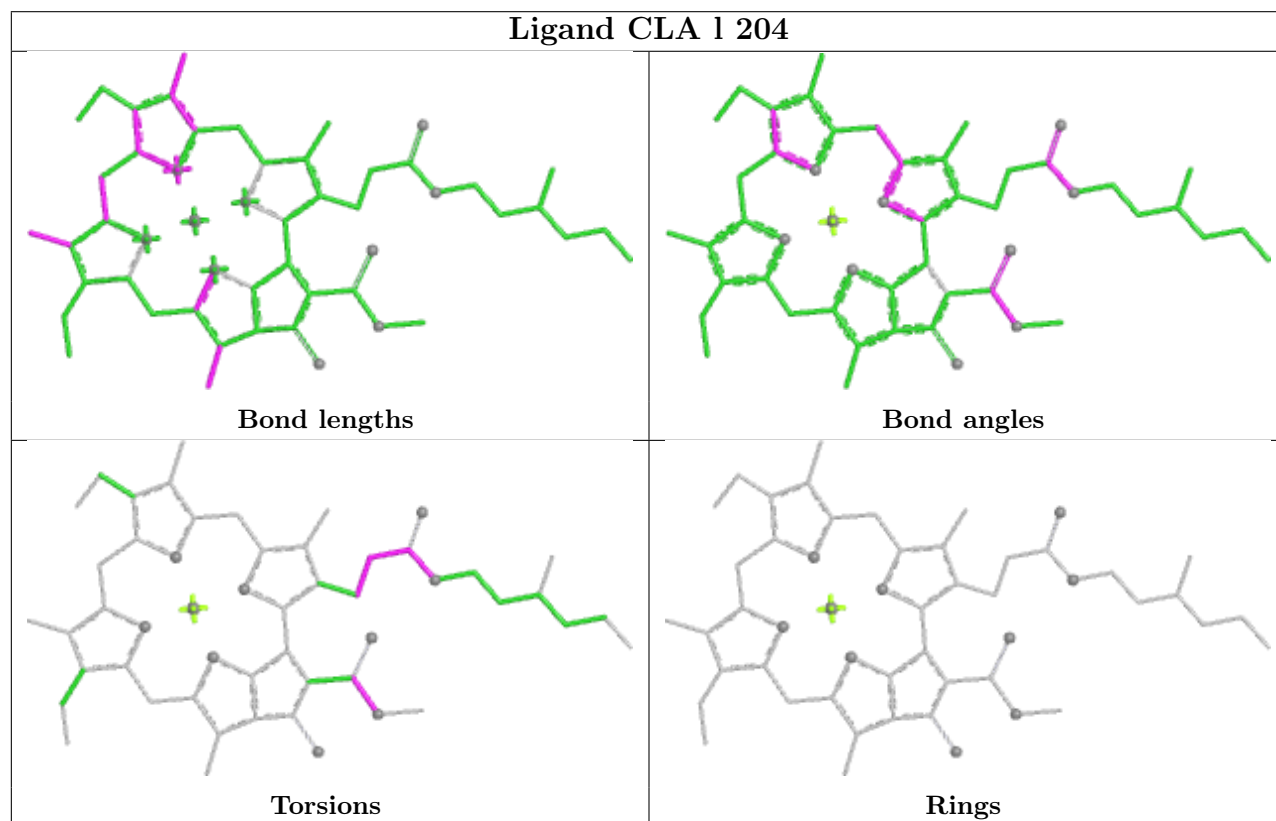
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|-----|-------|-----|------|---------|--------------|
| 19  | a     | 819 | CLA  | 3       | 0            |
| 19  | b     | 840 | CLA  | 2       | 0            |
| 19  | a     | 824 | CLA  | 4       | 0            |
| 19  | b     | 828 | CLA  | 11      | 0            |
| 21  | l     | 205 | BCR  | 4       | 0            |
| 19  | a     | 838 | CLA  | 1       | 0            |
| 19  | a     | 841 | CLA  | 7       | 0            |
| 24  | b     | 841 | PQN  | 3       | 0            |
| 19  | b     | 803 | CLA  | 3       | 0            |
| 19  | a     | 827 | CLA  | 5       | 0            |
| 21  | b     | 843 | BCR  | 1       | 0            |
| 19  | a     | 822 | CLA  | 10      | 0            |
| 19  | b     | 806 | CLA  | 6       | 0            |
| 19  | a     | 835 | CLA  | 8       | 0            |
| 29  | m     | 101 | ECH  | 4       | 0            |
| 19  | a     | 807 | CLA  | 6       | 0            |
| 19  | a     | 825 | CLA  | 6       | 0            |
| 19  | a     | 802 | CLA  | 2       | 0            |
| 19  | a     | 813 | CLA  | 6       | 0            |
| 19  | a     | 818 | CLA  | 5       | 0            |
| 26  | f     | 206 | LHG  | 4       | 0            |
| 19  | b     | 837 | CLA  | 8       | 0            |
| 19  | j     | 103 | CLA  | 4       | 0            |
| 27  | l     | 201 | LMG  | 3       | 0            |
| 19  | a     | 832 | CLA  | 9       | 0            |
| 19  | a     | 828 | CLA  | 6       | 0            |
| 29  | b     | 844 | ECH  | 4       | 0            |
| 19  | l     | 202 | CLA  | 2       | 0            |
| 19  | a     | 806 | CLA  | 7       | 0            |
| 19  | a     | 803 | CLA  | 8       | 0            |
| 19  | a     | 839 | CLA  | 6       | 0            |
| 20  | D     | 401 | PHO  | 3       | 0            |
| 19  | b     | 831 | CLA  | 4       | 0            |
| 21  | i     | 102 | BCR  | 4       | 0            |
| 27  | b     | 848 | LMG  | 9       | 0            |
| 21  | a     | 851 | BCR  | 1       | 0            |
| 19  | b     | 827 | CLA  | 4       | 0            |
| 19  | a     | 820 | CLA  | 6       | 0            |
| 19  | a     | 857 | CLA  | 2       | 0            |
| 19  | b     | 823 | CLA  | 8       | 0            |
| 19  | b     | 815 | CLA  | 6       | 0            |
| 21  | a     | 859 | BCR  | 6       | 0            |

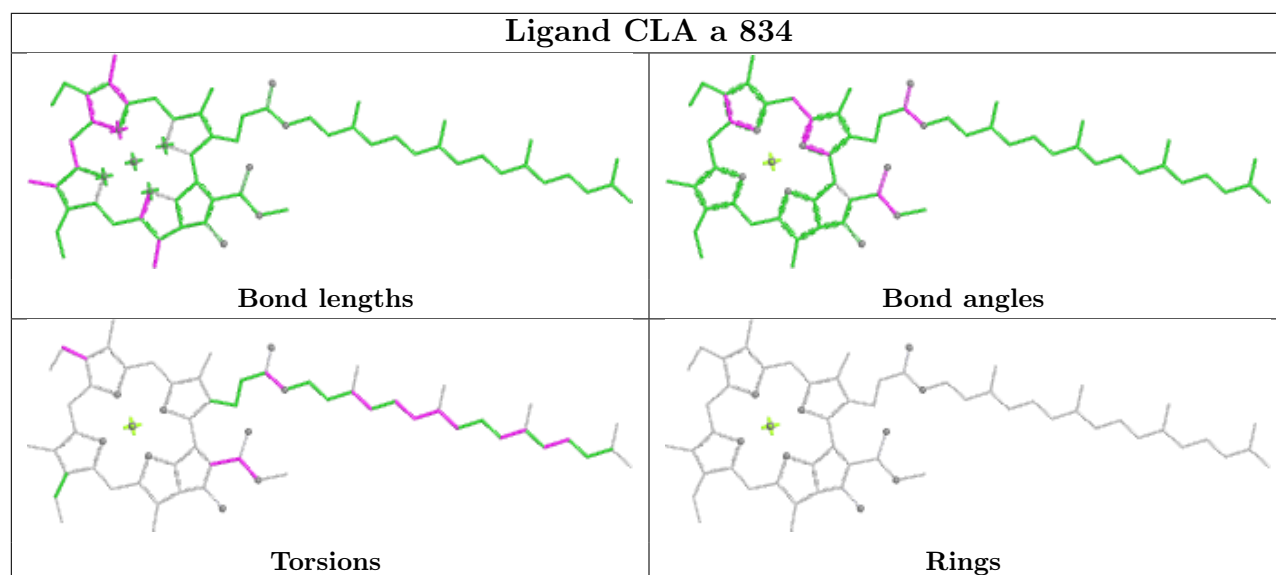
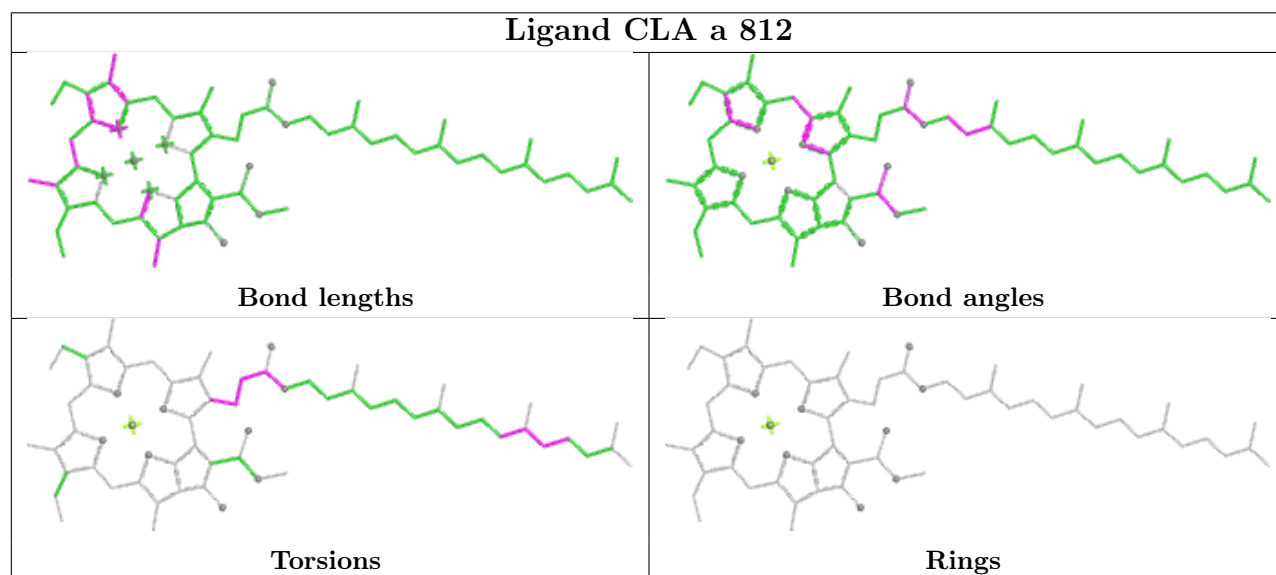
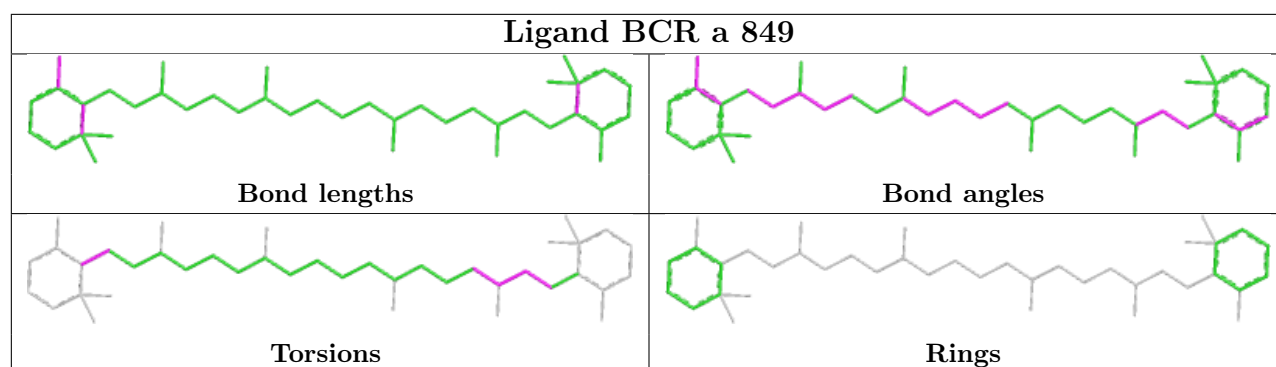
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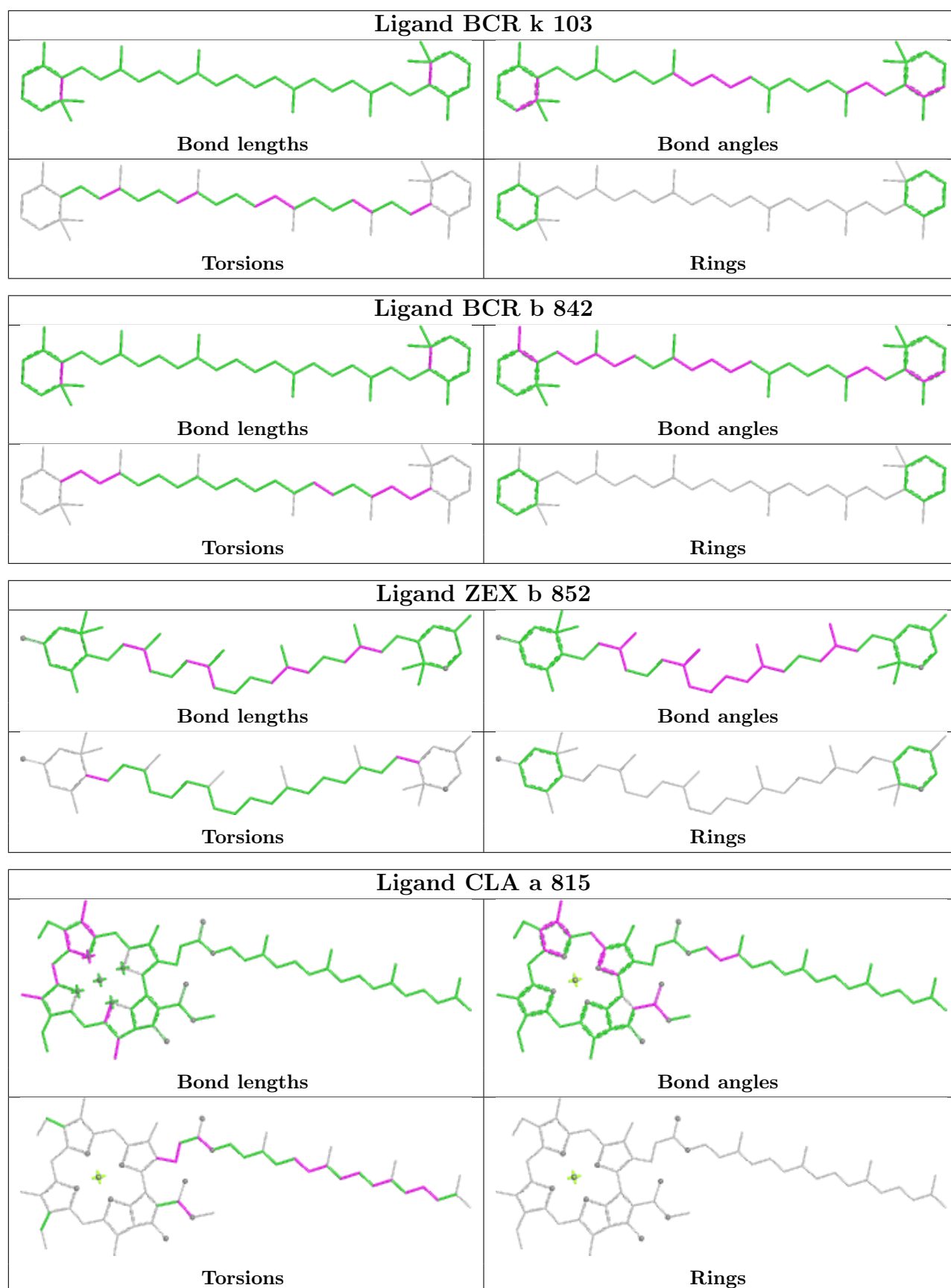
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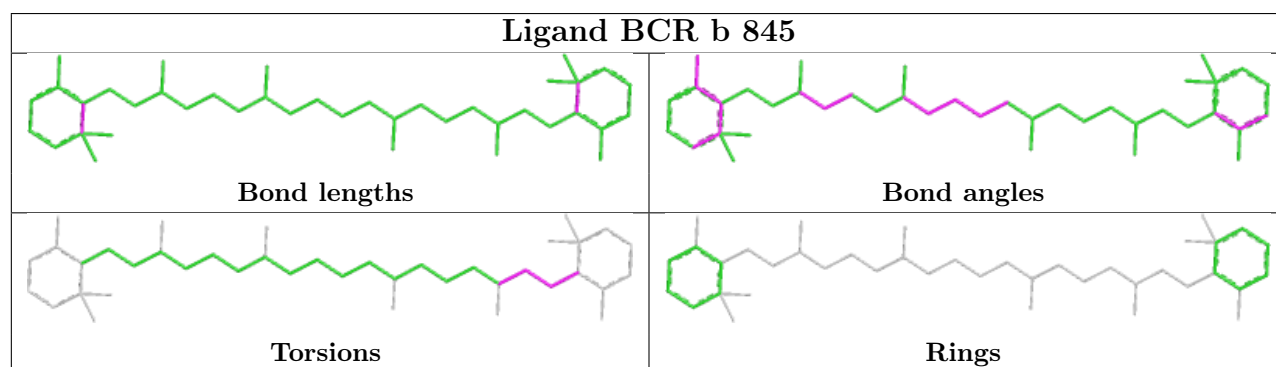
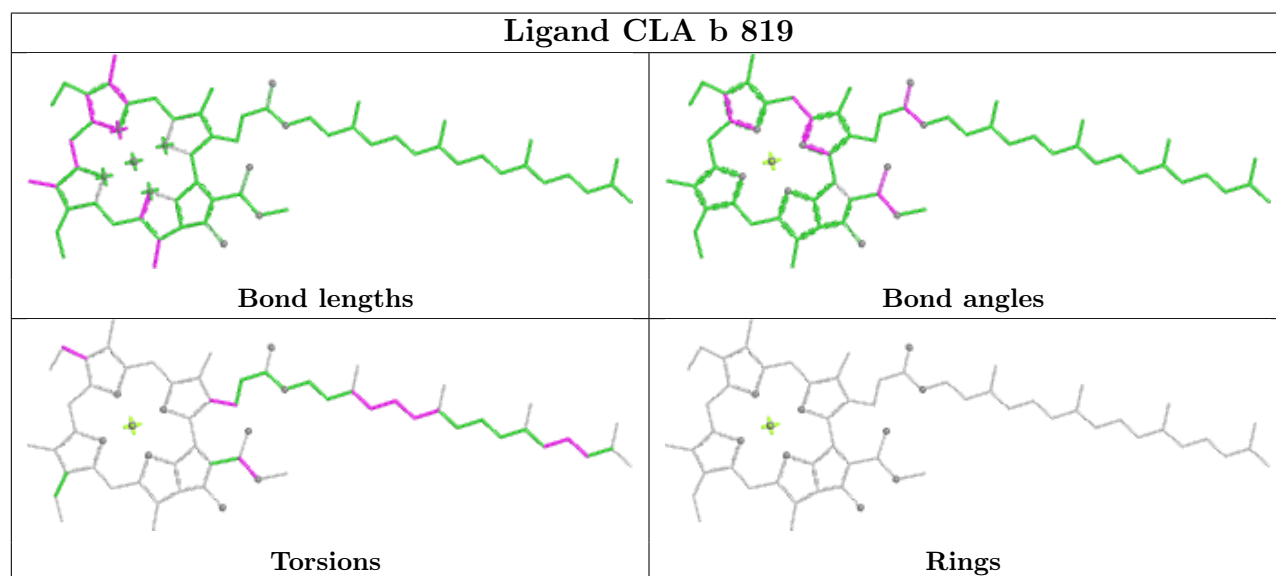
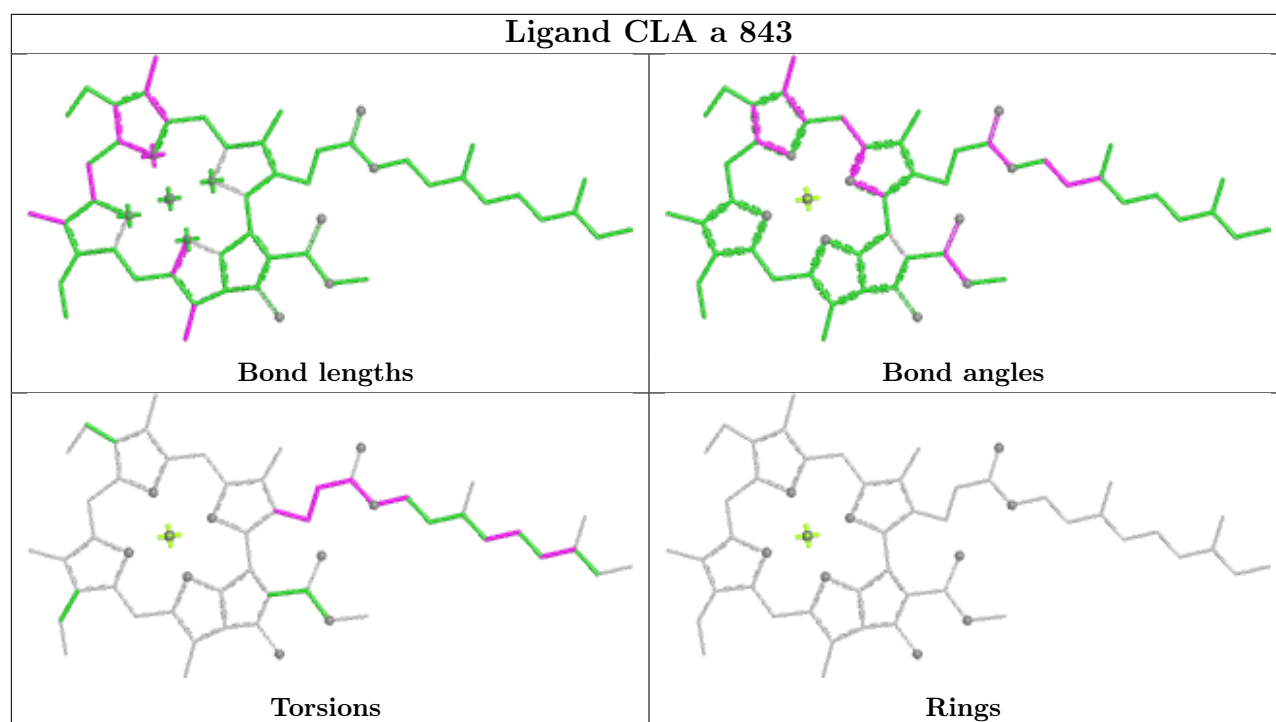
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 19  | b     | 816 | CLA  | 9       | 0            |

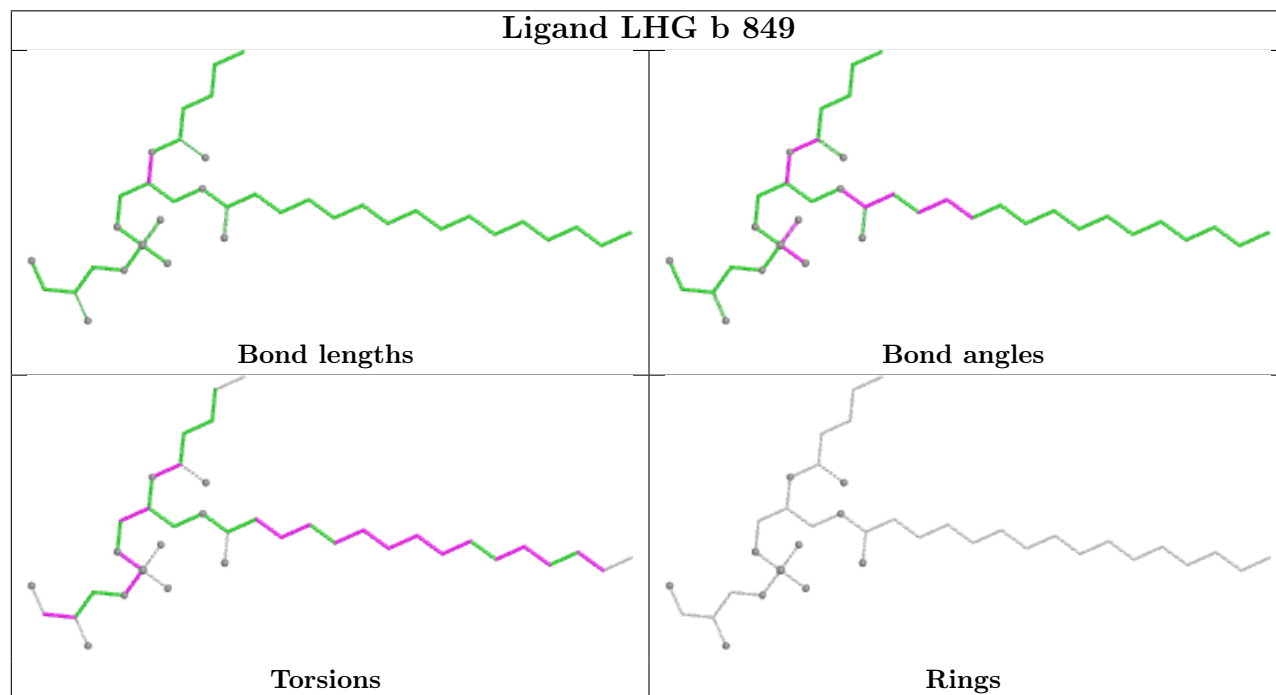
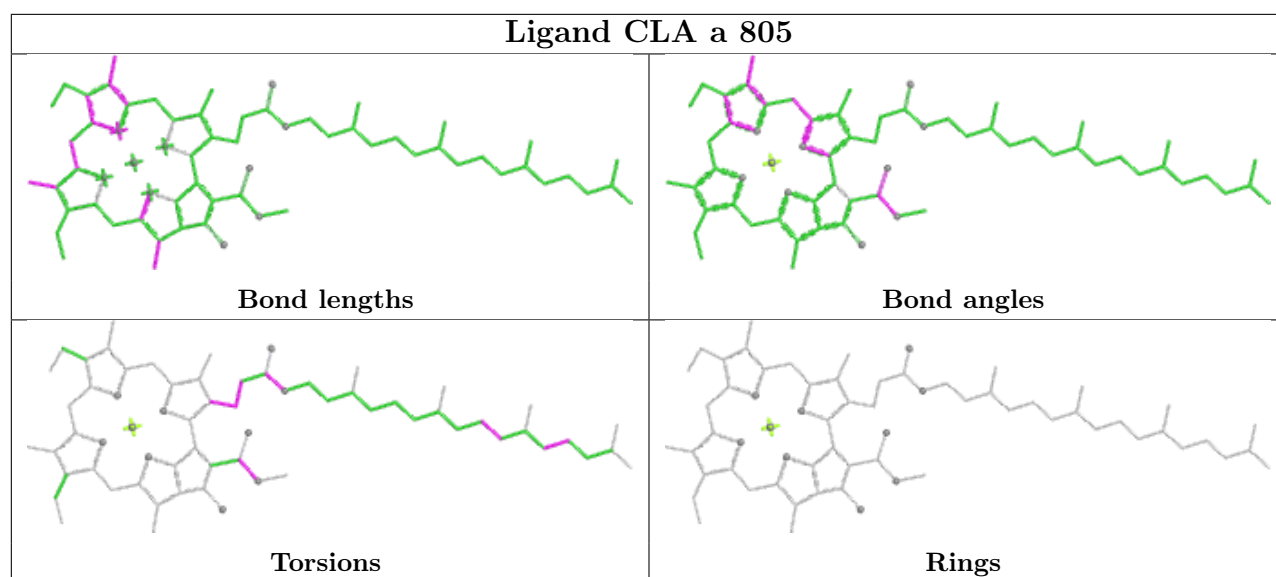
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

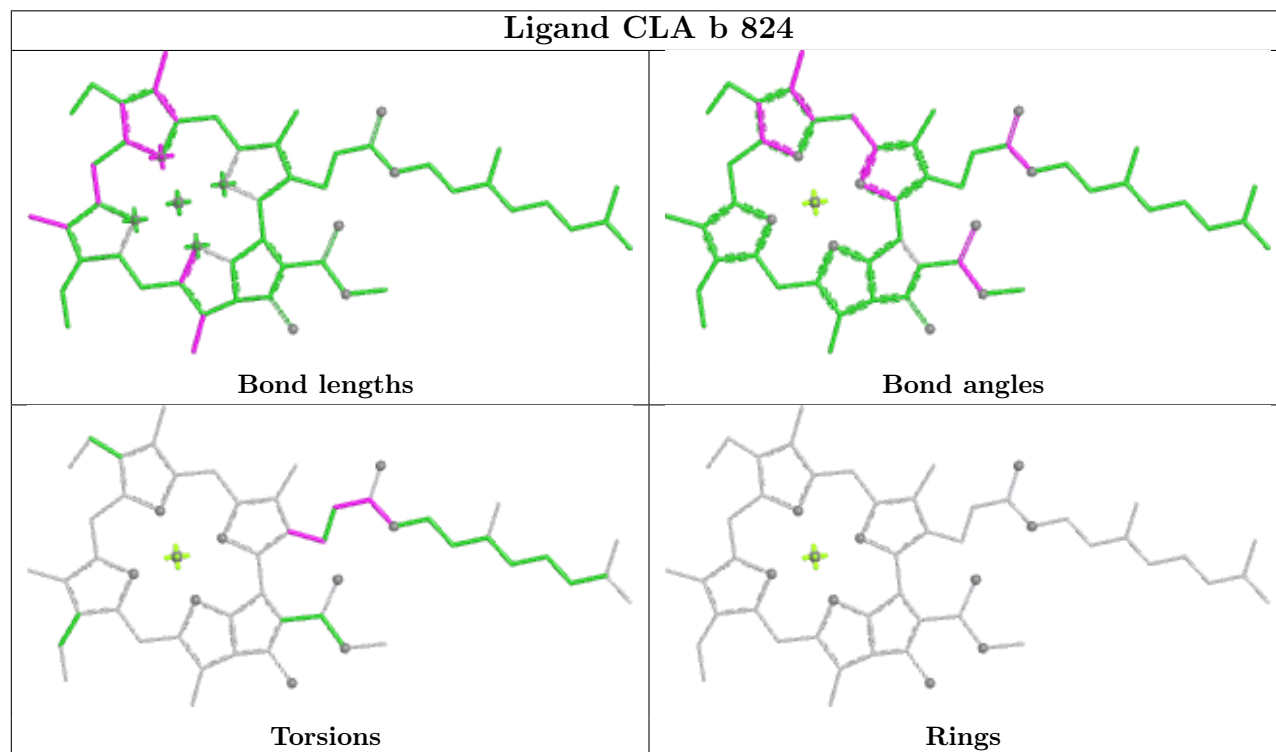
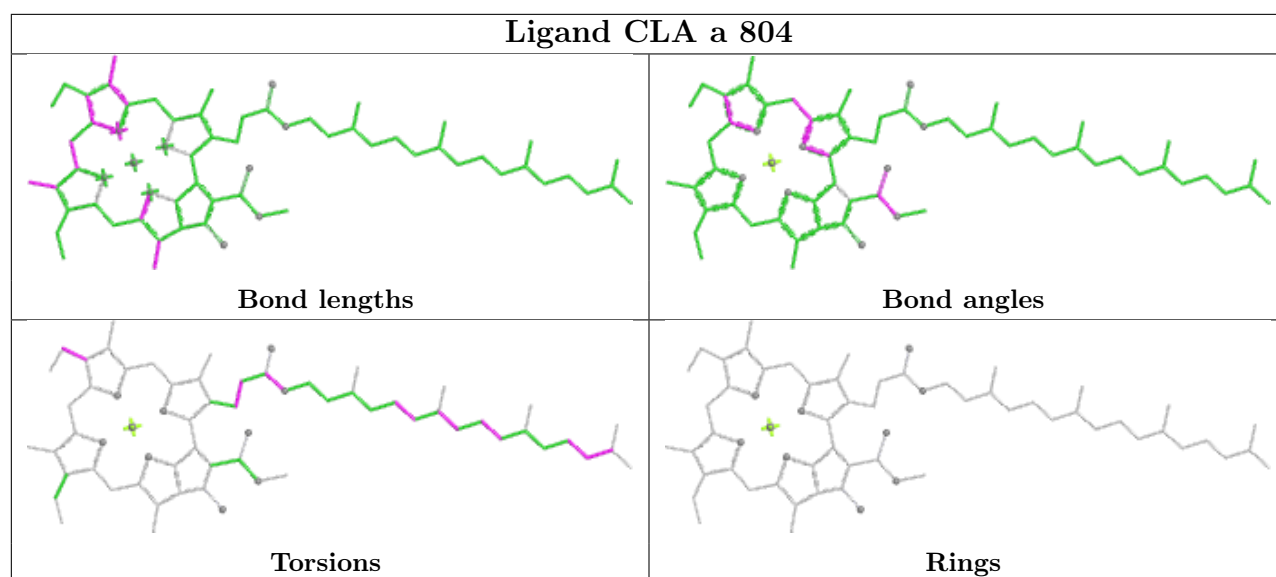




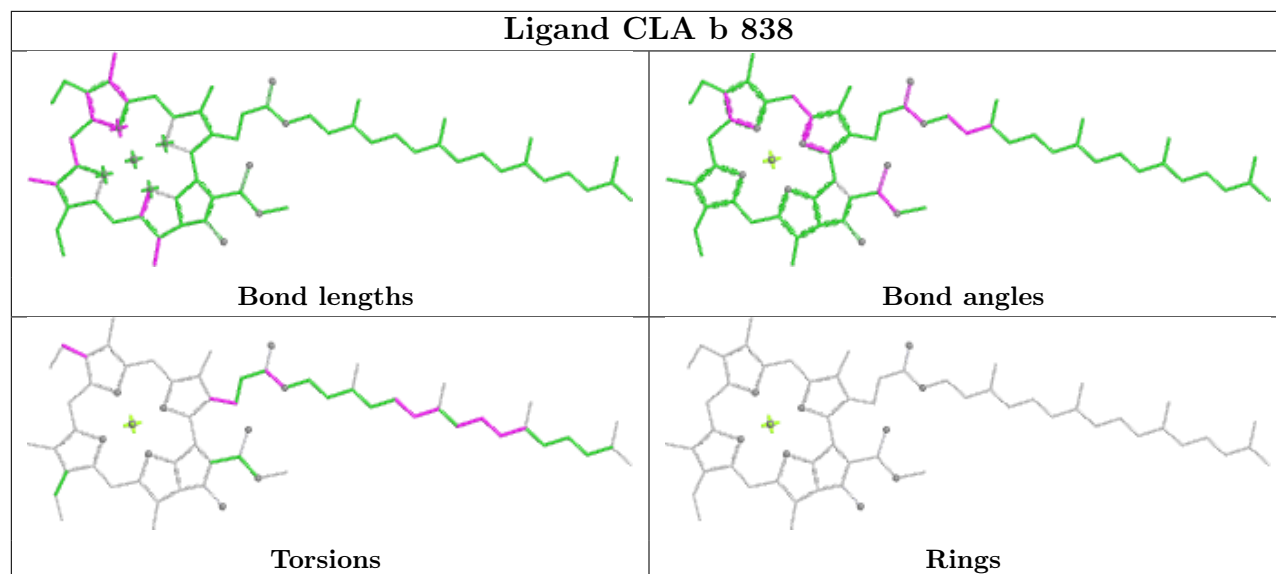




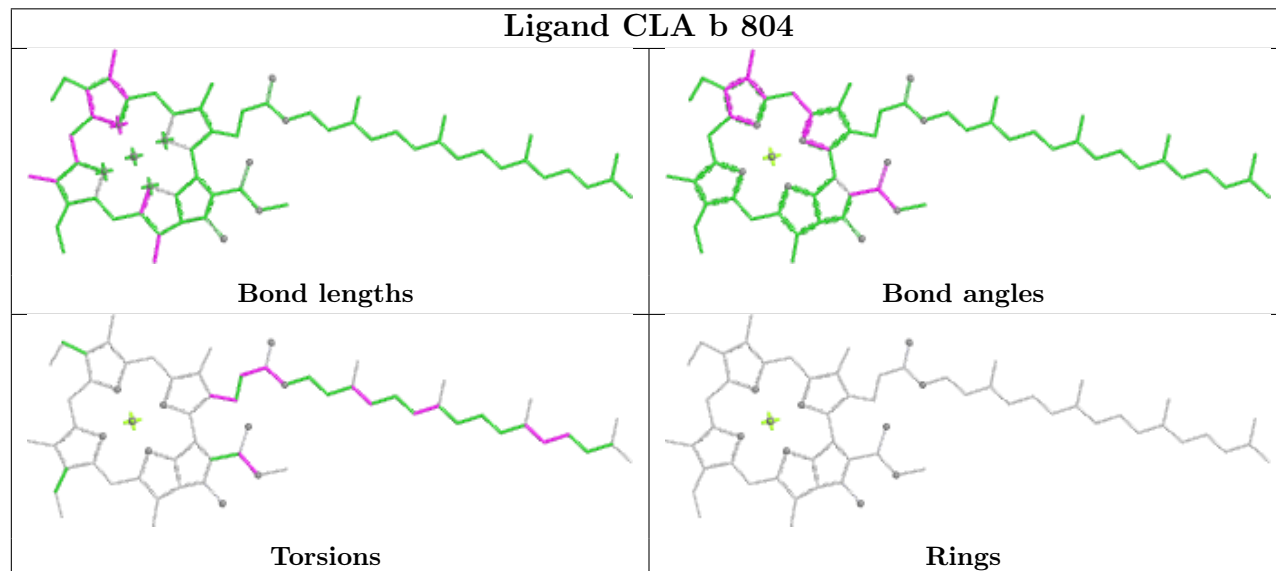




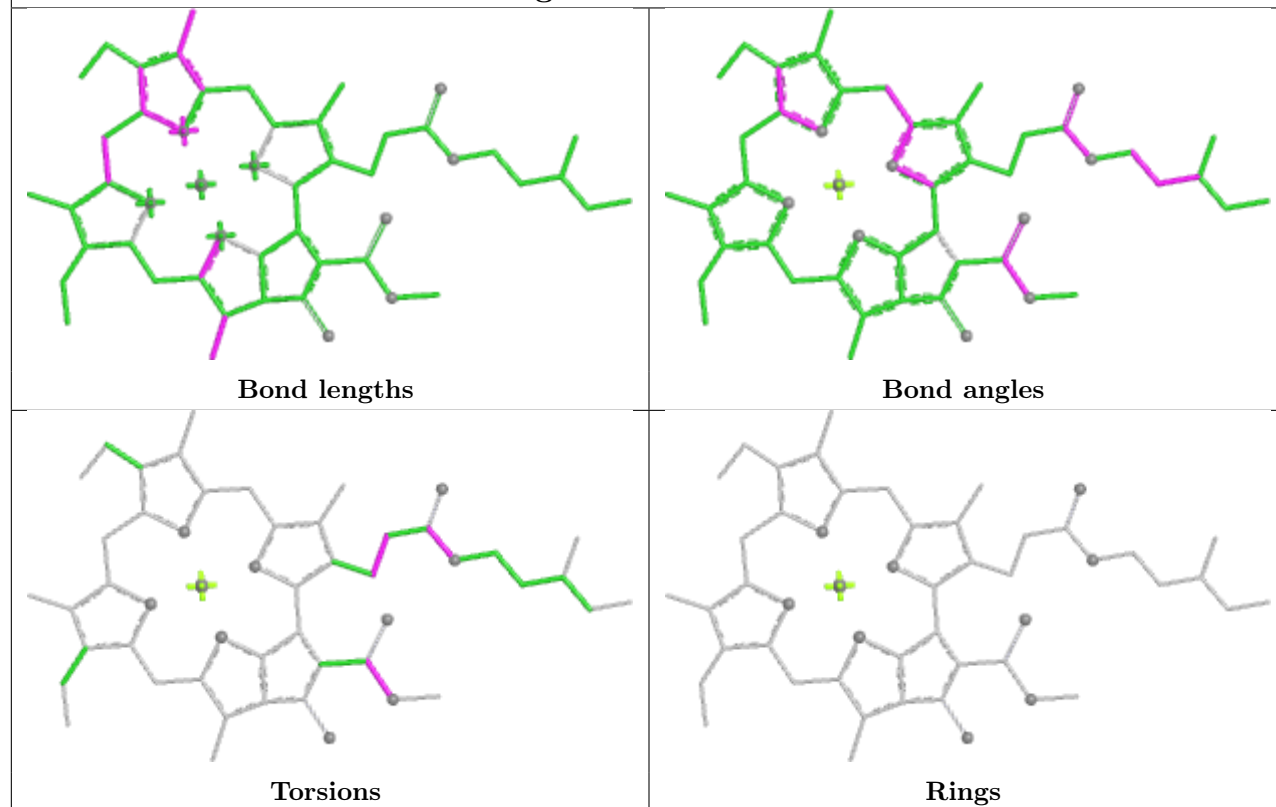
## Ligand CLA b 838



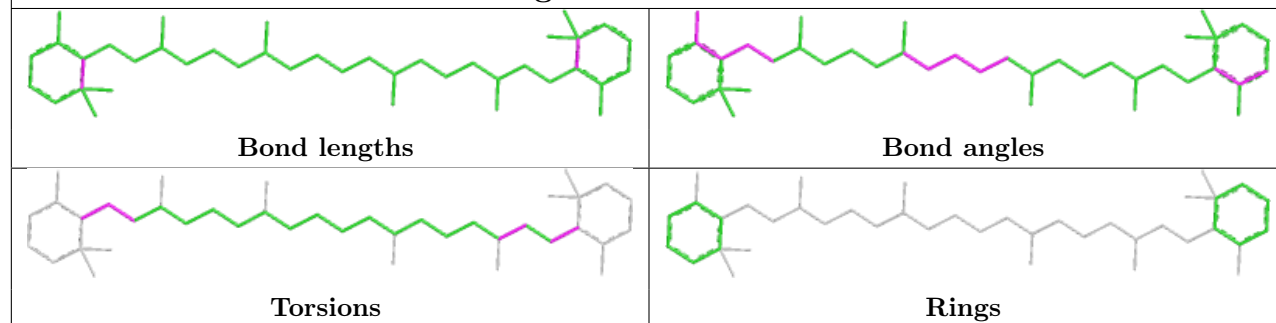
## Ligand CLA b 804

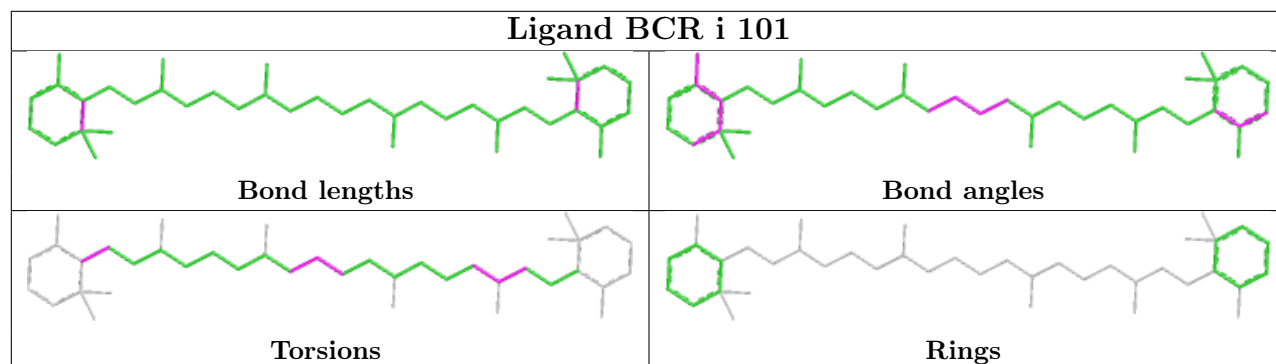
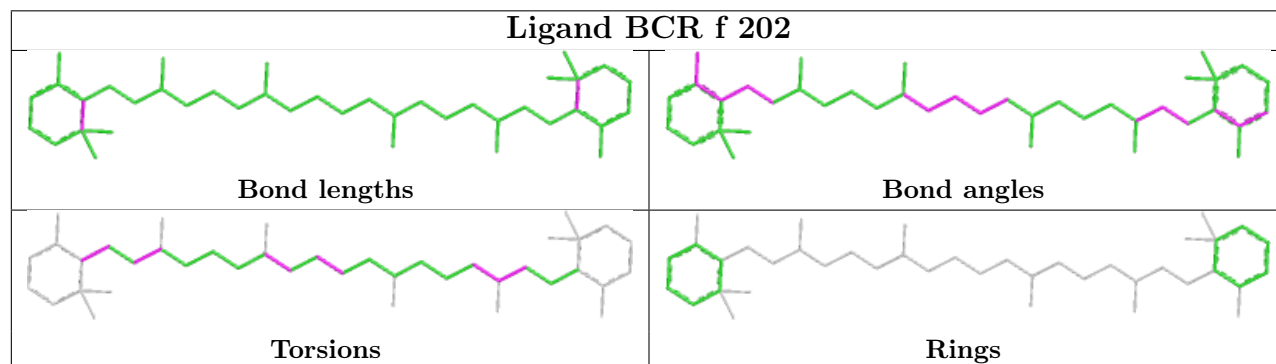
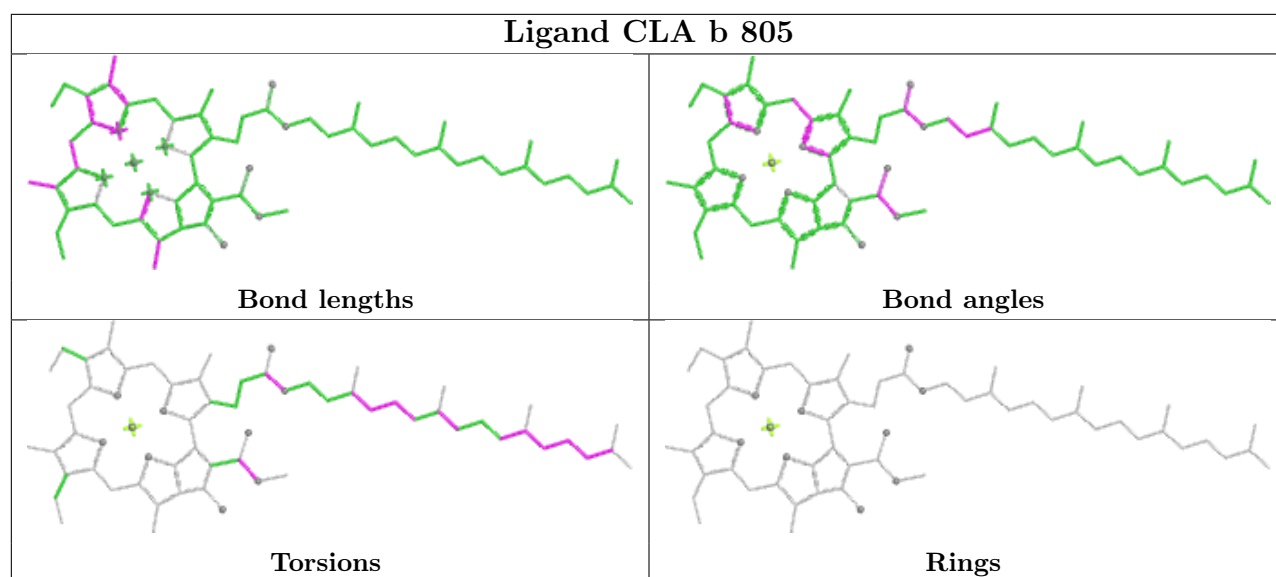


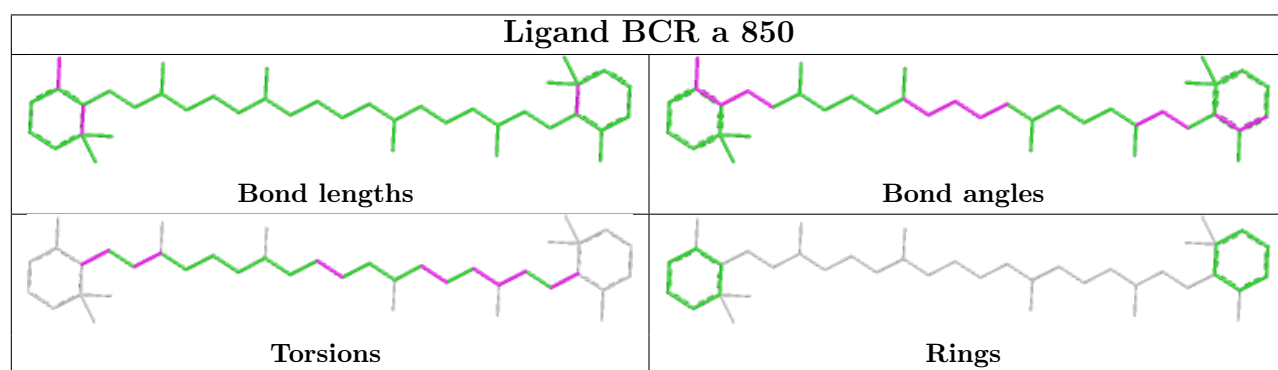
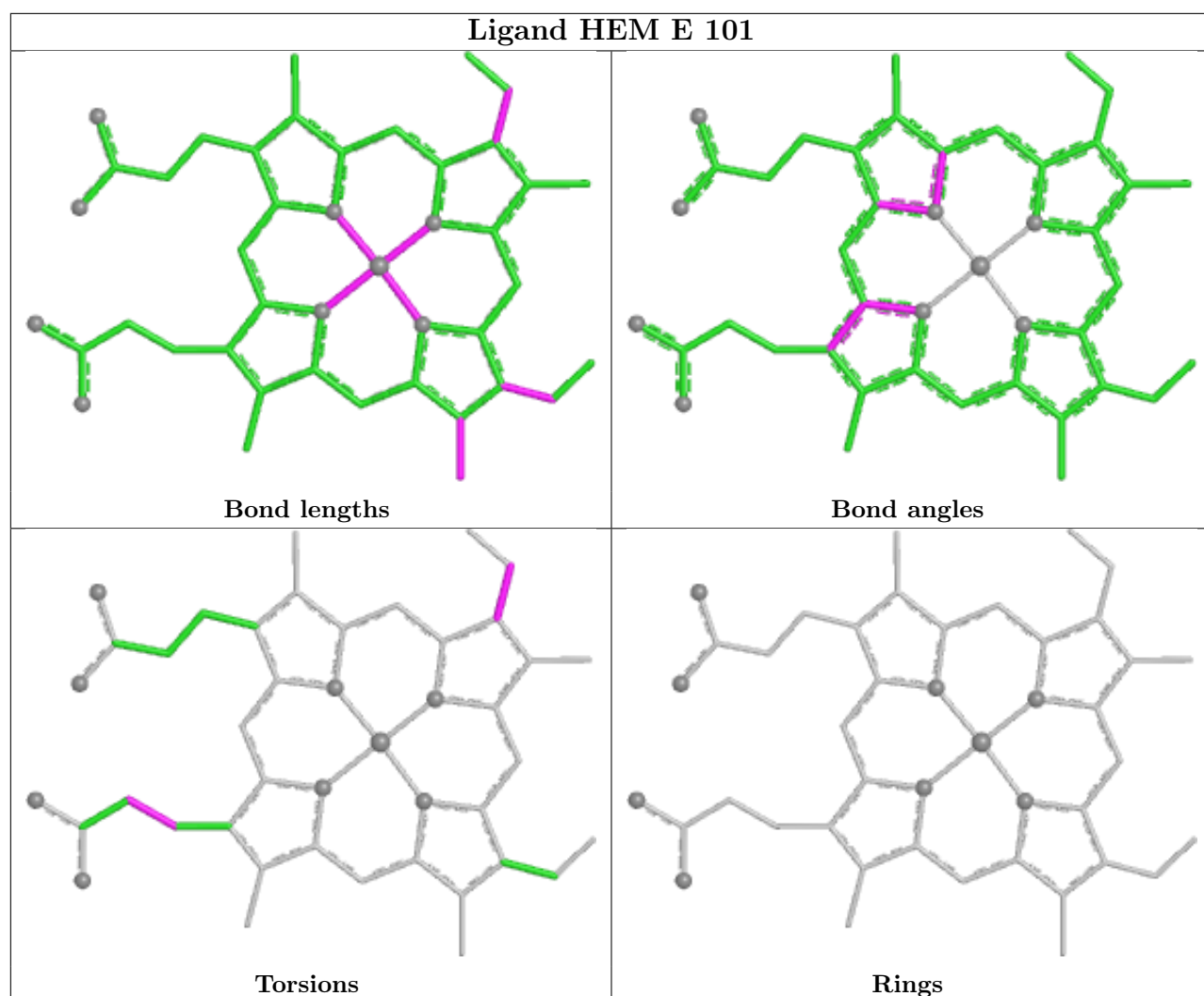
## Ligand CLA b 829

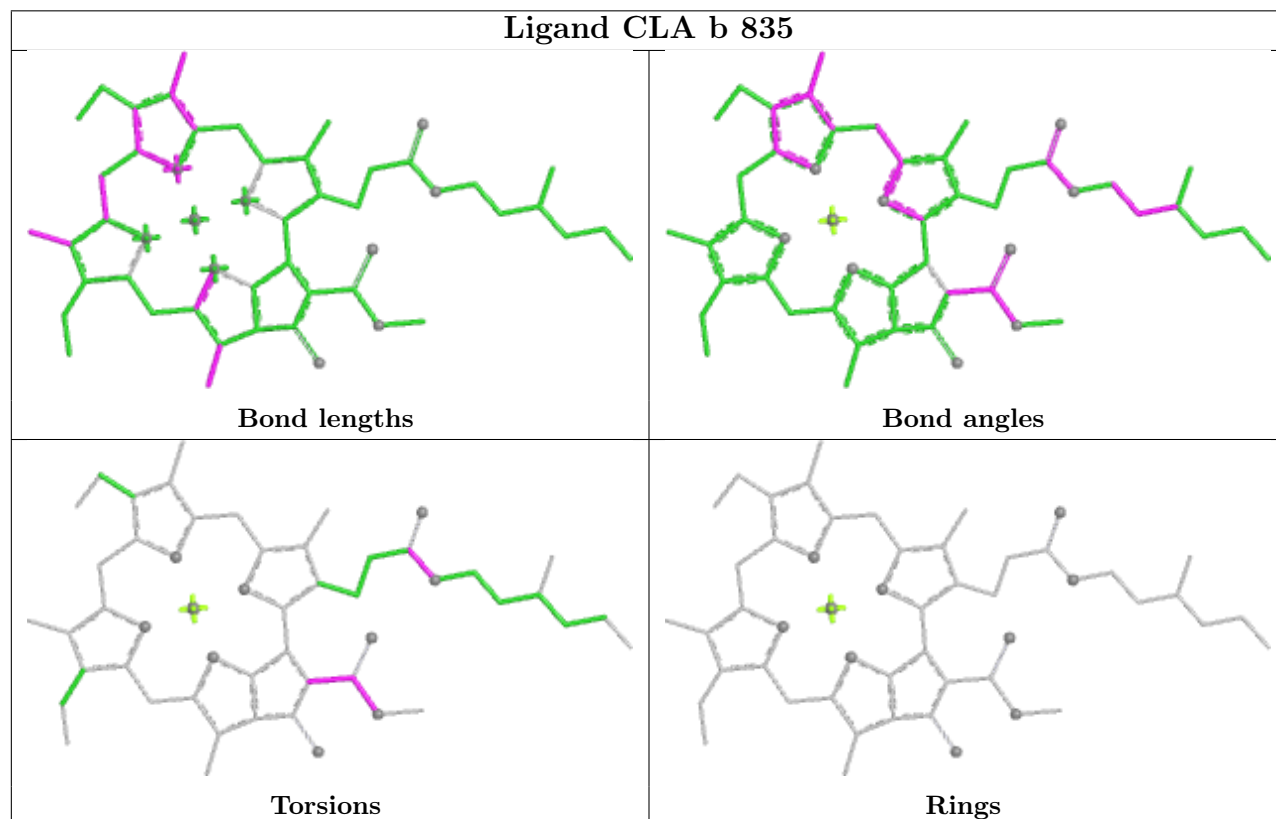
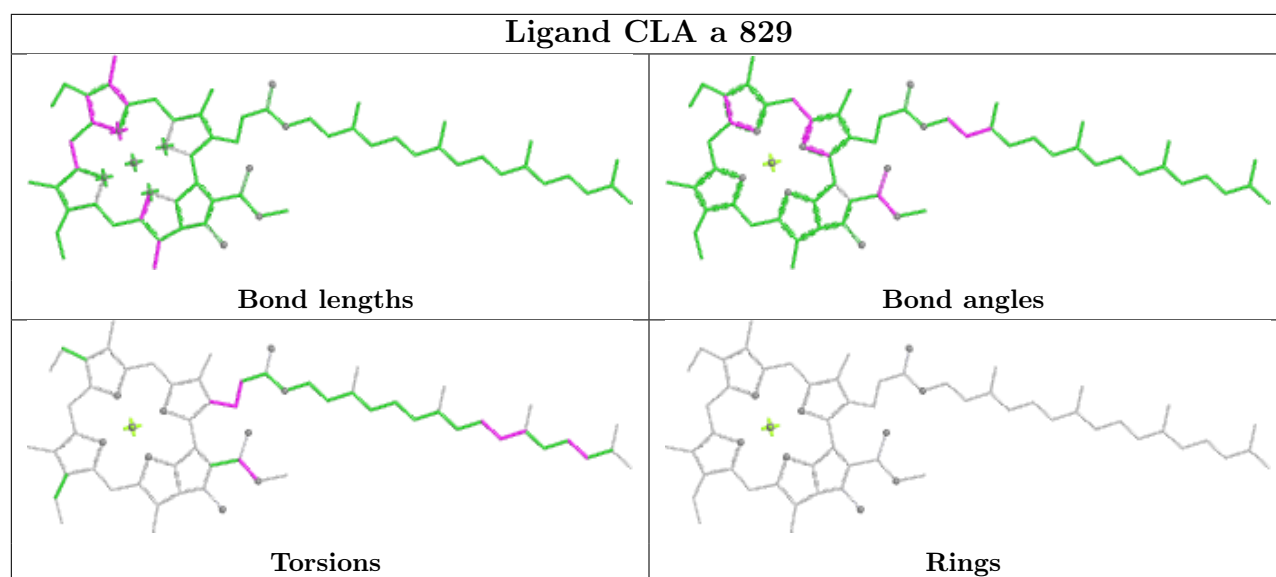


## Ligand BCR a 848

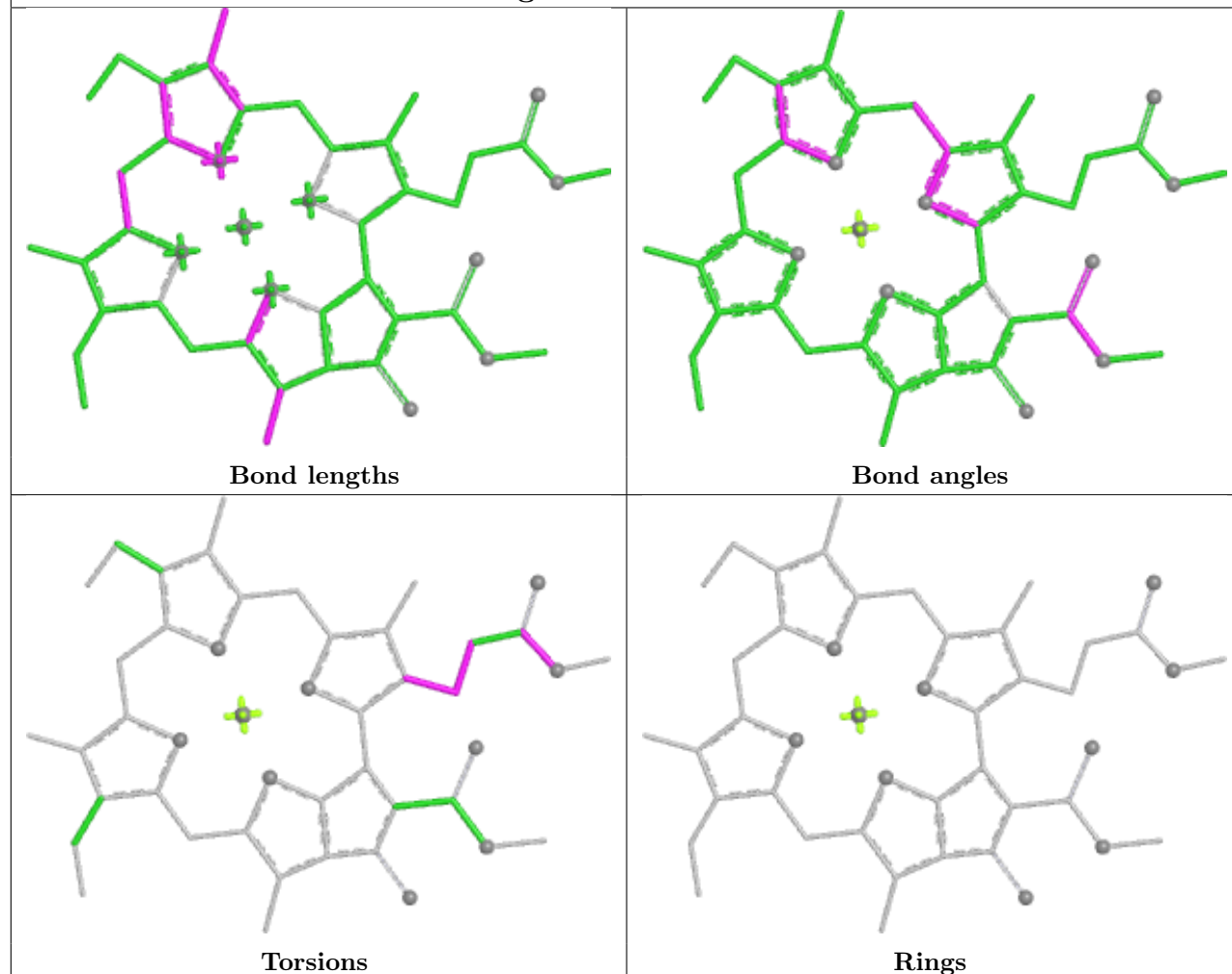




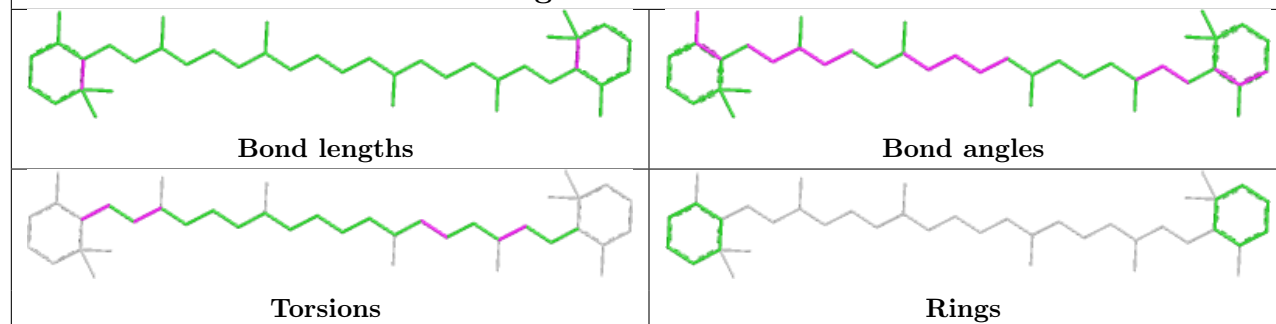




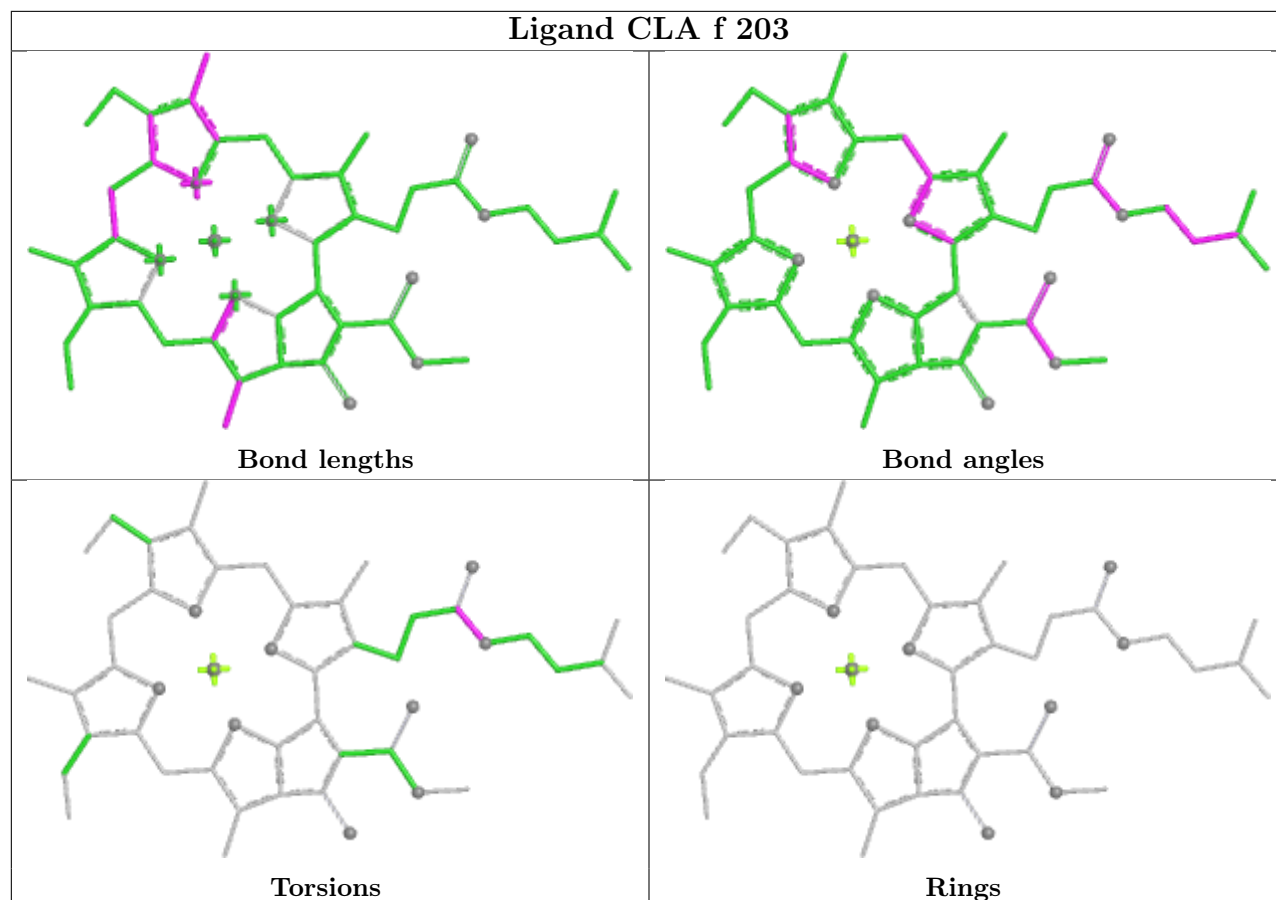
## Ligand CLA a 817



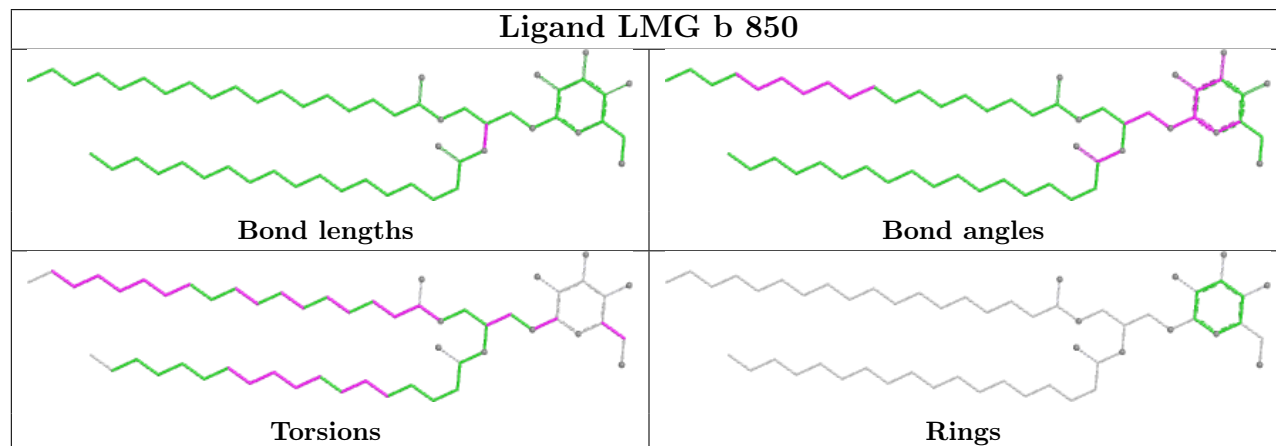
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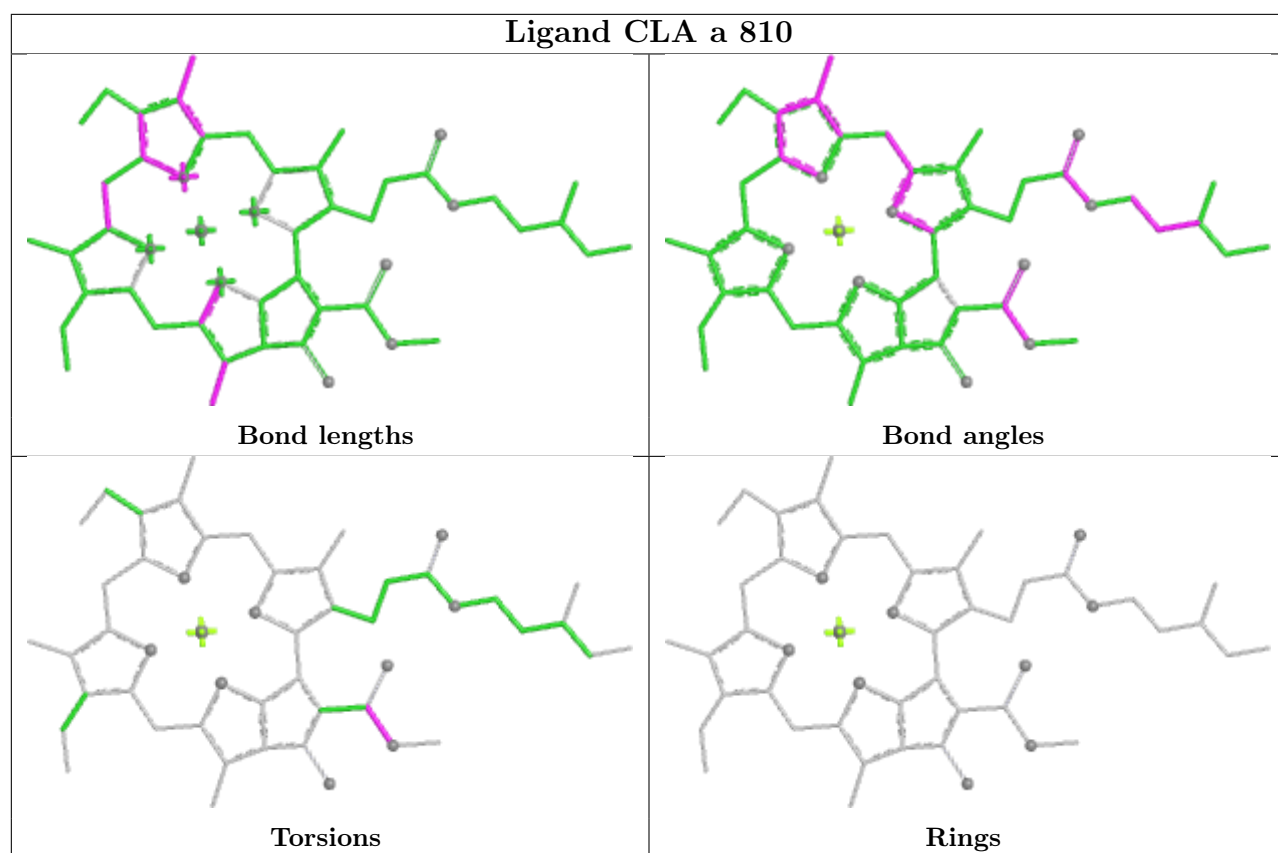


## Ligand CLA f 203

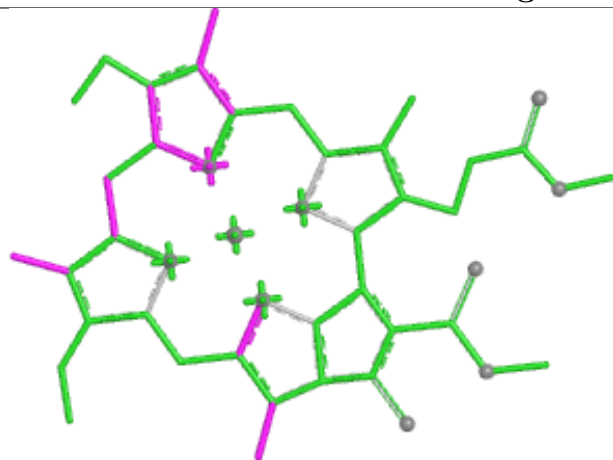


## Ligand LMG b 850

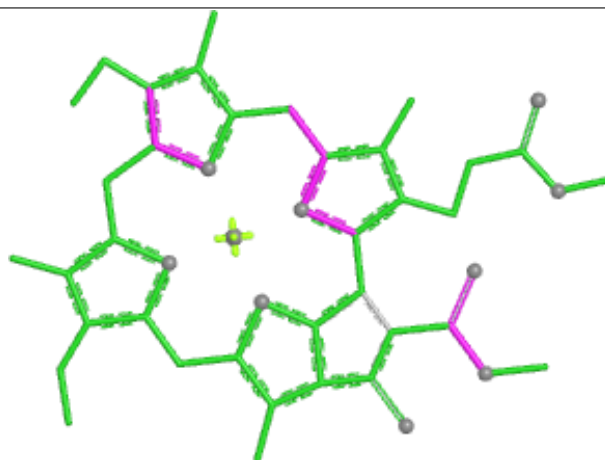




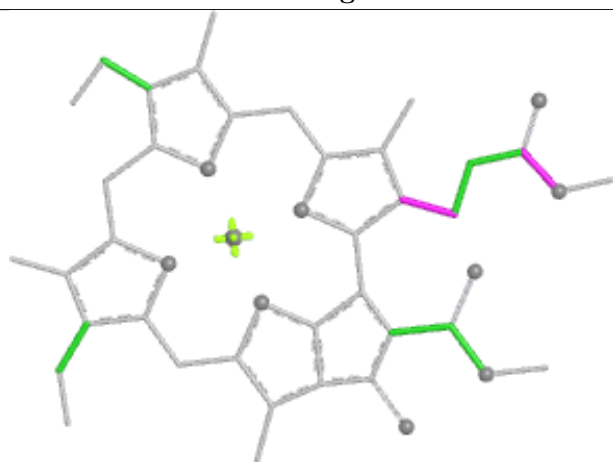
## Ligand CLA b 821



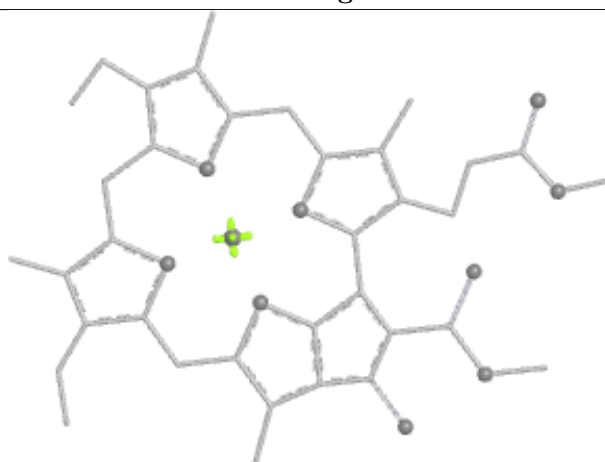
Bond lengths



Bond angles

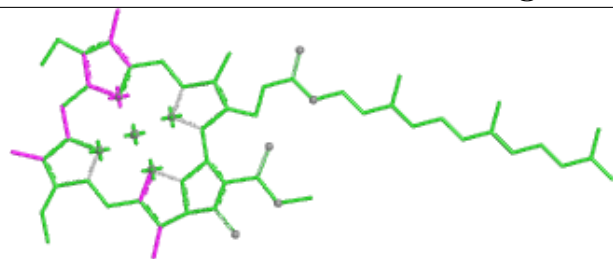


Torsions

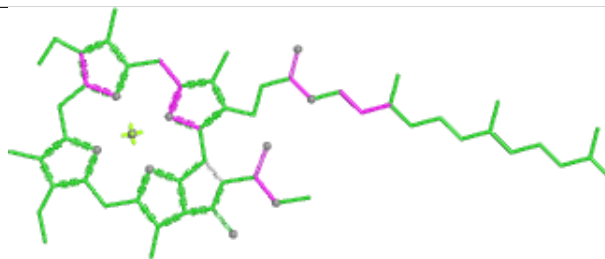


Rings

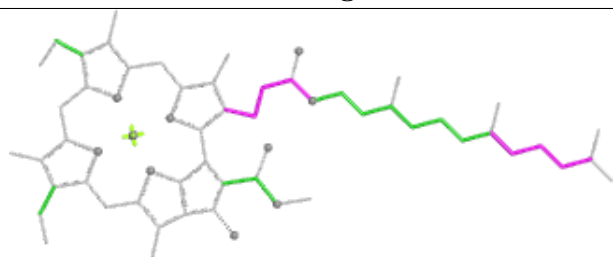
## Ligand CLA a 833



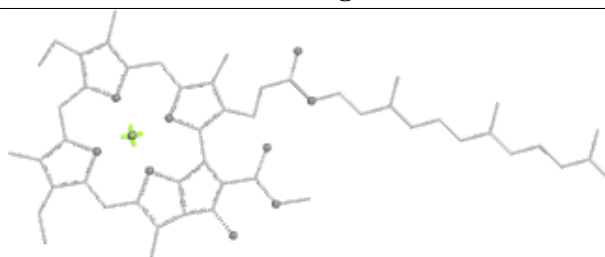
Bond lengths



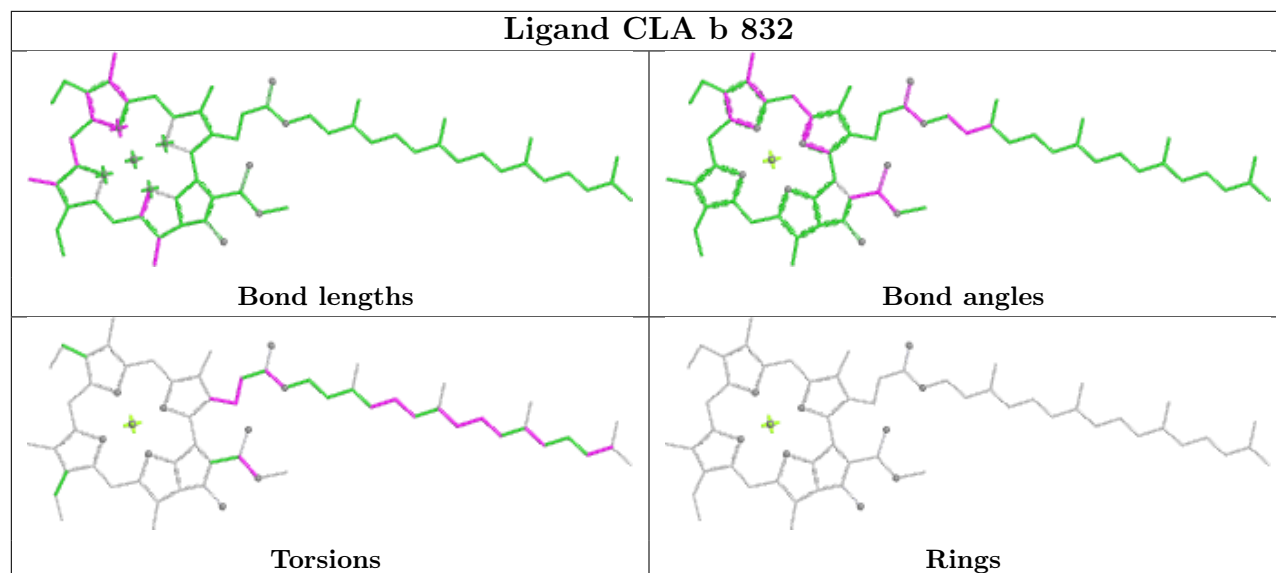
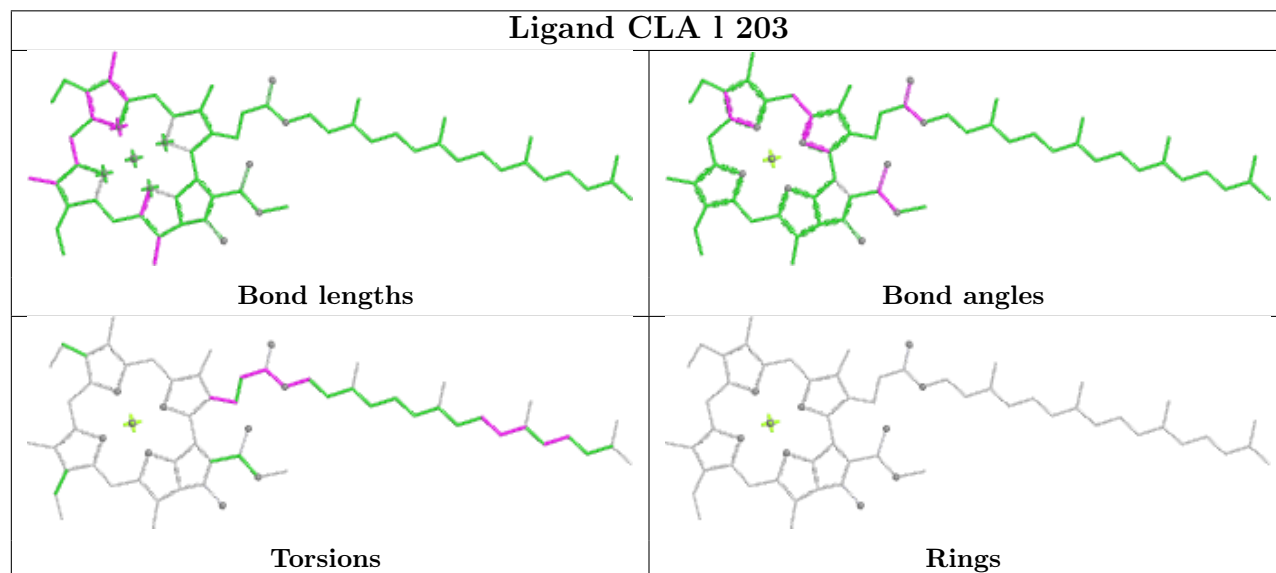
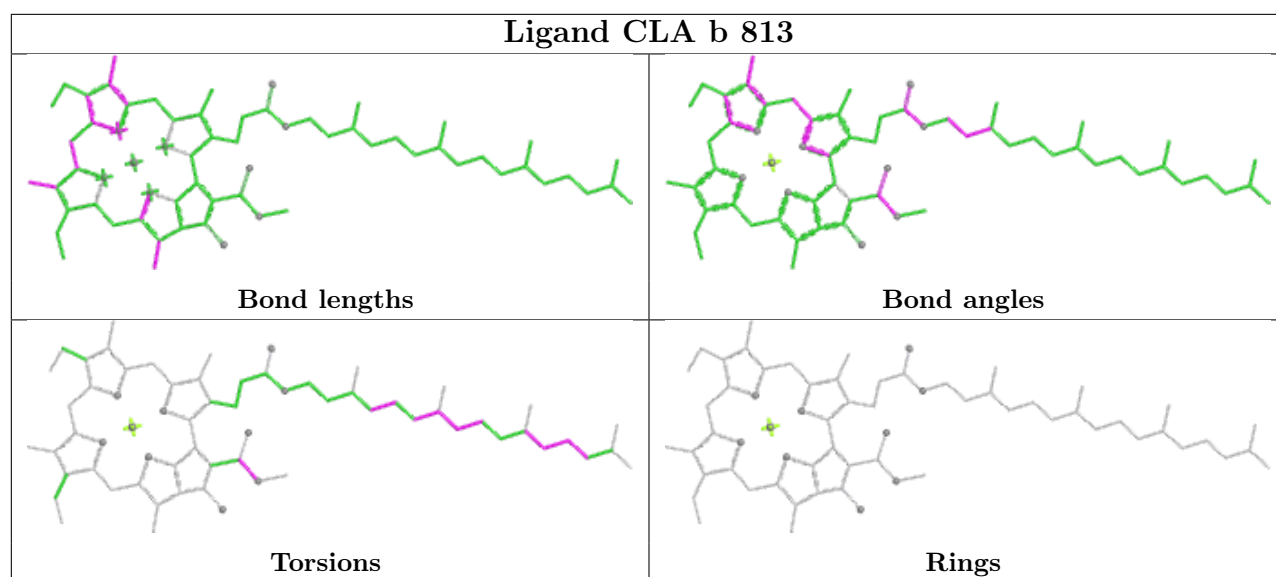
Bond angles

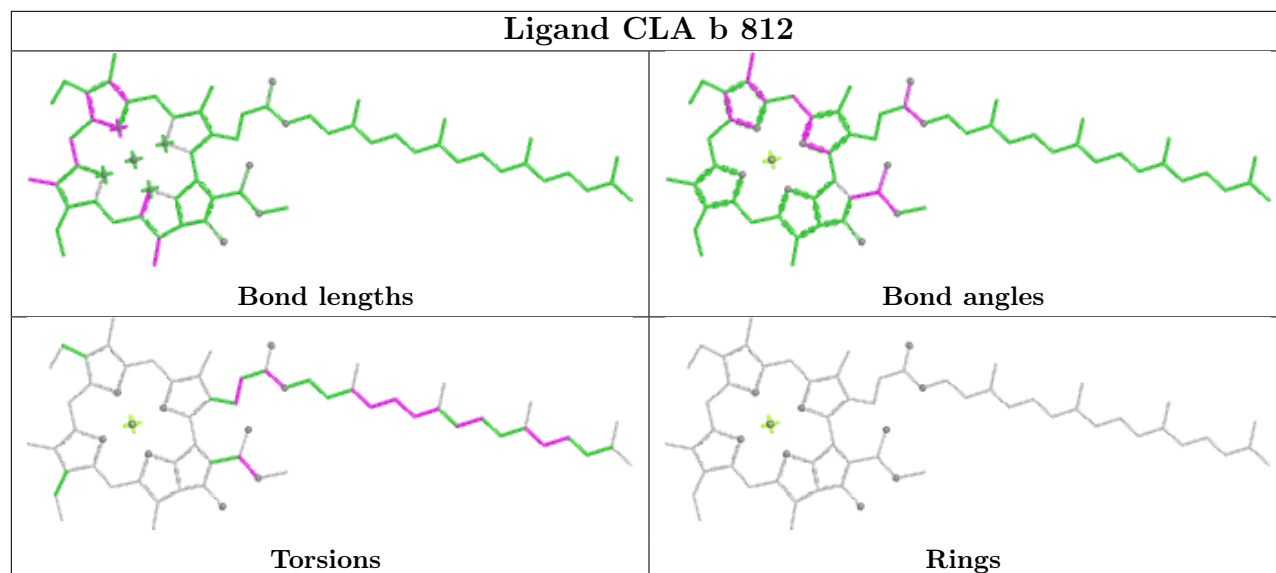
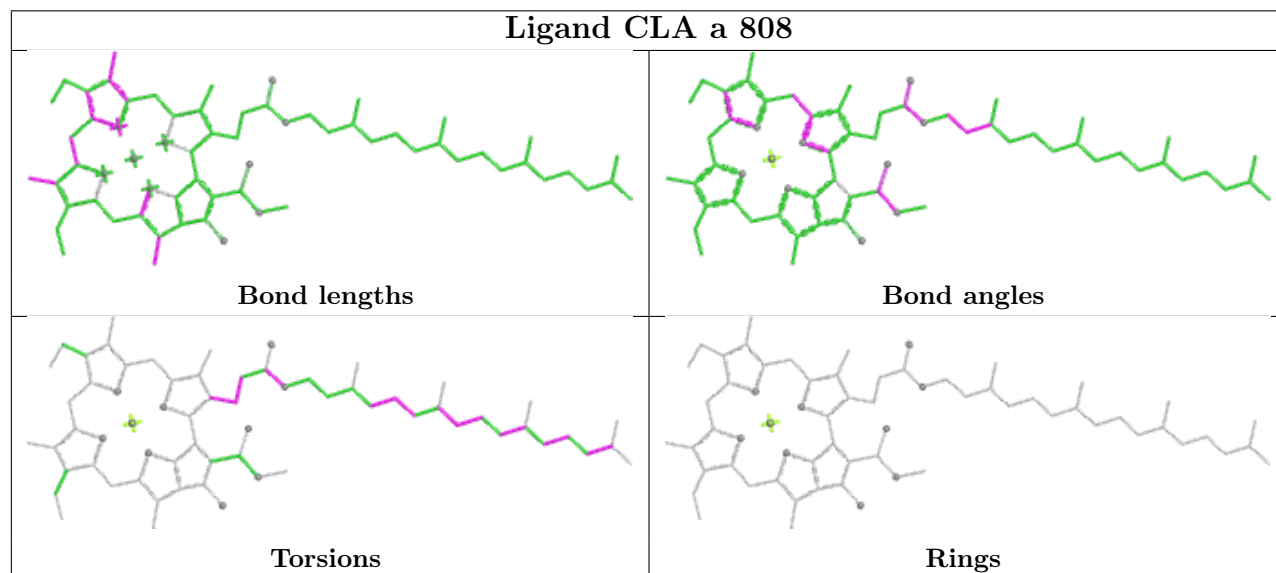
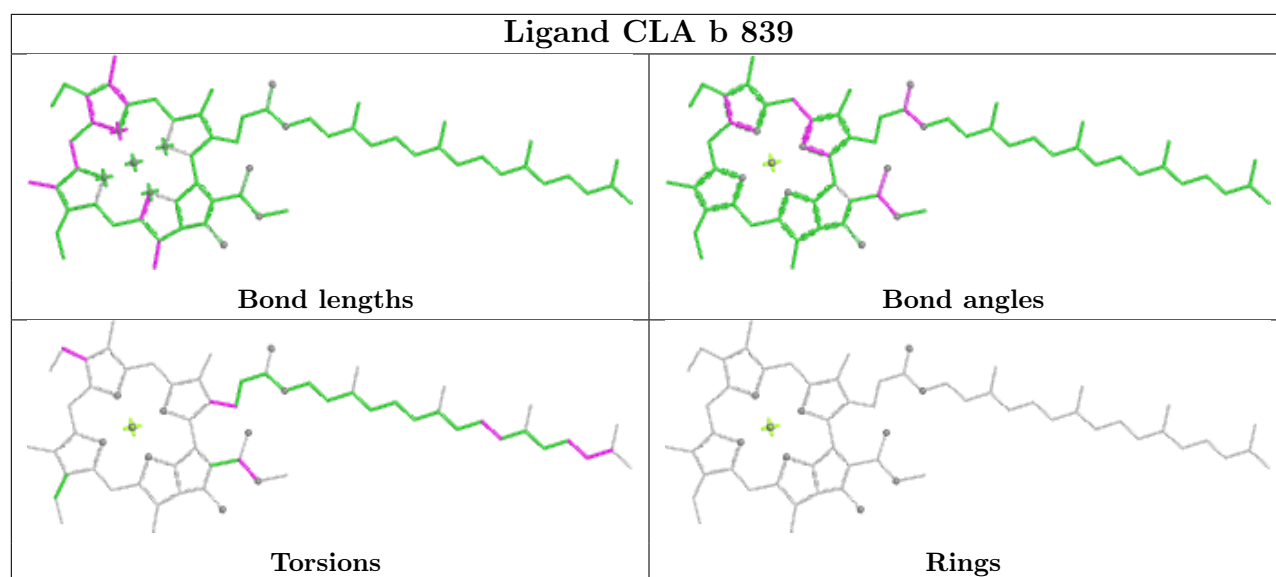


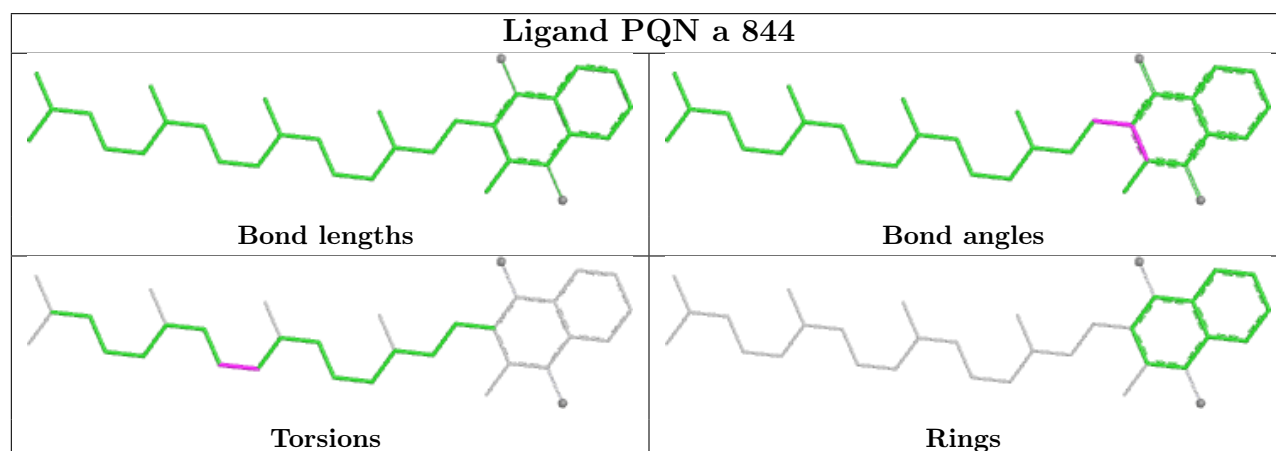
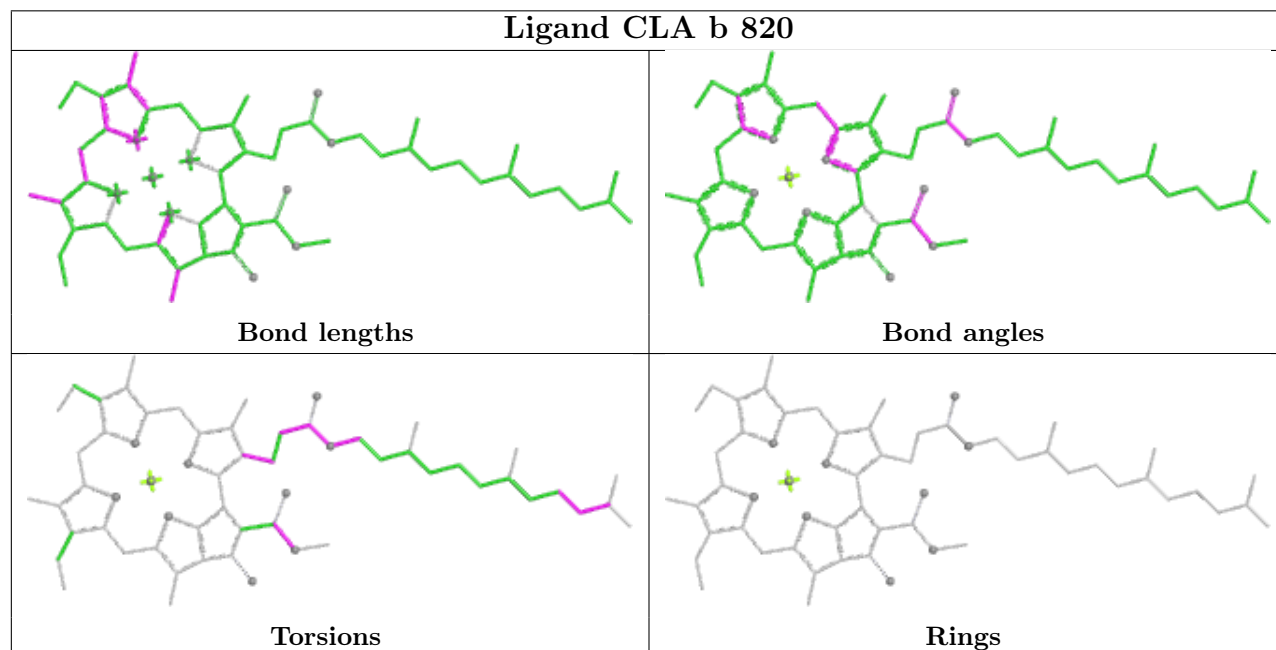
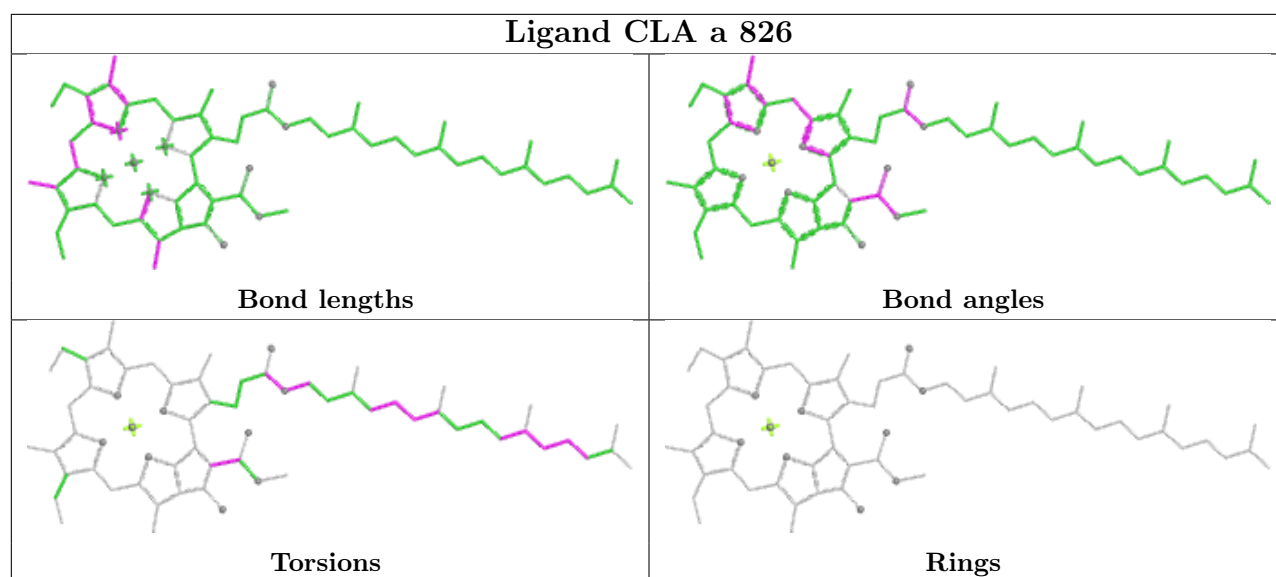
Torsions

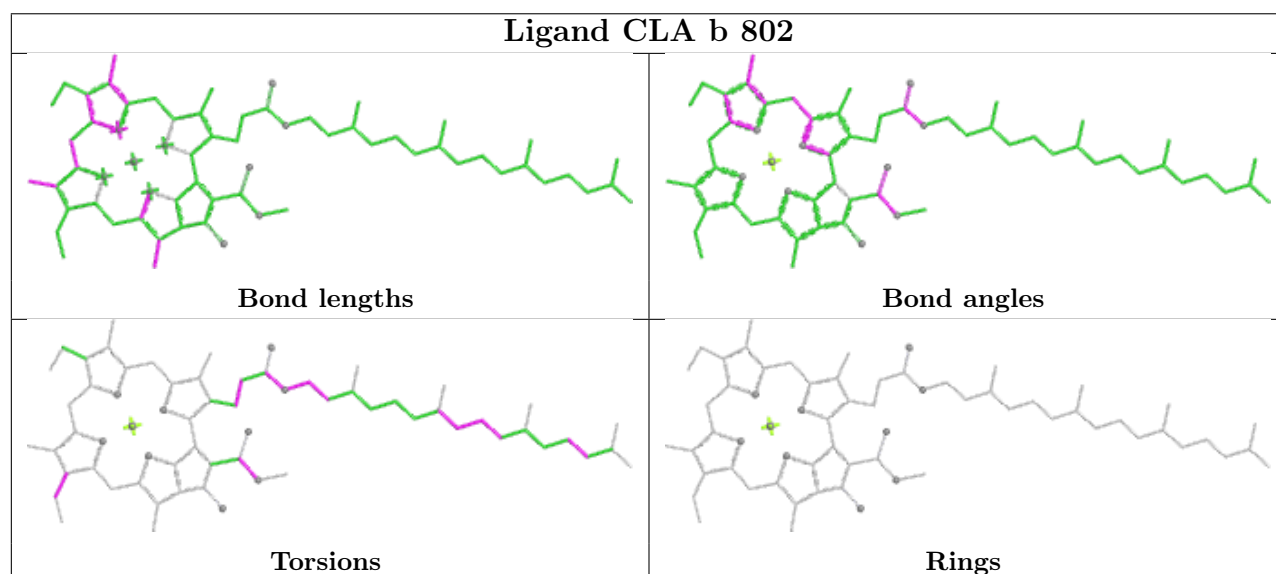
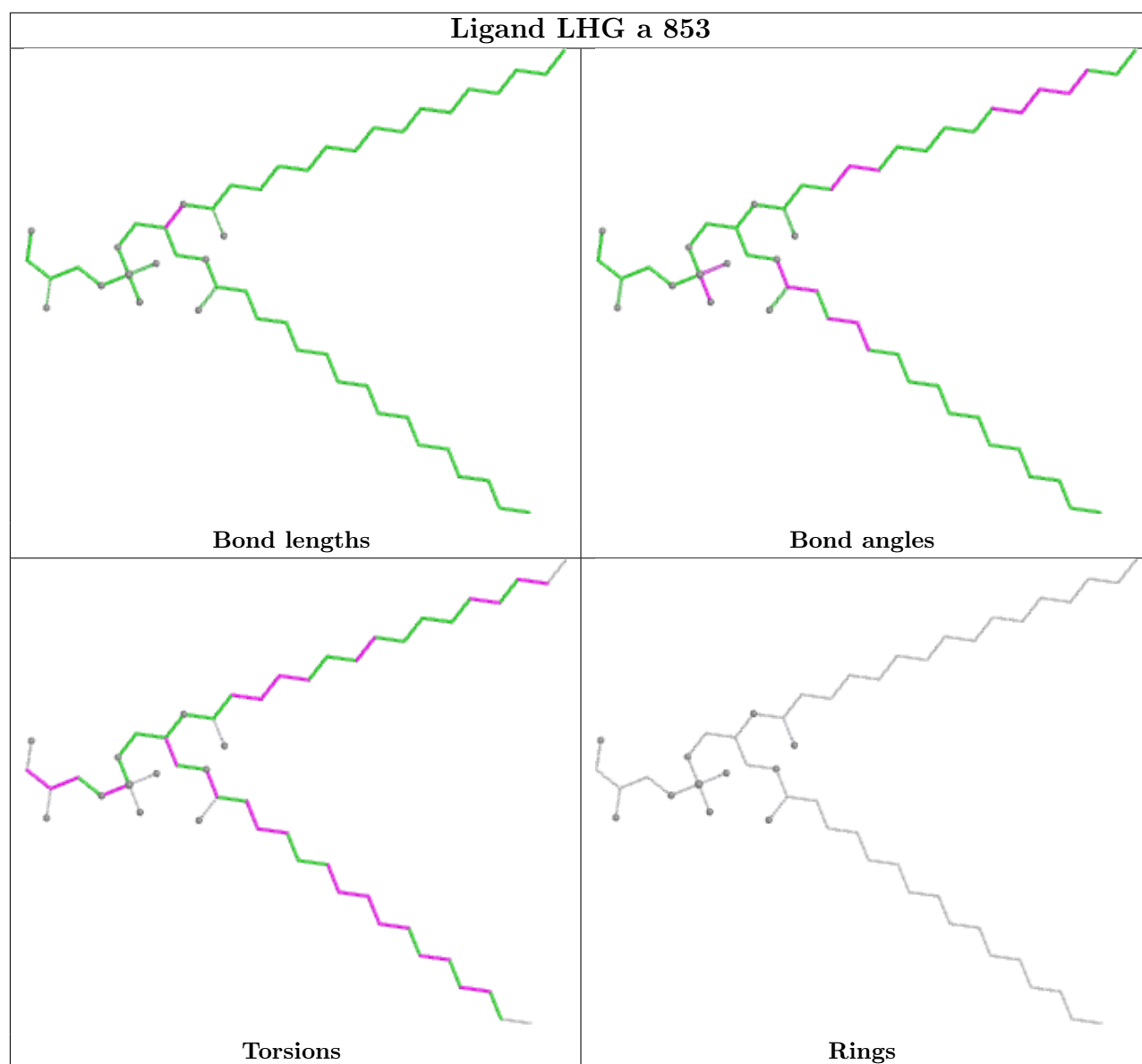


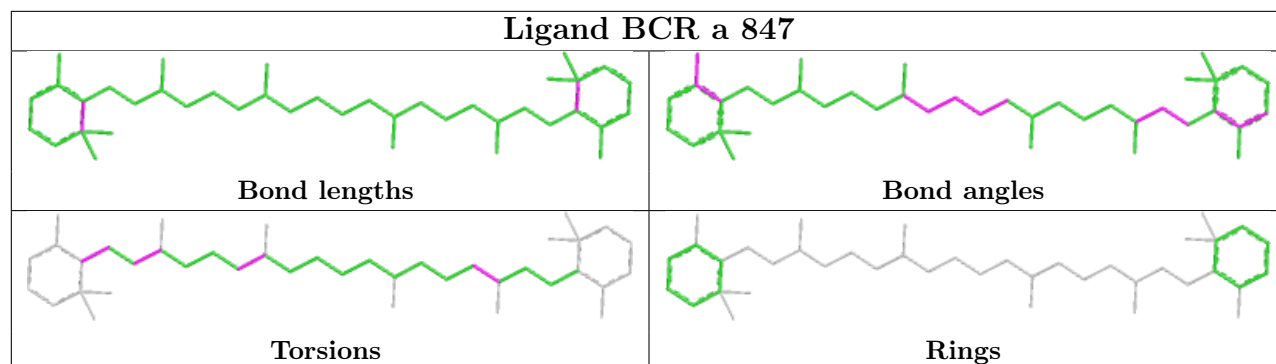
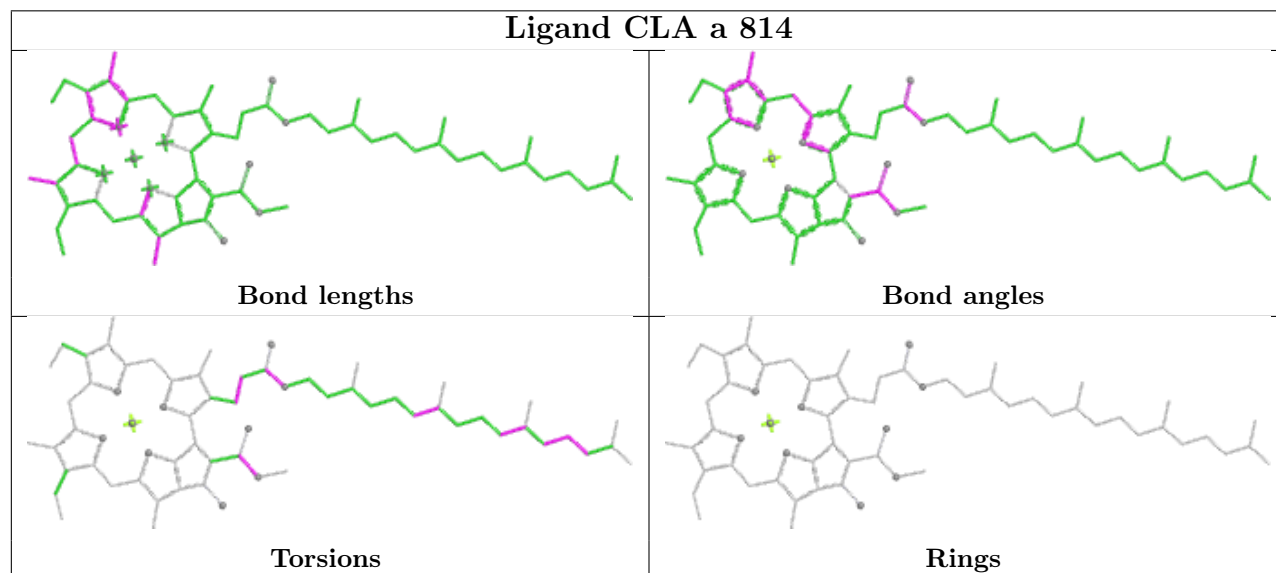
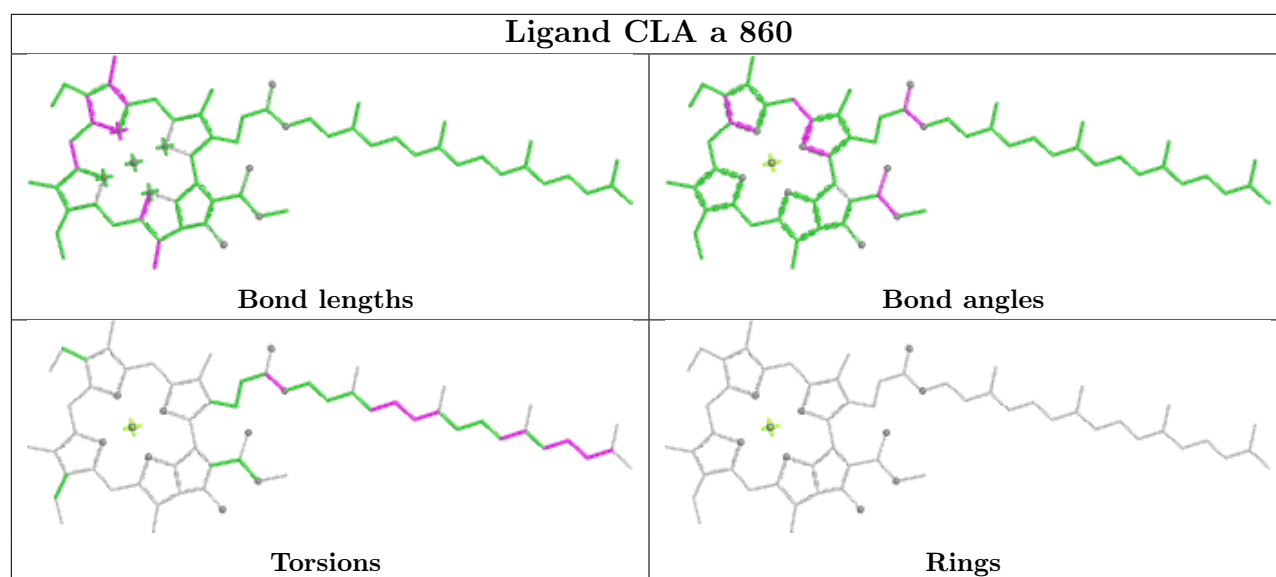
Rings



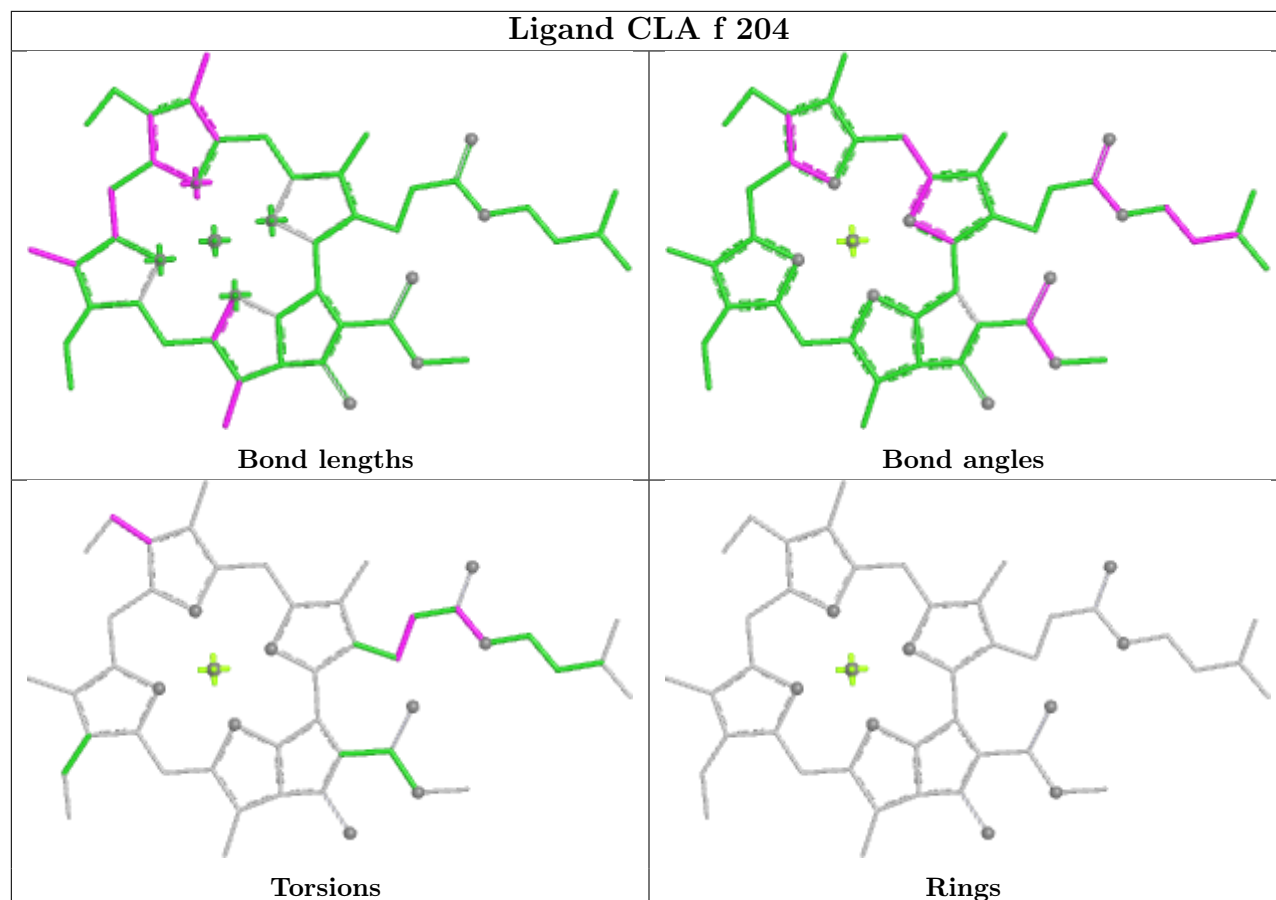




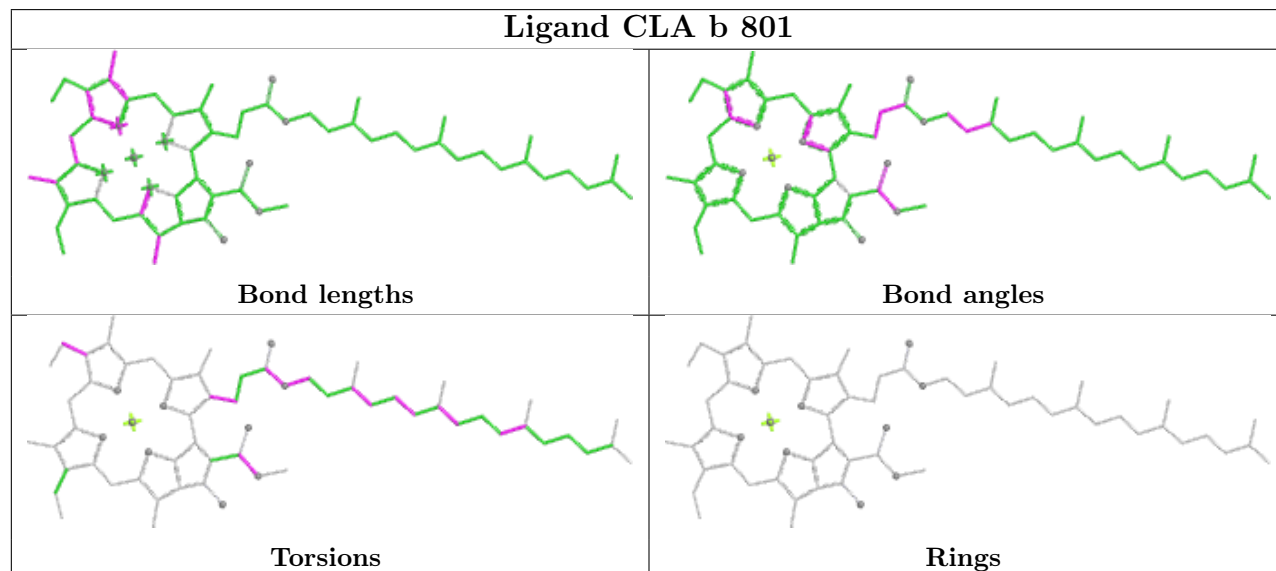


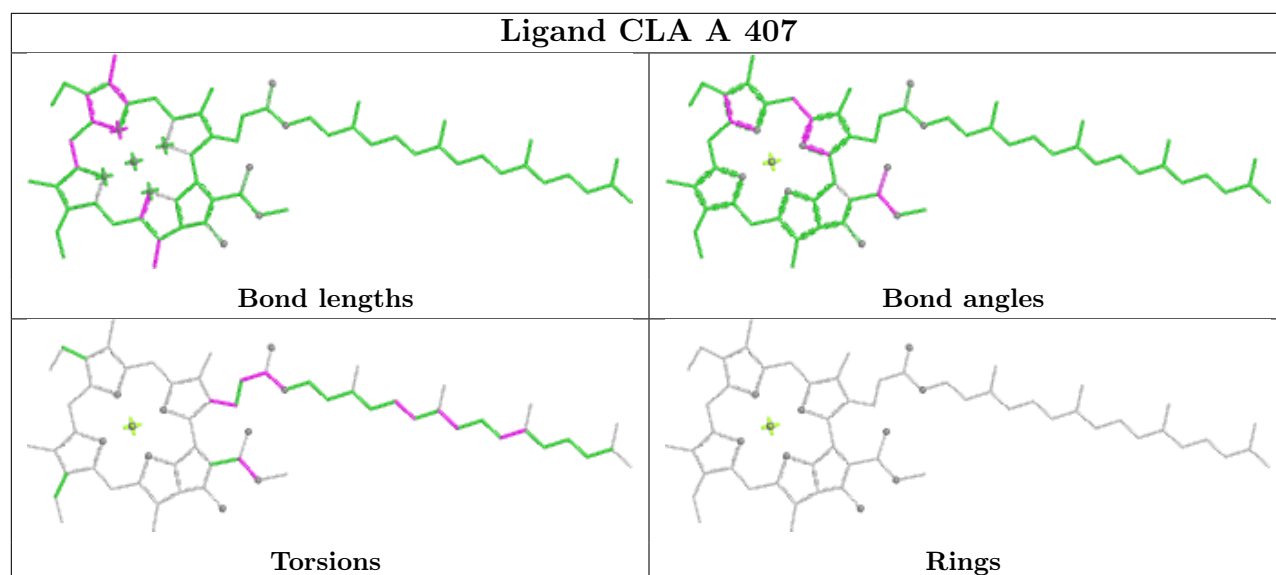
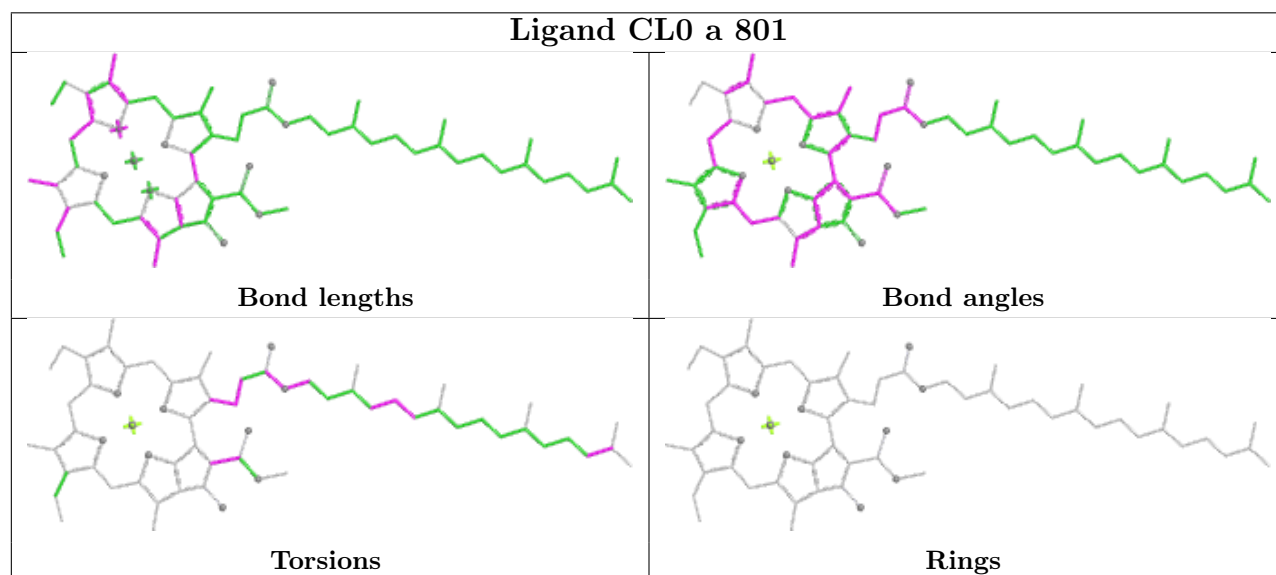
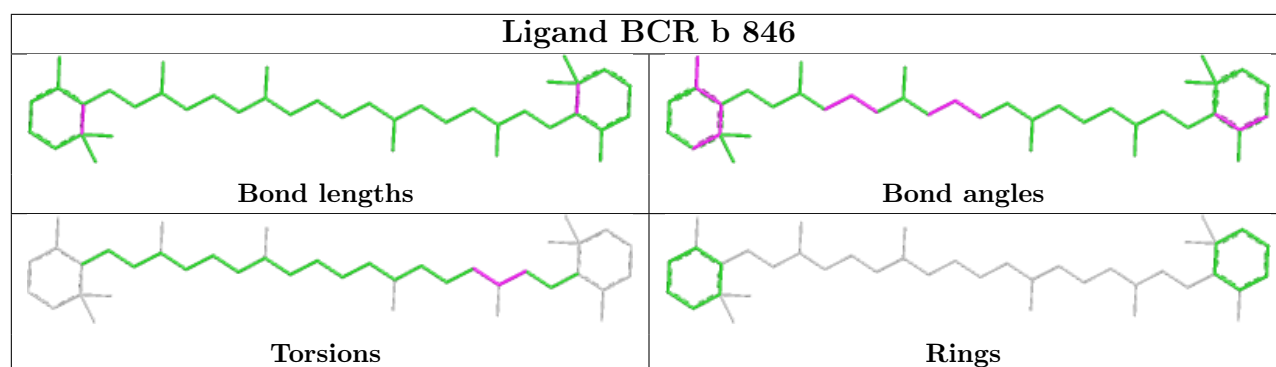


## Ligand CLA f 204

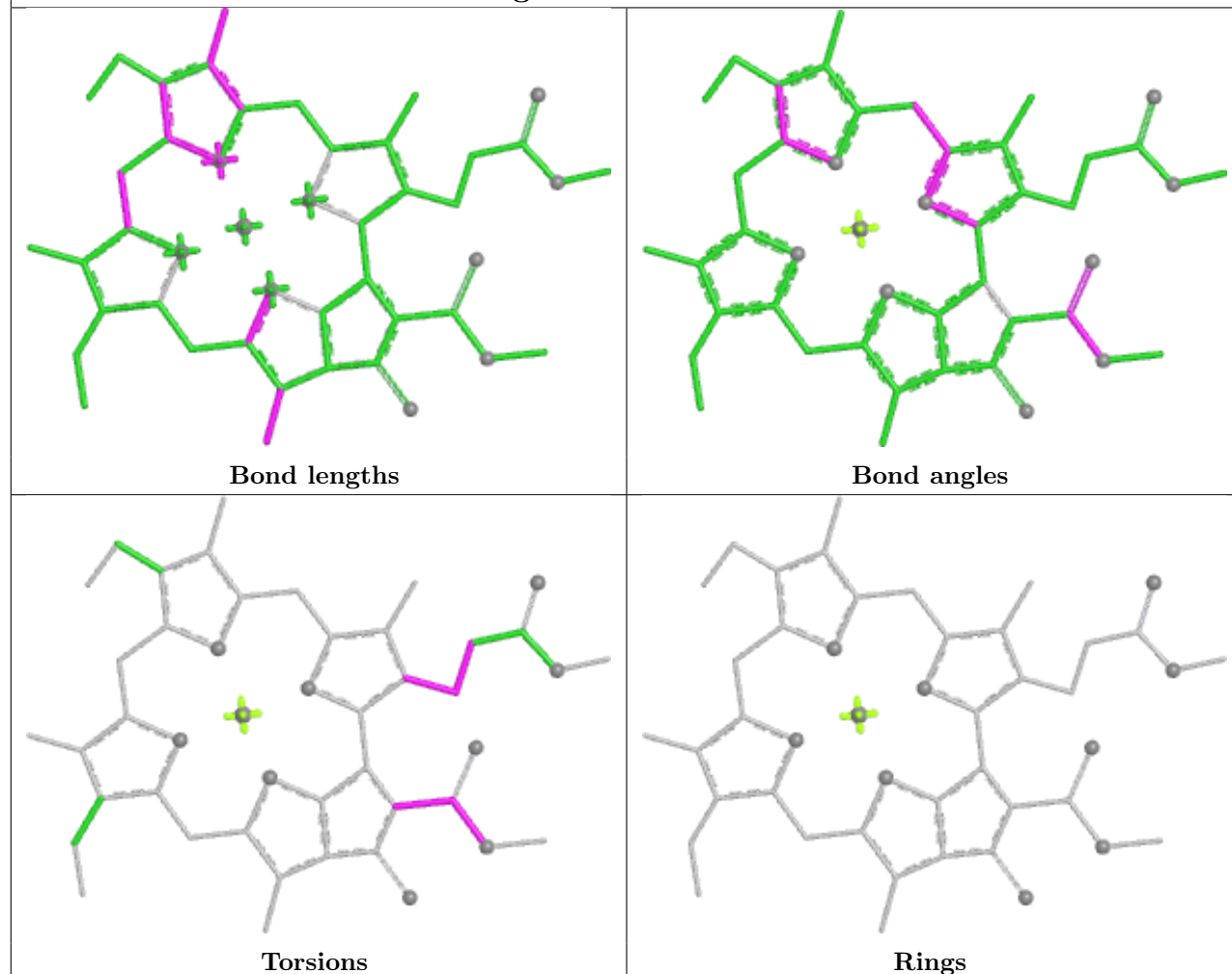


## Ligand CLA b 801

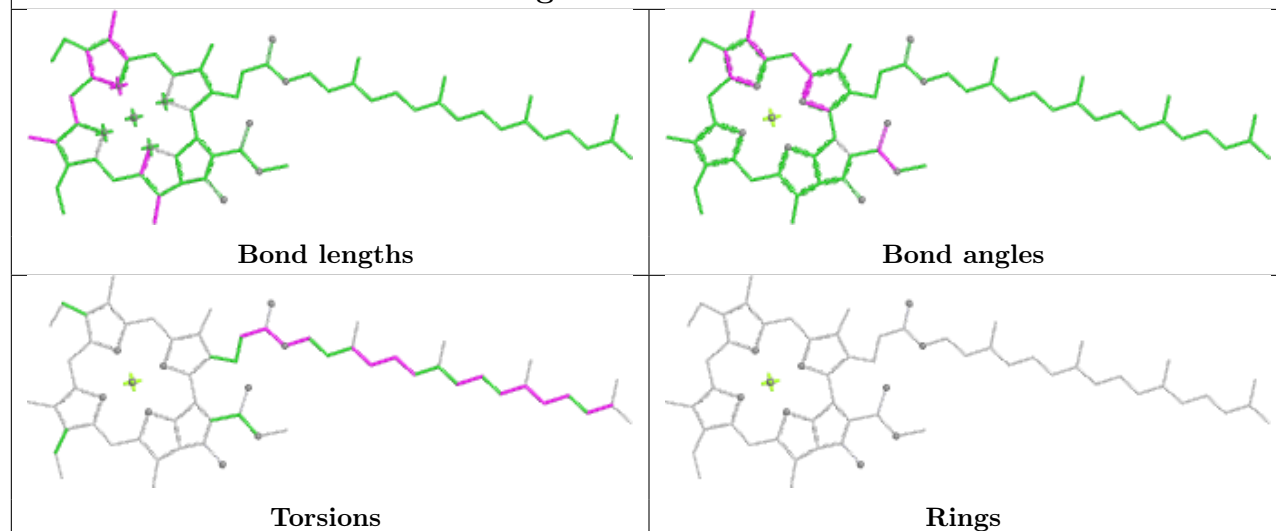


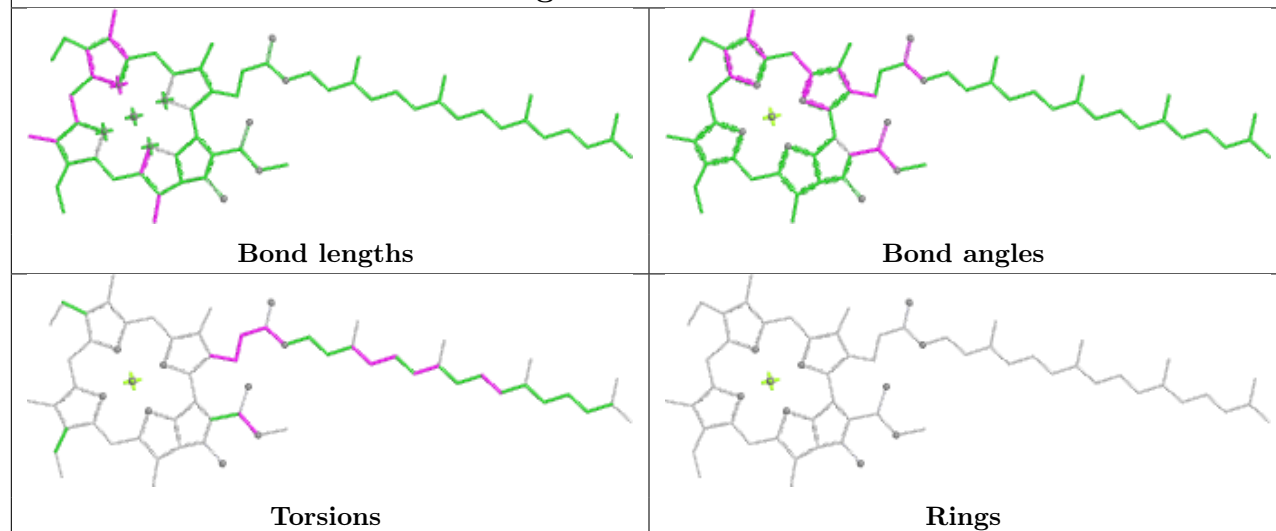
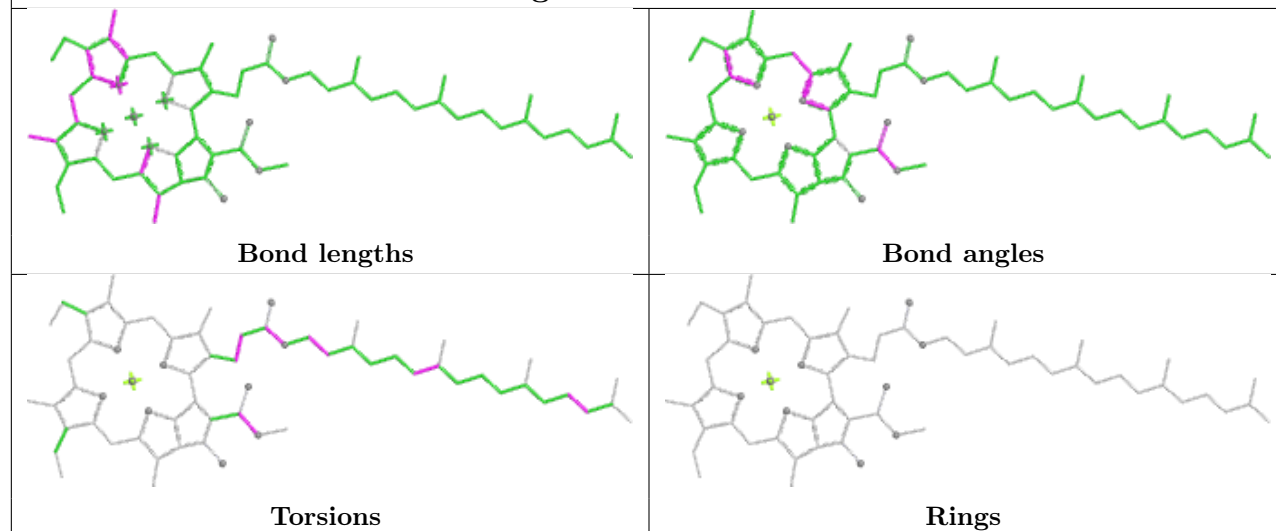


## Ligand CLA D 403

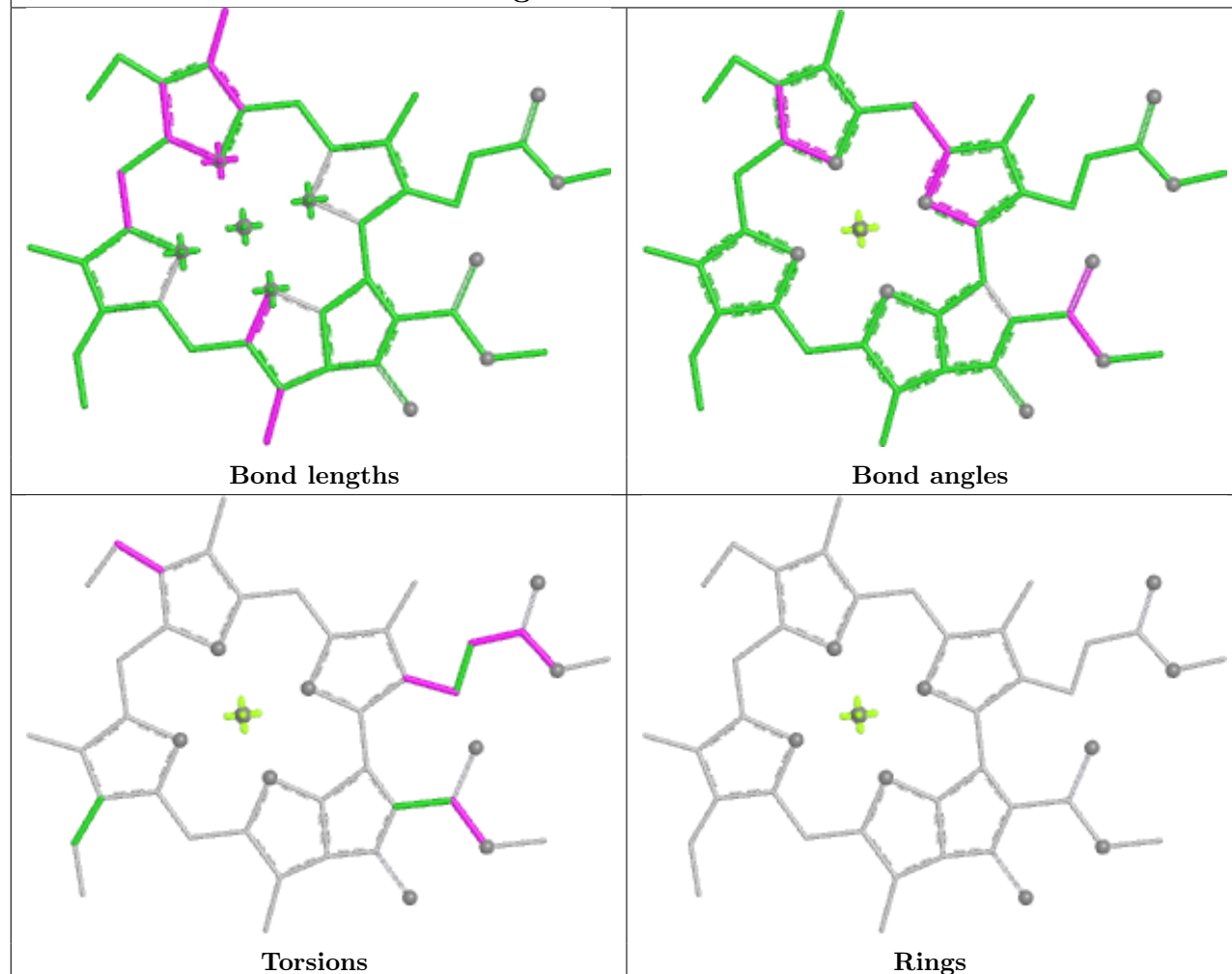


## Ligand CLA a 830

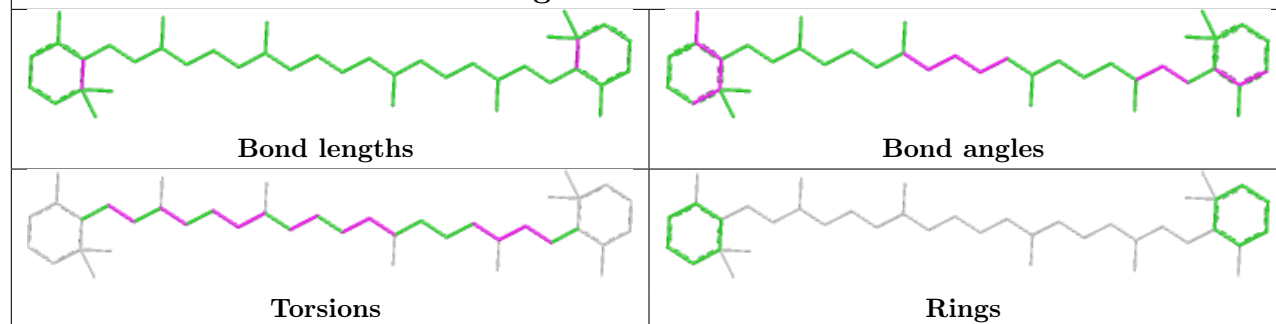


**Ligand CLA a 831****Ligand CLA A 402**

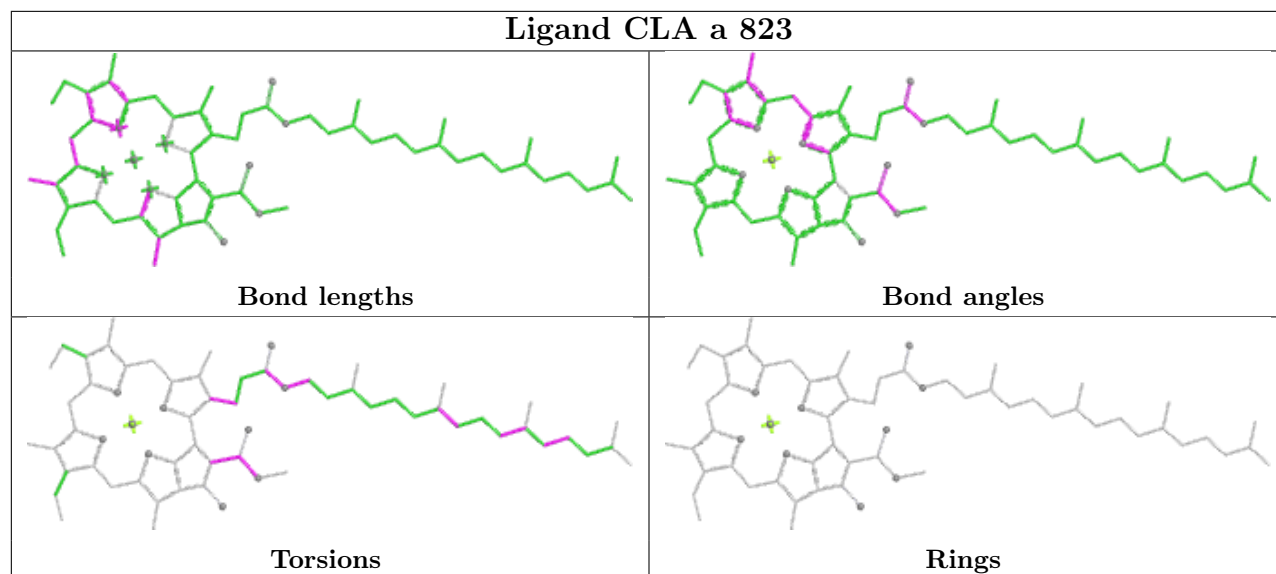
## Ligand CLA A 403



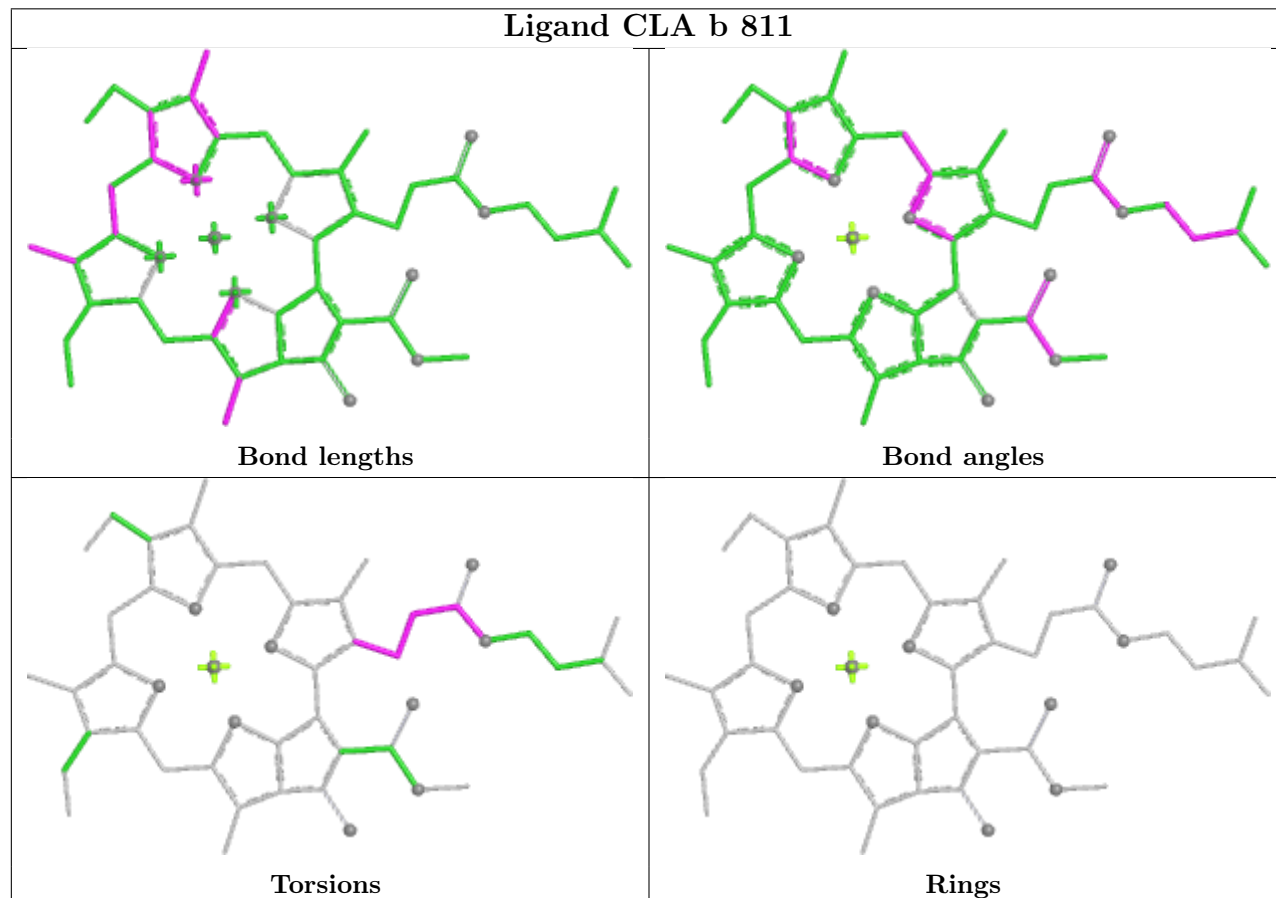
## Ligand BCR b 847

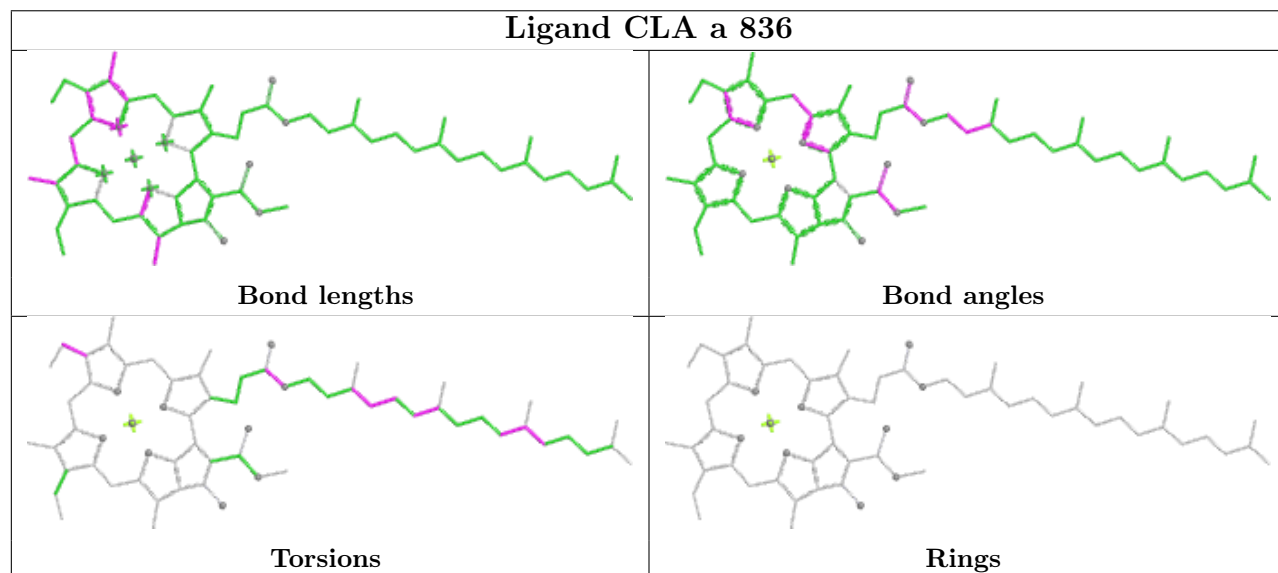
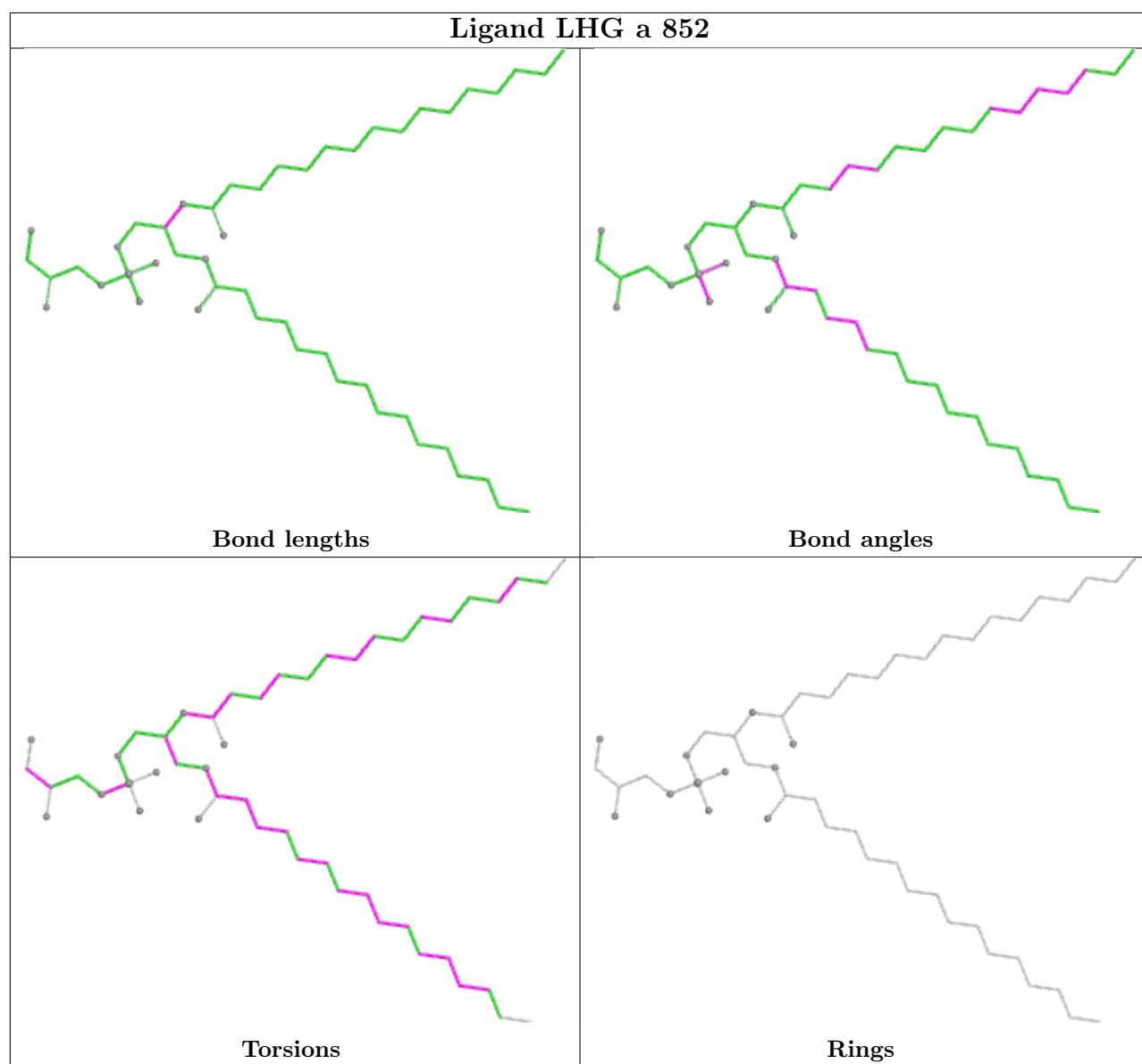


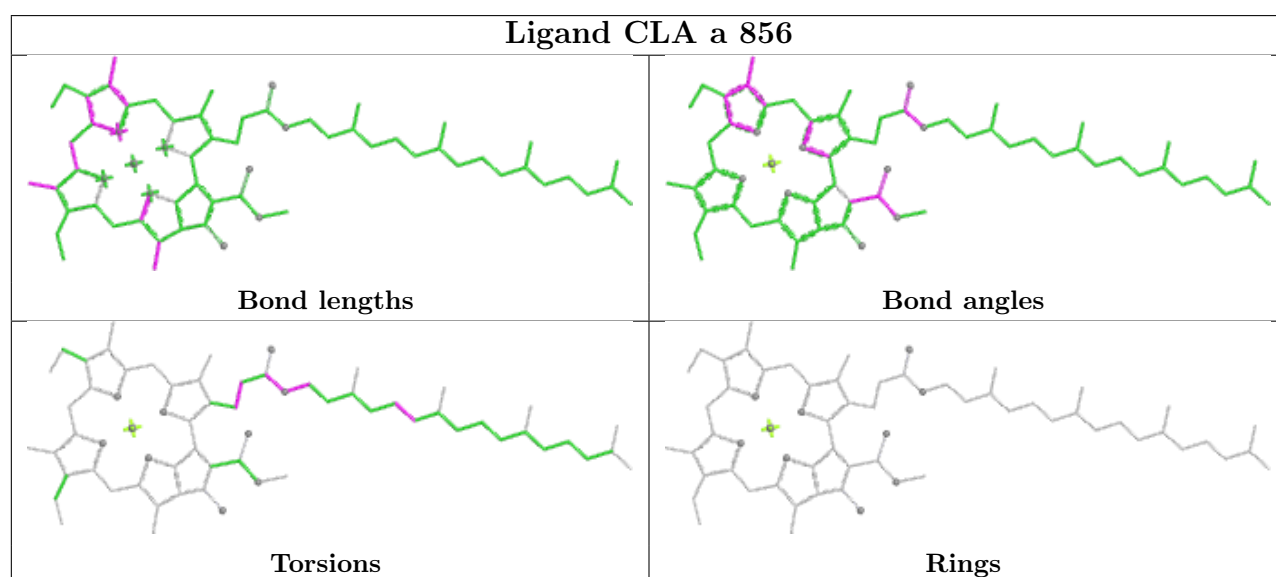
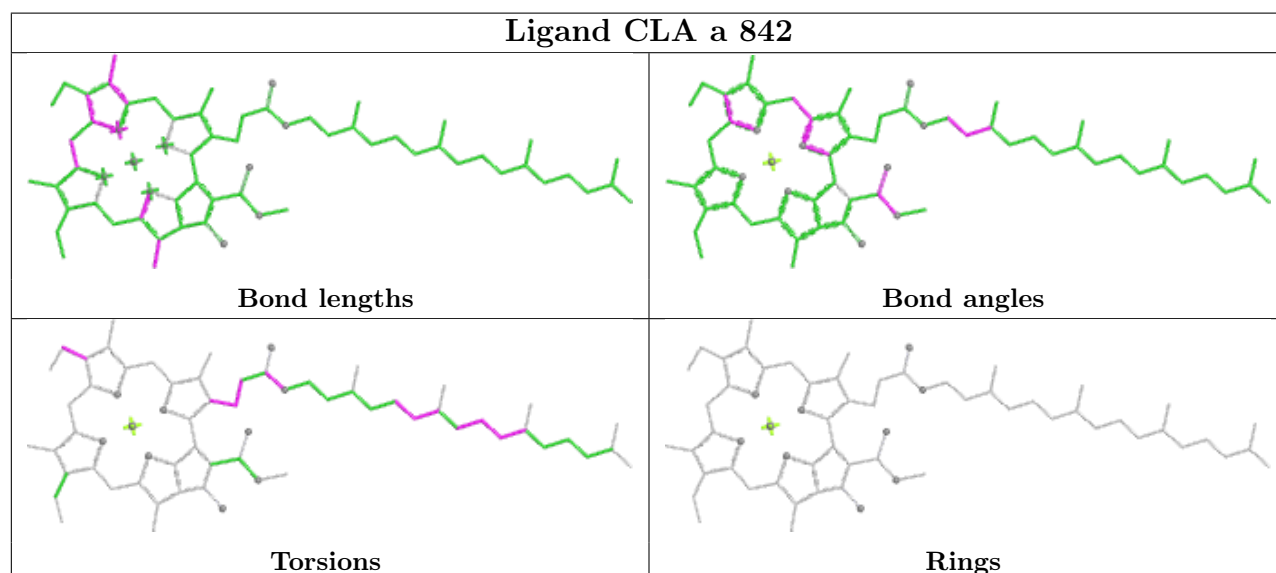
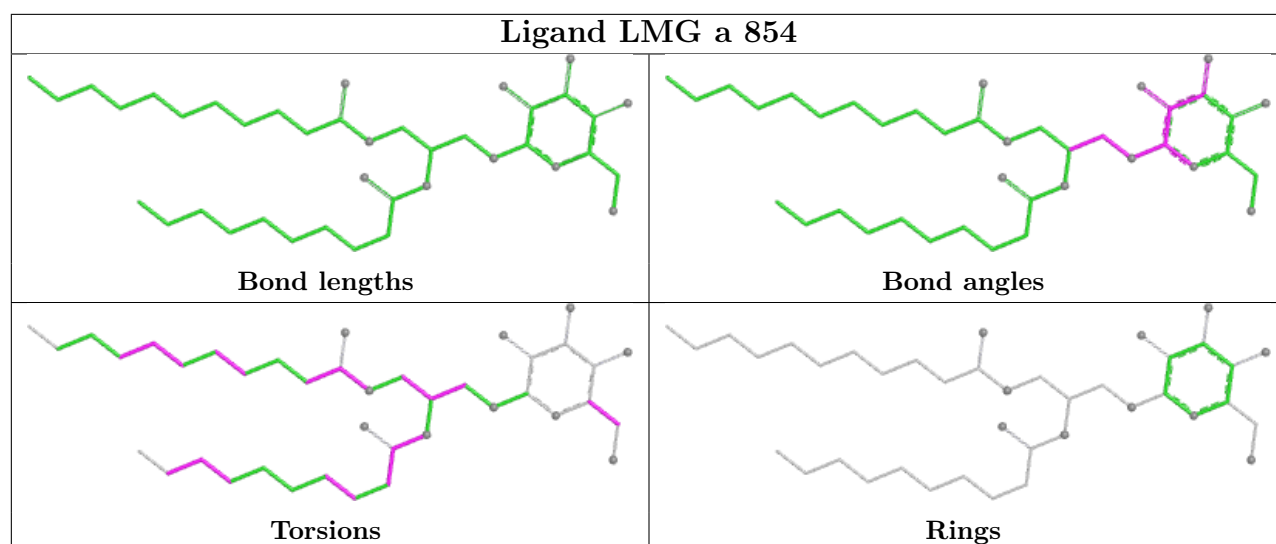
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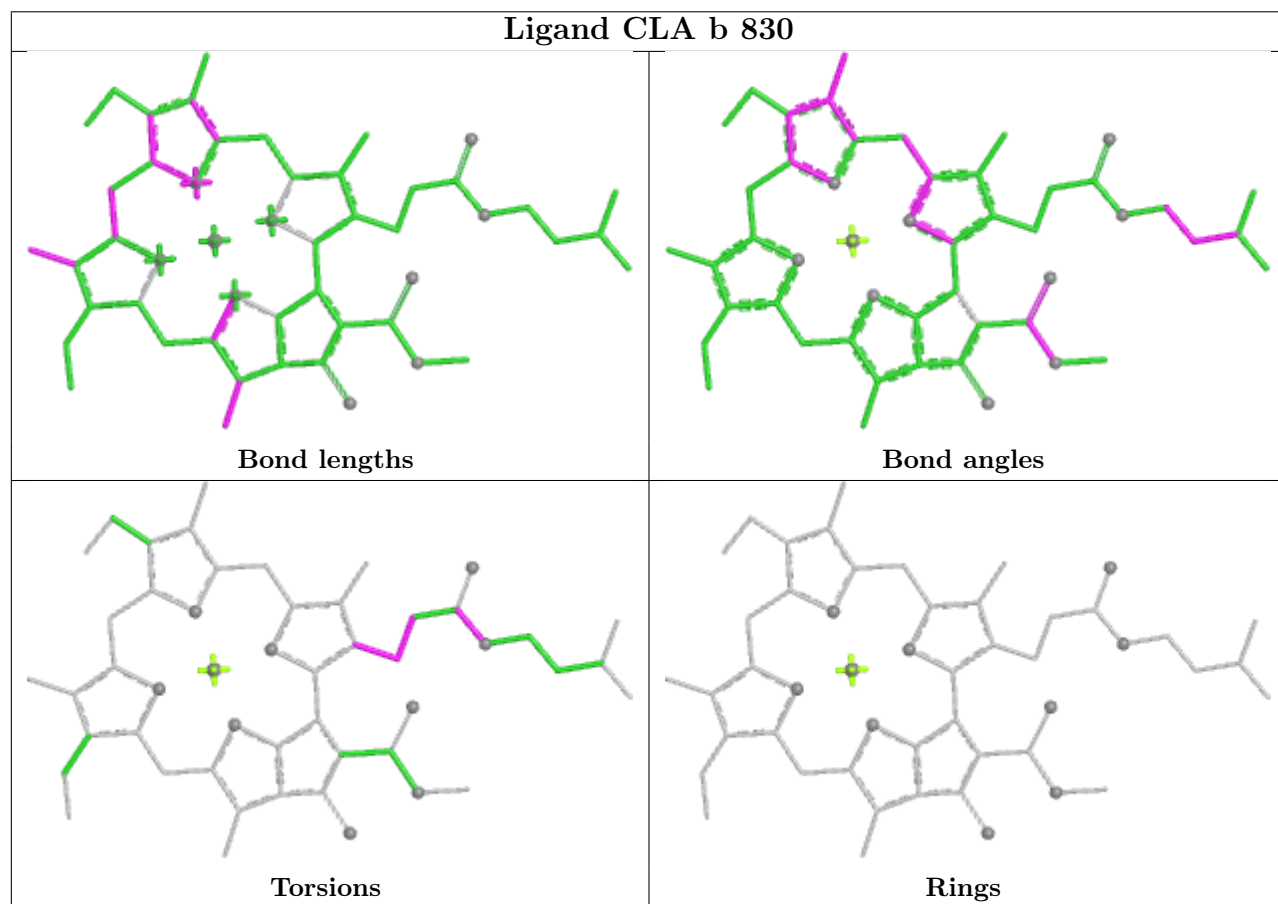
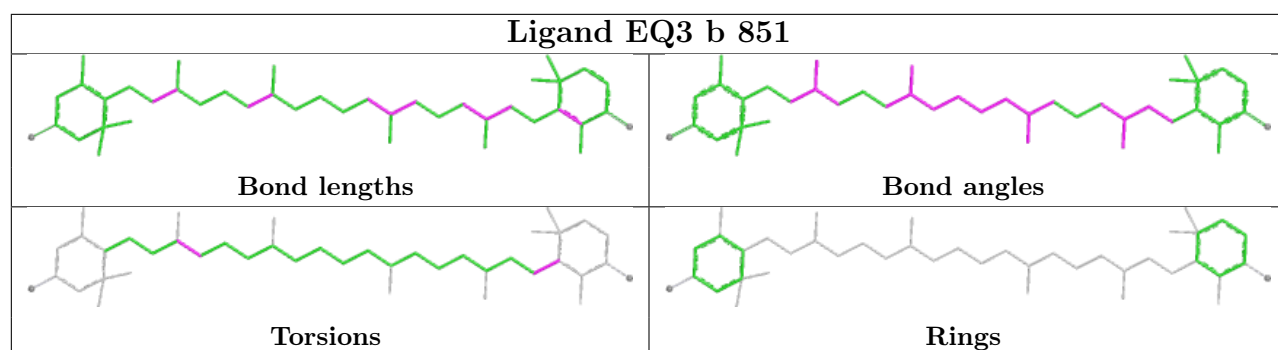


## Ligand CLA b 811

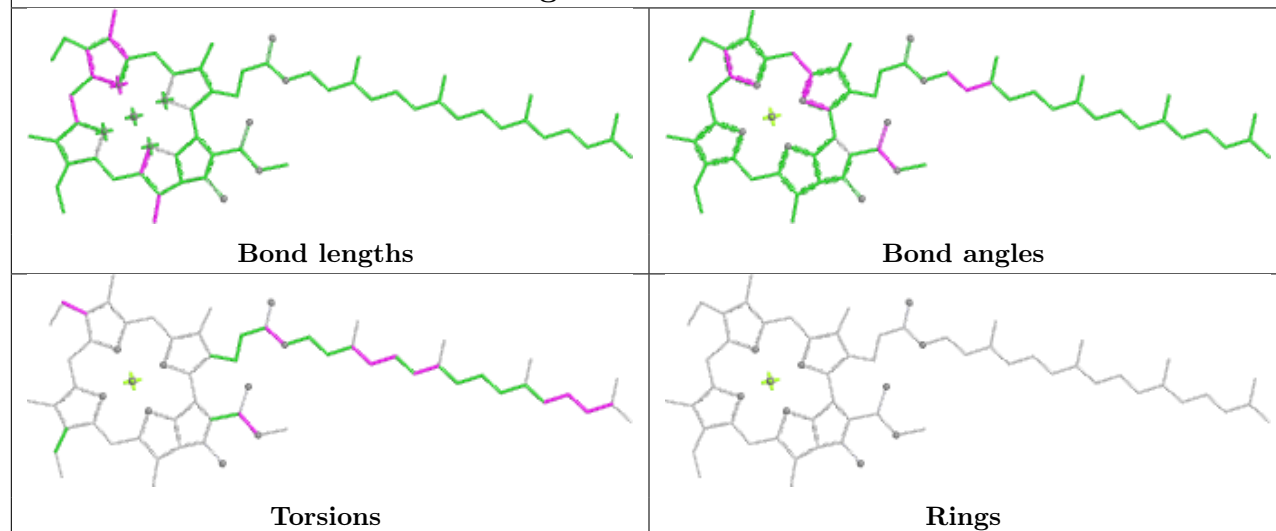




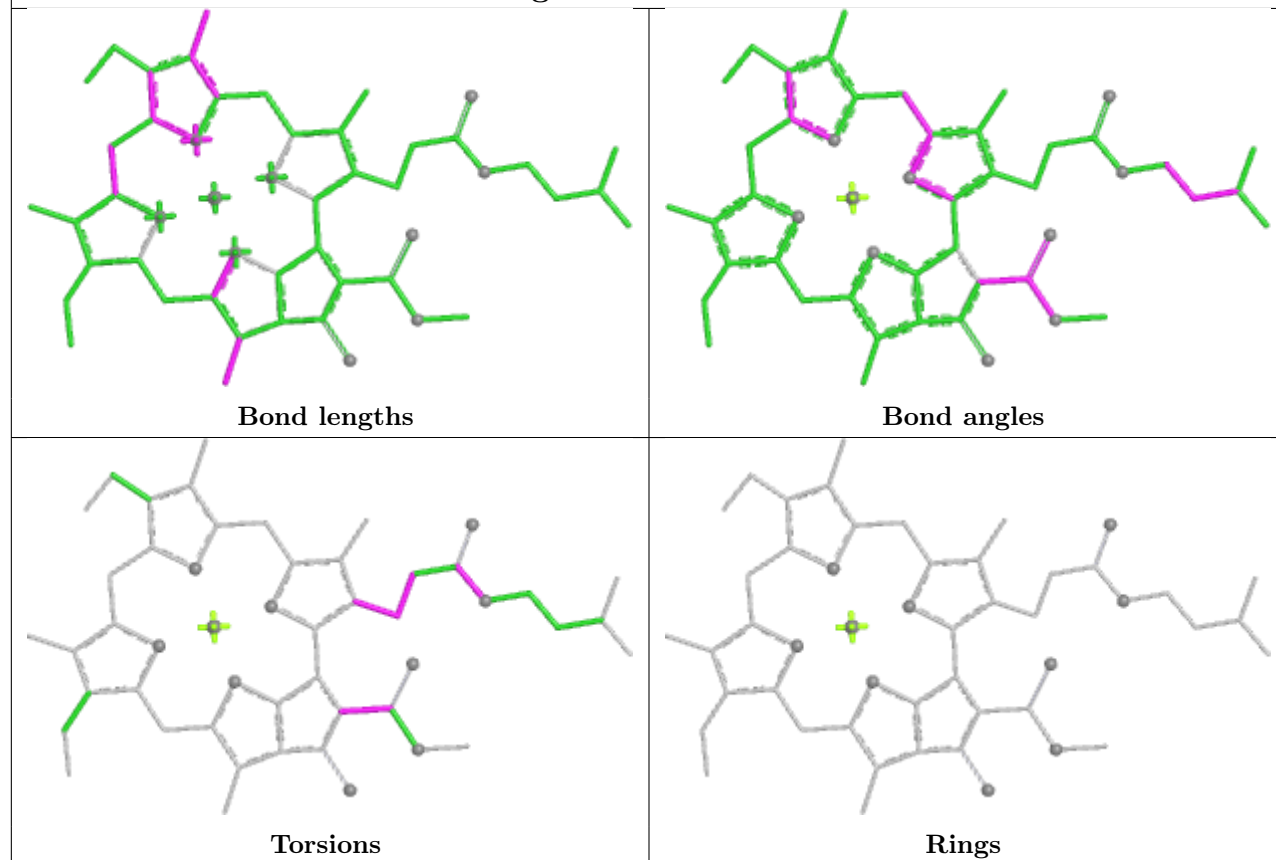


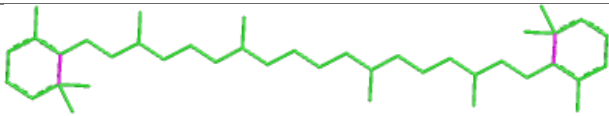
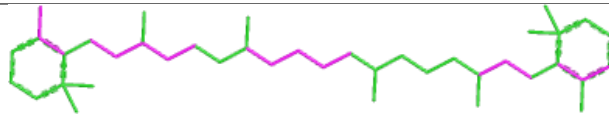
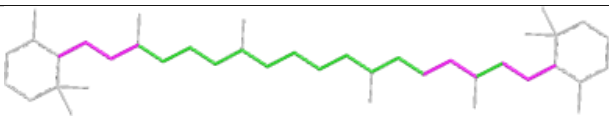
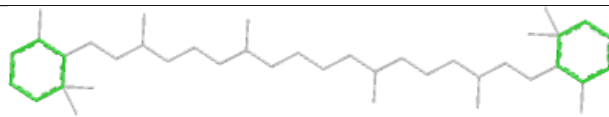


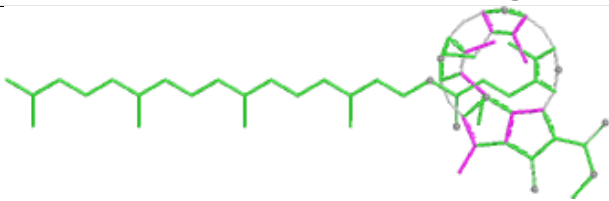
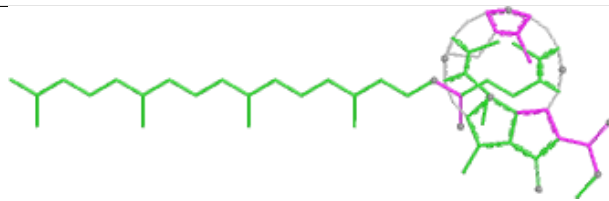
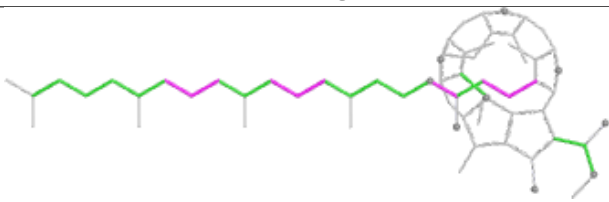
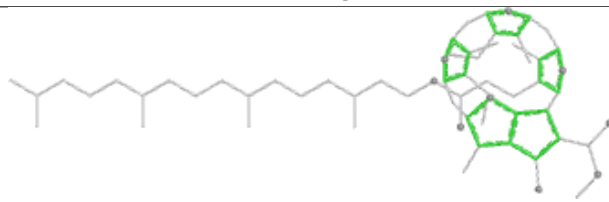
## Ligand CLA f 201

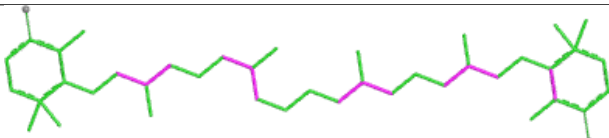
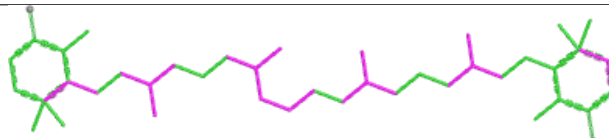
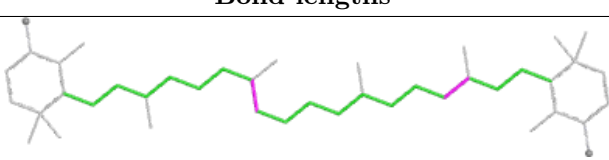
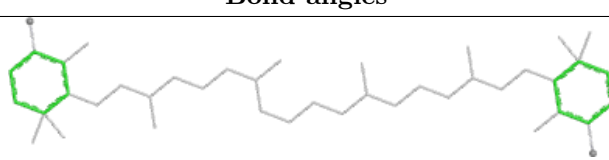


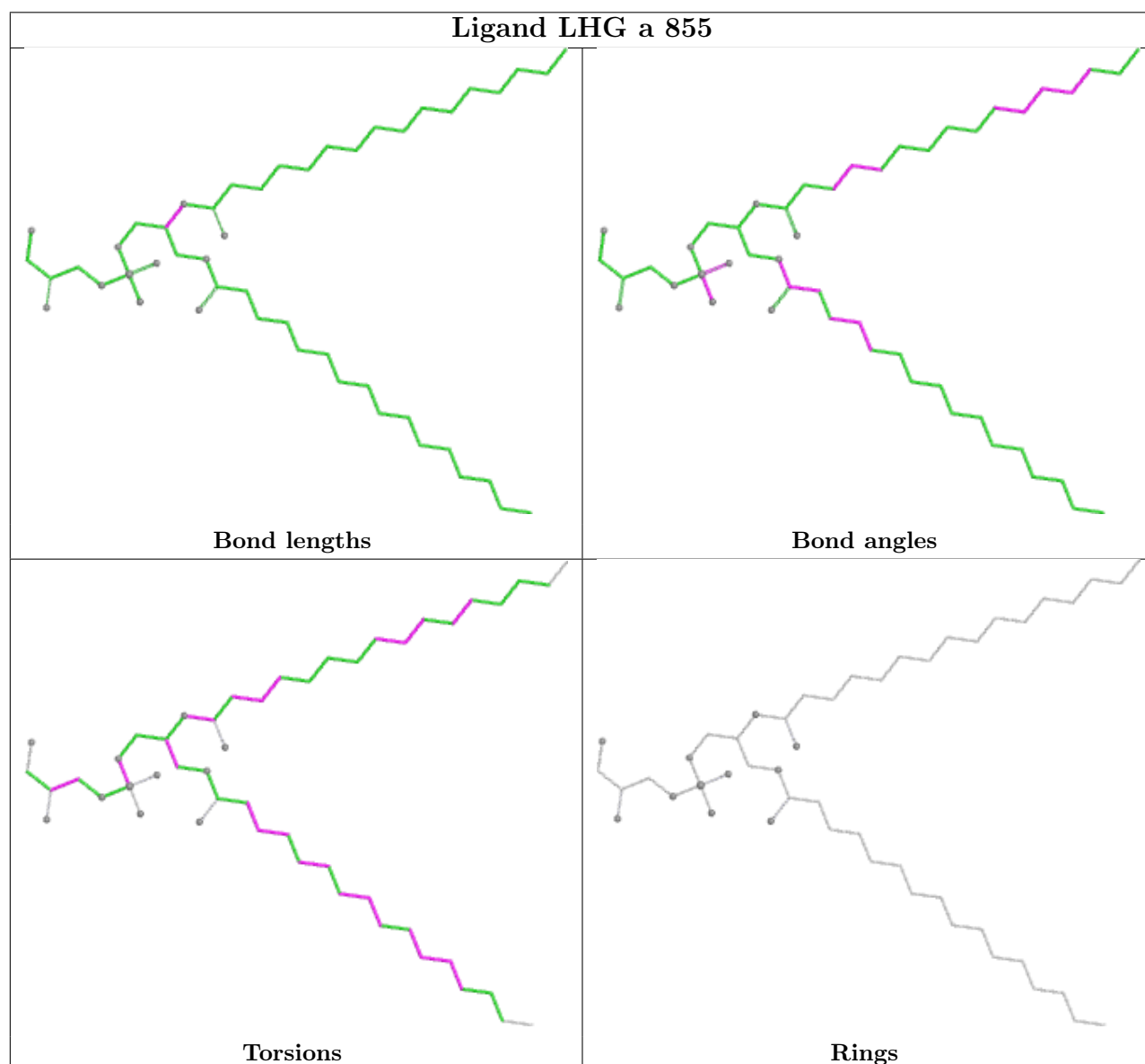
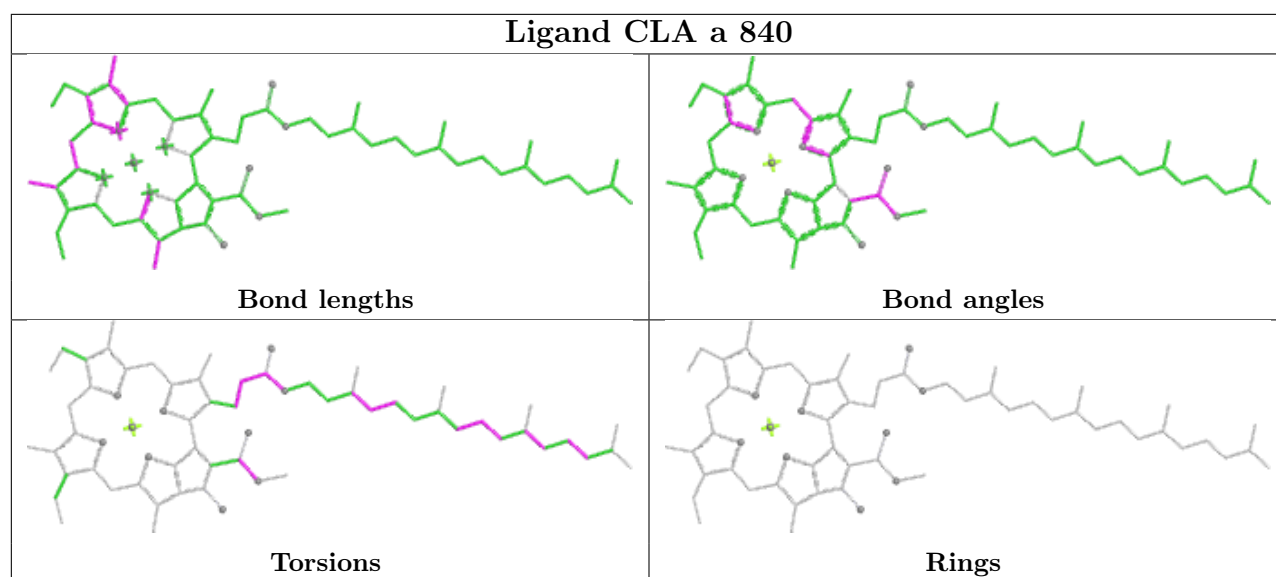
## Ligand CLA A 405



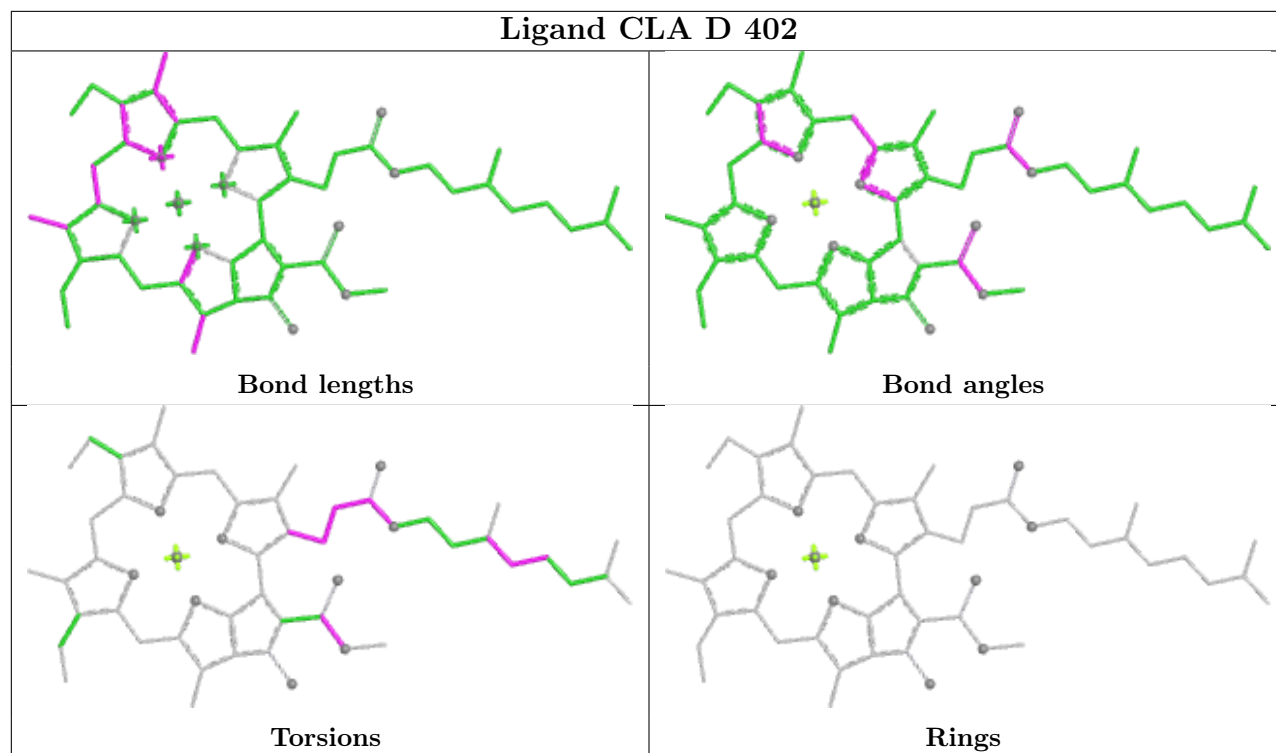
| Ligand BCR A 406                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

| Ligand PHO A 404                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

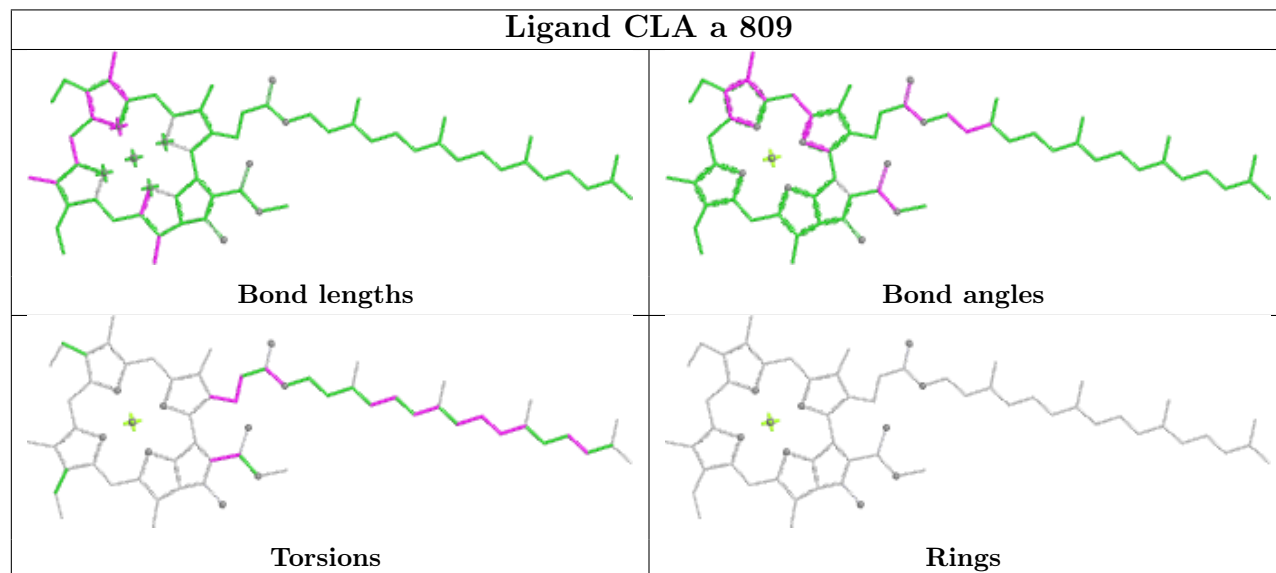
| Ligand 45D a 858                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |



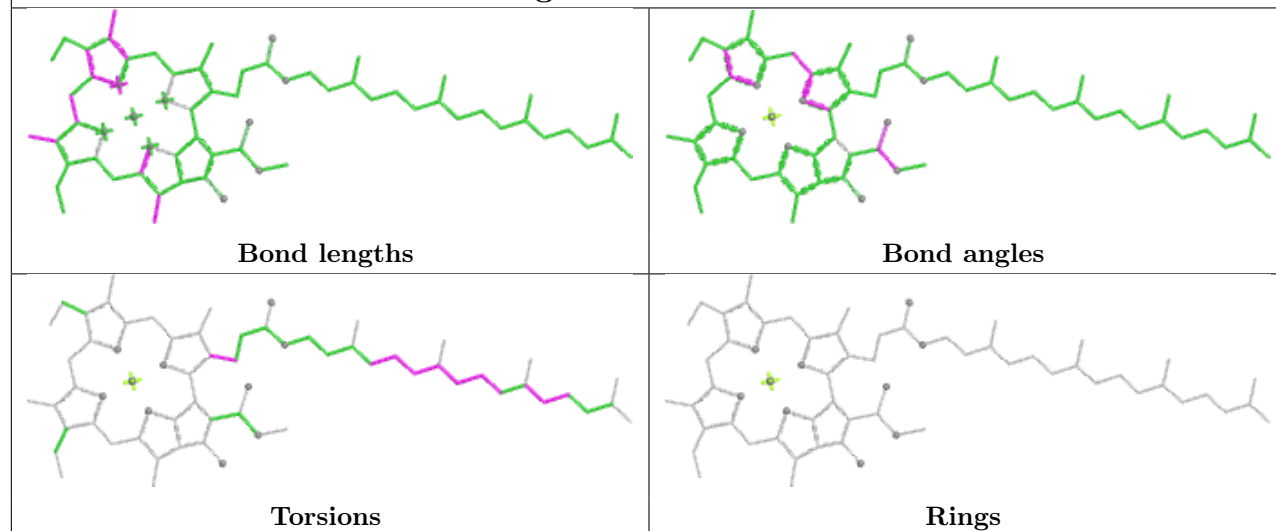
## Ligand CLA D 402



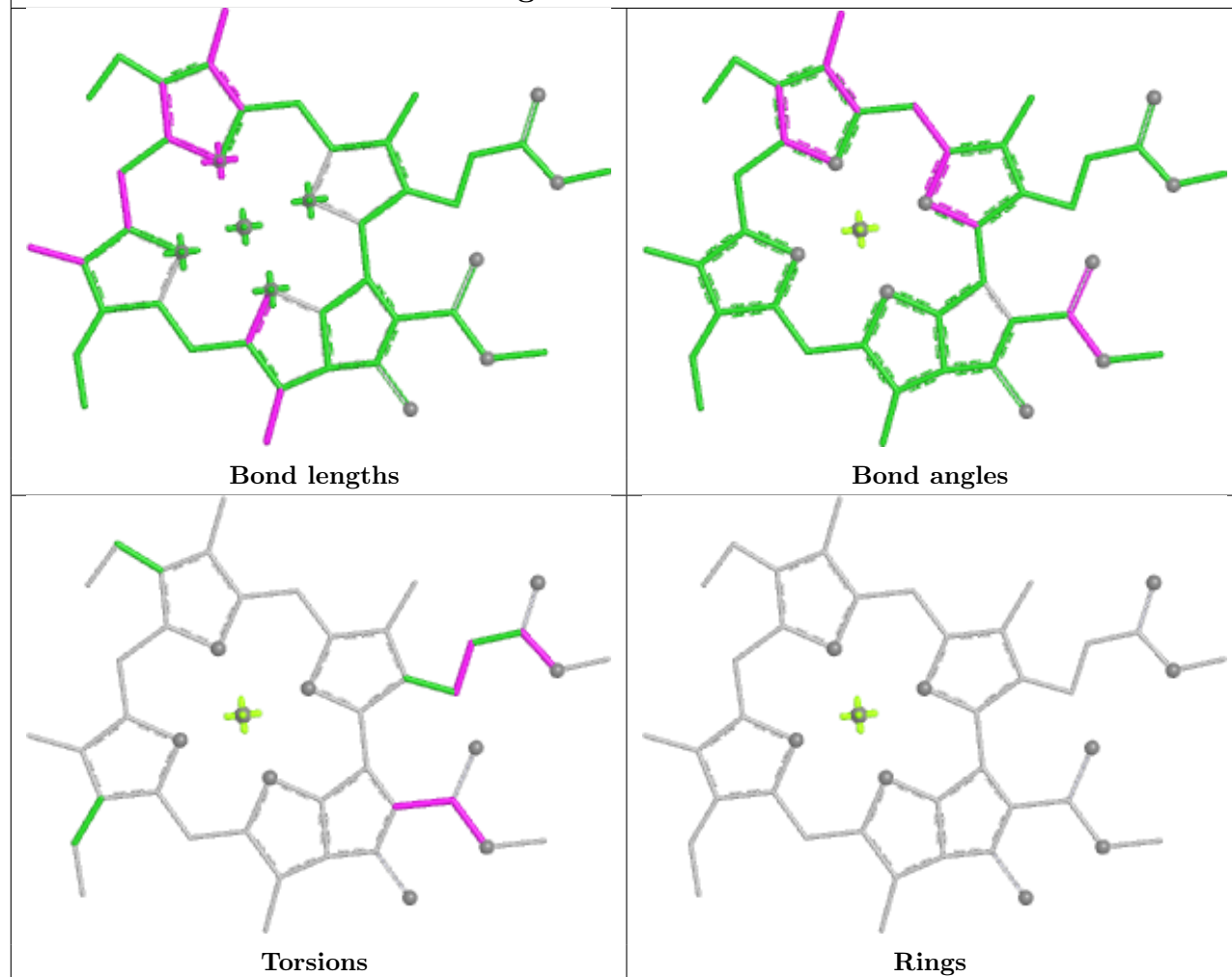
## Ligand CLA a 809

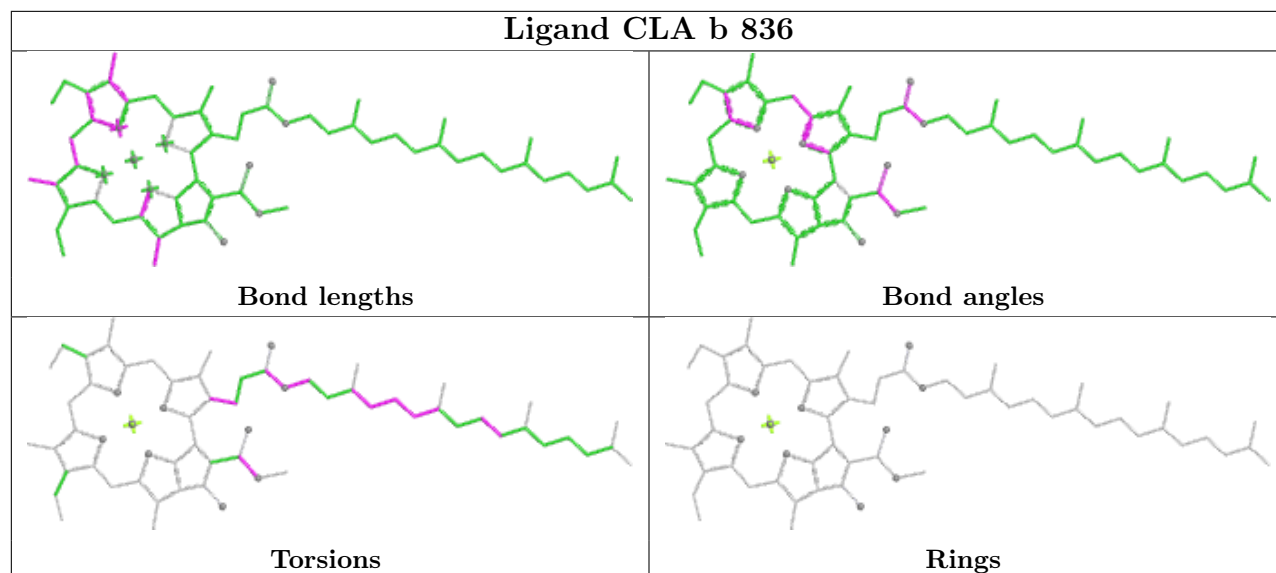
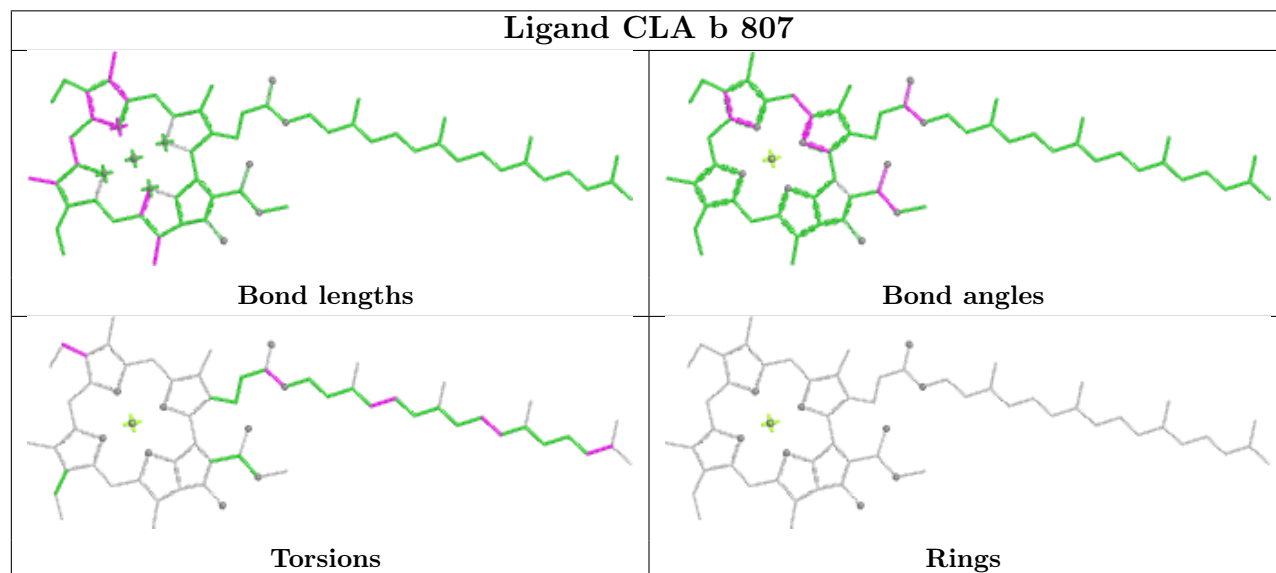
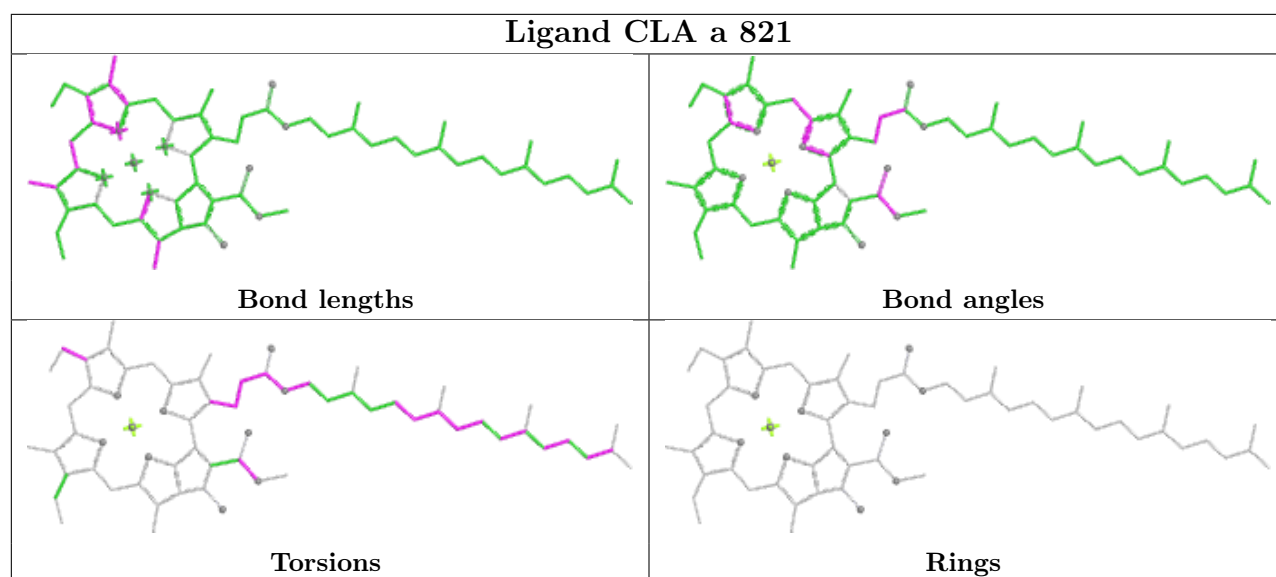


## Ligand CLA b 817

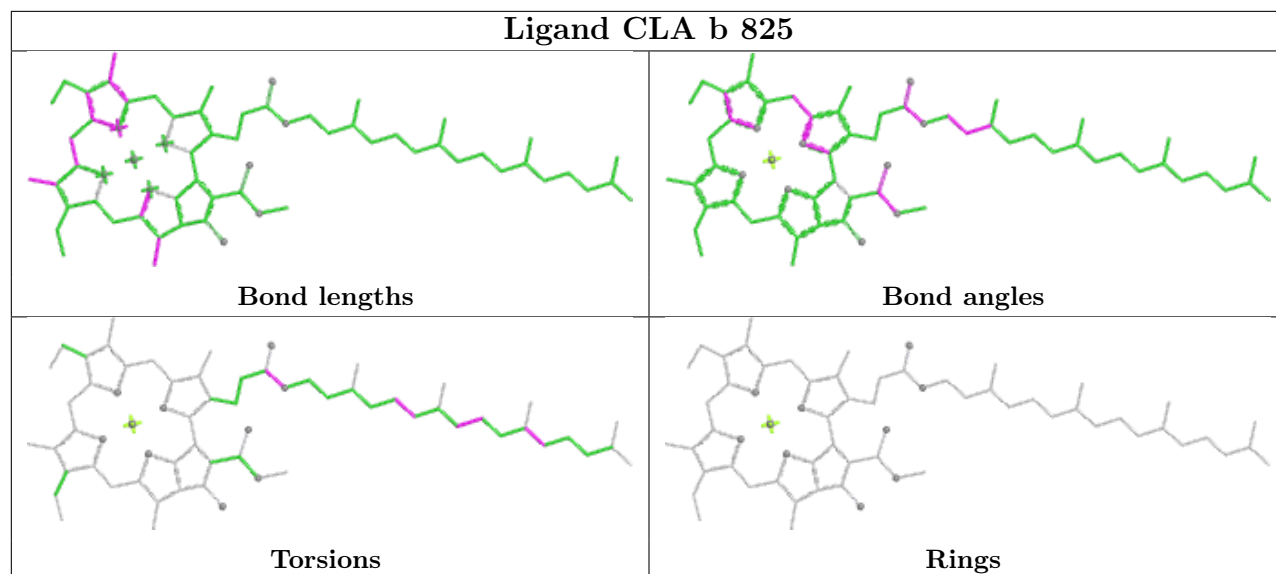


## Ligand CLA a 816

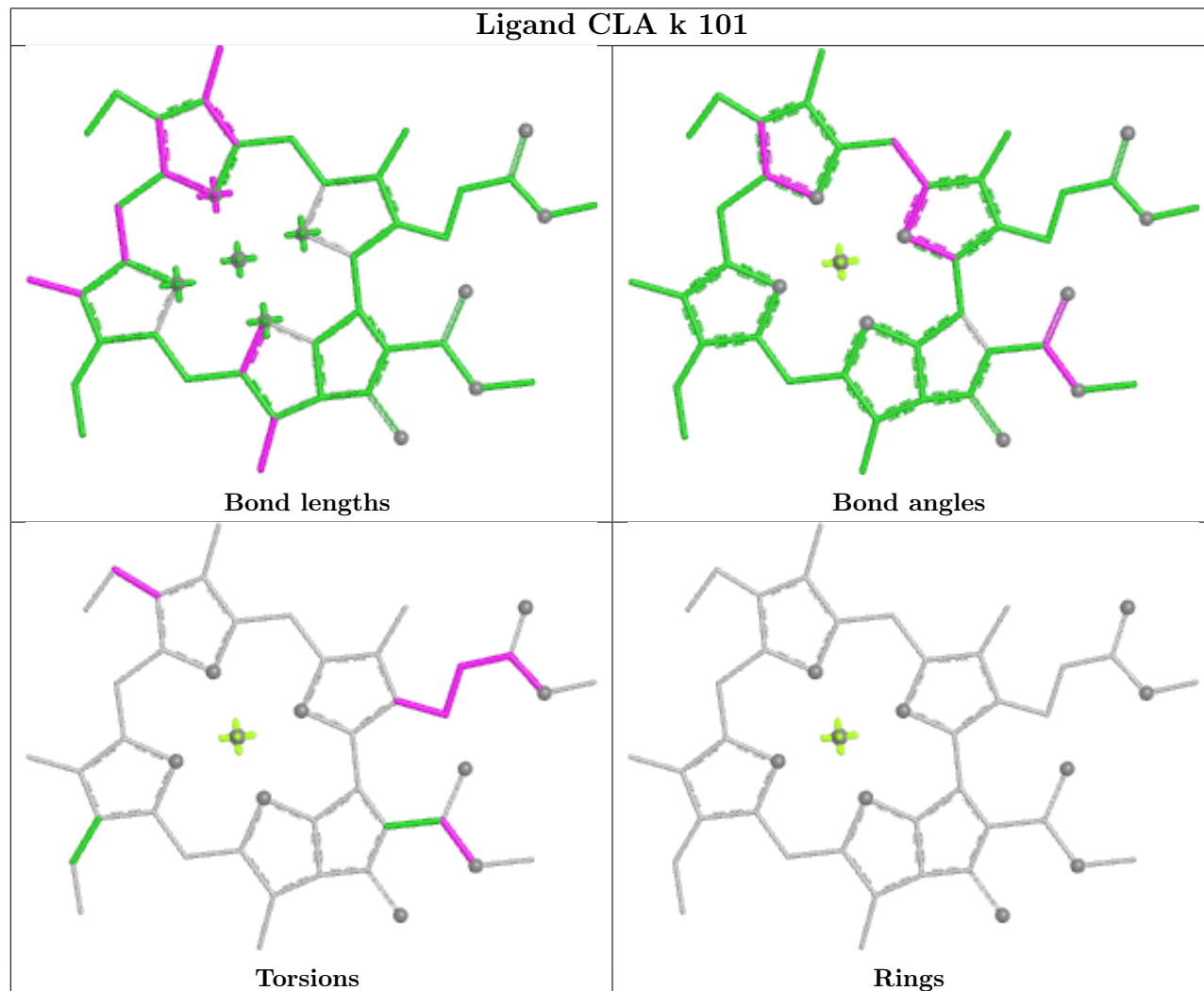


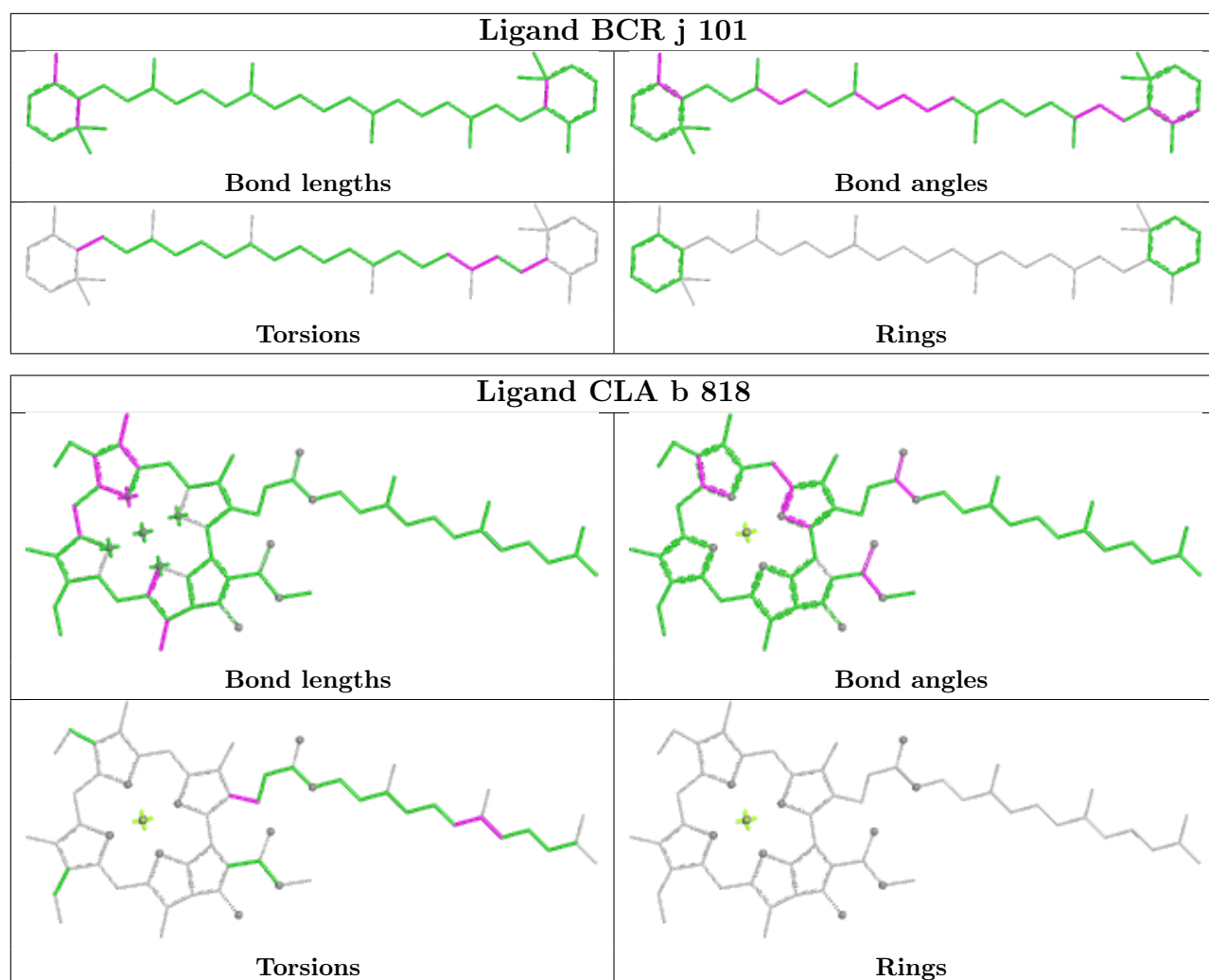


## Ligand CLA b 825

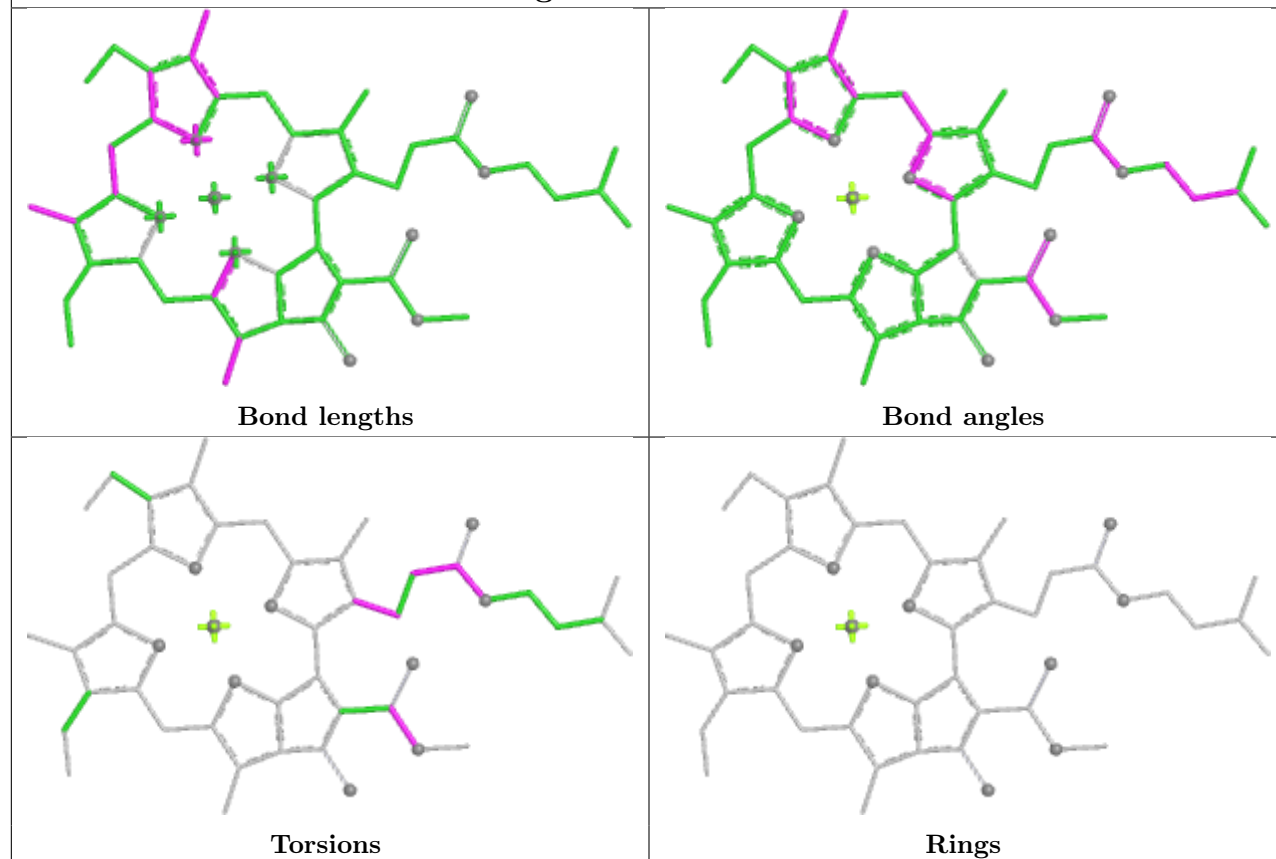


## Ligand CLA k 101

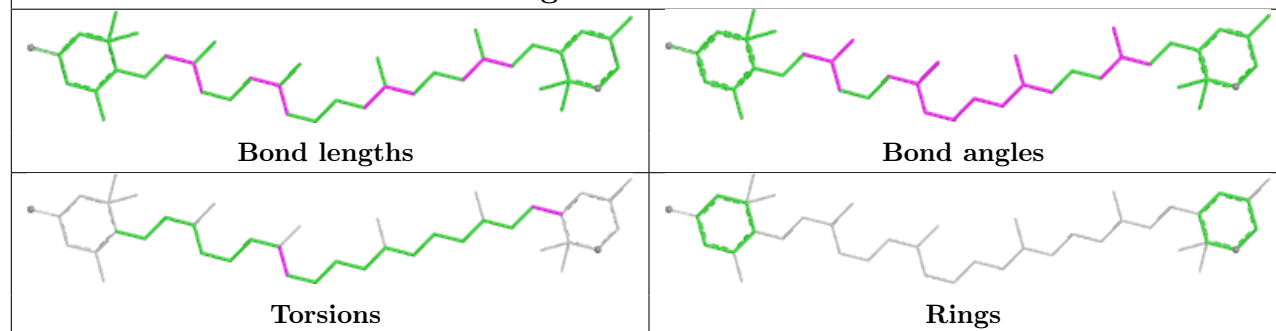




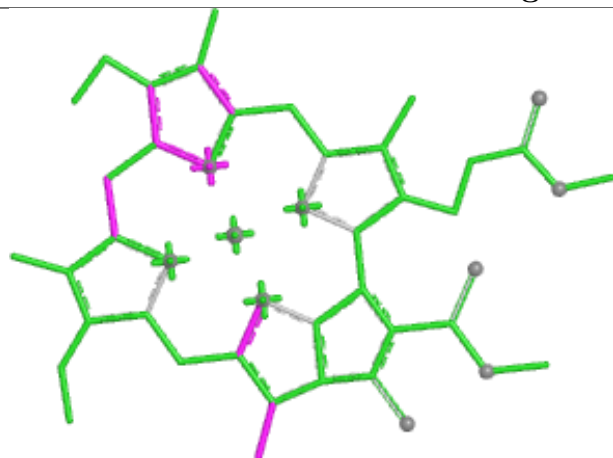
## Ligand CLA b 834



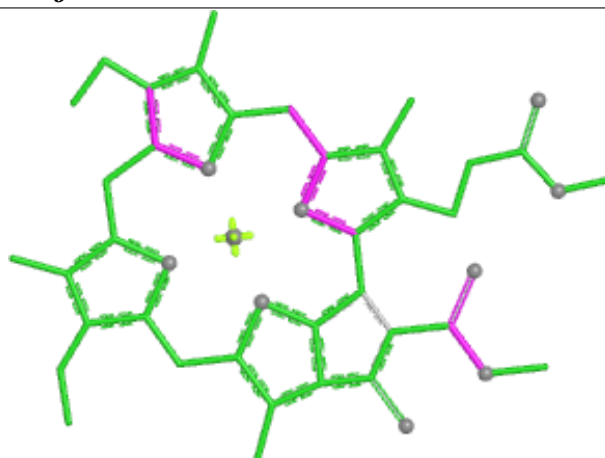
## Ligand ZEX f 205



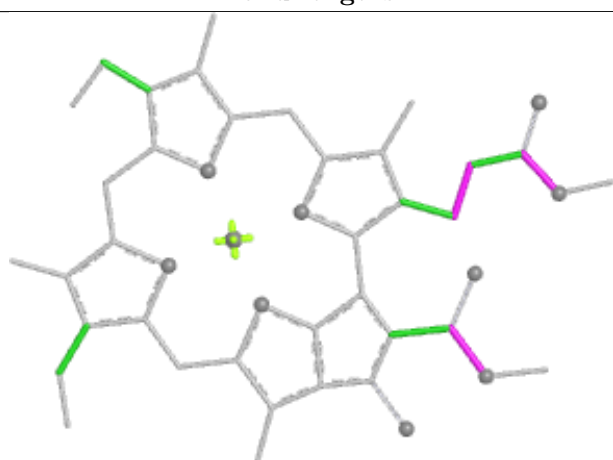
## Ligand CLA j 104



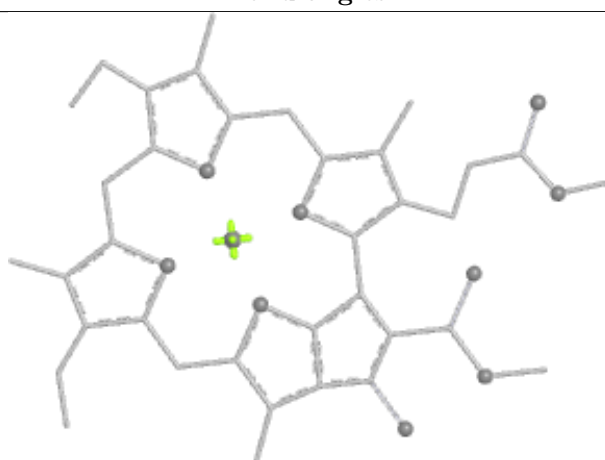
Bond lengths



Bond angles

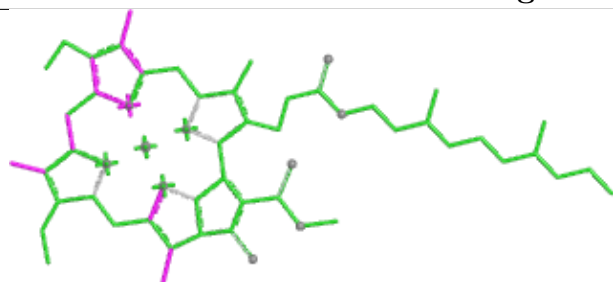


Torsions

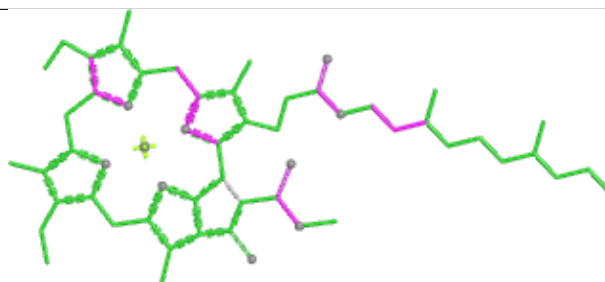


Rings

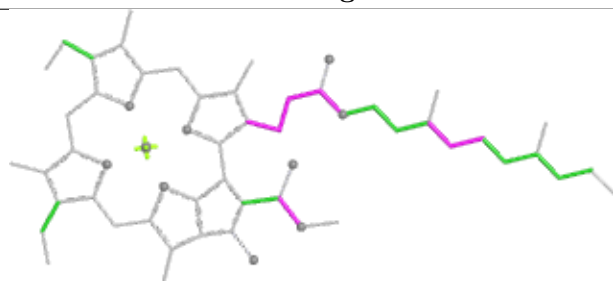
## Ligand CLA b 822



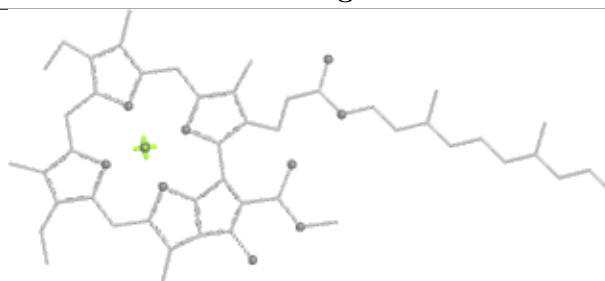
Bond lengths



Bond angles

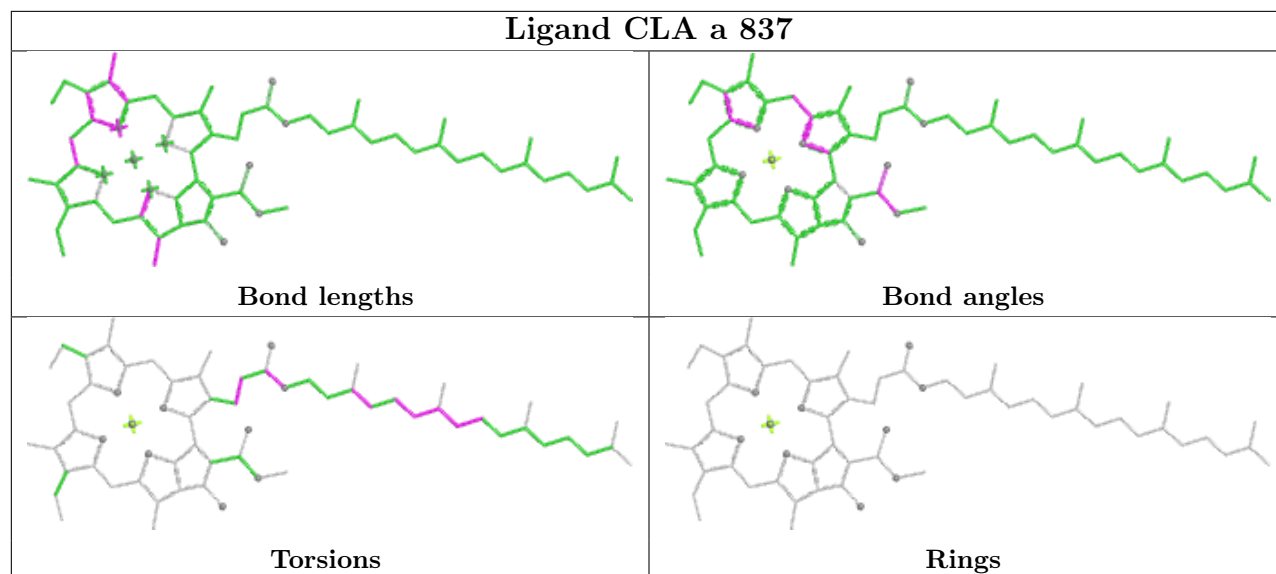


Torsions

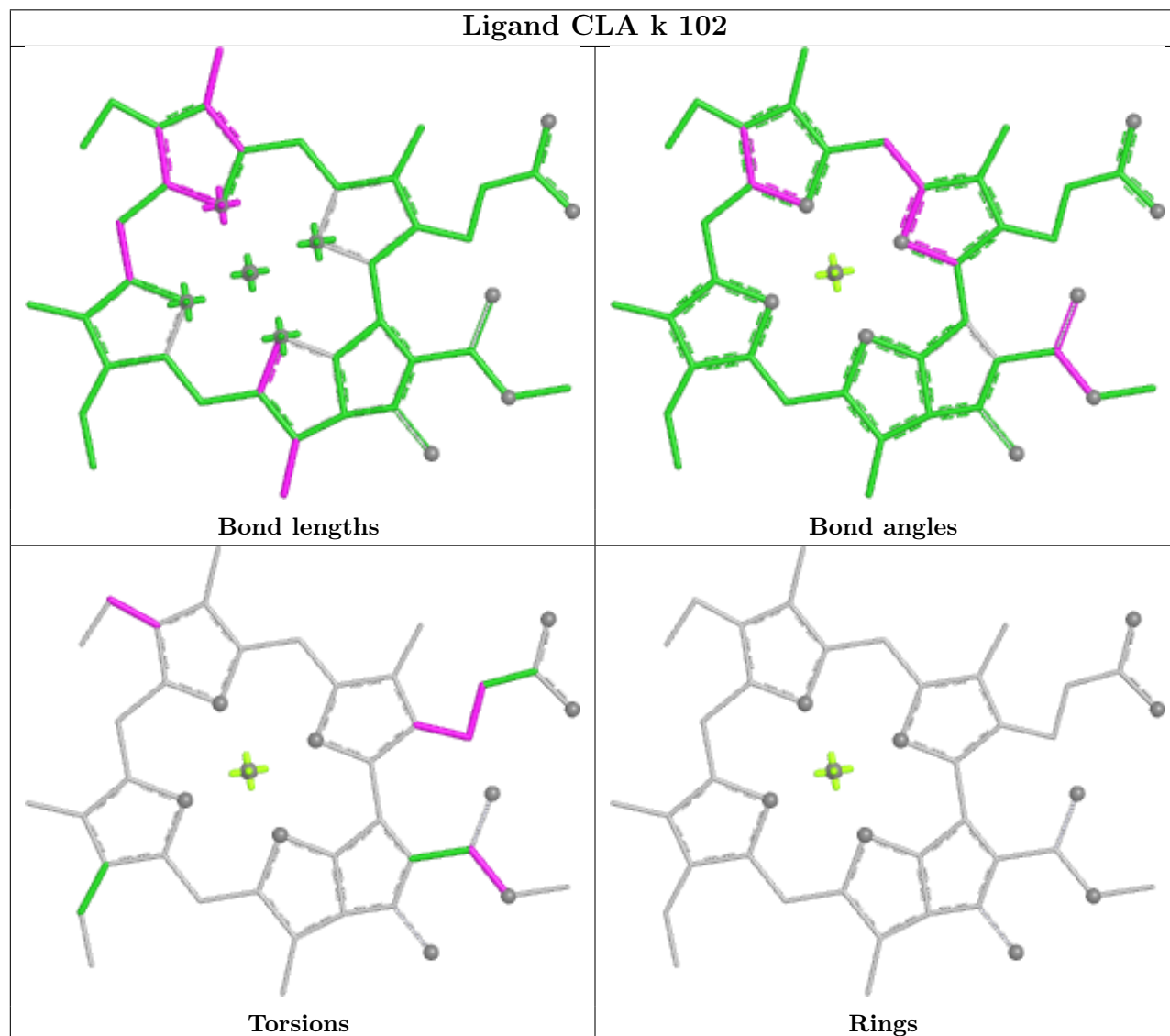


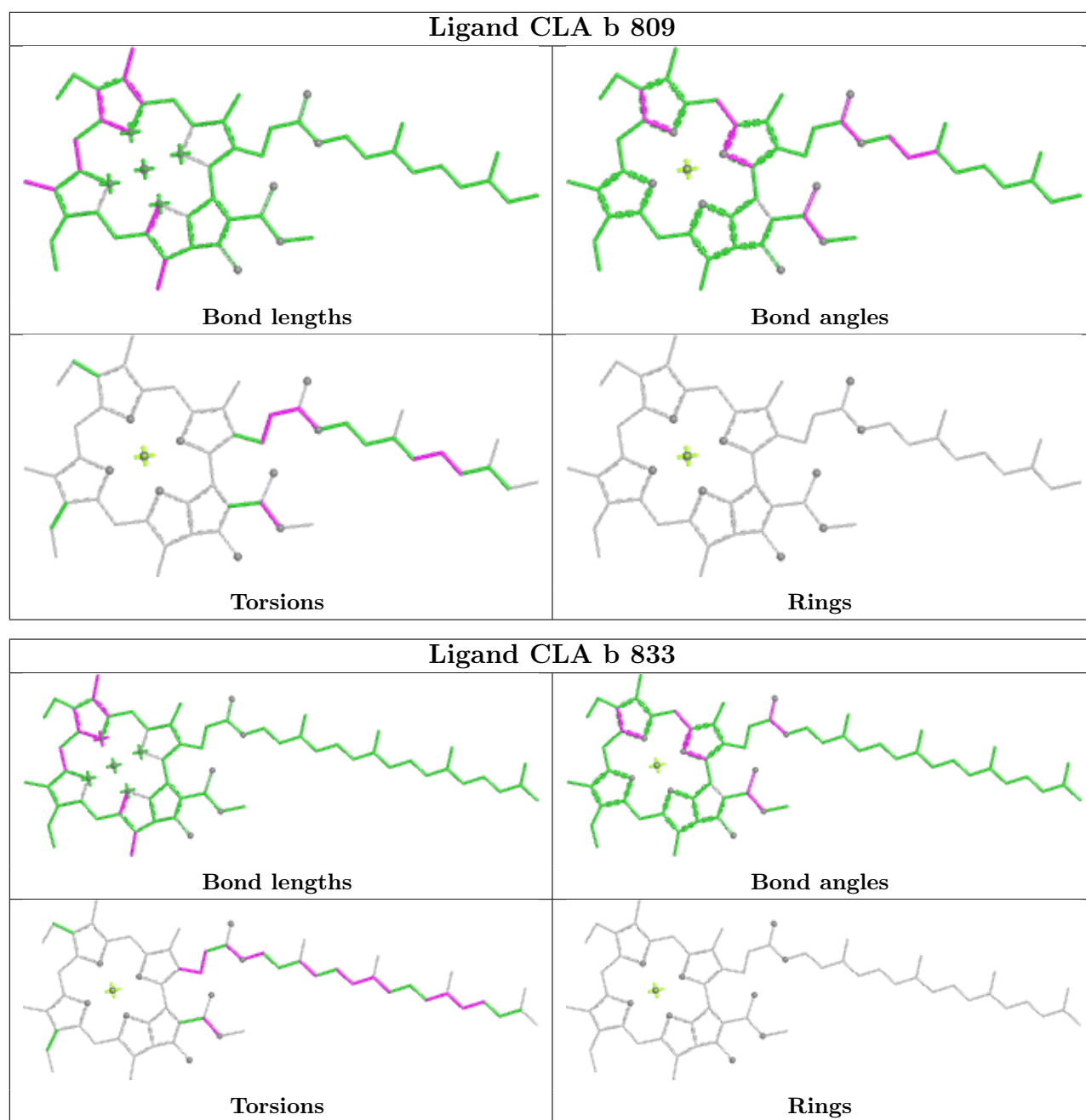
Rings

## Ligand CLA a 837

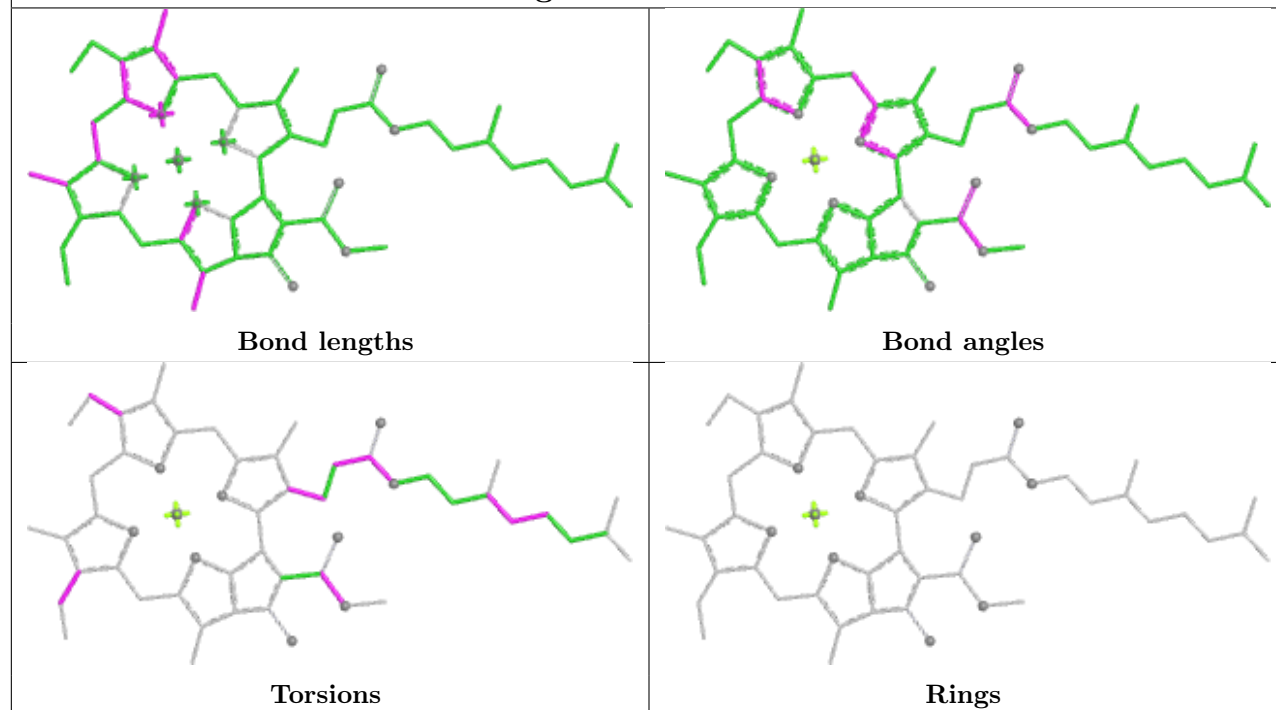


## Ligand CLA k 102

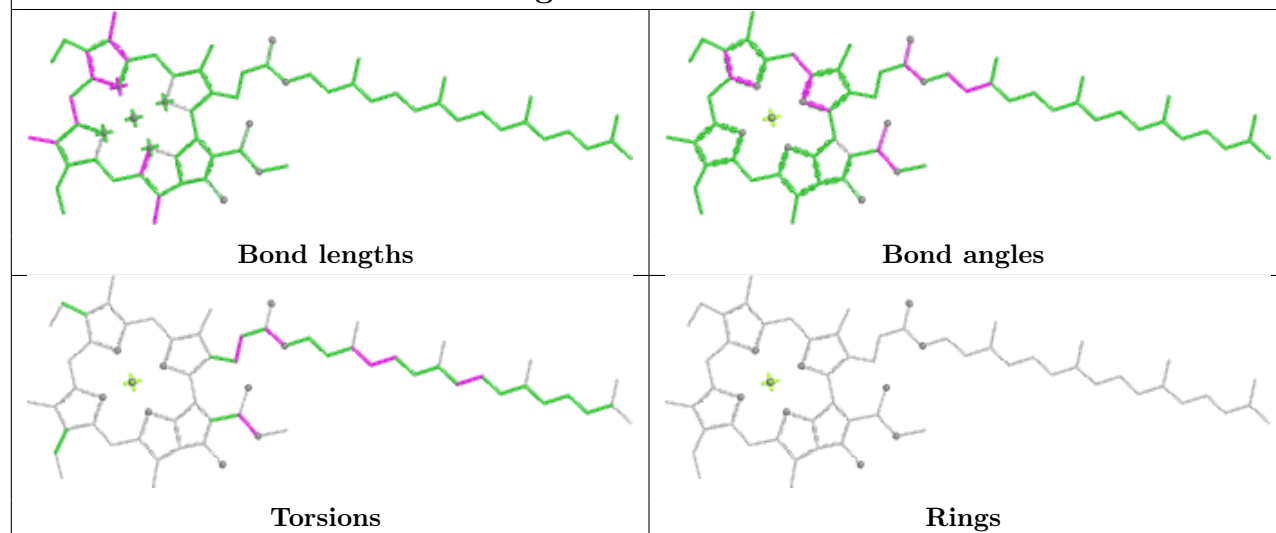




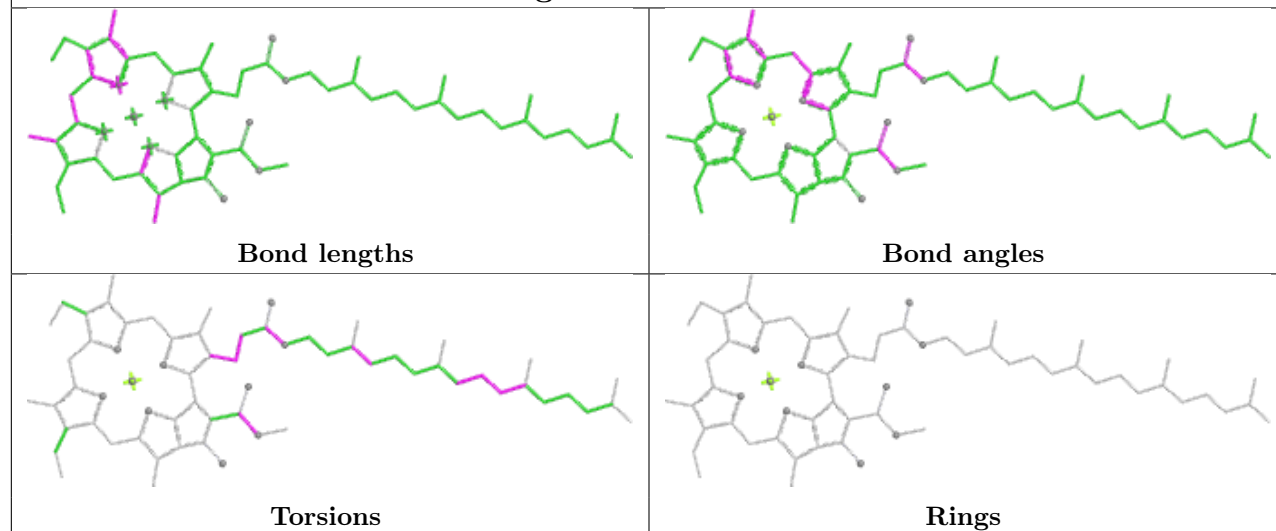
## Ligand CLA b 814



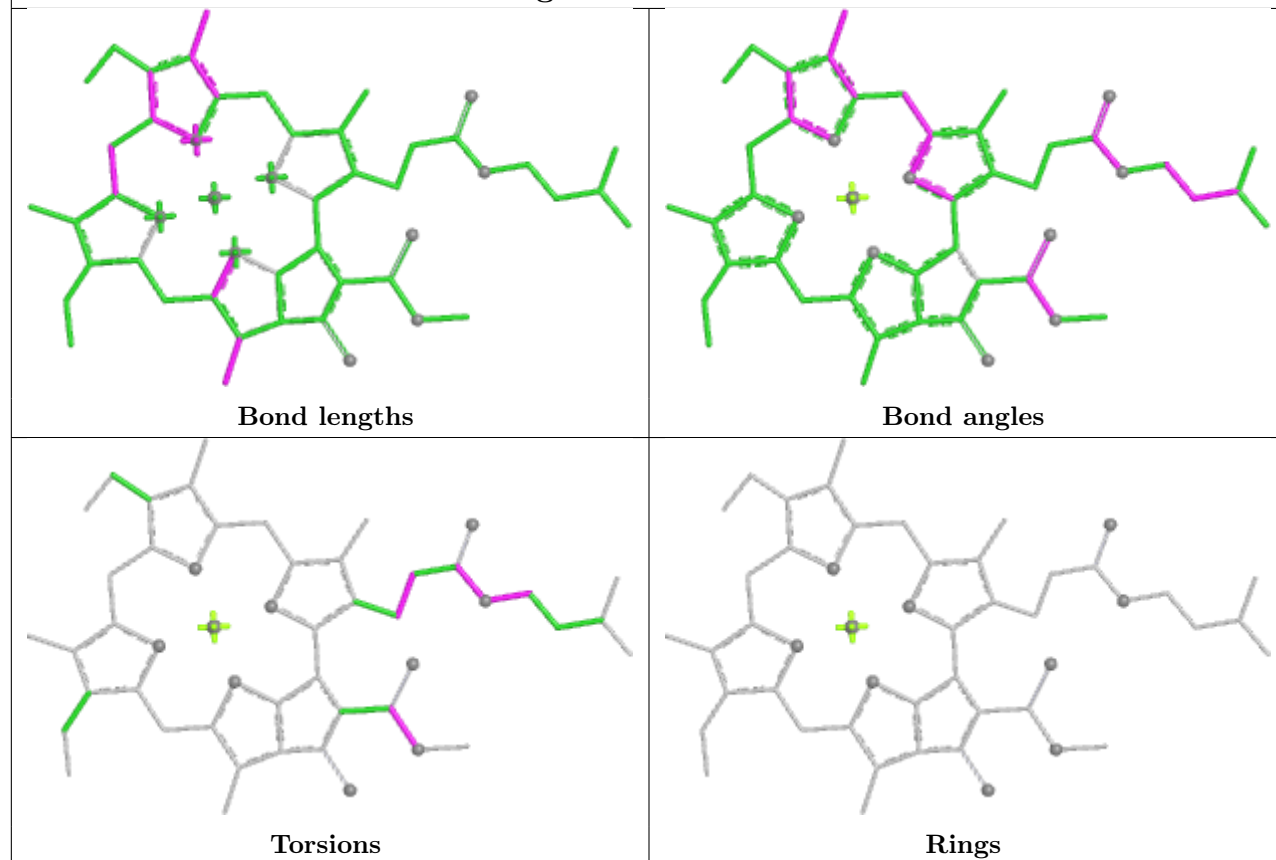
## Ligand CLA b 808



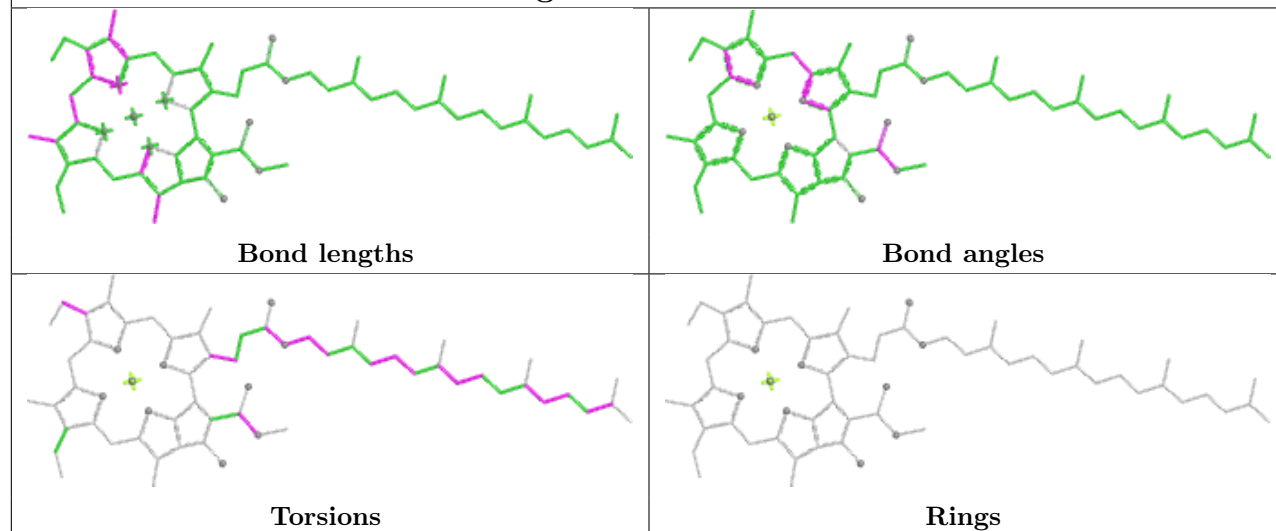
## Ligand CLA b 826



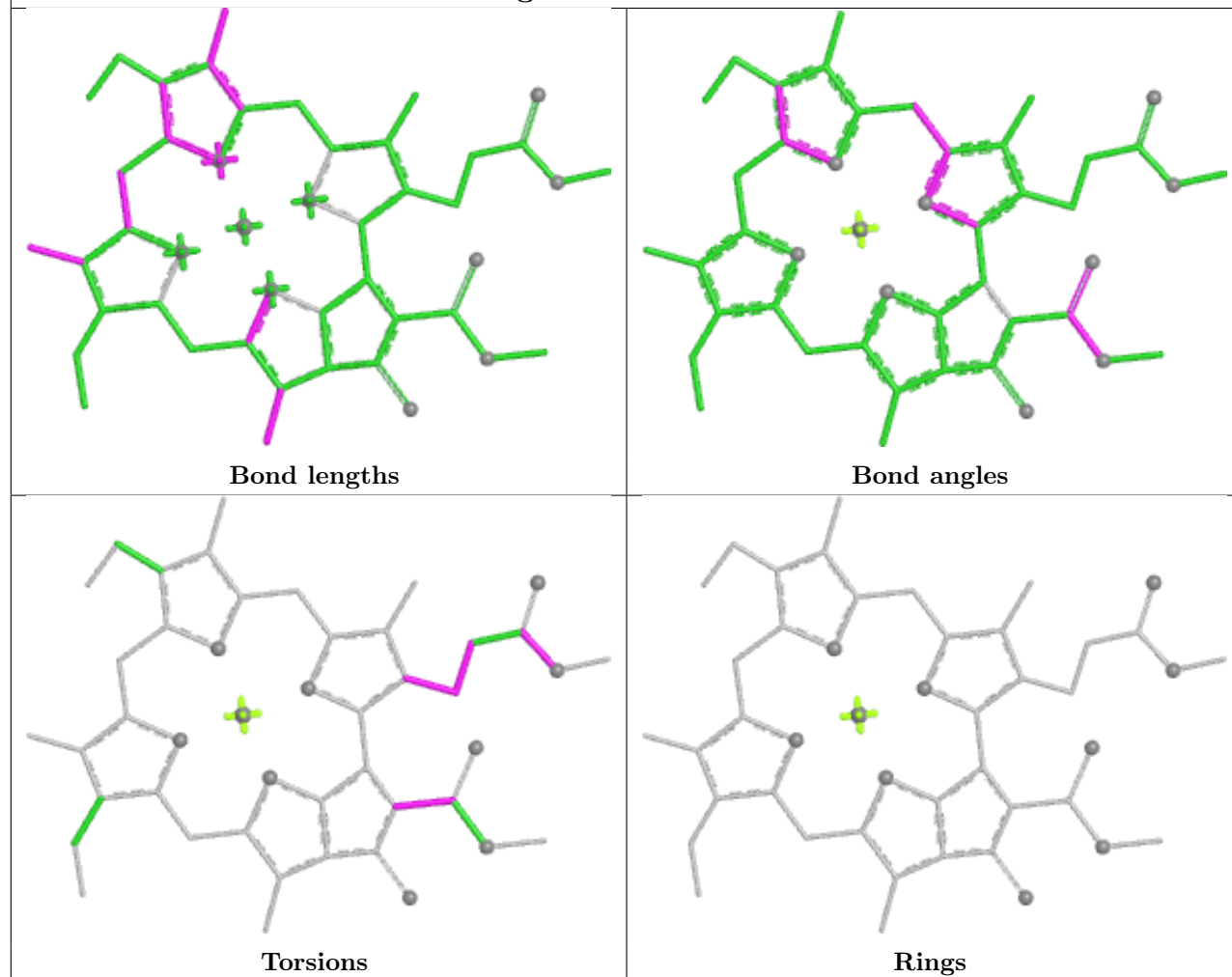
## Ligand CLA a 811

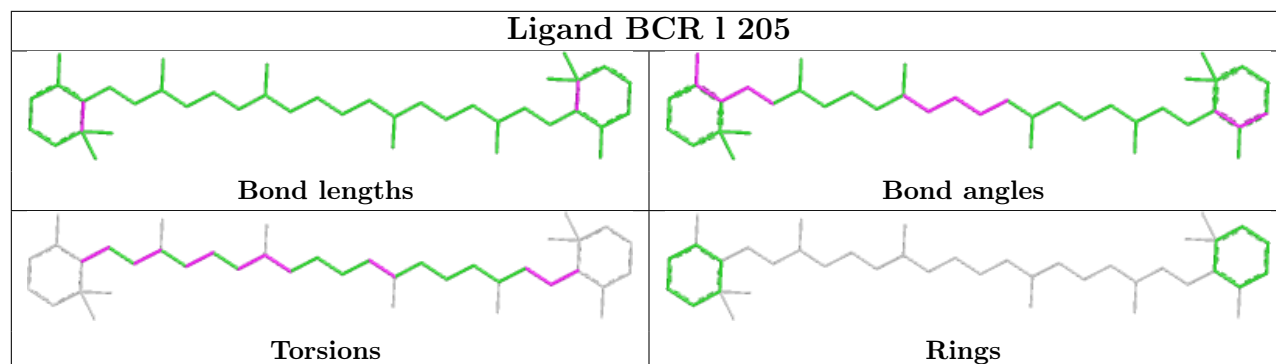
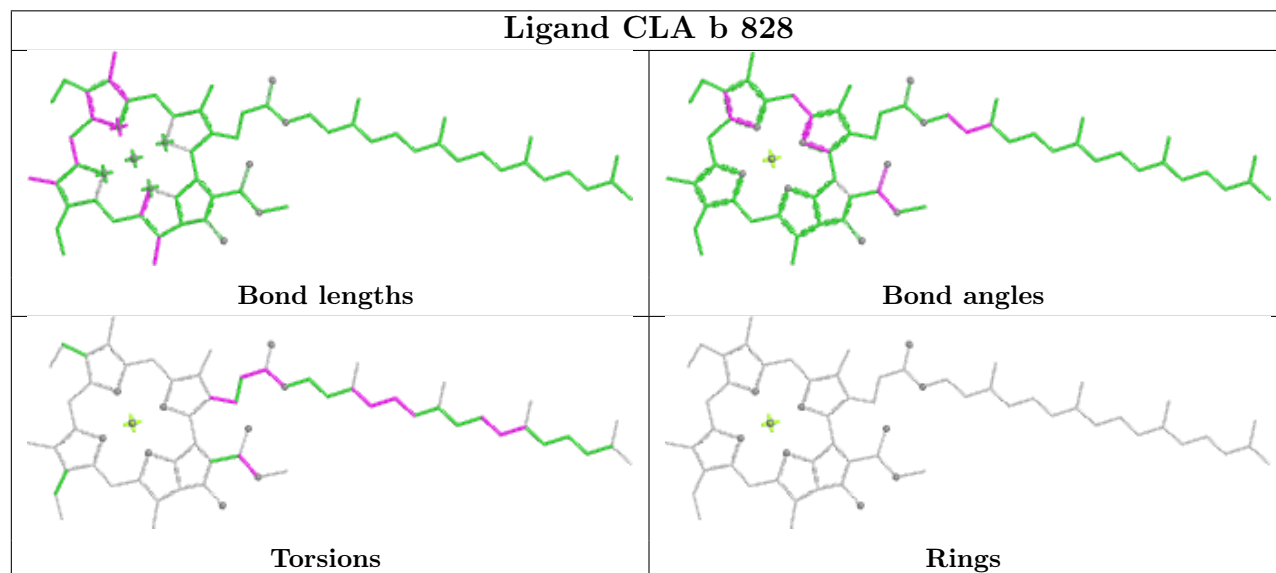
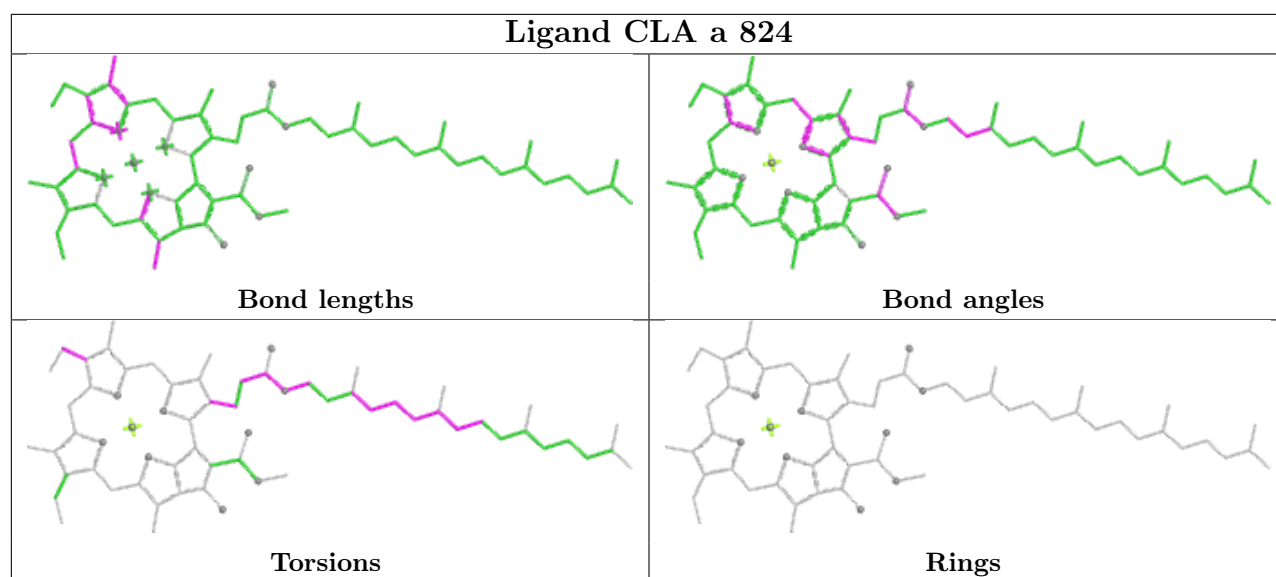


## Ligand CLA a 819

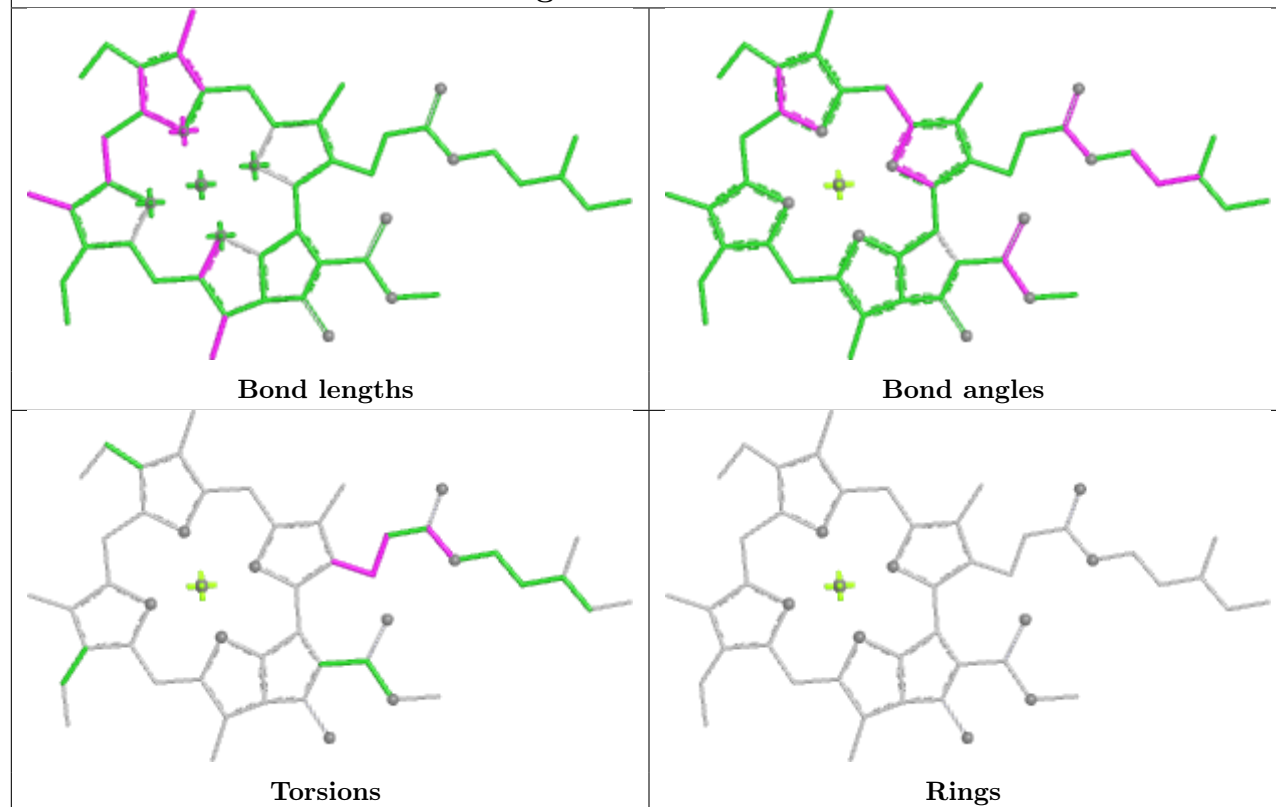


## Ligand CLA b 840

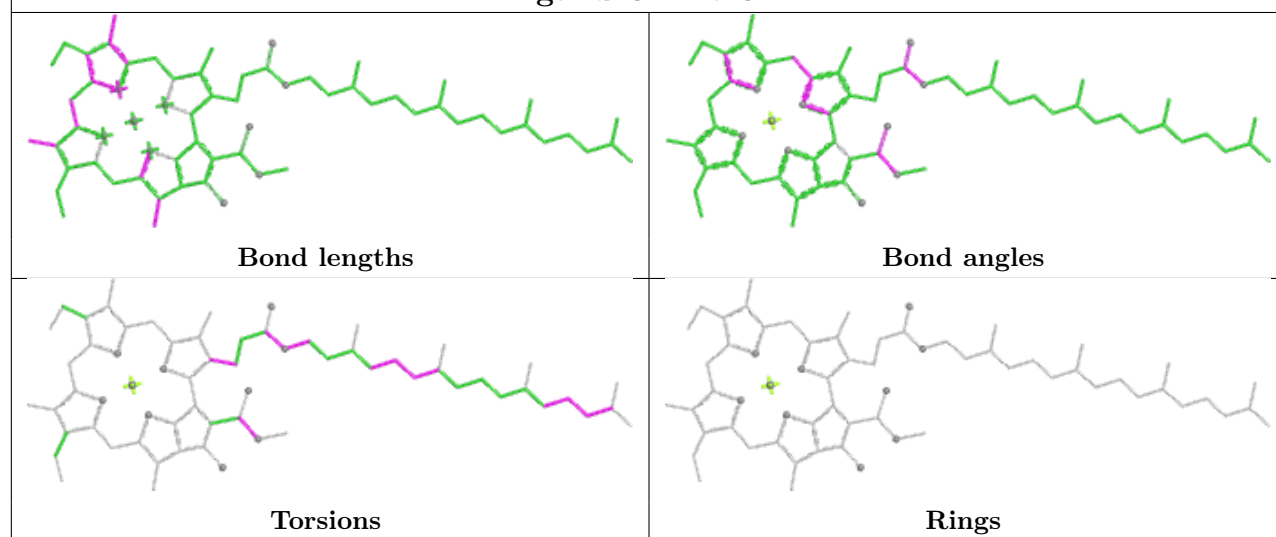


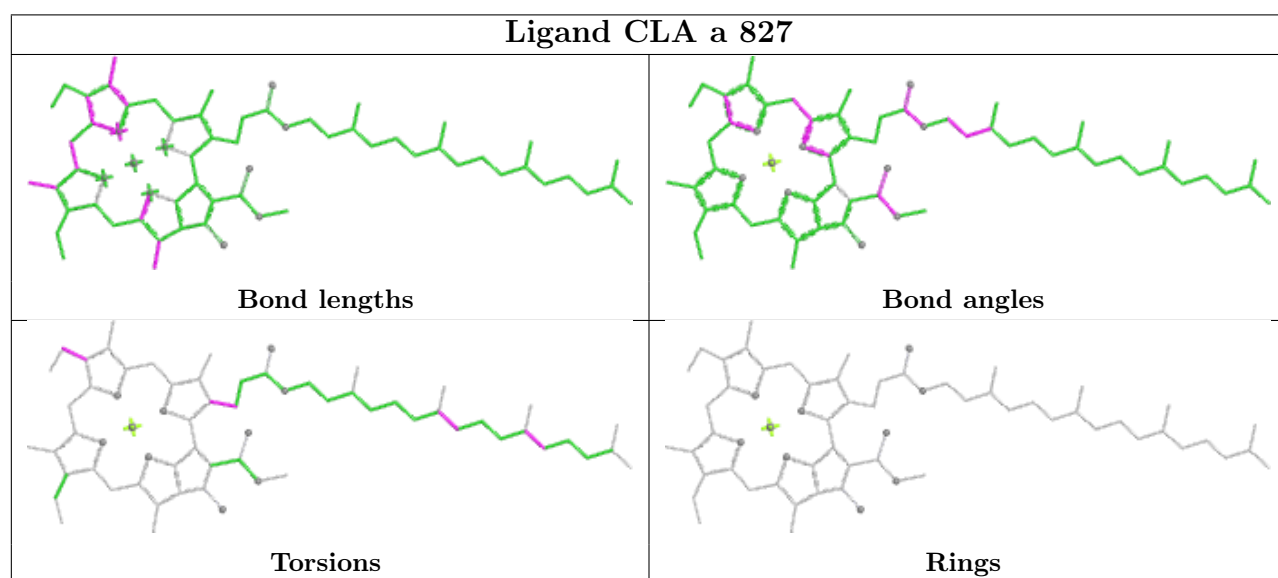
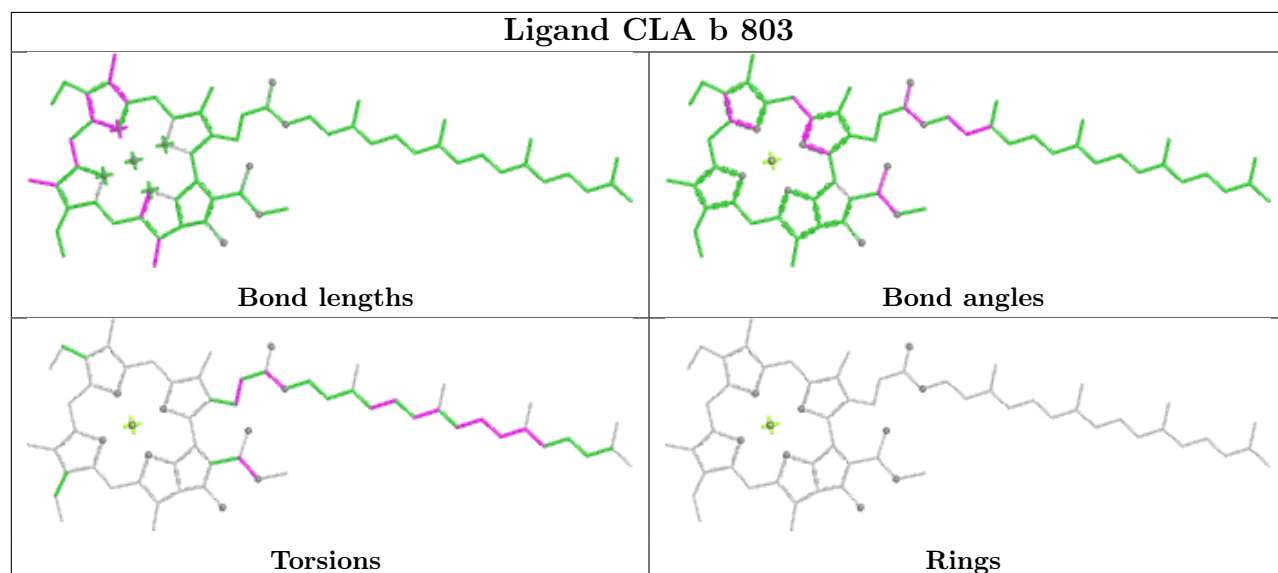
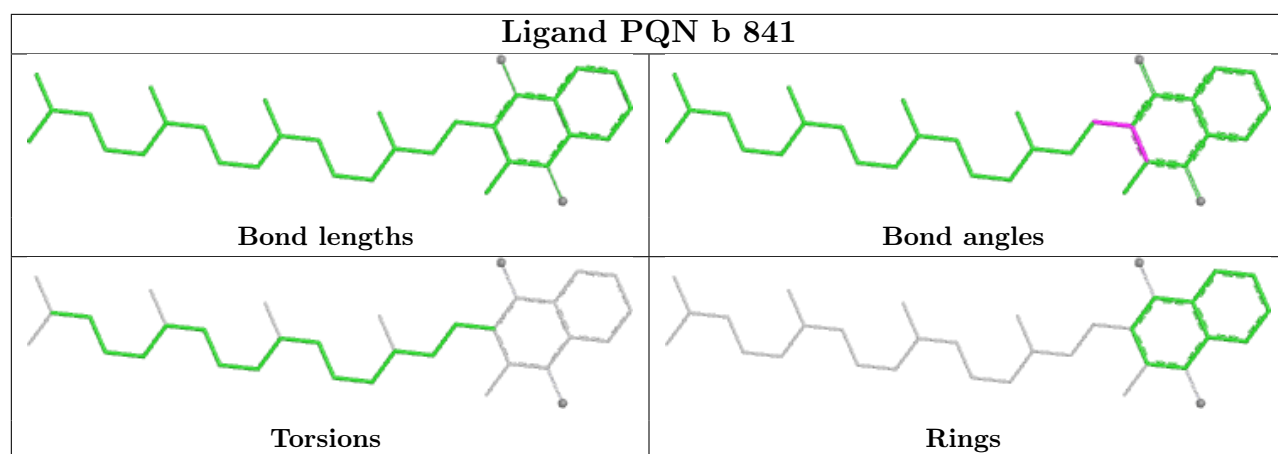


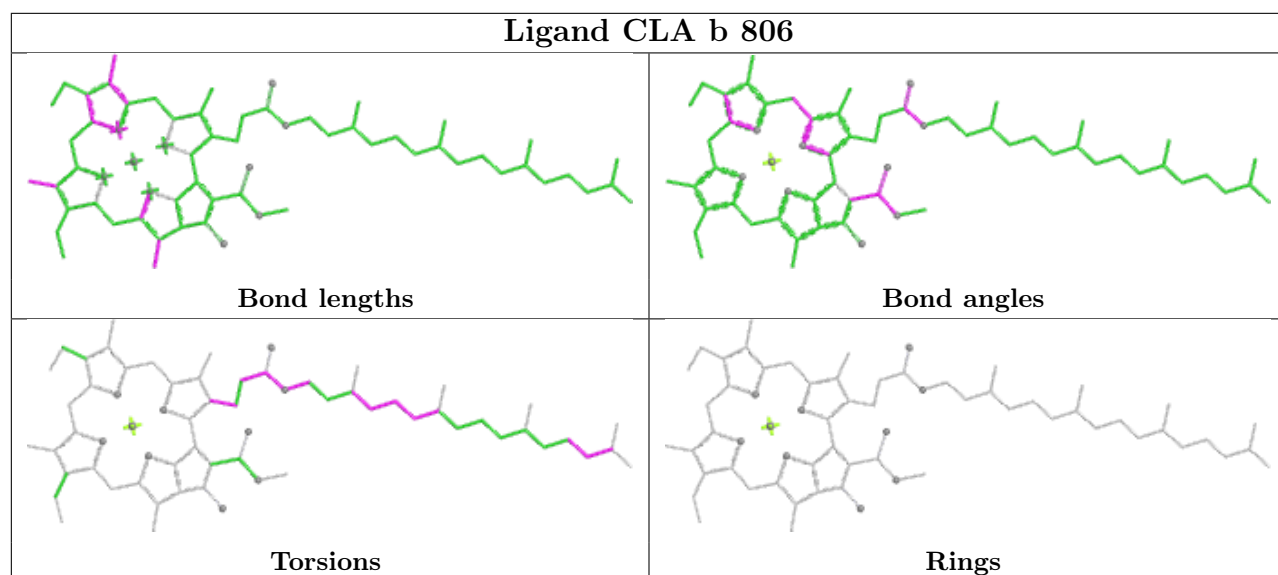
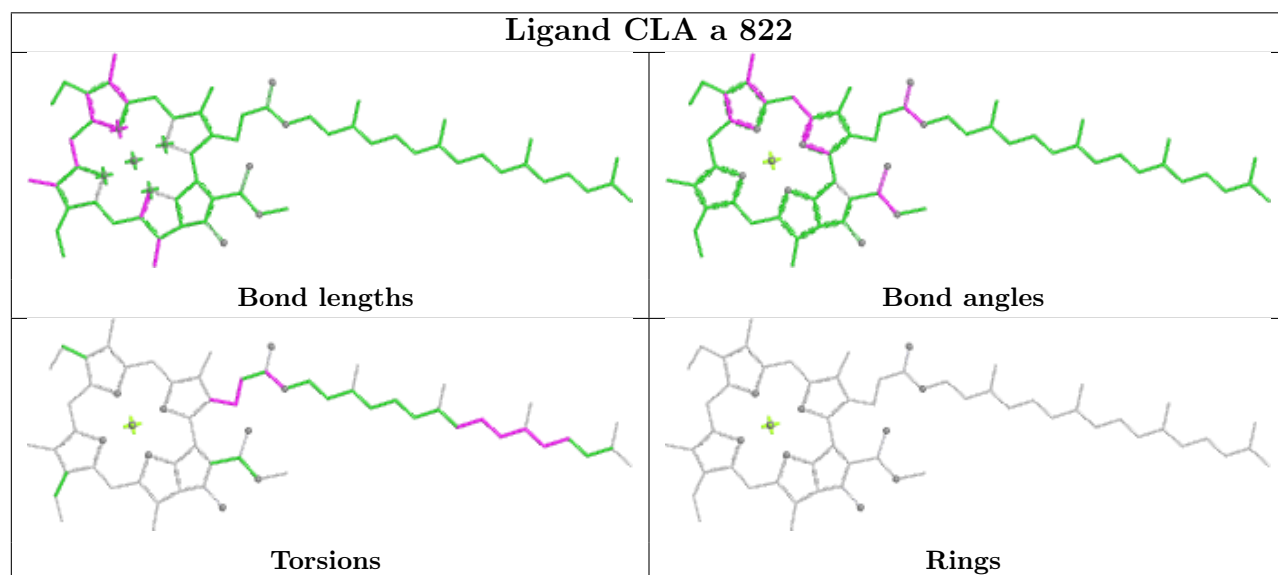
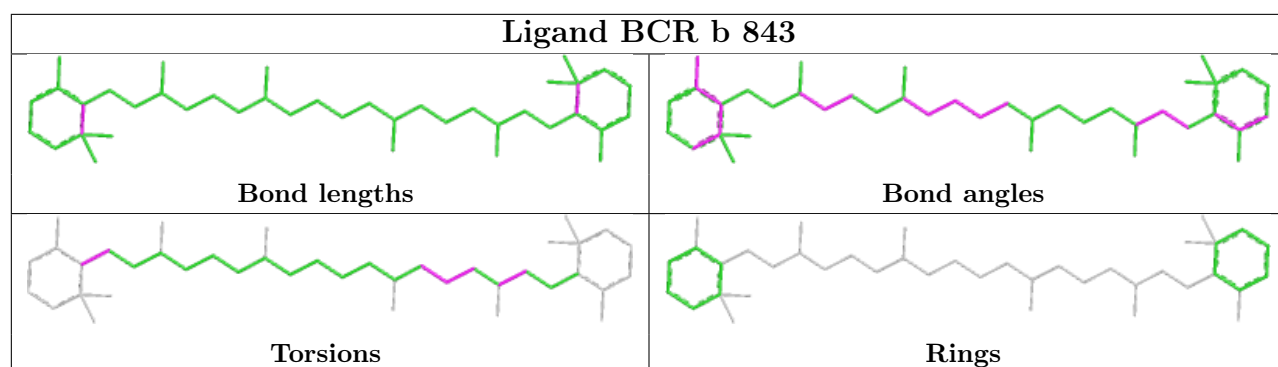
## Ligand CLA a 838

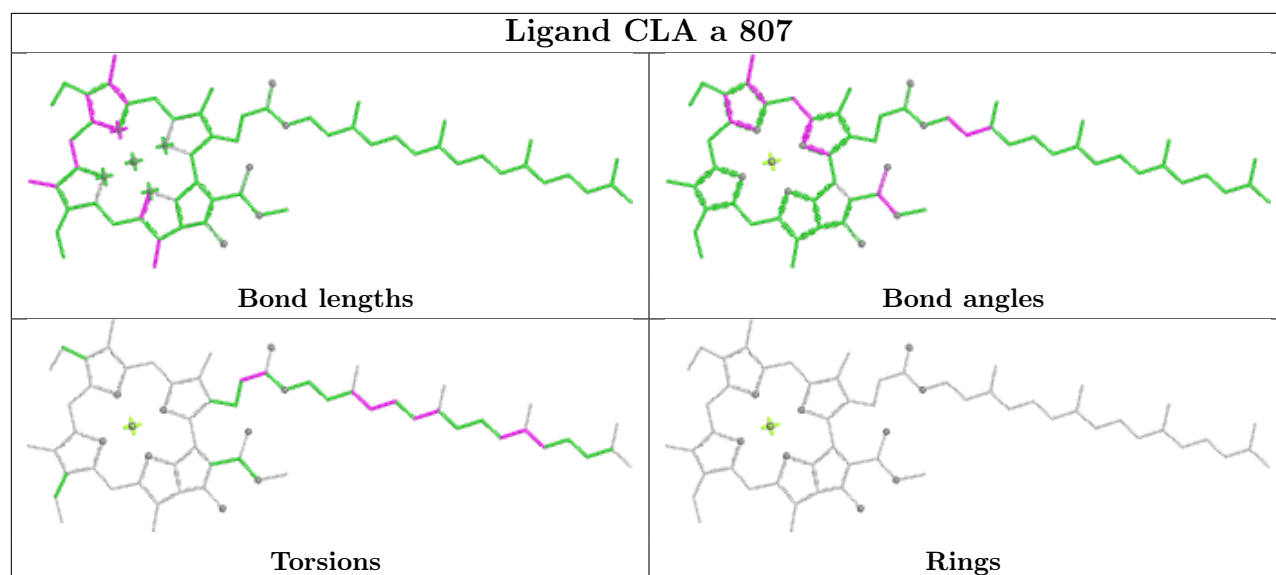
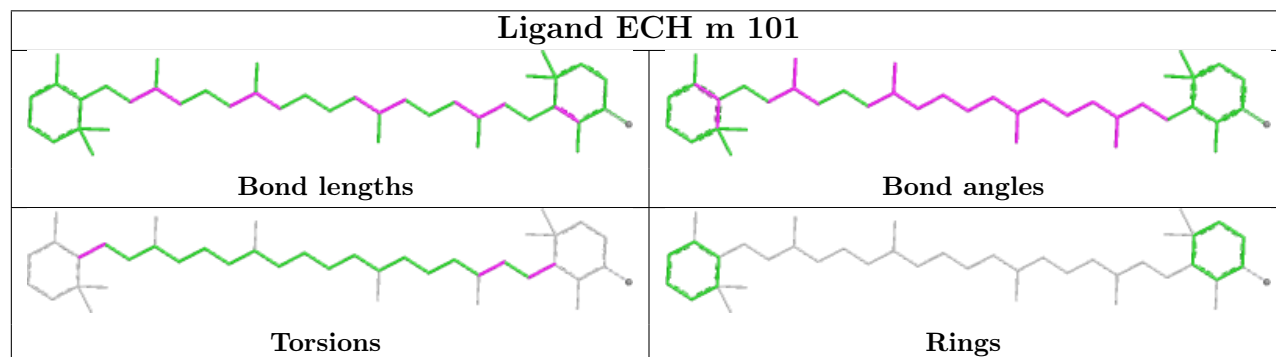
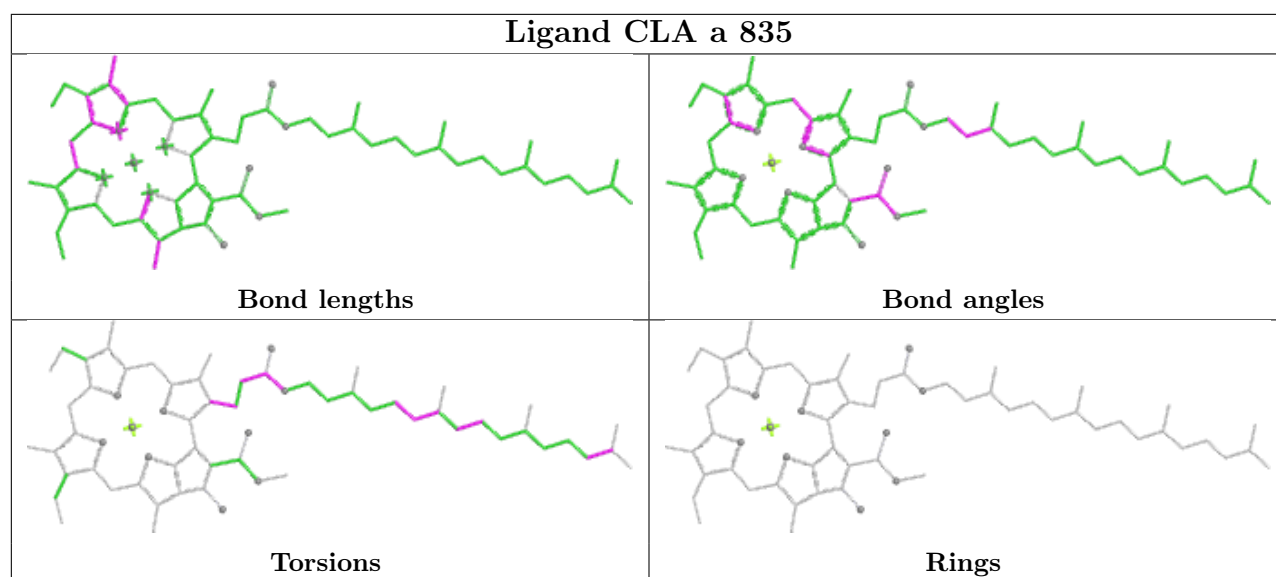


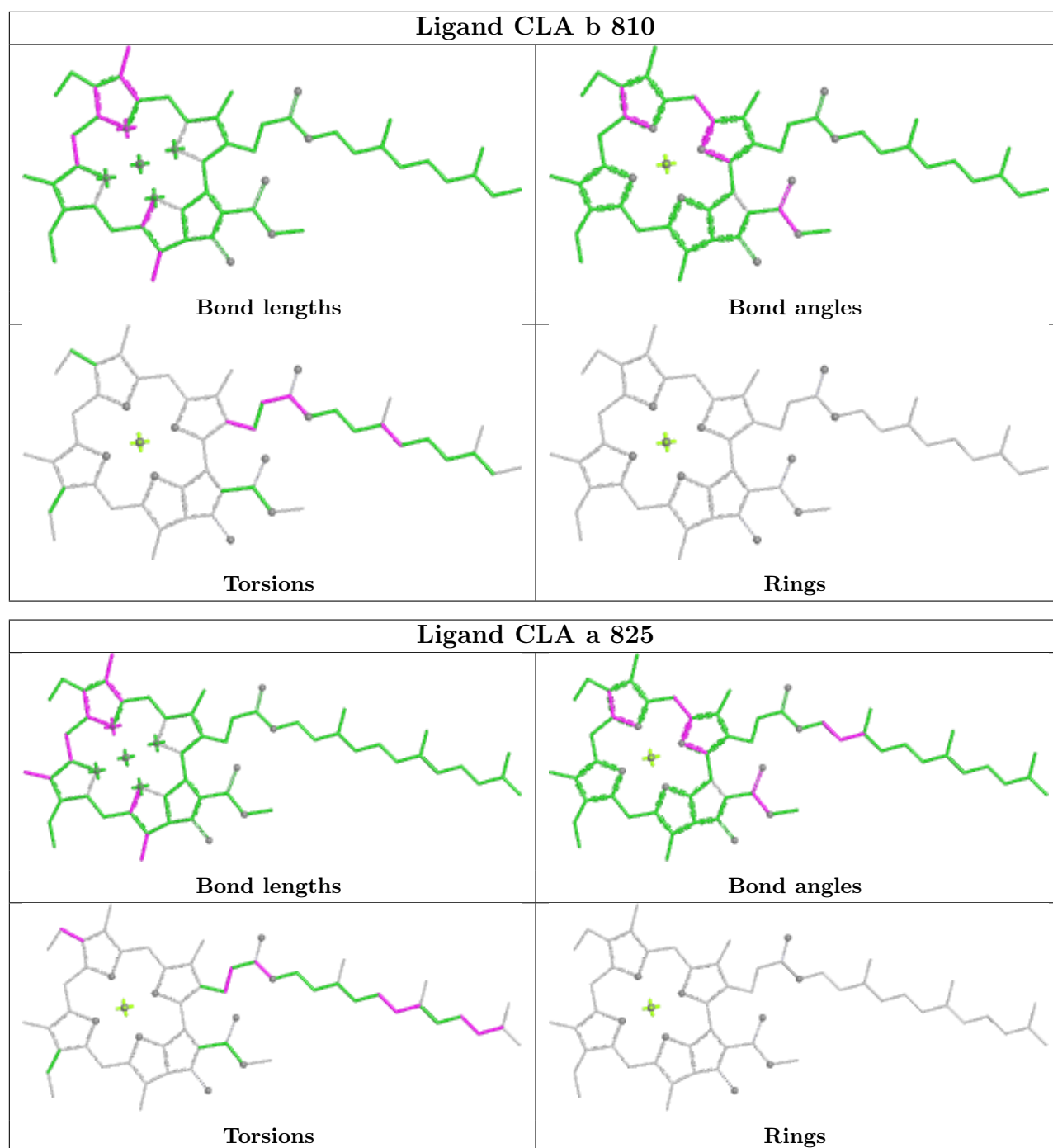
## Ligand CLA a 841

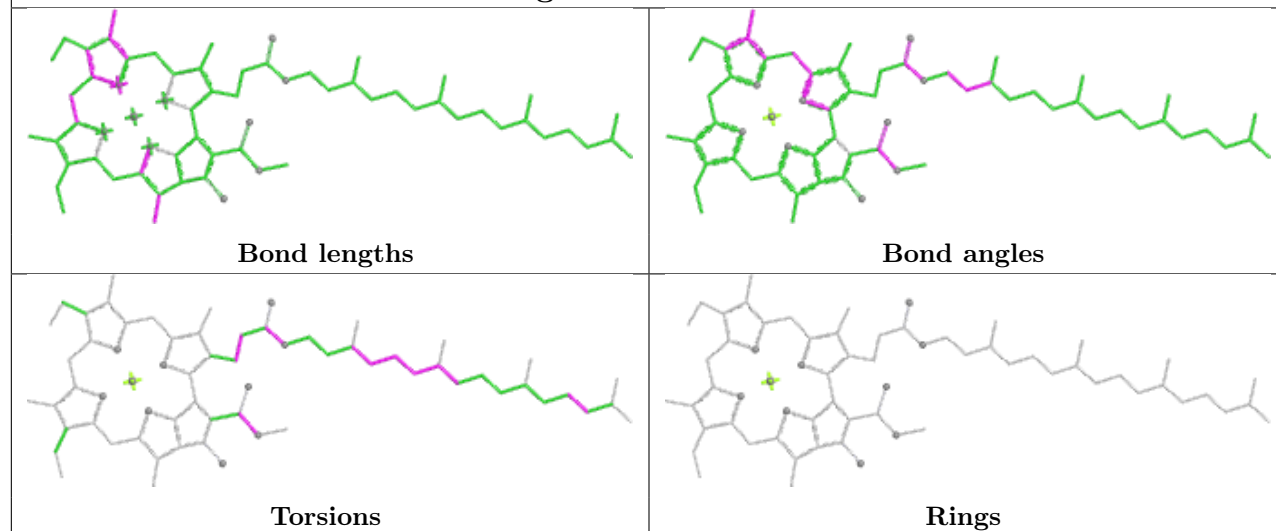
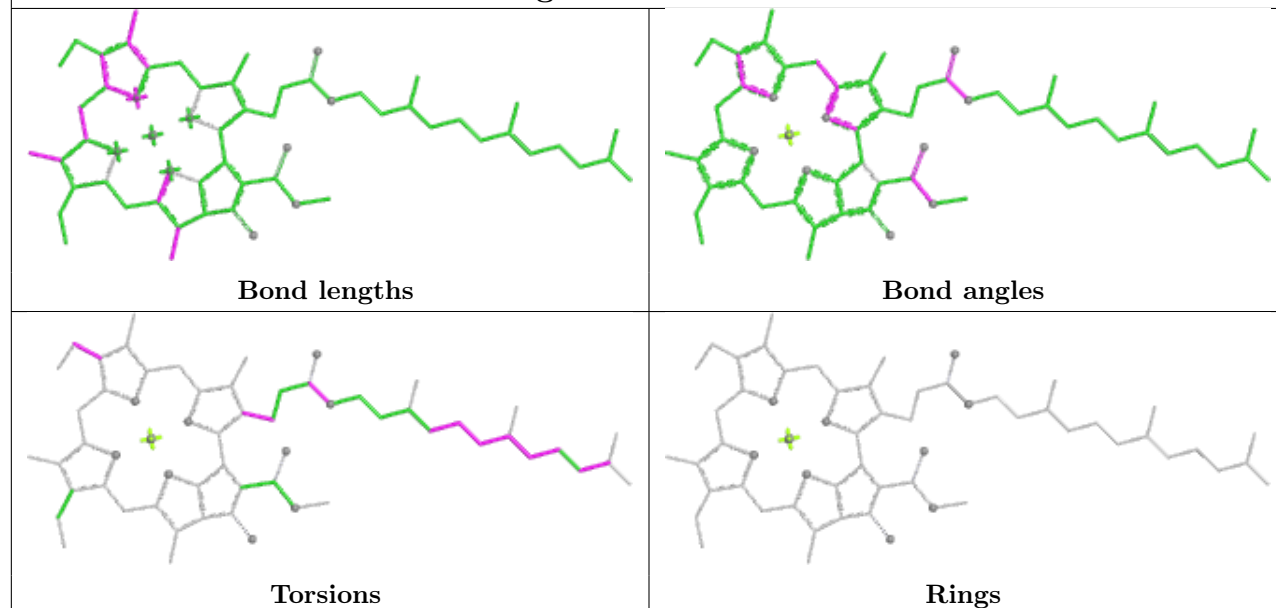


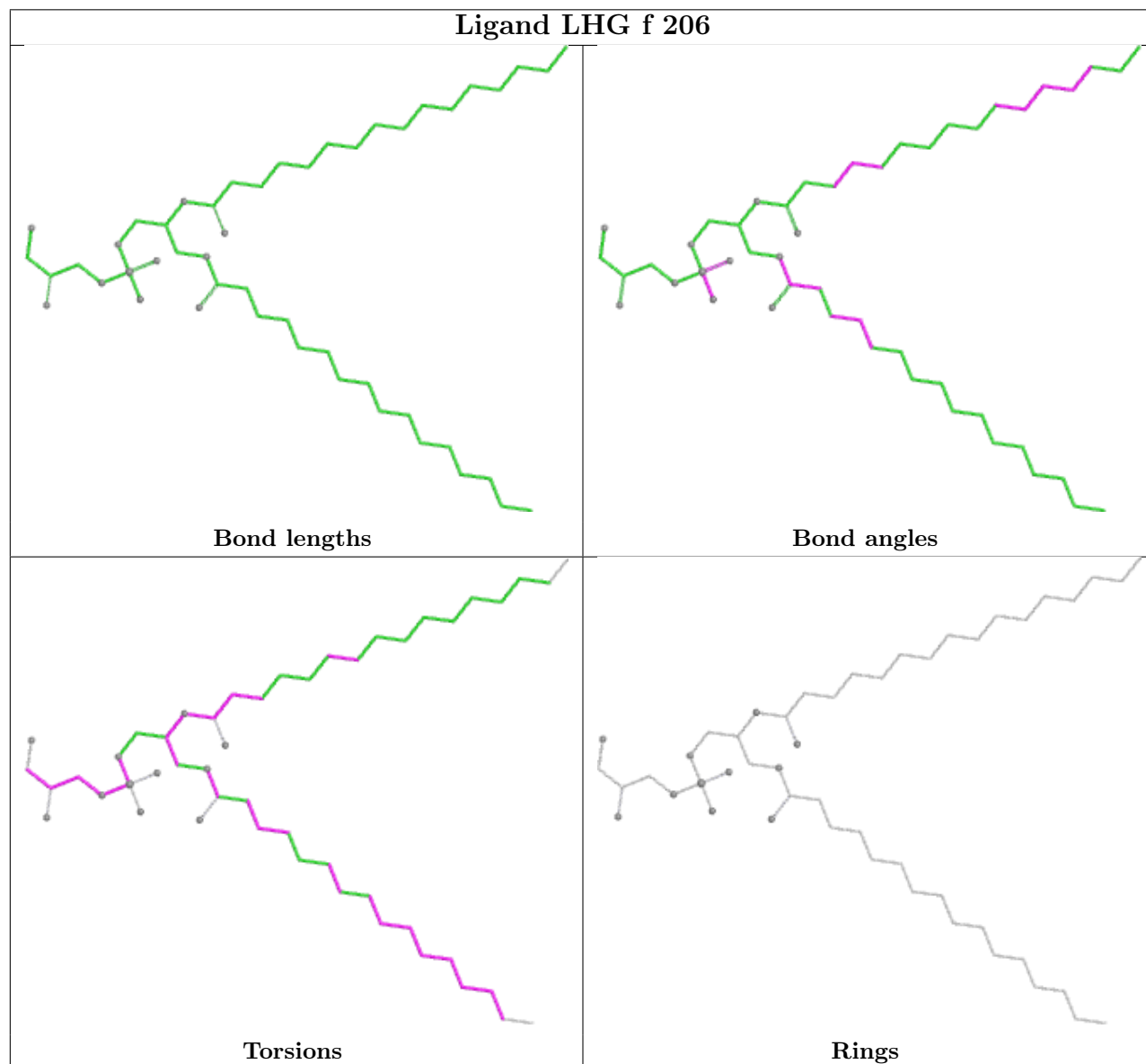
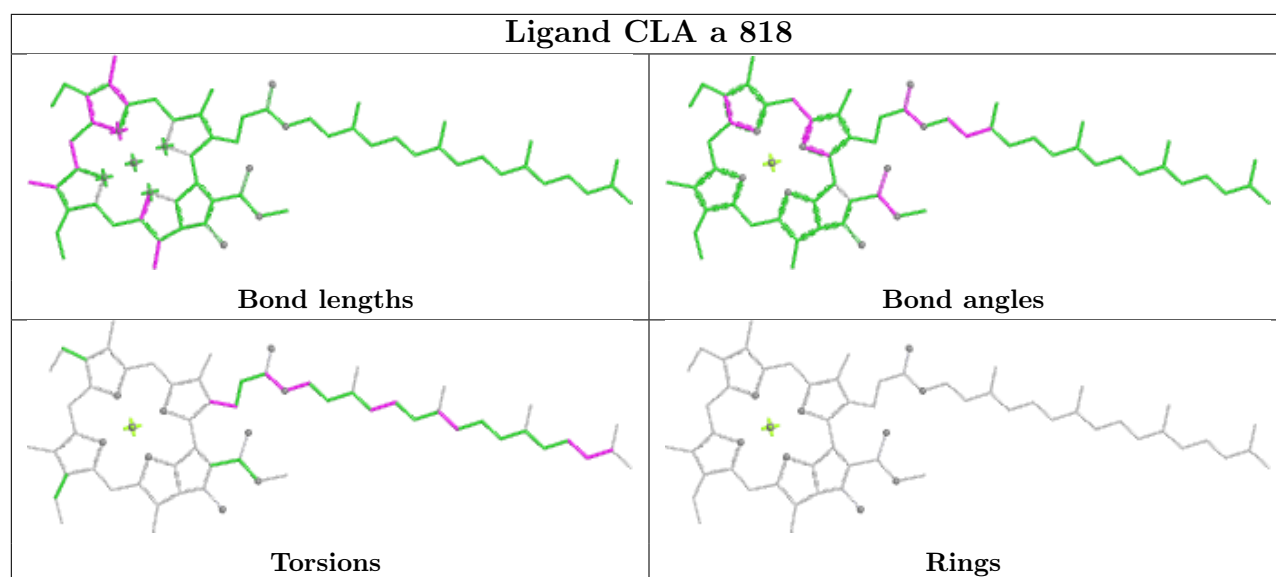




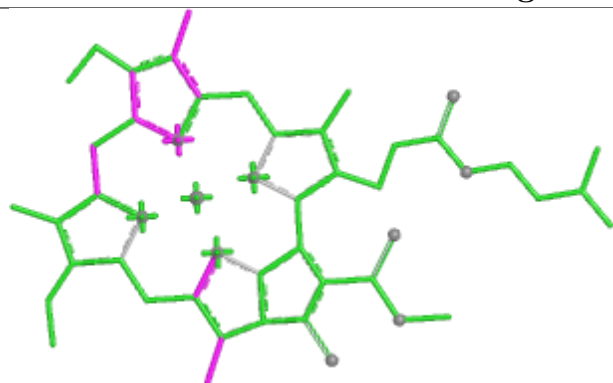




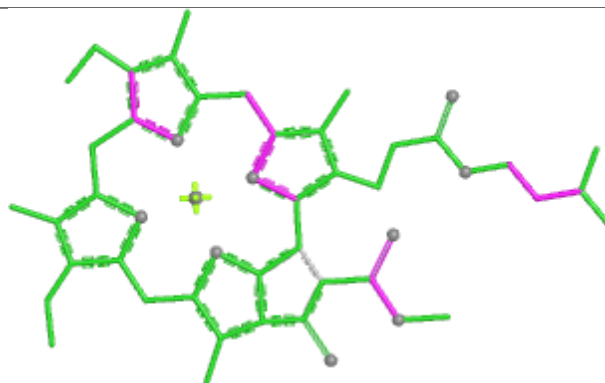
**Ligand CLA a 802****Ligand CLA a 813**



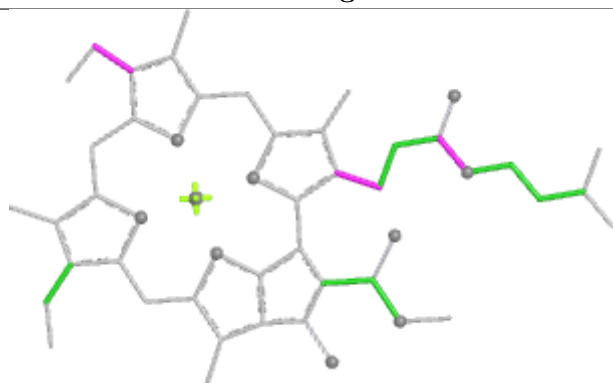
## Ligand CLA b 837



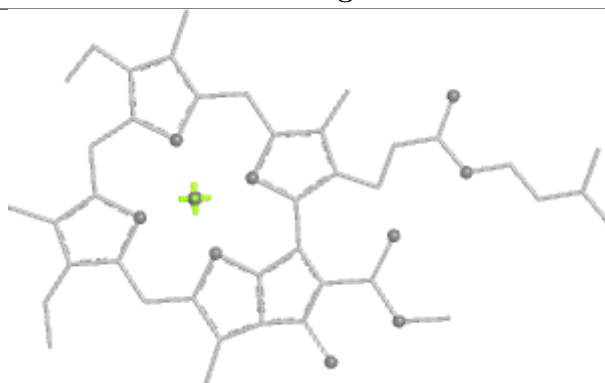
Bond lengths



Bond angles

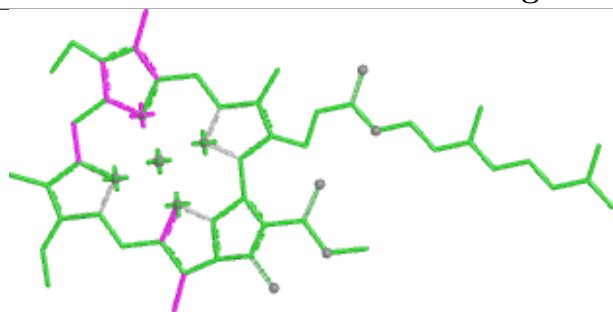


Torsions

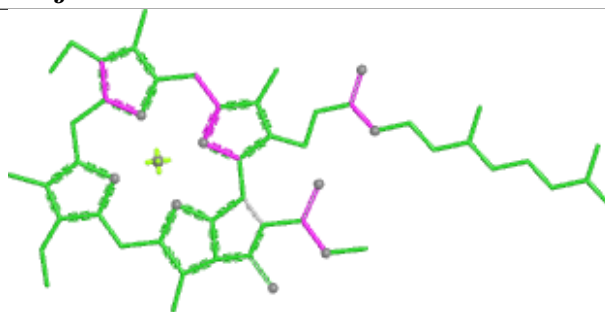


Rings

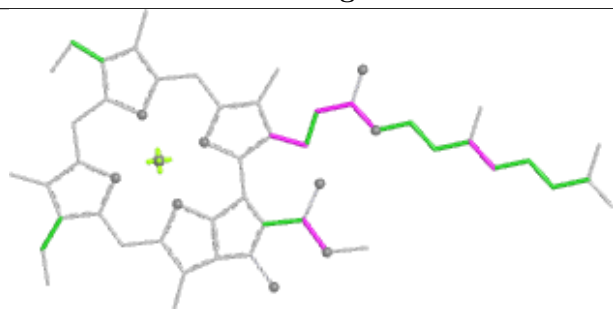
## Ligand CLA j 103



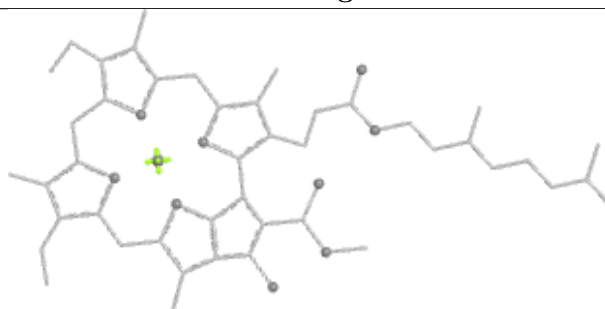
Bond lengths



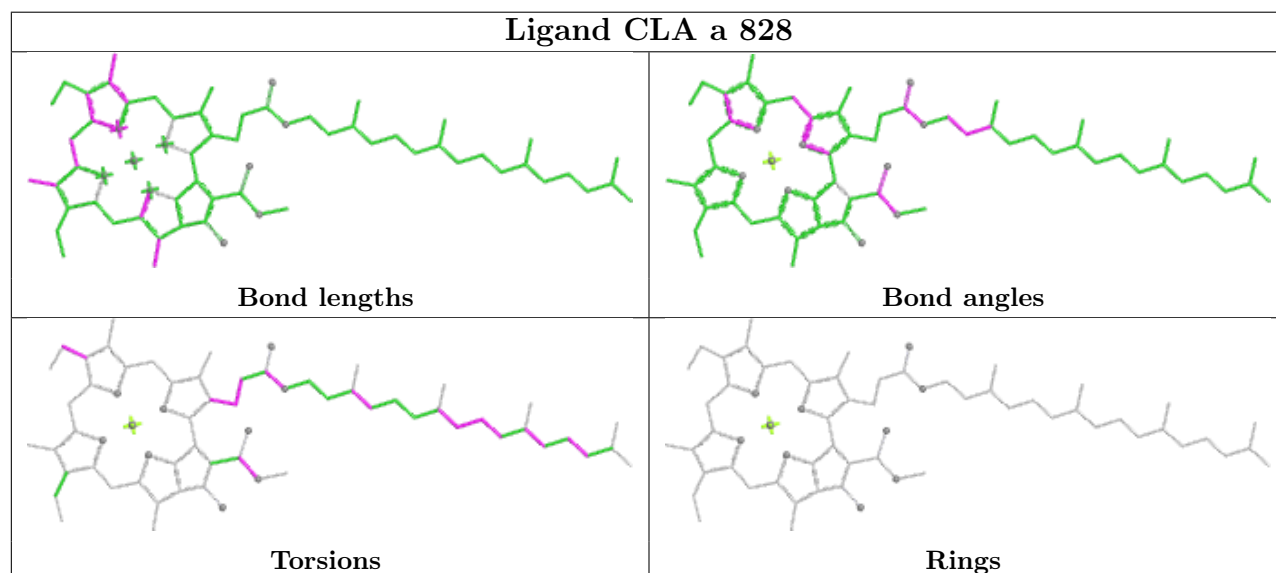
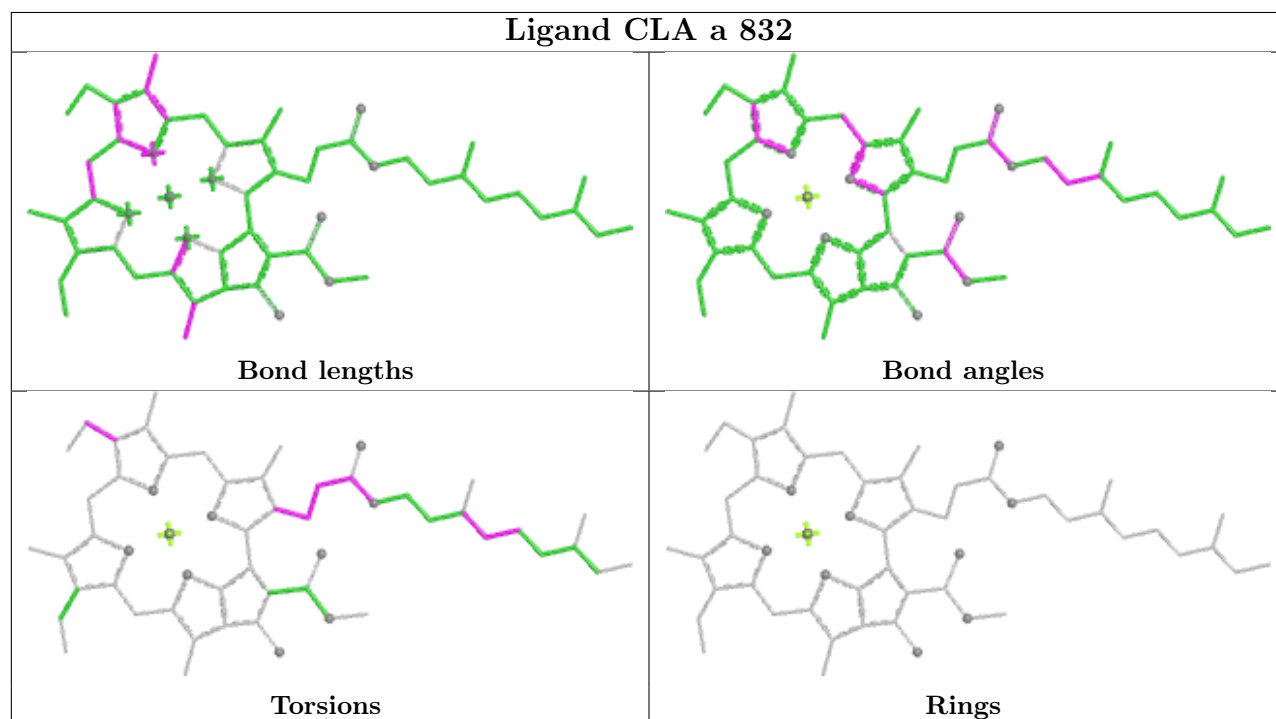
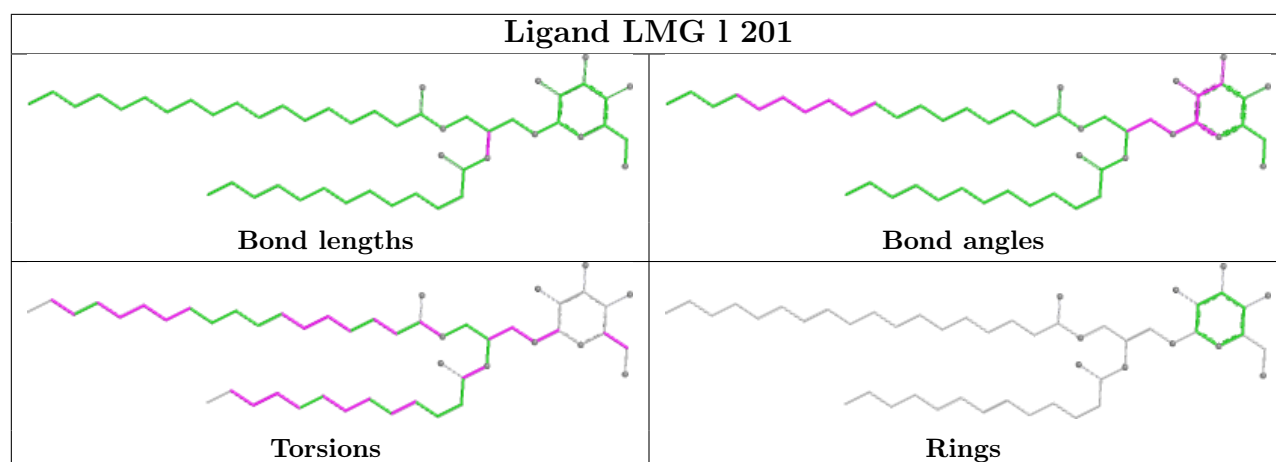
Bond angles

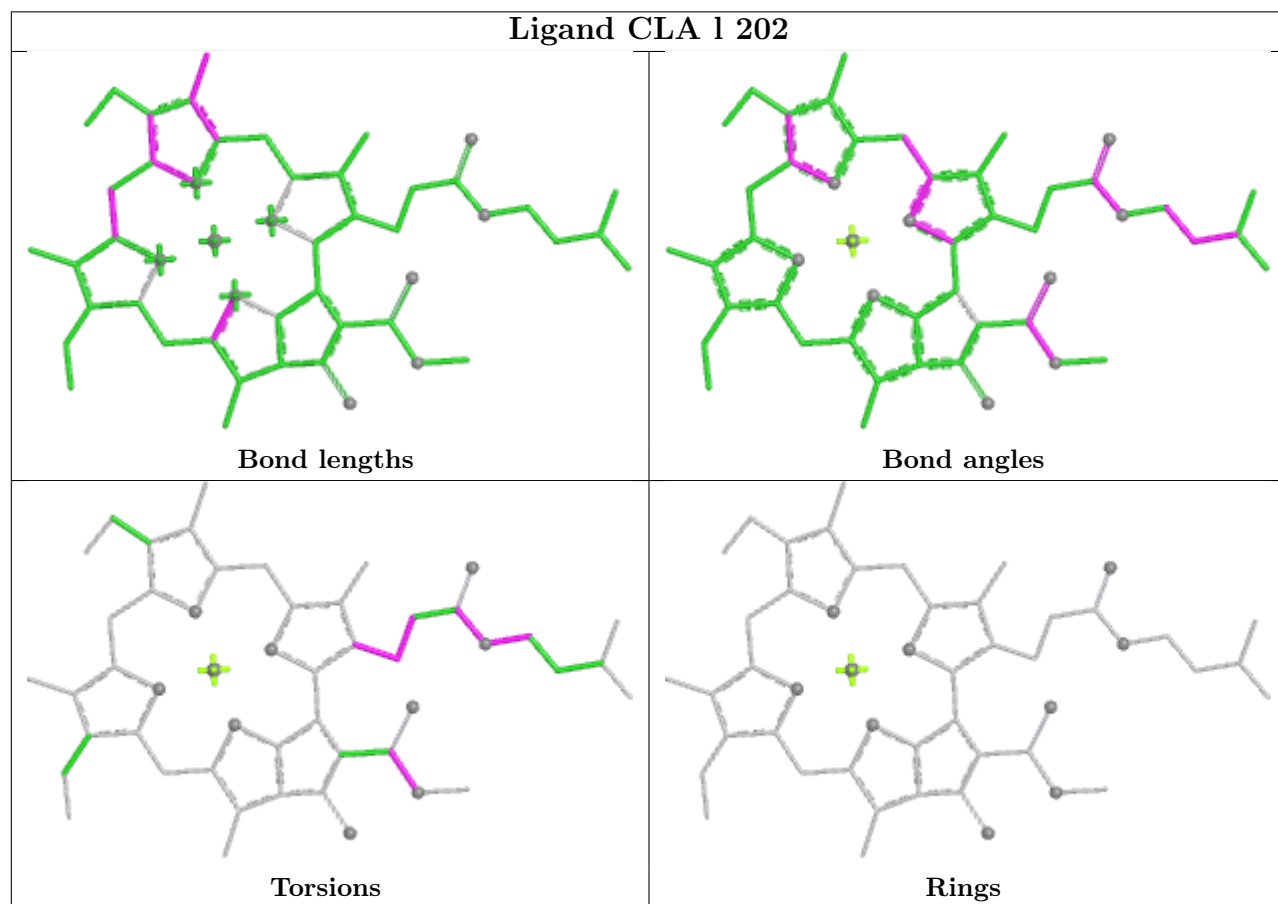
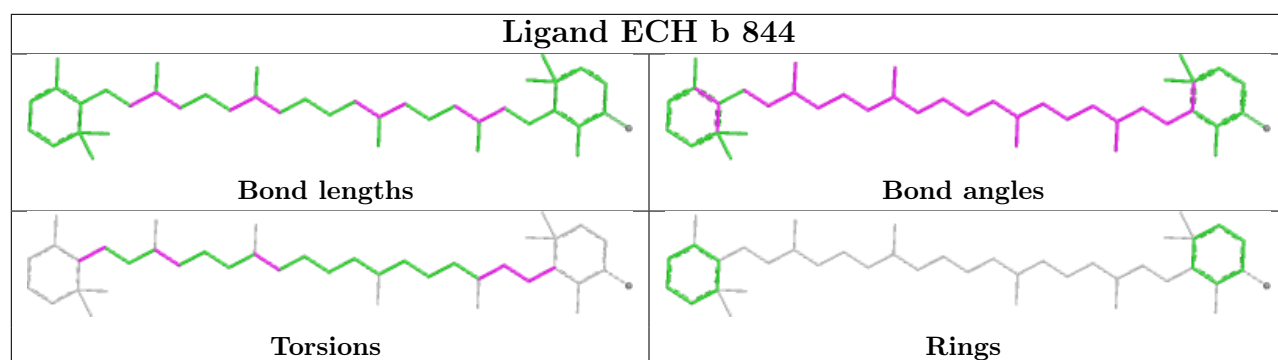


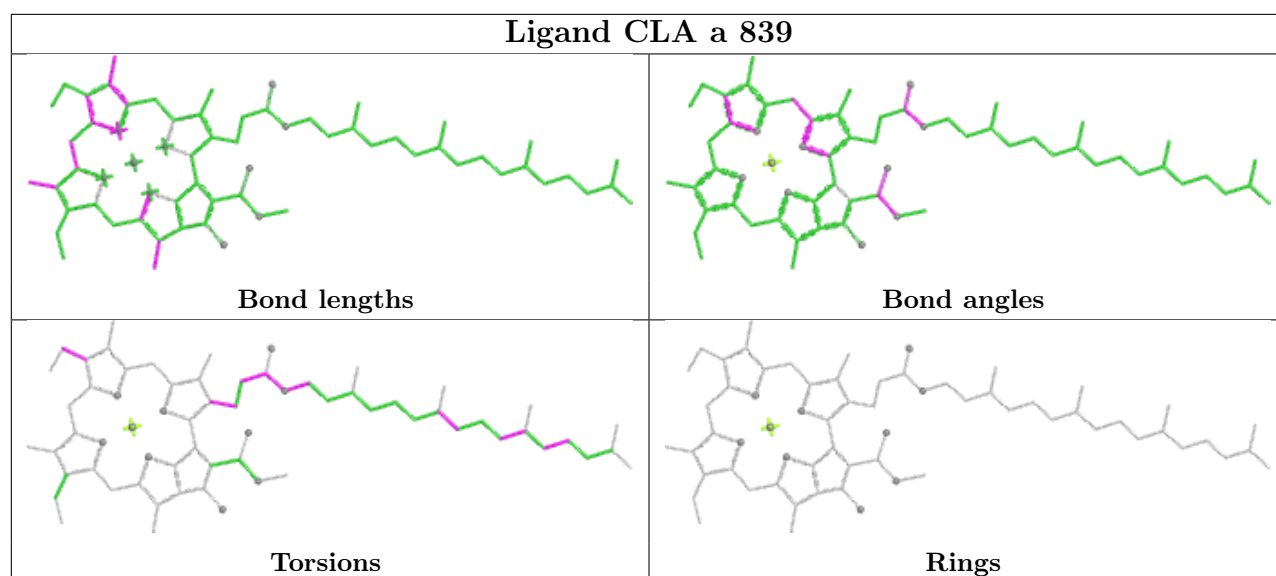
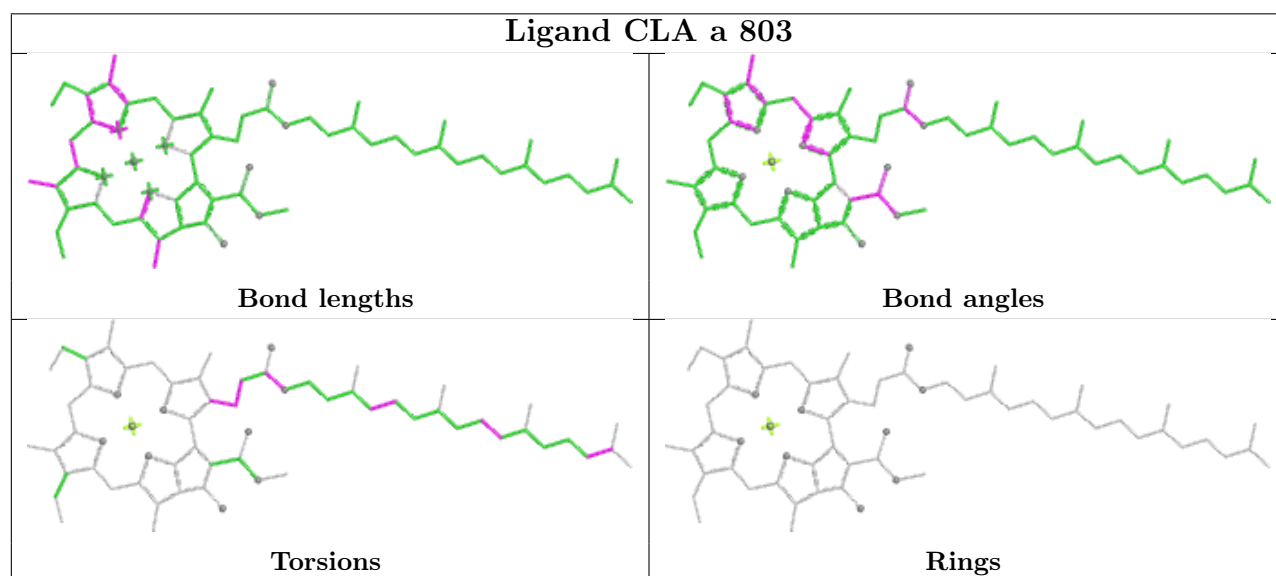
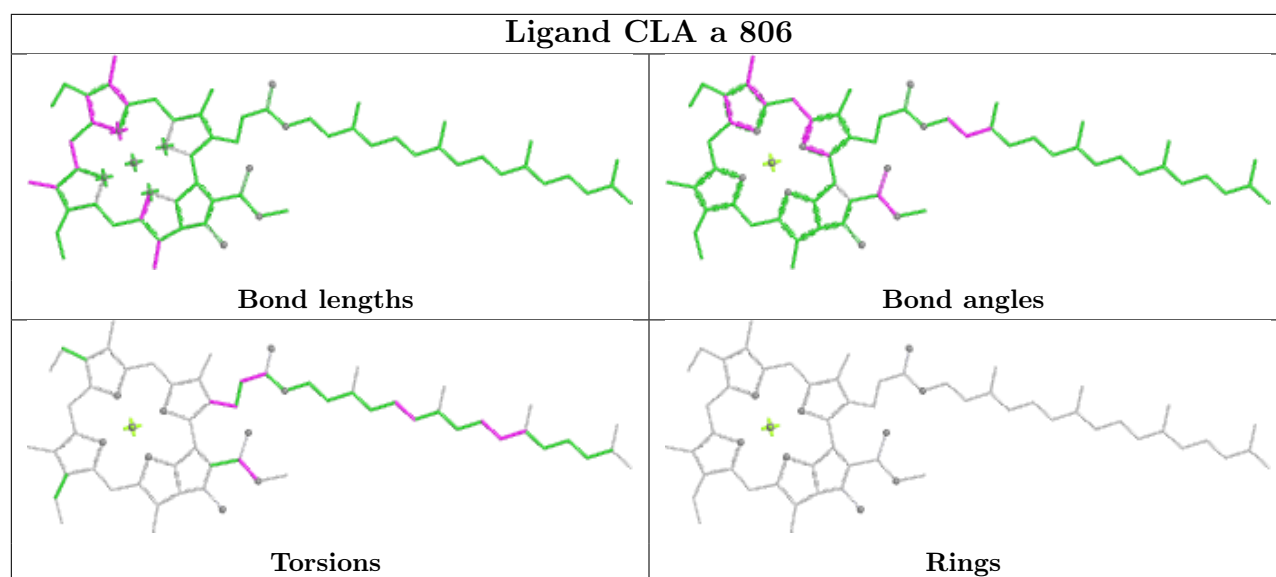
Torsions

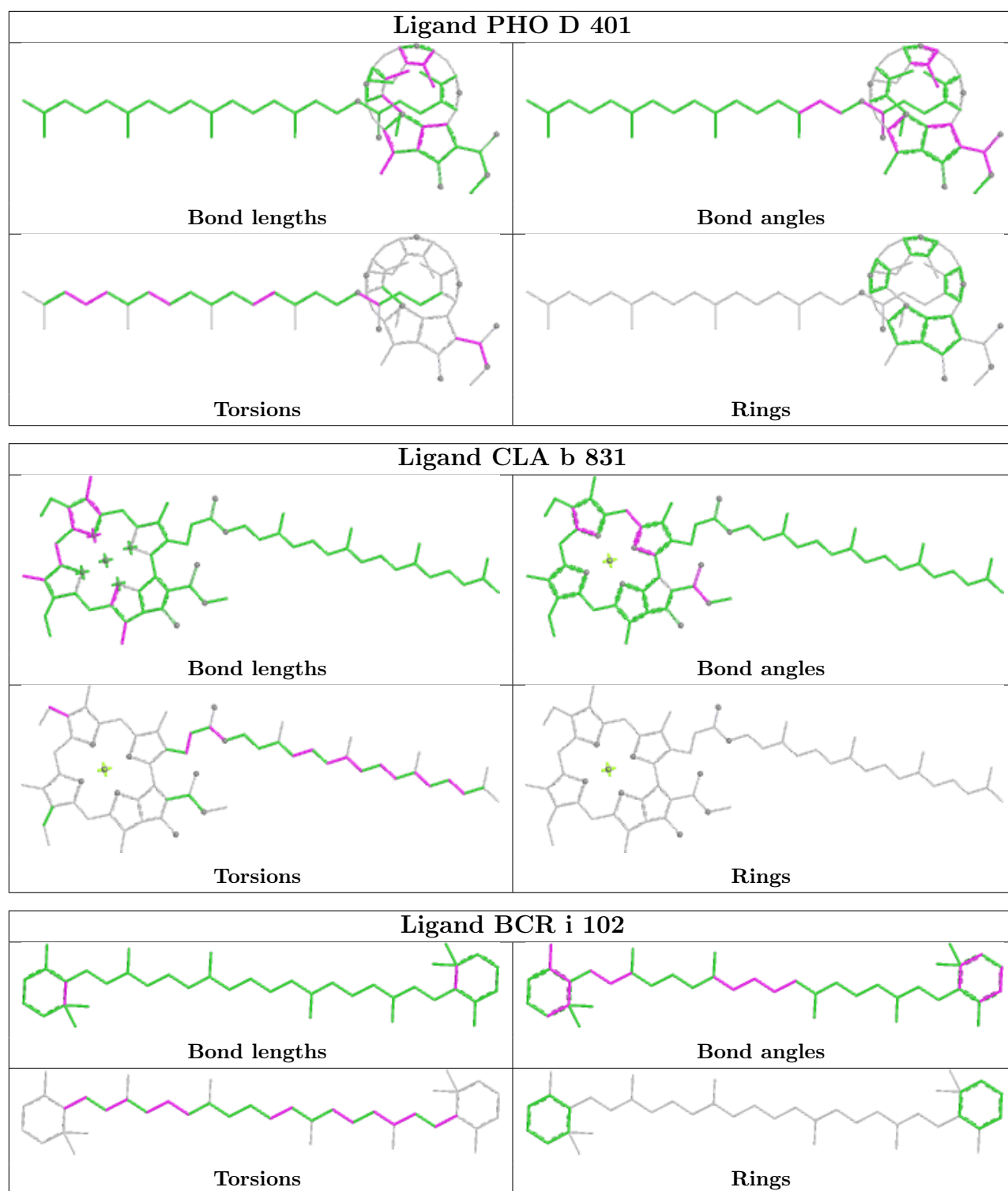


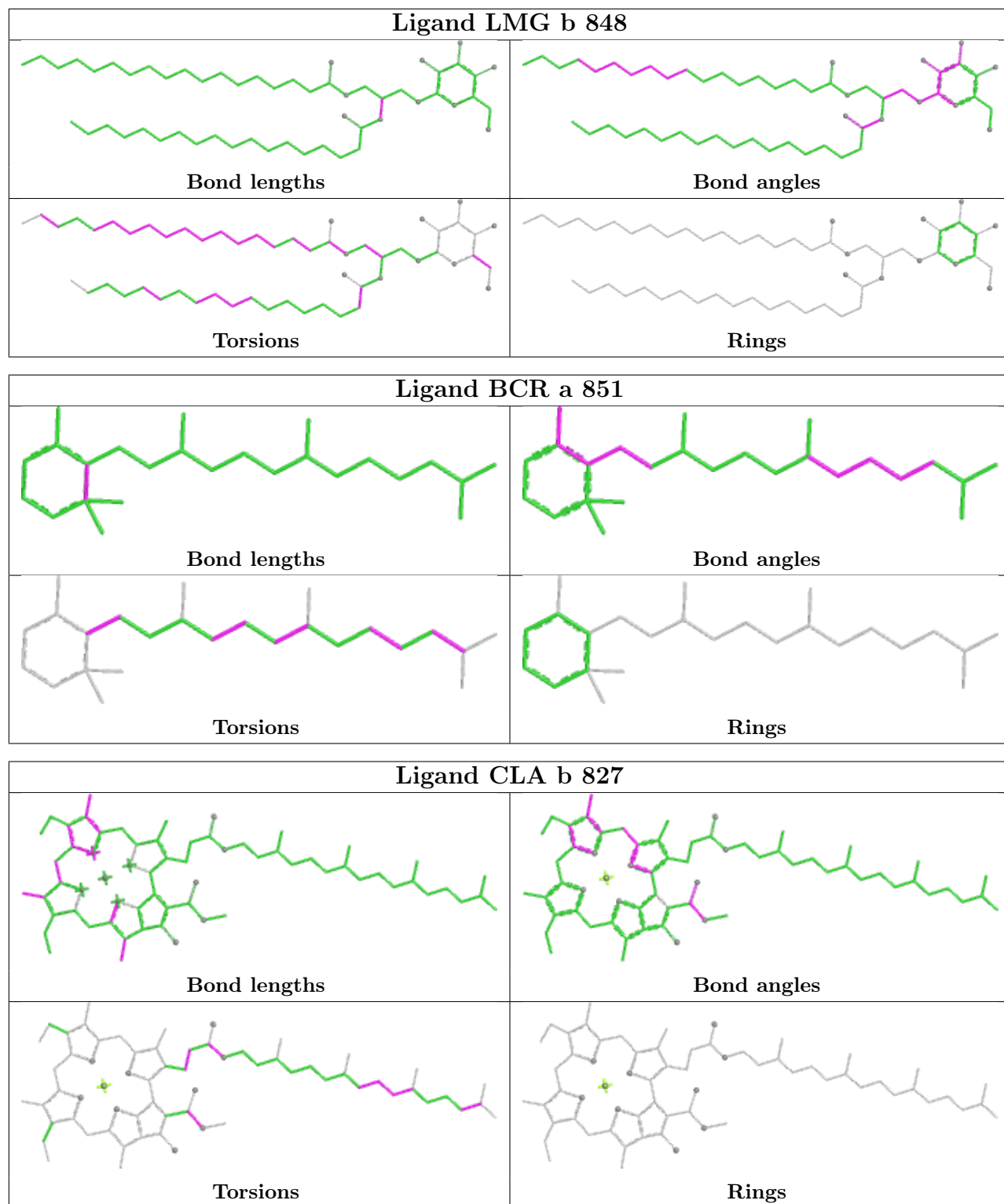
Rings

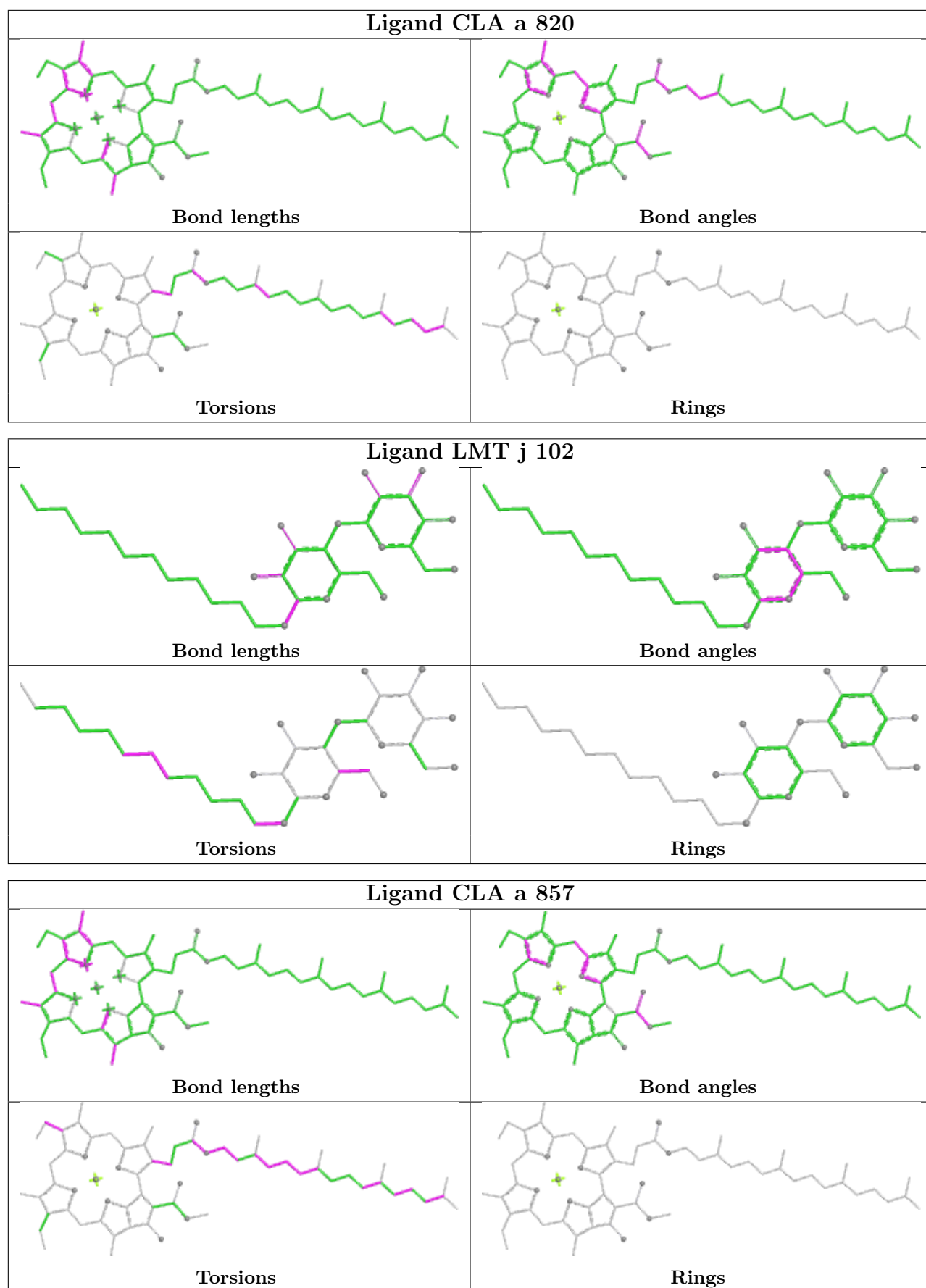


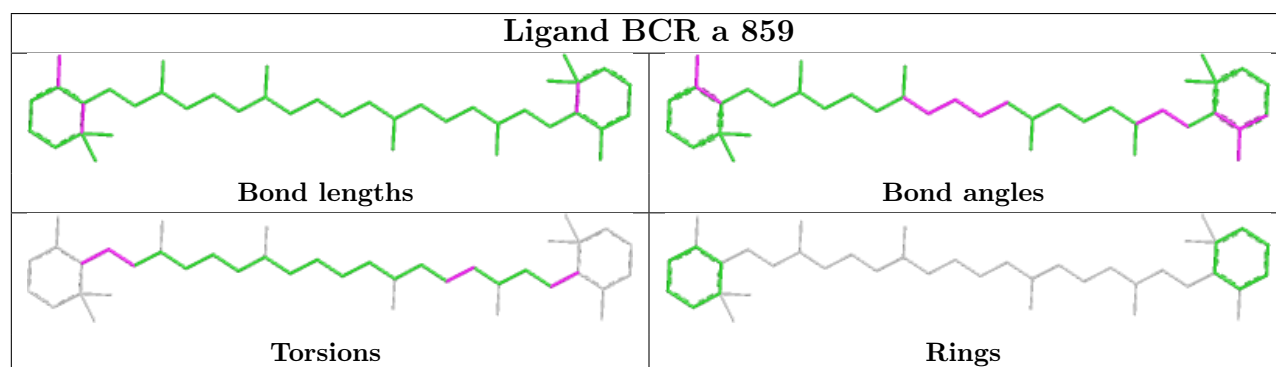
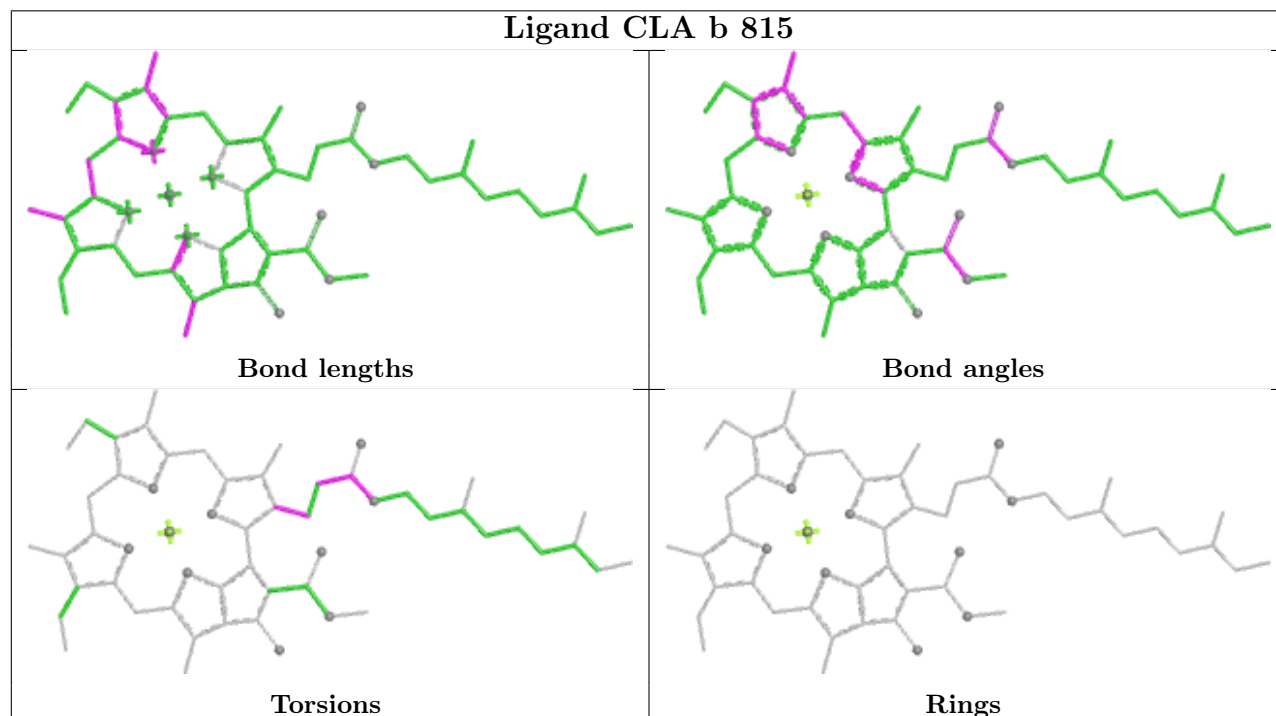
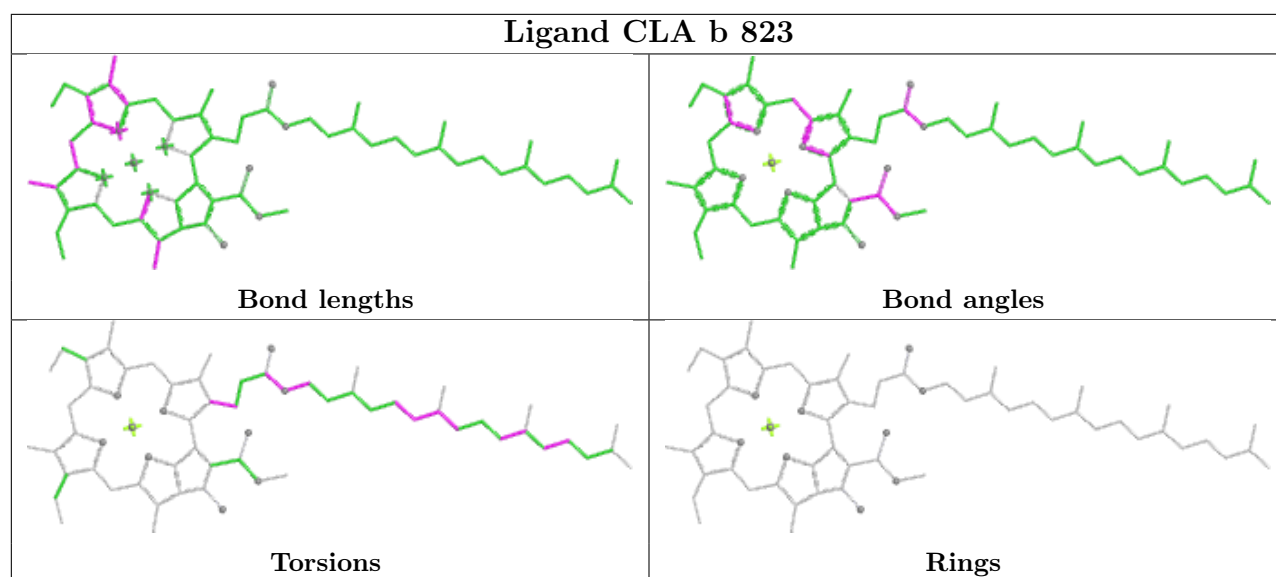


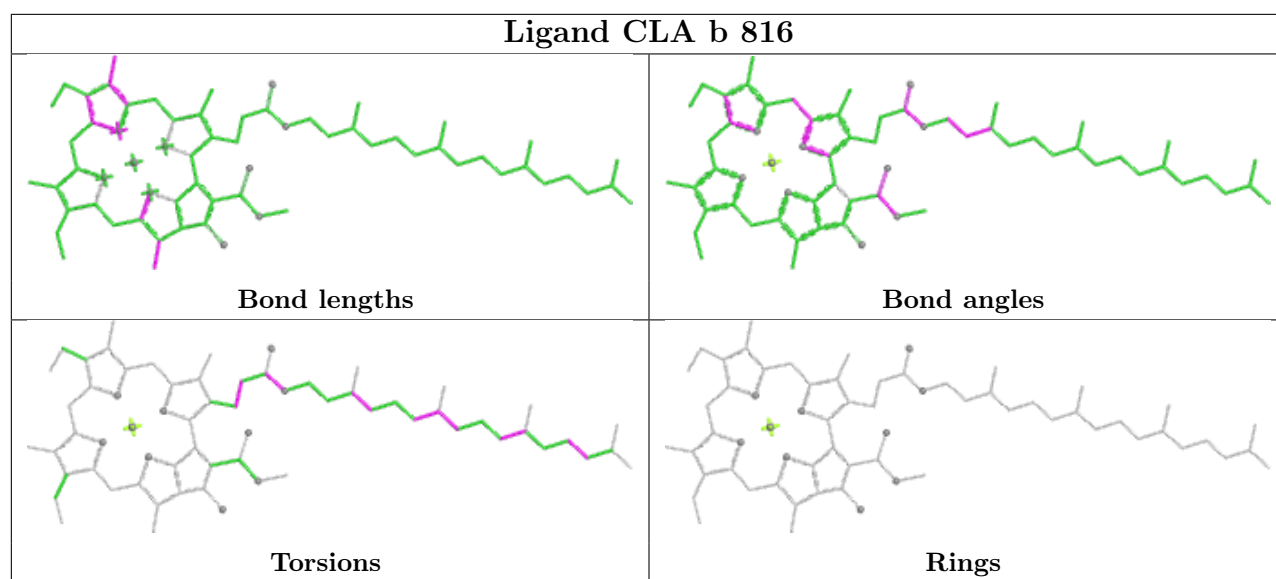












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

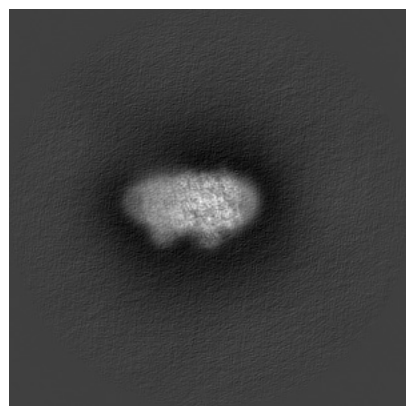
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15522. These allow visual inspection of the internal detail of the map and identification of artifacts.

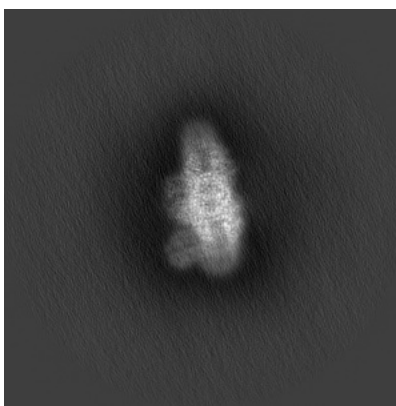
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

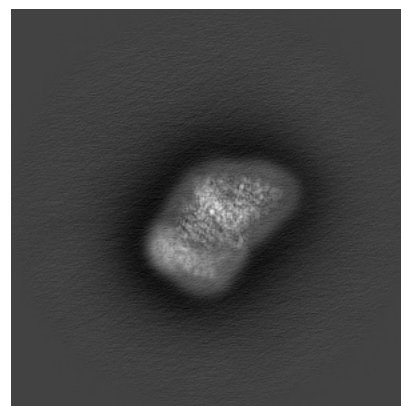
#### 6.1.1 Primary map



X

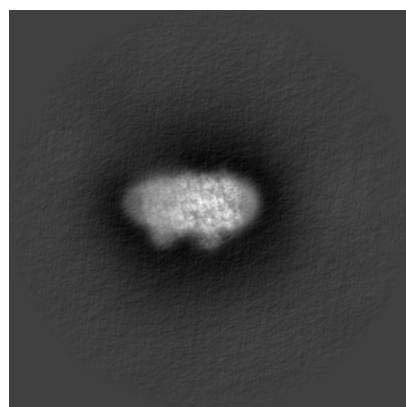


Y

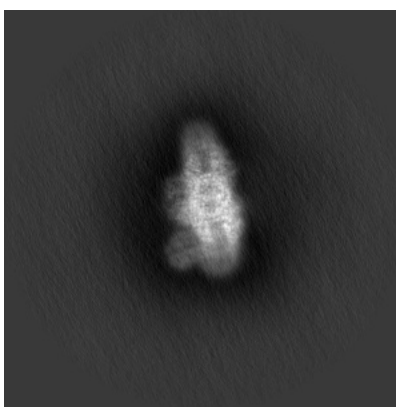


Z

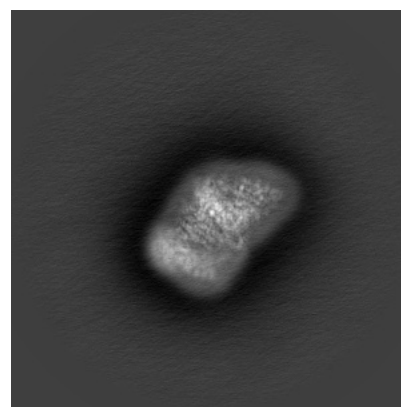
#### 6.1.2 Raw map



X



Y

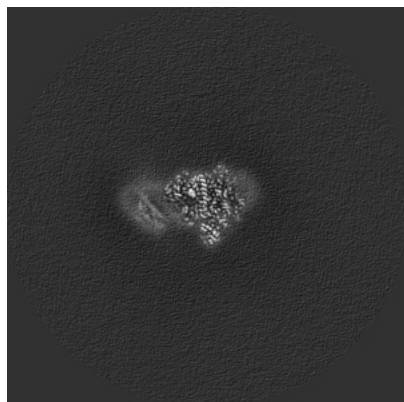


Z

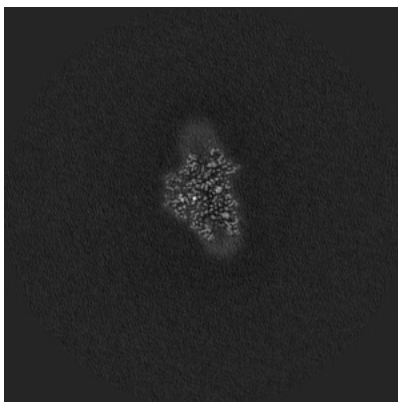
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

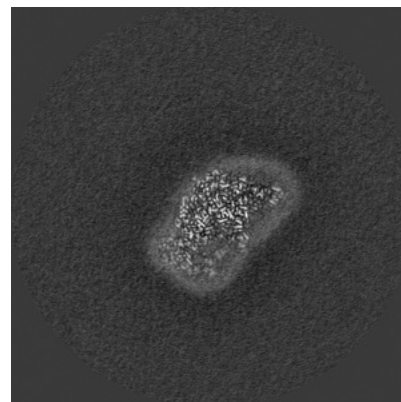
### 6.2.1 Primary map



X Index: 200

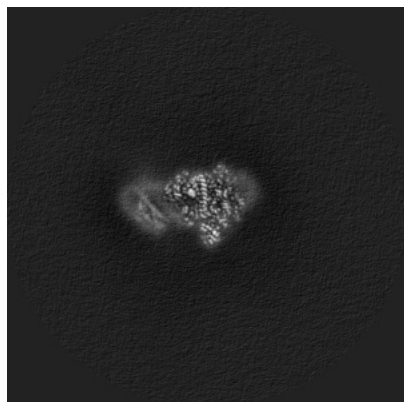


Y Index: 200

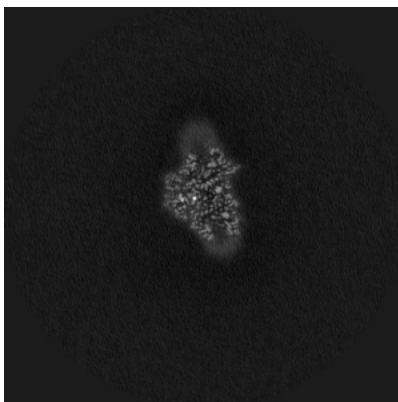


Z Index: 200

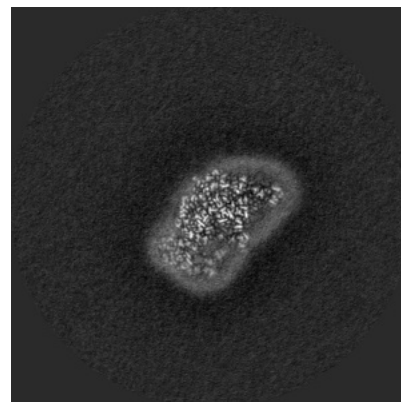
### 6.2.2 Raw map



X Index: 200



Y Index: 200

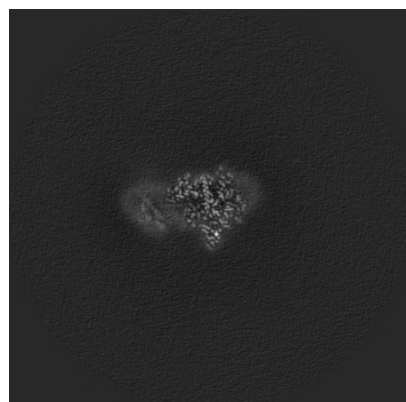


Z Index: 200

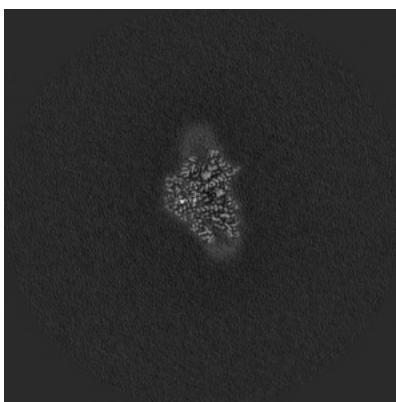
The images above show central slices of the map in three orthogonal directions.

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

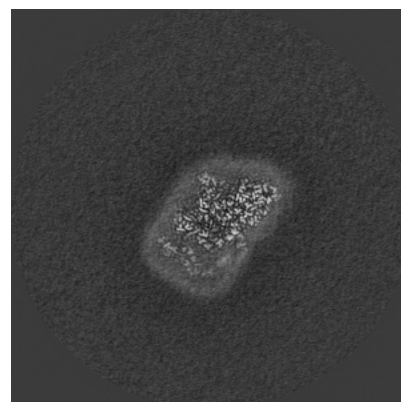
### 6.3.1 Primary map



X Index: 201

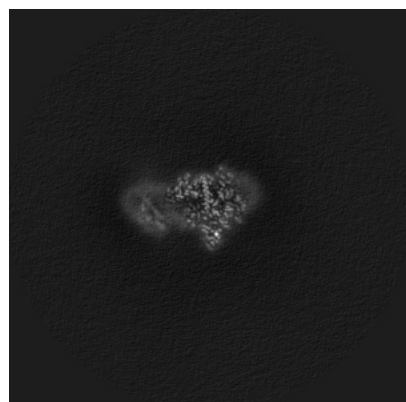


Y Index: 199

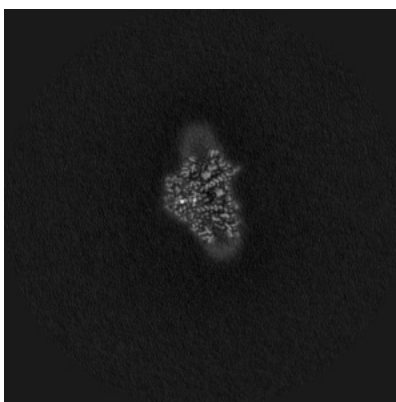


Z Index: 210

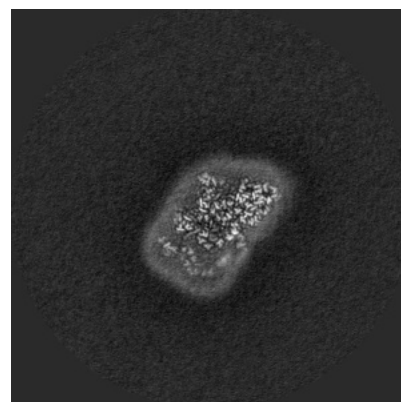
### 6.3.2 Raw map



X Index: 201



Y Index: 199

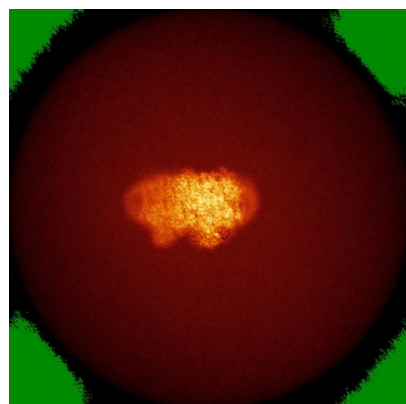


Z Index: 210

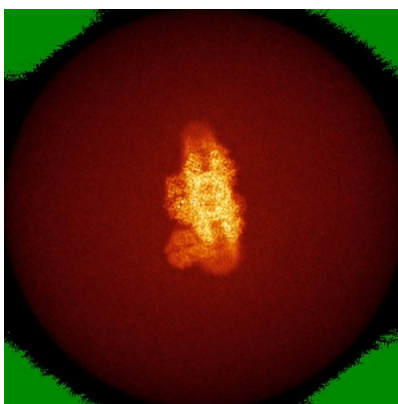
The images above show the largest variance slices of the map in three orthogonal directions.

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

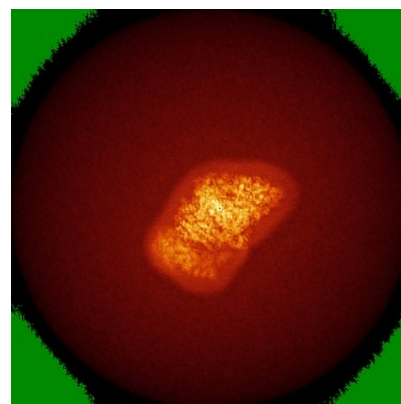
### 6.4.1 Primary map



X

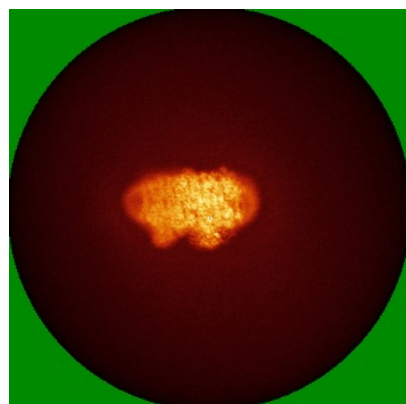


Y

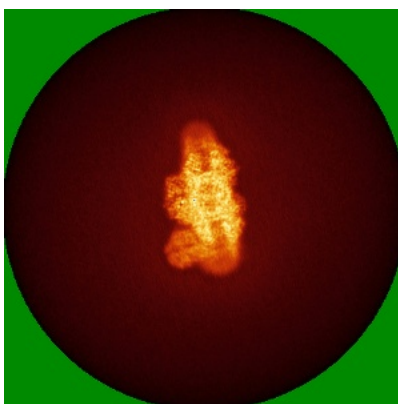


Z

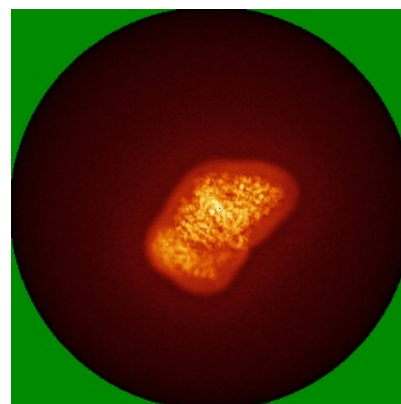
### 6.4.2 Raw map



X



Y



Z

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

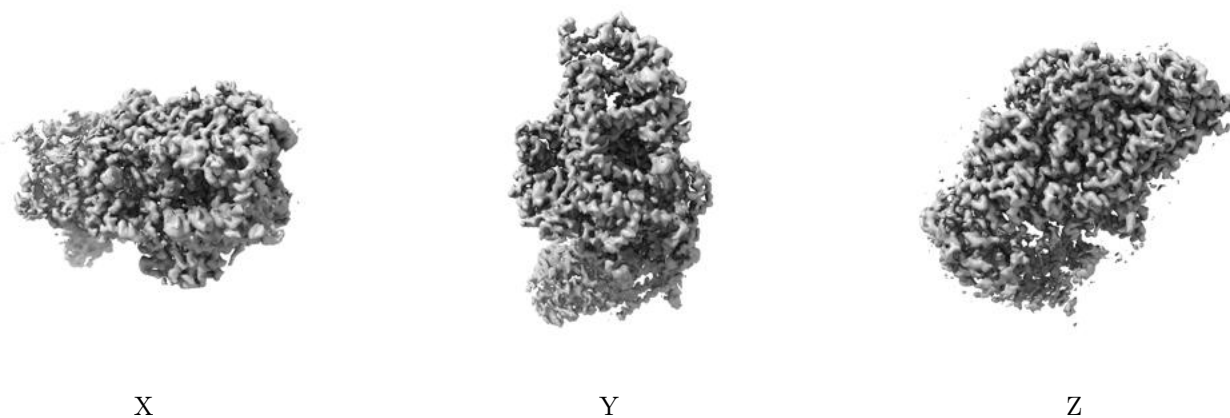
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0845. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

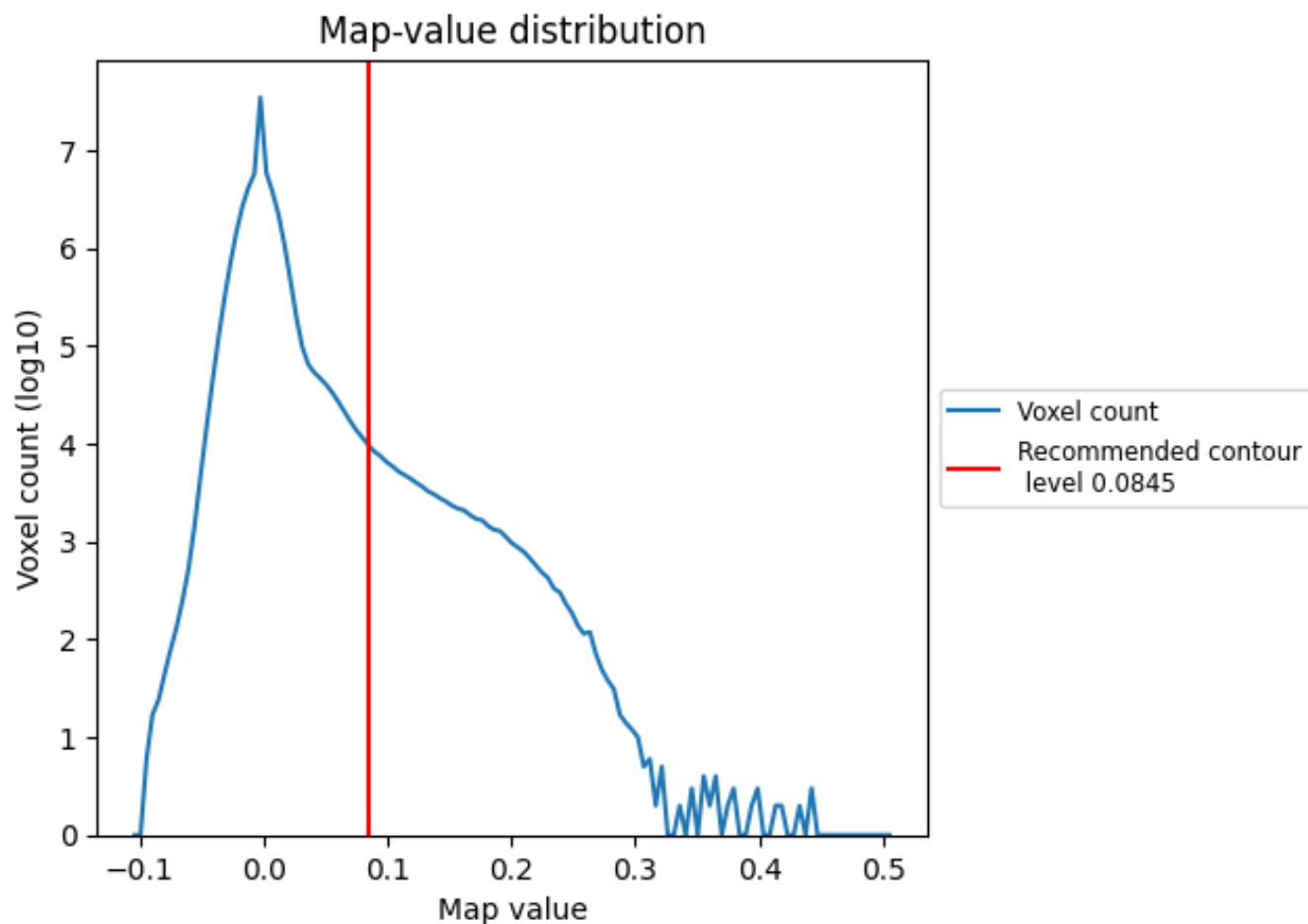
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

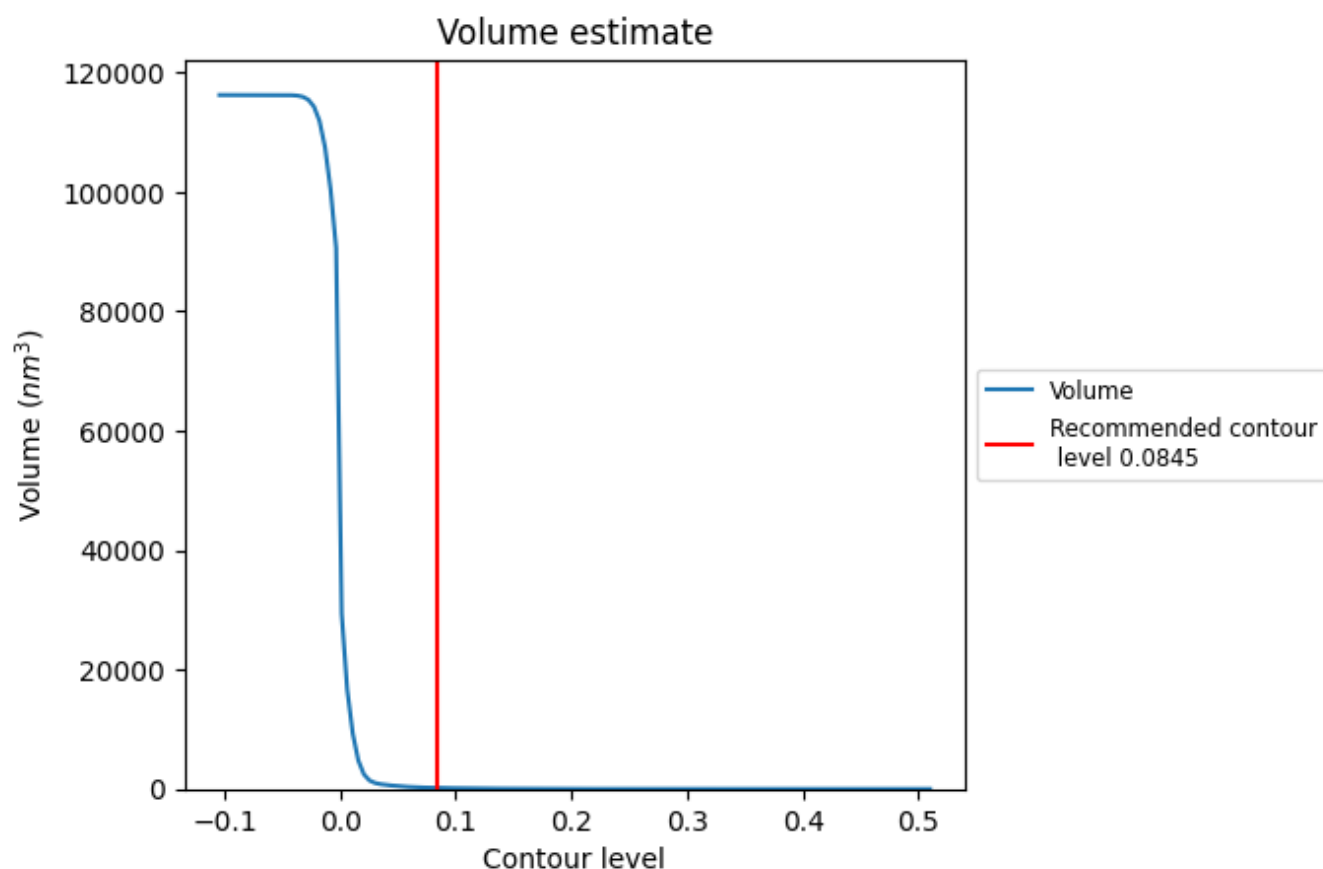
This section contains the results of statistical analysis of the map.

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



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

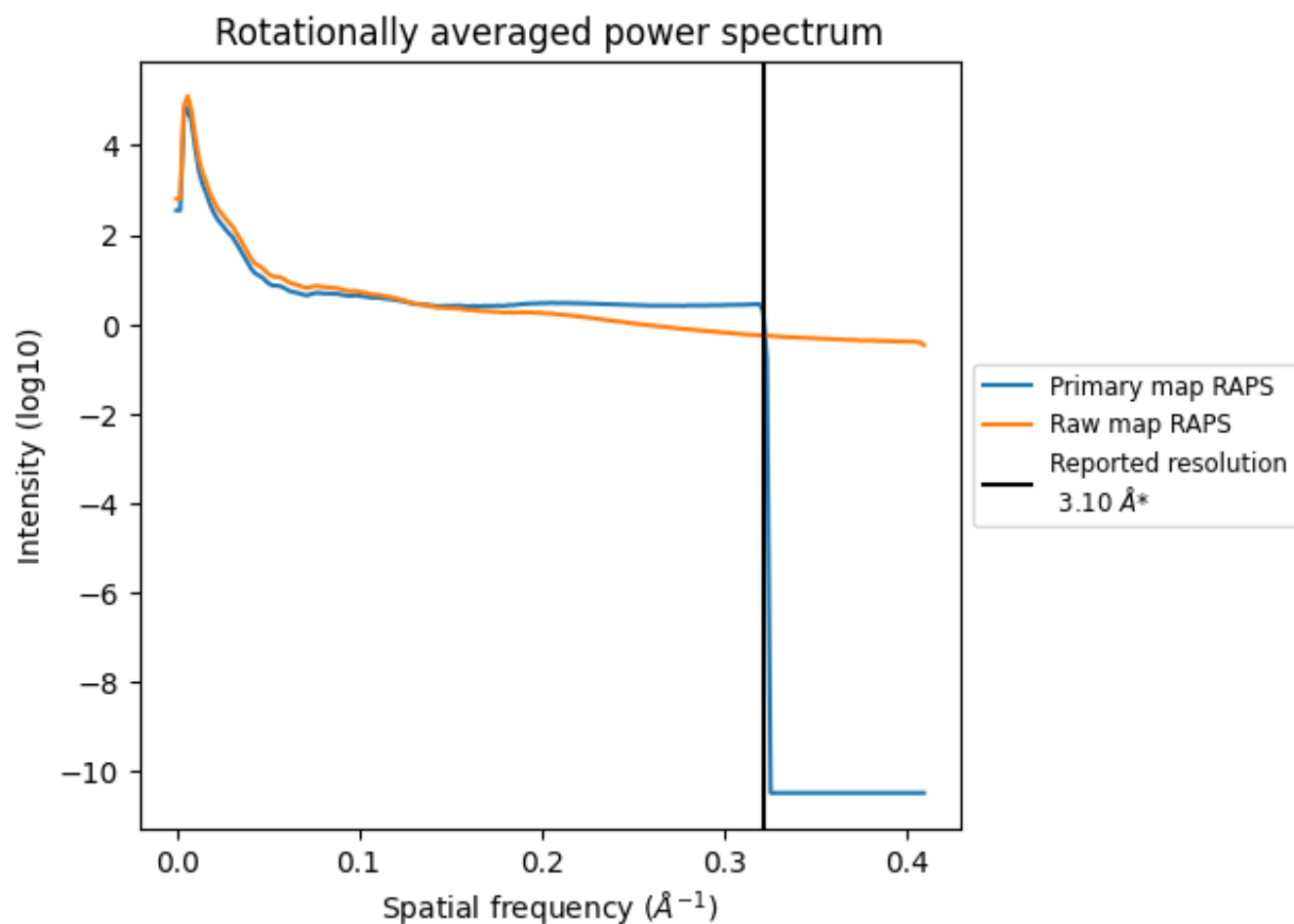
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173  $\text{nm}^3$ ; this corresponds to an approximate mass of 156 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

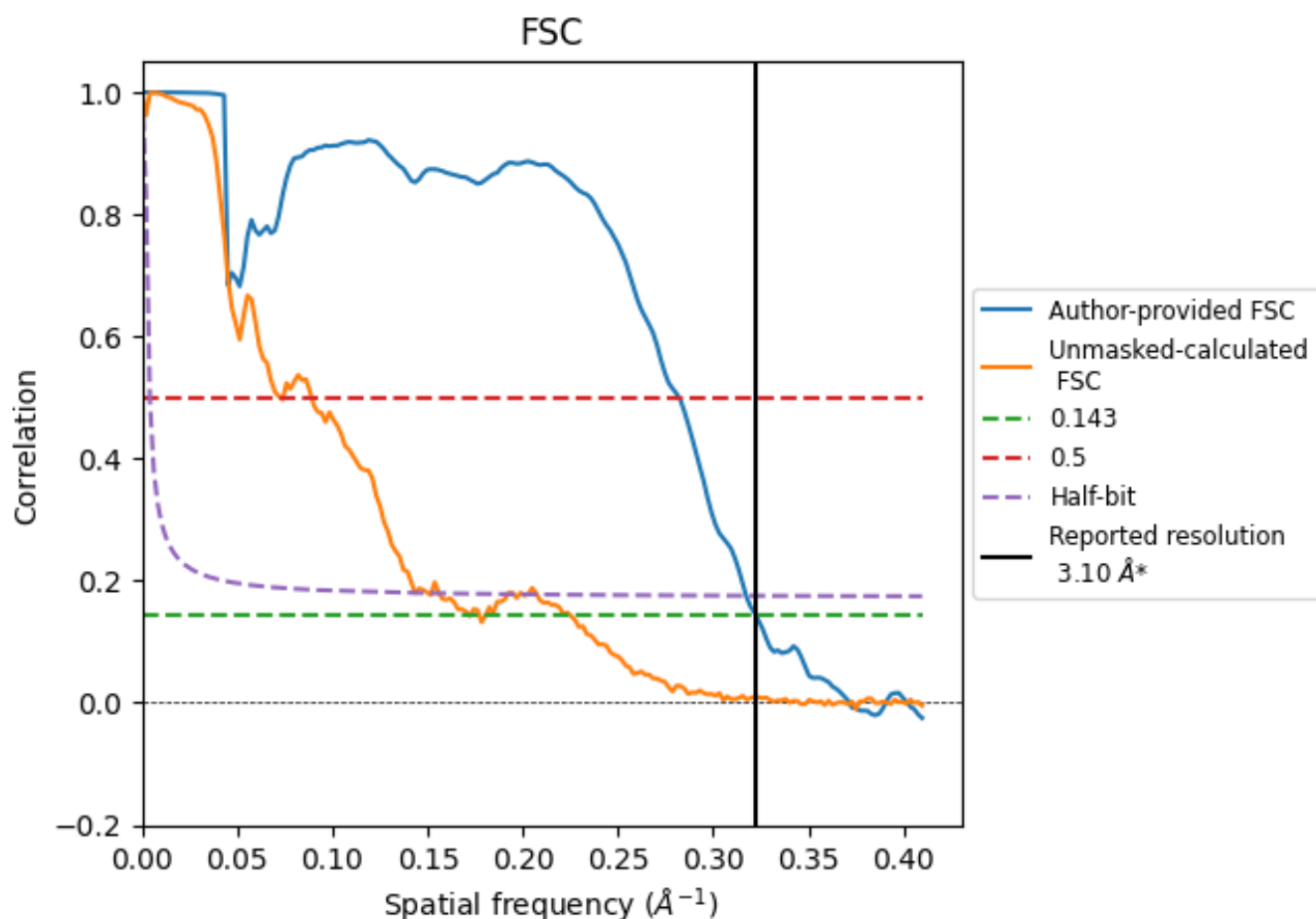


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

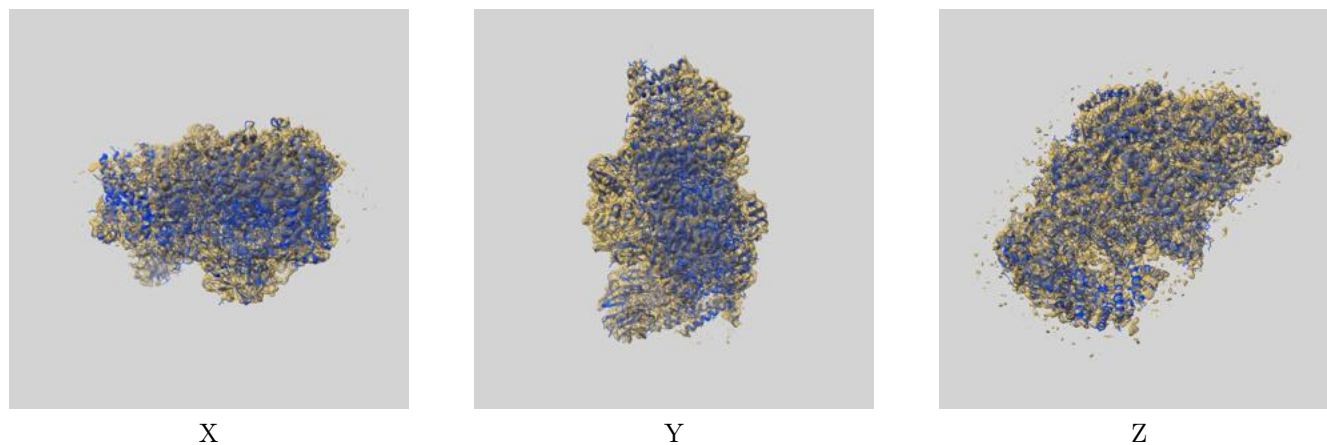
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.10                               | -     | -        |
| Author-provided FSC curve | 3.10                               | 3.55  | 3.15     |
| Unmasked-calculated*      | 5.82                               | 13.79 | 6.97     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.82 differs from the reported value 3.1 by more than 10 %

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

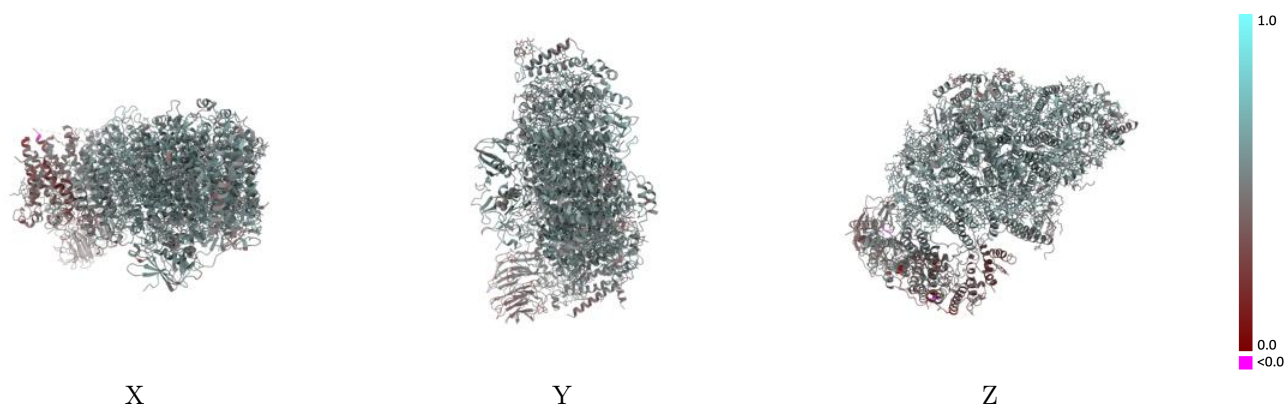
This section contains information regarding the fit between EMDB map EMD-15522 and PDB model 8AM5. Per-residue inclusion information can be found in section 3 on page 24.

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



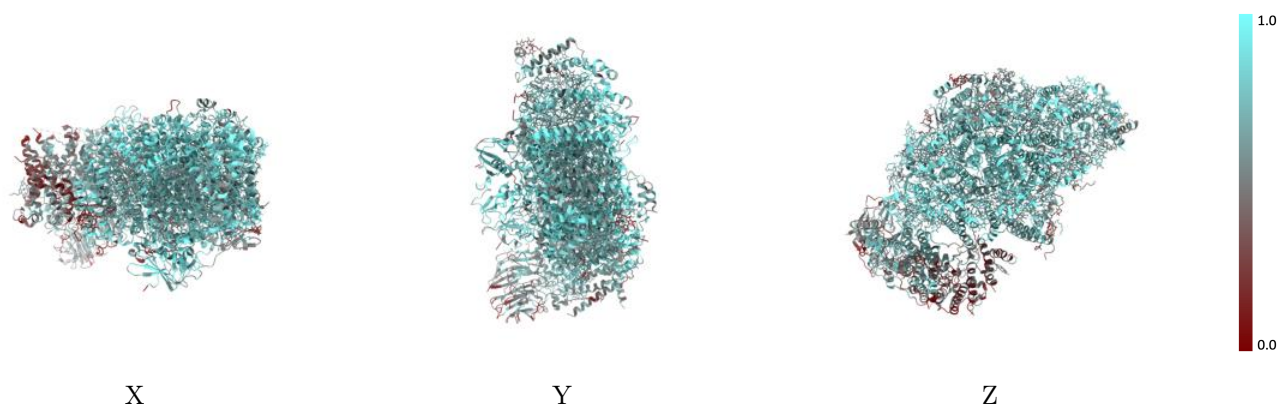
The images above show the 3D surface view of the map at the recommended contour level 0.0845 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



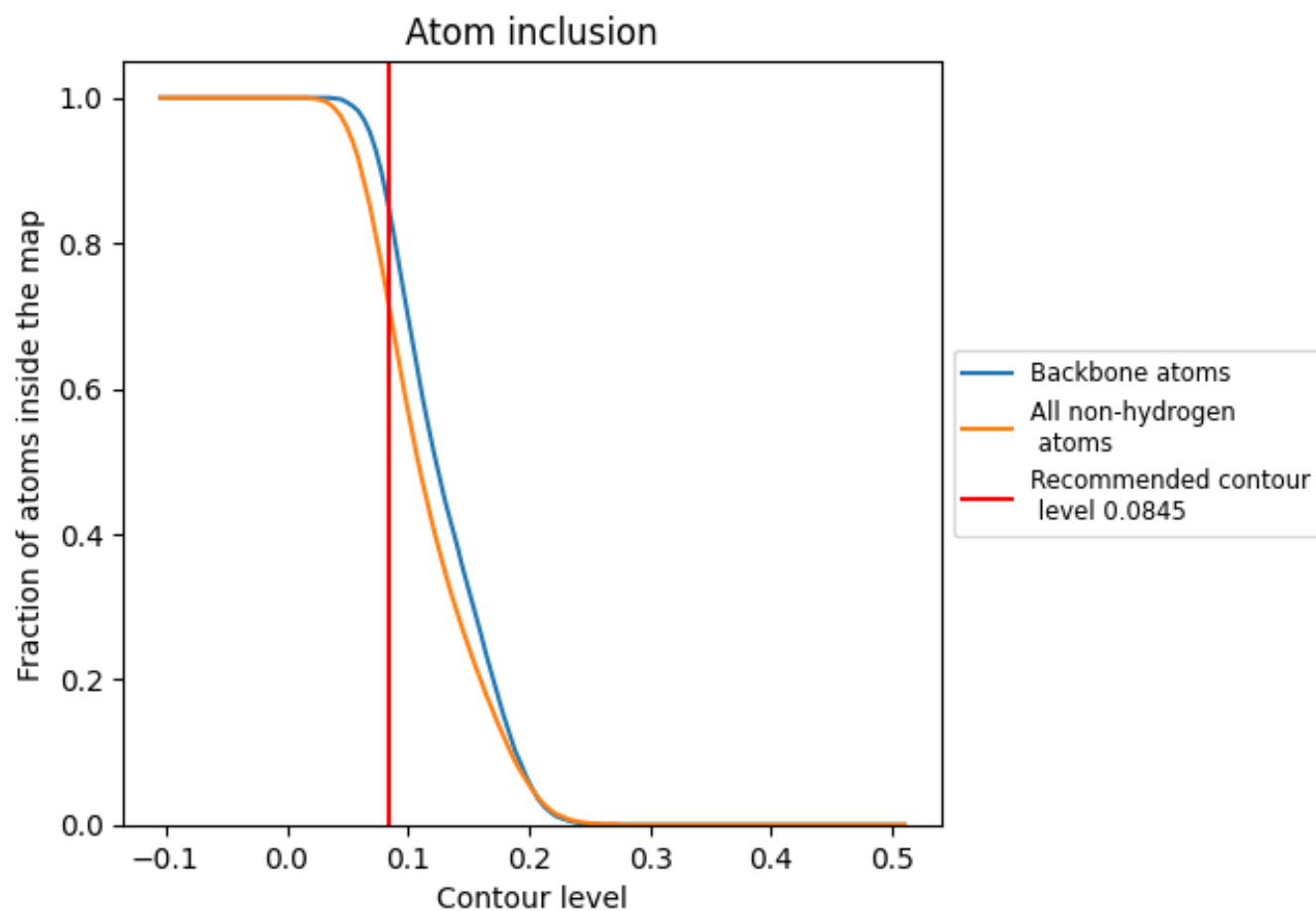
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0845).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0845) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.7120</div> | <div><div></div>0.5200</div> |
| A     | <div><div></div>0.6090</div> | <div><div></div>0.4720</div> |
| D     | <div><div></div>0.4770</div> | <div><div></div>0.4120</div> |
| E     | <div><div></div>0.4100</div> | <div><div></div>0.3530</div> |
| F     | <div><div></div>0.3460</div> | <div><div></div>0.3150</div> |
| I     | <div><div></div>0.4820</div> | <div><div></div>0.4130</div> |
| S     | <div><div></div>0.4850</div> | <div><div></div>0.4110</div> |
| a     | <div><div></div>0.7970</div> | <div><div></div>0.5600</div> |
| b     | <div><div></div>0.8220</div> | <div><div></div>0.5610</div> |
| c     | <div><div></div>0.8970</div> | <div><div></div>0.5540</div> |
| d     | <div><div></div>0.7830</div> | <div><div></div>0.5440</div> |
| e     | <div><div></div>0.7480</div> | <div><div></div>0.5360</div> |
| f     | <div><div></div>0.6720</div> | <div><div></div>0.5250</div> |
| i     | <div><div></div>0.7080</div> | <div><div></div>0.5450</div> |
| j     | <div><div></div>0.5850</div> | <div><div></div>0.5060</div> |
| k     | <div><div></div>0.5770</div> | <div><div></div>0.4970</div> |
| l     | <div><div></div>0.6190</div> | <div><div></div>0.4990</div> |
| m     | <div><div></div>0.6920</div> | <div><div></div>0.5460</div> |

1.0

0.0

<0.0