



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 01:24 AM JST

PDB ID : 6JO5
EMDB ID : EMD-9853
Title : Structure of the green algal photosystem I supercomplex with light-harvesting complex I
Authors : Suga, M.; Miyazaki, N.; Takahashi, Y.
Deposited on : 2019-03-20
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

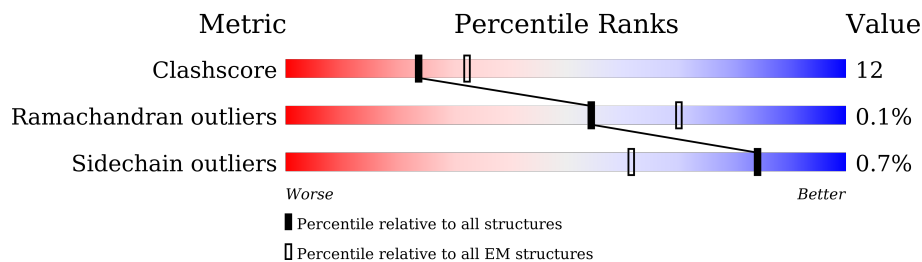
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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 (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 751 | |
| 2 | B | 755 | |
| 3 | C | 81 | |
| 4 | D | 161 | |
| 5 | E | 73 | |
| 6 | F | 165 | |
| 7 | G | 94 | |
| 8 | I | 106 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | J | 41 | |
| 10 | K | 87 | |
| 11 | L | 156 | |
| 12 | 1 | 194 | |
| 12 | Z | 194 | |
| 13 | 3 | 268 | |
| 14 | 7 | 215 | |
| 15 | 8 | 217 | |
| 16 | 4 | 236 | |
| 17 | 5 | 229 | |
| 18 | 6 | 232 | |
| 19 | 2 | 221 | |
| 20 | 9 | 189 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 21 | CL0 | A | 801 | X | - | - | - |
| 22 | CLA | 1 | 602 | X | - | - | - |
| 22 | CLA | 1 | 603 | X | - | - | - |
| 22 | CLA | 1 | 604 | X | - | - | - |
| 22 | CLA | 1 | 606 | X | - | - | - |
| 22 | CLA | 1 | 608 | X | - | - | - |
| 22 | CLA | 1 | 609 | X | - | - | - |
| 22 | CLA | 1 | 610 | X | - | - | - |
| 22 | CLA | 1 | 611 | X | - | - | - |
| 22 | CLA | 1 | 612 | X | - | - | - |
| 22 | CLA | 1 | 613 | X | - | - | - |
| 22 | CLA | 1 | 614 | X | - | - | - |
| 22 | CLA | 1 | 616 | X | - | - | - |
| 22 | CLA | 2 | 601 | X | - | - | - |
| 22 | CLA | 2 | 603 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | 2 | 606 | X | - | - | - |
| 22 | CLA | 2 | 609 | X | - | - | - |
| 22 | CLA | 2 | 612 | X | - | - | - |
| 22 | CLA | 3 | 602 | X | - | - | - |
| 22 | CLA | 3 | 603 | X | - | - | - |
| 22 | CLA | 3 | 604 | X | - | - | - |
| 22 | CLA | 3 | 606 | X | - | - | - |
| 22 | CLA | 3 | 607 | X | - | - | - |
| 22 | CLA | 3 | 609 | X | - | - | - |
| 22 | CLA | 3 | 610 | X | - | - | - |
| 22 | CLA | 3 | 611 | X | - | - | - |
| 22 | CLA | 3 | 612 | X | - | - | - |
| 22 | CLA | 3 | 617 | X | - | - | - |
| 22 | CLA | 3 | 620 | X | - | - | - |
| 22 | CLA | 4 | 601 | X | - | - | - |
| 22 | CLA | 4 | 603 | X | - | - | - |
| 22 | CLA | 4 | 609 | X | - | - | - |
| 22 | CLA | 4 | 610 | X | - | - | - |
| 22 | CLA | 4 | 611 | X | - | - | - |
| 22 | CLA | 4 | 612 | X | - | - | - |
| 22 | CLA | 4 | 614 | X | - | - | - |
| 22 | CLA | 4 | 616 | X | - | - | - |
| 22 | CLA | 5 | 601 | X | - | - | - |
| 22 | CLA | 5 | 603 | X | - | - | - |
| 22 | CLA | 5 | 606 | X | - | - | - |
| 22 | CLA | 5 | 609 | X | - | - | - |
| 22 | CLA | 5 | 610 | X | - | - | - |
| 22 | CLA | 5 | 611 | X | - | - | - |
| 22 | CLA | 5 | 612 | X | - | - | - |
| 22 | CLA | 5 | 613 | X | - | - | - |
| 22 | CLA | 5 | 616 | X | - | - | - |
| 22 | CLA | 5 | 617 | X | - | - | - |
| 22 | CLA | 5 | 621 | X | - | - | - |
| 22 | CLA | 6 | 601 | X | - | - | - |
| 22 | CLA | 6 | 602 | X | - | - | - |
| 22 | CLA | 6 | 603 | X | - | - | - |
| 22 | CLA | 6 | 604 | X | - | - | - |
| 22 | CLA | 6 | 609 | X | - | - | - |
| 22 | CLA | 6 | 610 | X | - | - | - |
| 22 | CLA | 6 | 611 | X | - | - | - |
| 22 | CLA | 6 | 612 | X | - | - | - |
| 22 | CLA | 6 | 613 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | 6 | 614 | X | - | - | - |
| 22 | CLA | 6 | 616 | X | - | - | - |
| 22 | CLA | 6 | 617 | X | - | - | - |
| 22 | CLA | 6 | 622 | X | - | - | - |
| 22 | CLA | 7 | 601 | X | - | - | - |
| 22 | CLA | 7 | 602 | X | - | - | - |
| 22 | CLA | 7 | 603 | X | - | - | - |
| 22 | CLA | 7 | 604 | X | - | - | - |
| 22 | CLA | 7 | 606 | X | - | - | - |
| 22 | CLA | 7 | 609 | X | - | - | - |
| 22 | CLA | 7 | 610 | X | - | - | - |
| 22 | CLA | 7 | 611 | X | - | - | - |
| 22 | CLA | 7 | 612 | X | - | - | - |
| 22 | CLA | 7 | 614 | X | - | - | - |
| 22 | CLA | 7 | 616 | X | - | - | - |
| 22 | CLA | 7 | 620 | X | - | - | - |
| 22 | CLA | 8 | 601 | X | - | - | - |
| 22 | CLA | 8 | 602 | X | - | - | - |
| 22 | CLA | 8 | 603 | X | - | - | - |
| 22 | CLA | 8 | 604 | X | - | - | - |
| 22 | CLA | 8 | 606 | X | - | - | - |
| 22 | CLA | 8 | 608 | X | - | - | - |
| 22 | CLA | 8 | 609 | X | - | - | - |
| 22 | CLA | 8 | 610 | X | - | - | - |
| 22 | CLA | 8 | 611 | X | - | - | - |
| 22 | CLA | 8 | 612 | X | - | - | - |
| 22 | CLA | 8 | 614 | X | - | - | - |
| 22 | CLA | 8 | 616 | X | - | - | - |
| 22 | CLA | 9 | 601 | X | - | - | - |
| 22 | CLA | 9 | 602 | X | - | - | - |
| 22 | CLA | 9 | 603 | X | - | - | - |
| 22 | CLA | 9 | 609 | X | - | - | - |
| 22 | CLA | 9 | 611 | X | - | - | - |
| 22 | CLA | 9 | 612 | X | - | - | - |
| 22 | CLA | 9 | 613 | X | - | - | - |
| 22 | CLA | A | 802 | X | - | X | - |
| 22 | CLA | A | 803 | X | - | - | - |
| 22 | CLA | A | 804 | X | - | - | - |
| 22 | CLA | A | 805 | X | - | X | - |
| 22 | CLA | A | 806 | X | - | - | - |
| 22 | CLA | A | 807 | X | - | - | - |
| 22 | CLA | A | 808 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | A | 809 | X | - | - | - |
| 22 | CLA | A | 811 | X | - | - | - |
| 22 | CLA | A | 812 | X | - | - | - |
| 22 | CLA | A | 813 | X | - | - | - |
| 22 | CLA | A | 814 | X | - | - | - |
| 22 | CLA | A | 815 | X | - | X | - |
| 22 | CLA | A | 816 | X | - | - | - |
| 22 | CLA | A | 817 | X | - | - | - |
| 22 | CLA | A | 819 | X | - | - | - |
| 22 | CLA | A | 820 | X | - | - | - |
| 22 | CLA | A | 821 | X | - | - | - |
| 22 | CLA | A | 822 | X | - | - | - |
| 22 | CLA | A | 824 | X | - | - | - |
| 22 | CLA | A | 826 | X | - | - | - |
| 22 | CLA | A | 827 | X | - | - | - |
| 22 | CLA | A | 828 | X | - | - | - |
| 22 | CLA | A | 829 | X | - | - | - |
| 22 | CLA | A | 830 | X | - | - | - |
| 22 | CLA | A | 831 | X | - | - | - |
| 22 | CLA | A | 832 | X | - | - | - |
| 22 | CLA | A | 833 | X | - | - | - |
| 22 | CLA | A | 834 | X | - | - | - |
| 22 | CLA | A | 835 | X | - | X | - |
| 22 | CLA | A | 837 | X | - | - | - |
| 22 | CLA | A | 838 | X | - | - | - |
| 22 | CLA | A | 839 | X | - | - | - |
| 22 | CLA | A | 840 | X | - | - | - |
| 22 | CLA | A | 841 | X | - | - | - |
| 22 | CLA | A | 842 | X | - | - | - |
| 22 | CLA | A | 843 | X | - | - | - |
| 22 | CLA | A | 845 | X | - | - | - |
| 22 | CLA | A | 854 | X | - | - | - |
| 22 | CLA | B | 802 | X | - | - | - |
| 22 | CLA | B | 803 | X | - | - | - |
| 22 | CLA | B | 804 | X | - | - | - |
| 22 | CLA | B | 805 | X | - | - | - |
| 22 | CLA | B | 806 | X | - | - | - |
| 22 | CLA | B | 807 | X | - | - | - |
| 22 | CLA | B | 808 | X | - | - | - |
| 22 | CLA | B | 809 | X | - | - | - |
| 22 | CLA | B | 810 | X | - | - | - |
| 22 | CLA | B | 811 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22 | CLA | B | 812 | X | - | - | - |
| 22 | CLA | B | 813 | X | - | - | - |
| 22 | CLA | B | 814 | X | - | - | - |
| 22 | CLA | B | 815 | X | - | - | - |
| 22 | CLA | B | 816 | X | - | - | - |
| 22 | CLA | B | 817 | X | - | - | - |
| 22 | CLA | B | 818 | X | - | - | - |
| 22 | CLA | B | 819 | X | - | - | - |
| 22 | CLA | B | 820 | X | - | - | - |
| 22 | CLA | B | 823 | X | - | - | - |
| 22 | CLA | B | 824 | X | - | - | - |
| 22 | CLA | B | 825 | X | - | - | - |
| 22 | CLA | B | 826 | X | - | - | - |
| 22 | CLA | B | 827 | X | - | - | - |
| 22 | CLA | B | 828 | X | - | - | - |
| 22 | CLA | B | 829 | X | - | - | - |
| 22 | CLA | B | 831 | X | - | - | - |
| 22 | CLA | B | 832 | X | - | - | - |
| 22 | CLA | B | 833 | X | - | - | - |
| 22 | CLA | B | 834 | X | - | - | - |
| 22 | CLA | B | 835 | X | - | - | - |
| 22 | CLA | B | 836 | X | - | - | - |
| 22 | CLA | B | 837 | X | - | - | - |
| 22 | CLA | B | 838 | X | - | - | - |
| 22 | CLA | B | 839 | X | - | - | - |
| 22 | CLA | B | 841 | X | - | - | - |
| 22 | CLA | B | 852 | X | - | - | - |
| 22 | CLA | F | 301 | X | - | - | - |
| 22 | CLA | F | 303 | X | - | - | - |
| 22 | CLA | F | 304 | X | - | - | - |
| 22 | CLA | G | 203 | X | - | - | - |
| 22 | CLA | G | 204 | X | - | - | - |
| 22 | CLA | J | 3002 | X | - | - | - |
| 22 | CLA | K | 4003 | X | - | - | - |
| 22 | CLA | Z | 603 | X | - | - | - |
| 22 | CLA | Z | 604 | X | - | - | - |
| 22 | CLA | Z | 606 | X | - | - | - |
| 22 | CLA | Z | 608 | X | - | - | - |
| 22 | CLA | Z | 609 | X | - | - | - |
| 22 | CLA | Z | 610 | X | - | - | - |
| 22 | CLA | Z | 611 | X | - | - | - |
| 22 | CLA | Z | 612 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | Z | 613 | X | - | - | - |
| 22 | CLA | Z | 614 | X | - | - | - |
| 22 | CLA | Z | 616 | X | - | - | - |
| 25 | BCR | 4 | 621 | - | - | X | - |
| 29 | CHL | 1 | 601 | X | - | - | - |
| 29 | CHL | 1 | 607 | X | - | - | - |
| 29 | CHL | 3 | 608 | X | - | - | - |
| 29 | CHL | 4 | 606 | X | - | - | - |
| 29 | CHL | 4 | 607 | X | - | - | - |
| 29 | CHL | 4 | 608 | X | - | - | - |
| 29 | CHL | 4 | 618 | X | - | - | - |
| 29 | CHL | 5 | 607 | X | - | - | - |
| 29 | CHL | 5 | 608 | X | - | - | - |
| 29 | CHL | 5 | 618 | X | - | - | - |
| 29 | CHL | 6 | 606 | X | - | - | - |
| 29 | CHL | 6 | 607 | X | - | - | - |
| 29 | CHL | 6 | 608 | X | - | - | - |
| 29 | CHL | 6 | 618 | X | - | - | - |
| 29 | CHL | 7 | 607 | X | - | - | - |
| 29 | CHL | 8 | 607 | X | - | - | - |
| 29 | CHL | 9 | 606 | X | - | - | - |
| 29 | CHL | 9 | 607 | X | - | - | - |
| 29 | CHL | Z | 601 | X | - | - | - |
| 29 | CHL | Z | 607 | X | - | - | - |

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 48476 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 738 | 5800 | 3793 | 989 | 996 | 22 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 732 | 5822 | 3824 | 978 | 1002 | 18 | 0 | 0 |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| B | -16 | HIS | - | insertion | UNP P09144 |
| B | -15 | HIS | - | insertion | UNP P09144 |
| B | -14 | HIS | - | insertion | UNP P09144 |
| B | -13 | HIS | - | insertion | UNP P09144 |
| B | -12 | HIS | - | insertion | UNP P09144 |
| B | -11 | HIS | - | insertion | UNP P09144 |
| B | -10 | HIS | - | insertion | UNP P09144 |
| B | -9 | HIS | - | insertion | UNP P09144 |
| B | -8 | HIS | - | insertion | UNP P09144 |
| B | -7 | HIS | - | insertion | UNP P09144 |
| B | -6 | HIS | - | insertion | UNP P09144 |
| B | -5 | HIS | - | insertion | UNP P09144 |
| B | -4 | HIS | - | insertion | UNP P09144 |
| B | -3 | HIS | - | insertion | UNP P09144 |
| B | -2 | HIS | - | insertion | UNP P09144 |
| B | -1 | HIS | - | insertion | UNP P09144 |
| B | 0 | HIS | - | insertion | UNP P09144 |
| B | 1 | HIS | - | insertion | UNP P09144 |
| B | 2 | HIS | - | insertion | UNP P09144 |
| B | 3 | HIS | - | insertion | UNP P09144 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | C | 80 | 600 | 369 | 103 | 116 | 12 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | D | 144 | 1132 | 725 | 200 | 200 | 7 | 0 | 0 |

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 5 | E | 61 | 480 | 306 | 85 | 89 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 6 | F | 165 | 1265 | 817 | 213 | 232 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| | | | Total | C | N | O | | |
| 7 | G | 68 | 503 | 327 | 87 | 89 | 0 | 0 |

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 8 | I | 37 | 281 | 195 | 39 | 46 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 9 | J | 39 | 320 | 219 | 45 | 55 | 1 | 0 | 0 |

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10 | K | 45 | Total | C | N | O | S | 0 | 0 |
| | | | 297 | 190 | 49 | 56 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | L | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 853 | 561 | 136 | 153 | 3 | | |

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | 1 | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1444 | 941 | 240 | 260 | 3 | | |
| 12 | Z | 192 | Total | C | N | O | S | 0 | 0 |
| | | | 1436 | 937 | 238 | 258 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | 3 | 202 | Total | C | N | O | S | 0 | 0 |
| | | | 1555 | 1018 | 252 | 277 | 8 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | 7 | 212 | Total | C | N | O | S | 0 | 0 |
| | | | 1644 | 1069 | 273 | 296 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15 | 8 | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1649 | 1073 | 280 | 292 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16 | 4 | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1570 | 1029 | 254 | 282 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 17 | 5 | 223 | 1744 | 1137 | 291 | 308 | 8 | 0 | 0 |

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 18 | 6 | 229 | 1765 | 1164 | 292 | 303 | 6 | 0 | 0 |

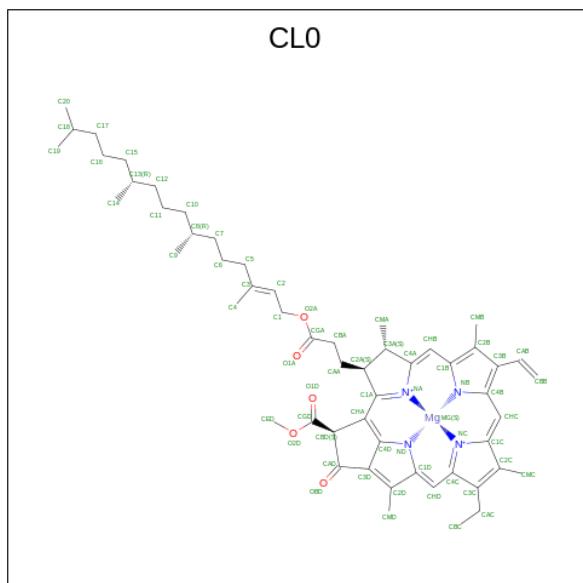
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 19 | 2 | 119 | 838 | 535 | 147 | 151 | 5 | 0 | 0 |

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

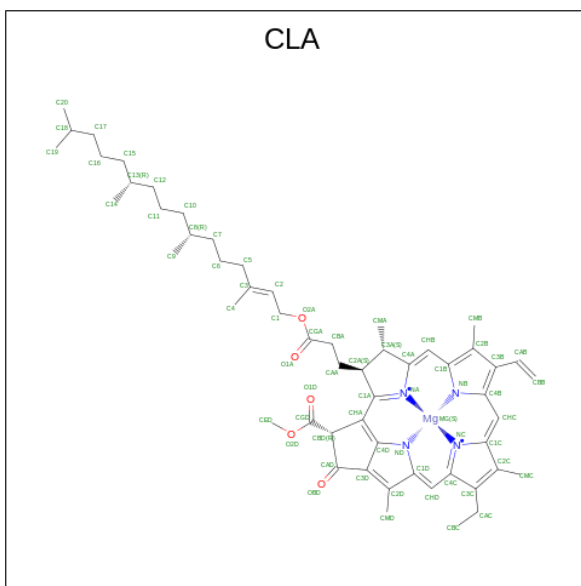
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 20 | 9 | 152 | 1180 | 766 | 195 | 213 | 6 | 0 | 0 |

- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CLO) (formula: $C_{55}H_{72}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| | | | Total | C | Mg | N | O | |
| 21 | A | 1 | 65 | 55 | 1 | 4 | 5 | 0 |

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|
| | | | Total | C | Mg | N | O | |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |
| 22 | A | 1 | Total 2689 | C 2249 | Mg 44 | N 176 | O 220 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | A | 1 | 2689 | 2249 | 44 | 176 | 220 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|------|----|-----|-----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | B | 1 | 2480 | 2070 | 41 | 164 | 205 | 0 |
| 22 | F | 1 | 175 | 145 | 3 | 12 | 15 | 0 |
| 22 | F | 1 | 175 | 145 | 3 | 12 | 15 | 0 |
| 22 | F | 1 | 175 | 145 | 3 | 12 | 15 | 0 |
| 22 | G | 1 | 96 | 76 | 2 | 8 | 10 | 0 |
| 22 | G | 1 | 96 | 76 | 2 | 8 | 10 | 0 |
| 22 | J | 1 | 42 | 34 | 1 | 4 | 3 | 0 |
| 22 | K | 1 | 91 | 71 | 2 | 8 | 10 | 0 |
| 22 | K | 1 | 91 | 71 | 2 | 8 | 10 | 0 |
| 22 | L | 1 | 115 | 95 | 2 | 8 | 10 | 0 |
| 22 | L | 1 | 115 | 95 | 2 | 8 | 10 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 1 | 1 | 722 | 602 | 12 | 48 | 60 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 3 | 1 | 696 | 570 | 13 | 52 | 61 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 7 | 1 | 741 | 607 | 14 | 56 | 64 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | 8 | 1 | 680 | 552 | 13 | 52 | 63 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | Z | 1 | 714 | 594 | 12 | 48 | 60 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| | | | Total | C | Mg | N | O | |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 4 | 1 | 576 | 468 | 11 | 44 | 53 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |
| 22 | 5 | 1 | 737 | 597 | 14 | 56 | 70 | 0 |

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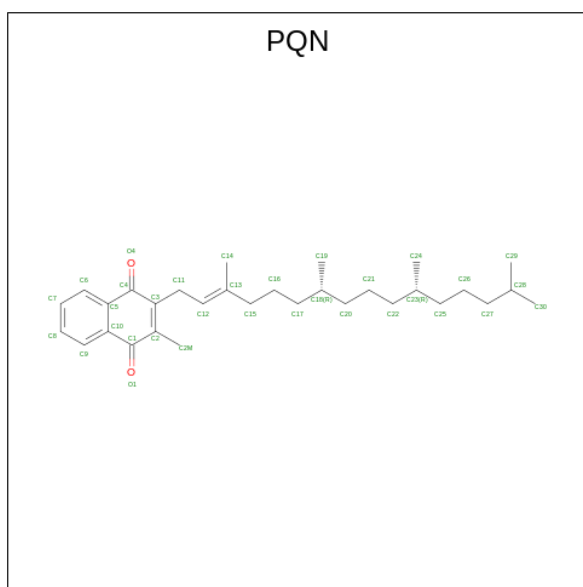
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| 22 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 737 | 597 | 14 | 56 | 70 | |
| 22 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 737 | 597 | 14 | 56 | 70 | |
| 22 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 737 | 597 | 14 | 56 | 70 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 696 | 566 | 13 | 52 | 65 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |

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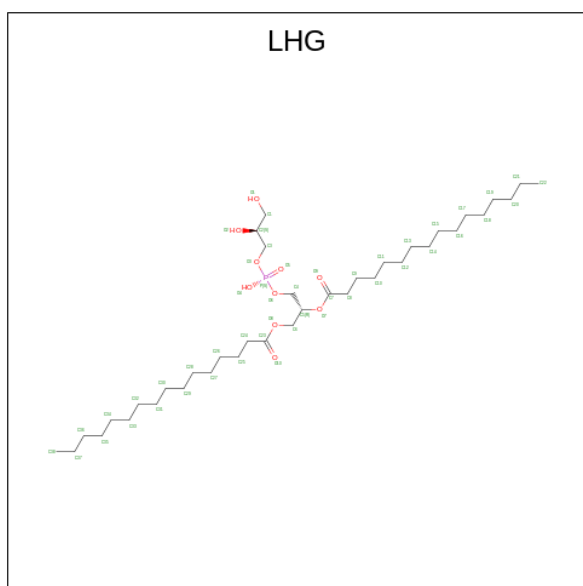
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 2 | 1 | Total | C | Mg | N | O | 0 |
| | | | 540 | 432 | 11 | 44 | 53 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |
| 22 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 514 | 414 | 10 | 40 | 50 | |

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 23 | A | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |
| 23 | B | 1 | Total | C | O | 0 |
| | | | 33 | 31 | 2 | |

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



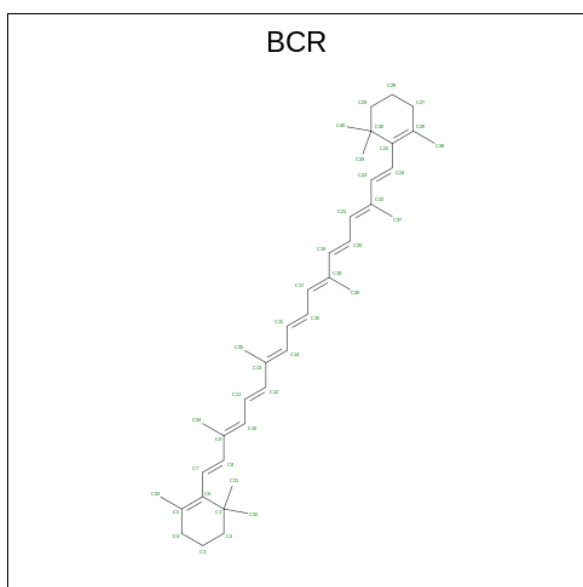
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 24 | A | 1 | Total | C | O | P | 0 |
| | | | 117 | 84 | 30 | 3 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|--------------|---------|---------|--------|---------|
| | | | Total | C | O | P | |
| 24 | A | 1 | Total 117 | C 84 | O 30 | P 3 | 0 |
| 24 | A | 1 | Total 117 | C 84 | O 30 | P 3 | 0 |
| 24 | B | 1 | Total 23 | C 12 | O 10 | P 1 | 0 |
| 24 | 1 | 1 | Total 43 | C 32 | O 10 | P 1 | 0 |
| 24 | 7 | 1 | Total 37 | C 26 | O 10 | P 1 | 0 |
| 24 | 8 | 1 | Total 37 | C 26 | O 10 | P 1 | 0 |
| 24 | Z | 1 | Total 43 | C 32 | O 10 | P 1 | 0 |
| 24 | 4 | 1 | Total 81 | C 59 | O 20 | P 2 | 0 |
| 24 | 4 | 1 | Total 81 | C 59 | O 20 | P 2 | 0 |
| 24 | 5 | 1 | Total 37 | C 26 | O 10 | P 1 | 0 |
| 24 | 6 | 1 | Total 49 | C 38 | O 10 | P 1 | 0 |

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



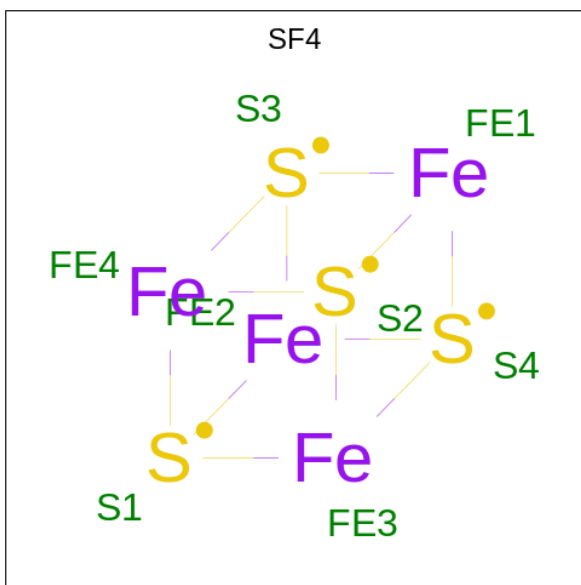
| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|--------------------|---------|
| 25 | A | 1 | Total C 240 240 | 0 |
| 25 | A | 1 | Total C 240 240 | 0 |
| 25 | A | 1 | Total C 240 240 | 0 |
| 25 | A | 1 | Total C 240 240 | 0 |
| 25 | A | 1 | Total C 240 240 | 0 |
| 25 | A | 1 | Total C 240 240 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | B | 1 | Total C 280 280 | 0 |
| 25 | F | 1 | Total C 40 40 | 0 |
| 25 | G | 1 | Total C 40 40 | 0 |
| 25 | I | 1 | Total C 40 40 | 0 |
| 25 | J | 1 | Total C 40 40 | 0 |
| 25 | K | 1 | Total C 80 80 | 0 |
| 25 | K | 1 | Total C 80 80 | 0 |
| 25 | L | 1 | Total C 80 80 | 0 |
| 25 | L | 1 | Total C 80 80 | 0 |
| 25 | 3 | 1 | Total C 120 120 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 25 | 3 | 1 | Total | C | 0 |
| | | | 120 | 120 | |
| 25 | 3 | 1 | Total | C | 0 |
| | | | 120 | 120 | |
| 25 | 7 | 1 | Total | C | 0 |
| | | | 80 | 80 | |
| 25 | 7 | 1 | Total | C | 0 |
| | | | 80 | 80 | |
| 25 | 8 | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 25 | 4 | 1 | Total | C | 0 |
| | | | 40 | 40 | |
| 25 | 5 | 1 | Total | C | 0 |
| | | | 80 | 80 | |
| 25 | 5 | 1 | Total | C | 0 |
| | | | 80 | 80 | |
| 25 | 6 | 1 | Total | C | 0 |
| | | | 80 | 80 | |
| 25 | 6 | 1 | Total | C | 0 |
| | | | 80 | 80 | |

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



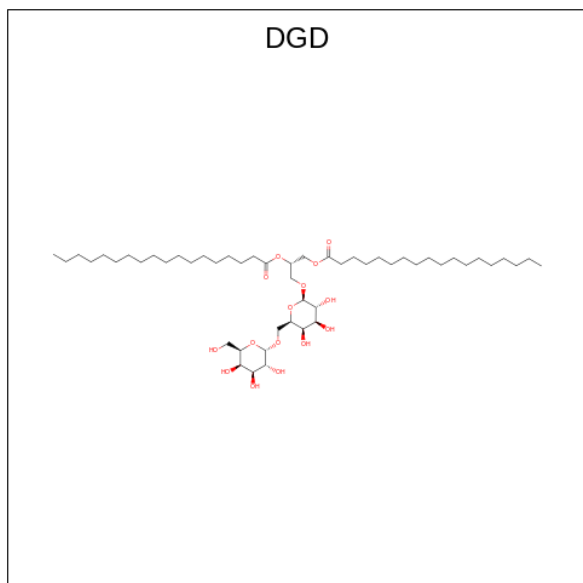
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 26 | A | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

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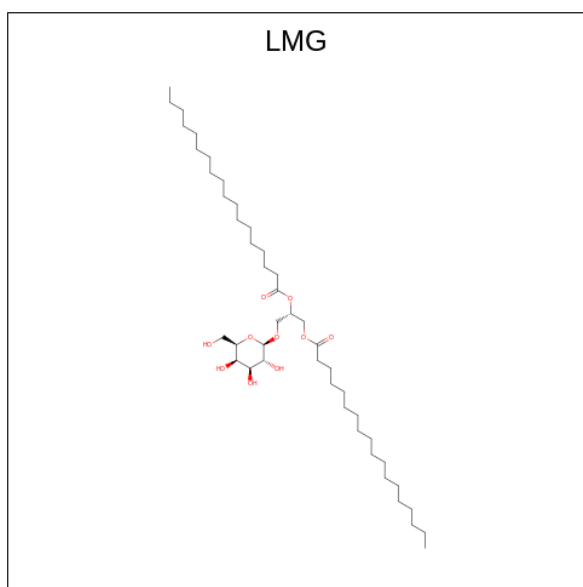
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | Fe | S | |
| 26 | C | 1 | 16 | 8 | 8 | 0 |
| 26 | C | 1 | 16 | 8 | 8 | 0 |

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



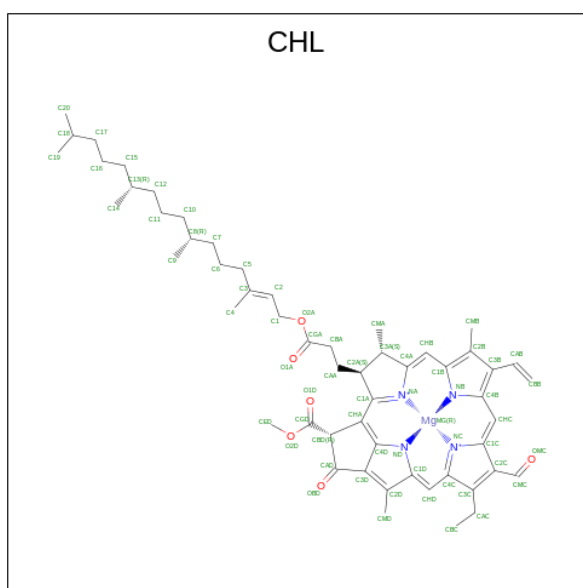
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|----|---------|
| | | | Total | C | O | |
| 27 | B | 1 | 66 | 51 | 15 | 0 |

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|--|---------|
| 28 | J | 1 | Total | C | O | | 0 |
| | | | 35 | 25 | 10 | | |
| 28 | 9 | 1 | Total | C | O | | 0 |
| | | | 44 | 34 | 10 | | |

- Molecule 29 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



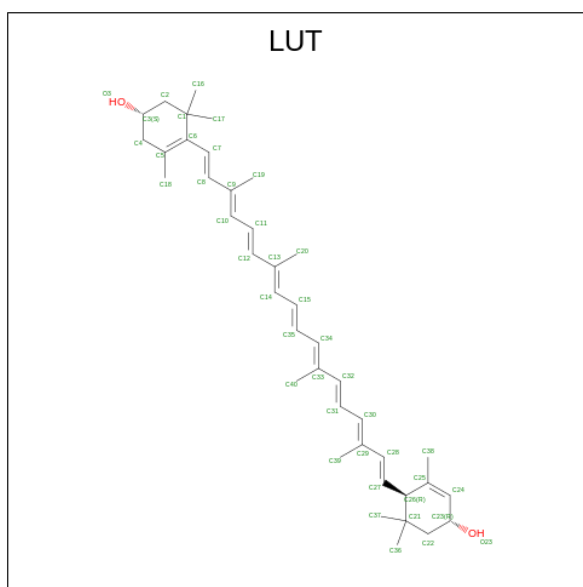
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|
| 29 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 101 | 79 | 2 | 8 | 12 | |
| 29 | 1 | 1 | Total | C | Mg | N | O | 0 |
| | | | 101 | 79 | 2 | 8 | 12 | |

Continued on next page...

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|-----|----|----|----|---------|
| 29 | 3 | 1 | Total | C | Mg | N | O | 0 |
| | | | 66 | 55 | 1 | 4 | 6 | |
| 29 | 7 | 1 | Total | C | Mg | N | O | 0 |
| | | | 54 | 43 | 1 | 4 | 6 | |
| 29 | 8 | 1 | Total | C | Mg | N | O | 0 |
| | | | 56 | 45 | 1 | 4 | 6 | |
| 29 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 101 | 79 | 2 | 8 | 12 | |
| 29 | Z | 1 | Total | C | Mg | N | O | 0 |
| | | | 101 | 79 | 2 | 8 | 12 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 201 | 159 | 4 | 16 | 22 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 201 | 159 | 4 | 16 | 22 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 201 | 159 | 4 | 16 | 22 | |
| 29 | 4 | 1 | Total | C | Mg | N | O | 0 |
| | | | 201 | 159 | 4 | 16 | 22 | |
| 29 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 145 | 114 | 3 | 12 | 16 | |
| 29 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 145 | 114 | 3 | 12 | 16 | |
| 29 | 5 | 1 | Total | C | Mg | N | O | 0 |
| | | | 145 | 114 | 3 | 12 | 16 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 206 | 164 | 4 | 16 | 22 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 206 | 164 | 4 | 16 | 22 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 206 | 164 | 4 | 16 | 22 | |
| 29 | 6 | 1 | Total | C | Mg | N | O | 0 |
| | | | 206 | 164 | 4 | 16 | 22 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 93 | 73 | 2 | 8 | 10 | |
| 29 | 9 | 1 | Total | C | Mg | N | O | 0 |
| | | | 93 | 73 | 2 | 8 | 10 | |

- Molecule 30 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|-----|---|---------|
| 30 | 1 | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 30 | 1 | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 30 | 1 | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 30 | 3 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 3 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 7 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 7 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 8 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 8 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | Z | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 30 | Z | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 30 | Z | 1 | Total | C | O | 0 |
| | | | 126 | 120 | 6 | |
| 30 | 4 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 4 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |

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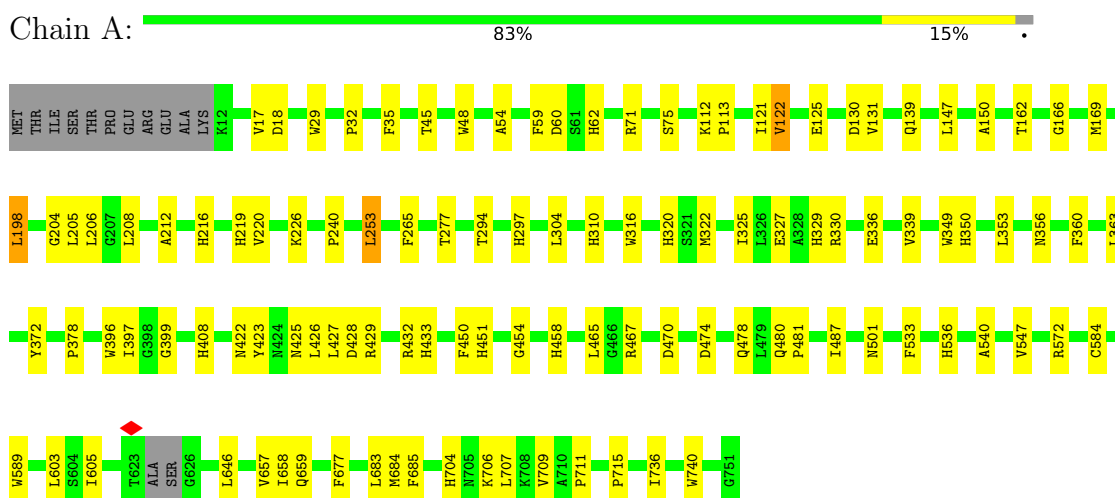
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 30 | 5 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 5 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 6 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 6 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 2 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 2 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 9 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |
| 30 | 9 | 1 | Total | C | O | 0 |
| | | | 84 | 80 | 4 | |

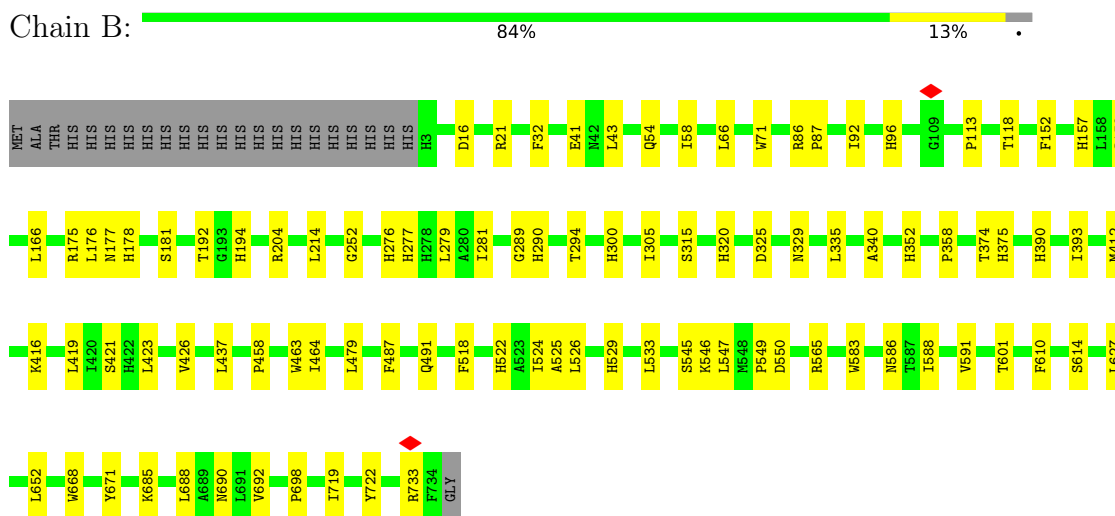
3 Residue-property plots

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

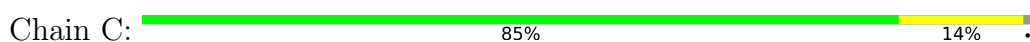
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center





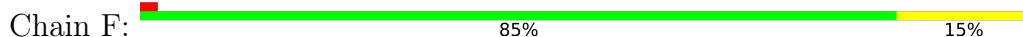
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



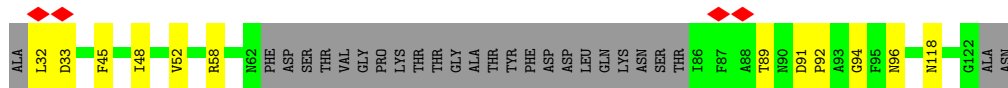
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



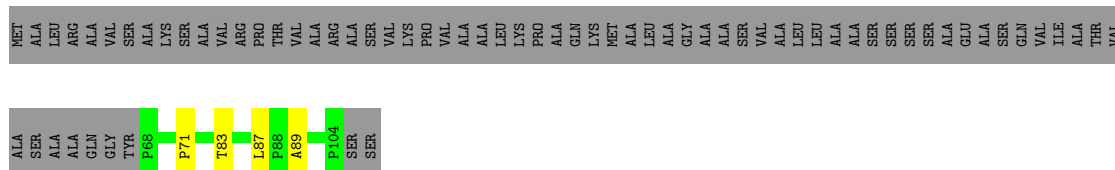
- Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic



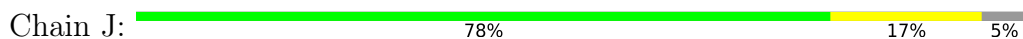
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction center subunit VIII

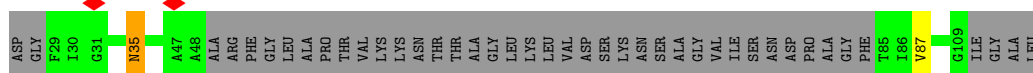


- Molecule 9: Photosystem I reaction center subunit IX





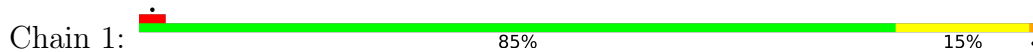
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic



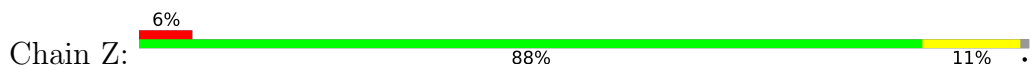
- Molecule 11: Photosystem I reaction center subunit XI



- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

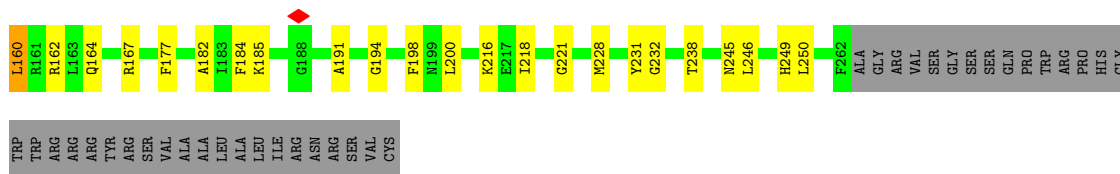


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

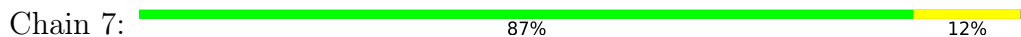


- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

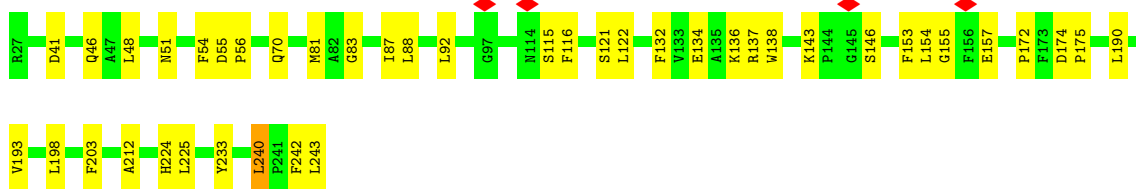
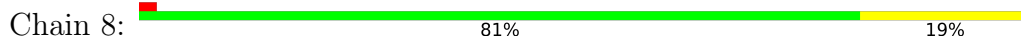




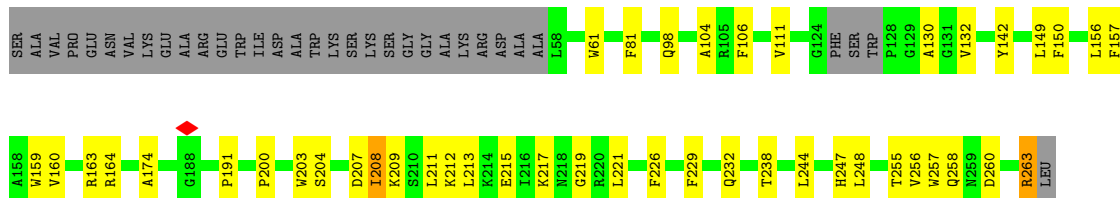
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



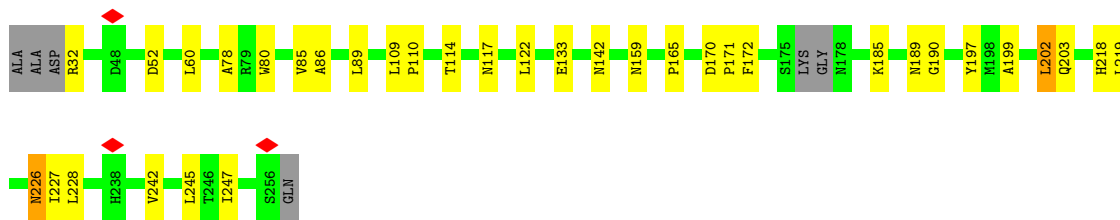
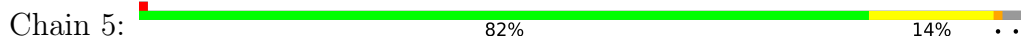
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



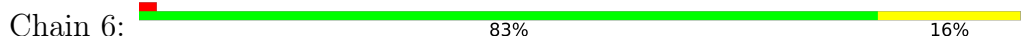
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

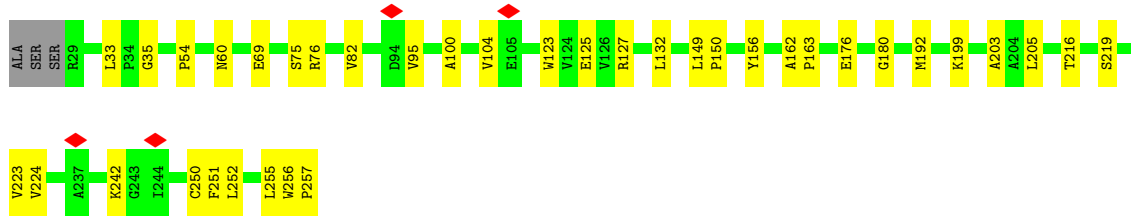


• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

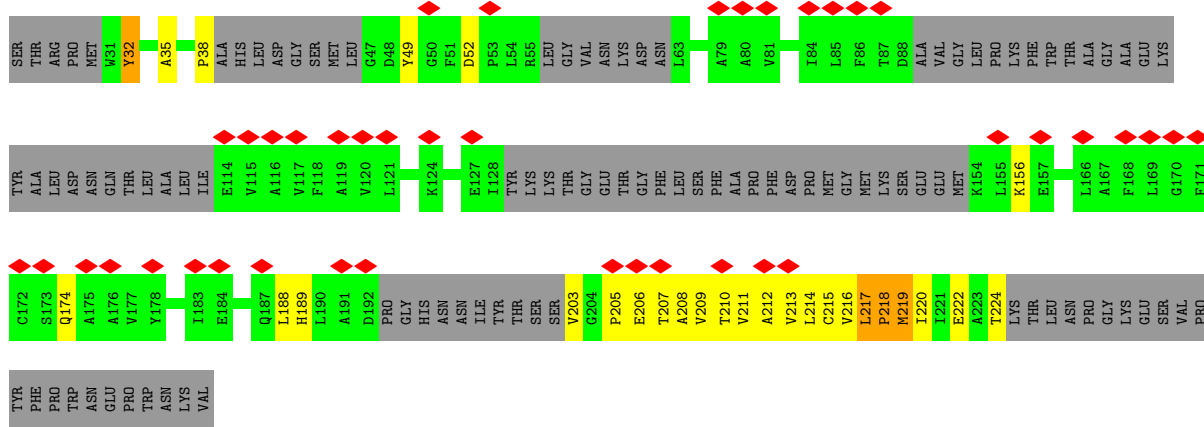
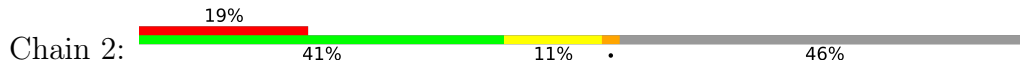


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

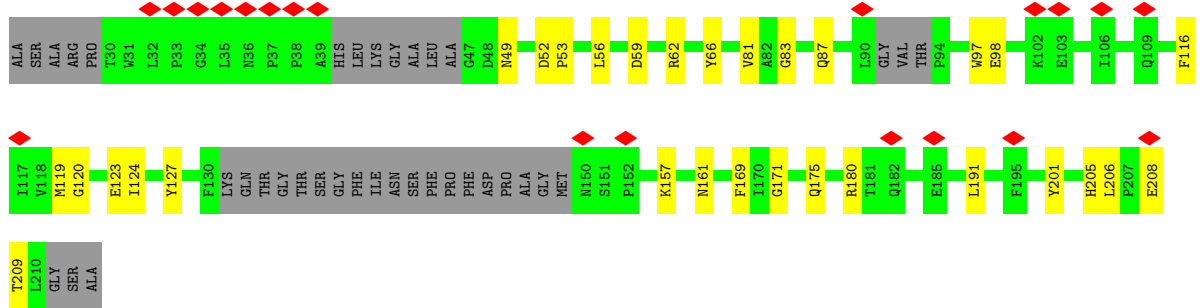




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic



• Molecule 20: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 338867 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.498 | Depositor |
| Minimum map value | -0.258 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.012 | Depositor |
| Recommended contour level | 0.05 | Depositor |
| Map size (\AA) | 358.4, 358.4, 358.4 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.12, 1.12, 1.12 | 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: LMG, PQN, LHG, LUT, CLA, CHL, SF4, CL0, BCR, DGD

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.37 | 0/5995 | 0.61 | 4/8172 (0.0%) |
| 2 | B | 0.36 | 0/6035 | 0.57 | 1/8240 (0.0%) |
| 3 | C | 0.36 | 0/610 | 0.61 | 0/826 |
| 4 | D | 0.36 | 0/1160 | 0.55 | 0/1567 |
| 5 | E | 0.33 | 0/490 | 0.47 | 0/667 |
| 6 | F | 0.33 | 0/1291 | 0.58 | 0/1747 |
| 7 | G | 0.29 | 0/513 | 0.51 | 0/696 |
| 8 | I | 0.34 | 0/293 | 0.60 | 0/406 |
| 9 | J | 0.35 | 0/331 | 0.55 | 0/454 |
| 10 | K | 0.28 | 0/297 | 0.54 | 0/401 |
| 11 | L | 0.33 | 0/874 | 0.59 | 0/1194 |
| 12 | 1 | 0.31 | 0/1490 | 0.52 | 1/2028 (0.0%) |
| 12 | Z | 0.31 | 0/1481 | 0.55 | 0/2015 |
| 13 | 3 | 0.36 | 0/1601 | 0.57 | 1/2173 (0.0%) |
| 14 | 7 | 0.34 | 0/1696 | 0.55 | 0/2303 |
| 15 | 8 | 0.34 | 0/1700 | 0.67 | 3/2315 (0.1%) |
| 16 | 4 | 0.33 | 0/1621 | 0.59 | 3/2209 (0.1%) |
| 17 | 5 | 0.31 | 0/1798 | 0.52 | 0/2450 |
| 18 | 6 | 0.30 | 0/1827 | 0.54 | 0/2497 |
| 19 | 2 | 0.36 | 0/851 | 0.63 | 2/1154 (0.2%) |
| 20 | 9 | 0.32 | 0/1211 | 0.56 | 0/1643 |
| All | All | 0.34 | 0/33165 | 0.58 | 15/45157 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | B | 0 | 1 |
| 14 | 7 | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All | 0 | 2 |

There are no bond length outliers.

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 19 | 2 | 217 | LEU | C-N-CD | 8.65 | 146.56 | 128.40 |
| 16 | 4 | 164 | ARG | NE-CZ-NH1 | 8.33 | 124.47 | 120.30 |
| 1 | A | 198 | LEU | CA-CB-CG | 7.99 | 133.68 | 115.30 |
| 15 | 8 | 137 | ARG | NE-CZ-NH1 | 7.33 | 123.97 | 120.30 |
| 19 | 2 | 218 | PRO | CA-N-CD | -6.93 | 101.79 | 111.50 |
| 15 | 8 | 240 | LEU | CA-CB-CG | 6.78 | 130.89 | 115.30 |
| 2 | B | 688 | LEU | CA-CB-CG | 5.82 | 128.69 | 115.30 |
| 16 | 4 | 238 | THR | C-N-CA | 5.76 | 136.09 | 121.70 |
| 15 | 8 | 137 | ARG | NE-CZ-NH2 | -5.73 | 117.43 | 120.30 |
| 1 | A | 253 | LEU | CB-CG-CD2 | -5.66 | 101.37 | 111.00 |
| 16 | 4 | 164 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 12 | 1 | 175 | LEU | CA-CB-CG | 5.49 | 127.92 | 115.30 |
| 13 | 3 | 200 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 1 | A | 253 | LEU | CB-CG-CD1 | 5.24 | 119.90 | 111.00 |
| 1 | A | 198 | LEU | CB-CG-CD2 | 5.13 | 119.72 | 111.00 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 14 | 7 | 150 | PHE | Peptide |
| 2 | B | 668 | TRP | Peptide |

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 | 5800 | 0 | 5646 | 111 | 0 |
| 2 | B | 5822 | 0 | 5574 | 97 | 0 |
| 3 | C | 600 | 0 | 581 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | D | 1132 | 0 | 1150 | 16 | 0 |
| 5 | E | 480 | 0 | 476 | 6 | 0 |
| 6 | F | 1265 | 0 | 1301 | 52 | 0 |
| 7 | G | 503 | 0 | 496 | 7 | 0 |
| 8 | I | 281 | 0 | 292 | 5 | 0 |
| 9 | J | 320 | 0 | 322 | 7 | 0 |
| 10 | K | 297 | 0 | 319 | 2 | 0 |
| 11 | L | 853 | 0 | 864 | 25 | 0 |
| 12 | 1 | 1444 | 0 | 1395 | 26 | 0 |
| 12 | Z | 1436 | 0 | 1388 | 19 | 0 |
| 13 | 3 | 1555 | 0 | 1522 | 30 | 0 |
| 14 | 7 | 1644 | 0 | 1582 | 23 | 0 |
| 15 | 8 | 1649 | 0 | 1628 | 36 | 0 |
| 16 | 4 | 1570 | 0 | 1526 | 72 | 0 |
| 17 | 5 | 1744 | 0 | 1715 | 39 | 0 |
| 18 | 6 | 1765 | 0 | 1767 | 38 | 0 |
| 19 | 2 | 838 | 0 | 767 | 65 | 0 |
| 20 | 9 | 1180 | 0 | 1160 | 35 | 0 |
| 21 | A | 65 | 0 | 72 | 3 | 0 |
| 22 | 1 | 722 | 0 | 735 | 34 | 0 |
| 22 | 2 | 540 | 0 | 426 | 19 | 0 |
| 22 | 3 | 696 | 0 | 630 | 26 | 0 |
| 22 | 4 | 576 | 0 | 490 | 42 | 0 |
| 22 | 5 | 737 | 0 | 632 | 34 | 0 |
| 22 | 6 | 696 | 0 | 620 | 44 | 0 |
| 22 | 7 | 741 | 0 | 658 | 32 | 0 |
| 22 | 8 | 680 | 0 | 592 | 24 | 0 |
| 22 | 9 | 514 | 0 | 426 | 19 | 0 |
| 22 | A | 2689 | 0 | 2796 | 204 | 0 |
| 22 | B | 2480 | 0 | 2545 | 122 | 0 |
| 22 | F | 175 | 0 | 177 | 8 | 0 |
| 22 | G | 96 | 0 | 72 | 0 | 0 |
| 22 | J | 42 | 0 | 31 | 1 | 0 |
| 22 | K | 91 | 0 | 66 | 2 | 0 |
| 22 | L | 115 | 0 | 111 | 1 | 0 |
| 22 | Z | 714 | 0 | 714 | 24 | 0 |
| 23 | A | 33 | 0 | 46 | 4 | 0 |
| 23 | B | 33 | 0 | 46 | 1 | 0 |
| 24 | 1 | 43 | 0 | 56 | 2 | 0 |
| 24 | 4 | 81 | 0 | 106 | 3 | 0 |
| 24 | 5 | 37 | 0 | 44 | 0 | 0 |
| 24 | 6 | 49 | 0 | 74 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24 | 7 | 37 | 0 | 44 | 0 | 0 |
| 24 | 8 | 37 | 0 | 44 | 1 | 0 |
| 24 | A | 117 | 0 | 153 | 5 | 0 |
| 24 | B | 23 | 0 | 16 | 0 | 0 |
| 24 | Z | 43 | 0 | 56 | 1 | 0 |
| 25 | 3 | 120 | 0 | 163 | 15 | 0 |
| 25 | 4 | 40 | 0 | 56 | 39 | 0 |
| 25 | 5 | 80 | 0 | 112 | 12 | 0 |
| 25 | 6 | 80 | 0 | 110 | 11 | 0 |
| 25 | 7 | 80 | 0 | 112 | 6 | 0 |
| 25 | 8 | 40 | 0 | 56 | 6 | 0 |
| 25 | A | 240 | 0 | 336 | 25 | 0 |
| 25 | B | 280 | 0 | 392 | 29 | 0 |
| 25 | F | 40 | 0 | 56 | 15 | 0 |
| 25 | G | 40 | 0 | 56 | 3 | 0 |
| 25 | I | 40 | 0 | 56 | 1 | 0 |
| 25 | J | 40 | 0 | 56 | 2 | 0 |
| 25 | K | 80 | 0 | 112 | 6 | 0 |
| 25 | L | 80 | 0 | 112 | 9 | 0 |
| 26 | A | 8 | 0 | 0 | 0 | 0 |
| 26 | C | 16 | 0 | 0 | 0 | 0 |
| 27 | B | 66 | 0 | 96 | 1 | 0 |
| 28 | 9 | 44 | 0 | 61 | 1 | 0 |
| 28 | J | 35 | 0 | 40 | 0 | 0 |
| 29 | 1 | 101 | 0 | 74 | 4 | 0 |
| 29 | 3 | 66 | 0 | 70 | 5 | 0 |
| 29 | 4 | 201 | 0 | 150 | 25 | 0 |
| 29 | 5 | 145 | 0 | 101 | 6 | 0 |
| 29 | 6 | 206 | 0 | 159 | 11 | 0 |
| 29 | 7 | 54 | 0 | 43 | 1 | 0 |
| 29 | 8 | 56 | 0 | 47 | 0 | 0 |
| 29 | 9 | 93 | 0 | 64 | 1 | 0 |
| 29 | Z | 101 | 0 | 73 | 1 | 0 |
| 30 | 1 | 126 | 0 | 168 | 14 | 0 |
| 30 | 2 | 84 | 0 | 112 | 6 | 0 |
| 30 | 3 | 84 | 0 | 112 | 7 | 0 |
| 30 | 4 | 84 | 0 | 112 | 16 | 0 |
| 30 | 5 | 84 | 0 | 112 | 20 | 0 |
| 30 | 6 | 84 | 0 | 112 | 7 | 0 |
| 30 | 7 | 84 | 0 | 112 | 8 | 0 |
| 30 | 8 | 84 | 0 | 112 | 13 | 0 |
| 30 | 9 | 84 | 0 | 112 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30 | Z | 126 | 0 | 168 | 10 | 0 |
| All | All | 48476 | 0 | 47944 | 1162 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1162) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:4:257:TRP:CD1 | 22:4:616:CLA:CBB | 1.75 | 1.60 |
| 19:2:32:TYR:CE2 | 19:2:35:ALA:HB2 | 1.37 | 1.59 |
| 22:A:802:CLA:C19 | 22:A:842:CLA:C4 | 1.79 | 1.53 |
| 19:2:32:TYR:CD2 | 19:2:35:ALA:HB2 | 1.41 | 1.50 |
| 1:A:198:LEU:HD23 | 1:A:322:MET:CE | 1.43 | 1.48 |
| 22:A:805:CLA:C4 | 22:A:812:CLA:HBB1 | 1.44 | 1.45 |
| 19:2:189:HIS:ND1 | 22:2:613:CLA:CAA | 1.80 | 1.41 |
| 19:2:189:HIS:ND1 | 22:2:613:CLA:HAA2 | 1.09 | 1.39 |
| 19:2:189:HIS:CE1 | 22:2:613:CLA:HAA2 | 1.63 | 1.33 |
| 2:B:416:LYS:NZ | 6:F:226:PRO:CG | 1.91 | 1.33 |
| 19:2:32:TYR:CE2 | 19:2:35:ALA:CB | 2.11 | 1.31 |
| 22:A:833:CLA:OBD | 11:L:57:THR:HG21 | 1.34 | 1.22 |
| 1:A:198:LEU:CD2 | 1:A:322:MET:CE | 2.17 | 1.21 |
| 17:5:185:LYS:O | 17:5:189:ASN:ND2 | 1.76 | 1.18 |
| 2:B:416:LYS:NZ | 6:F:226:PRO:HG2 | 1.50 | 1.17 |
| 2:B:416:LYS:HZ3 | 6:F:226:PRO:CG | 1.51 | 1.17 |
| 19:2:222:GLU:HG3 | 20:9:127:TYR:HE2 | 1.10 | 1.16 |
| 2:B:159:GLN:HE21 | 19:2:224:THR:HG21 | 1.09 | 1.15 |
| 17:5:85:VAL:HG11 | 30:5:620:LUT:H12 | 1.29 | 1.14 |
| 19:2:222:GLU:CG | 20:9:127:TYR:HE2 | 1.59 | 1.14 |
| 11:L:186:TYR:O | 11:L:188:CYS:N | 1.80 | 1.13 |
| 22:B:820:CLA:HHC | 22:B:820:CLA:HBB1 | 1.25 | 1.12 |
| 2:B:416:LYS:NZ | 6:F:226:PRO:HG3 | 1.61 | 1.11 |
| 18:6:257:PRO:HB2 | 22:6:616:CLA:HAB | 1.27 | 1.11 |
| 22:B:812:CLA:HBB2 | 22:B:820:CLA:C7 | 1.81 | 1.10 |
| 22:B:841:CLA:HHC | 22:B:841:CLA:HBB1 | 1.34 | 1.08 |
| 22:B:812:CLA:HBB2 | 22:B:820:CLA:H72 | 1.08 | 1.07 |
| 16:4:207:ASP:HB3 | 16:4:209:LYS:HE2 | 1.07 | 1.06 |
| 1:A:198:LEU:CD2 | 1:A:322:MET:HE3 | 1.84 | 1.05 |
| 22:A:805:CLA:HHC | 22:A:805:CLA:HBB1 | 1.38 | 1.05 |
| 22:A:805:CLA:H42 | 22:A:812:CLA:HBB1 | 1.37 | 1.04 |
| 19:2:209:VAL:O | 19:2:213:VAL:HG23 | 1.56 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:815:CLA:HHC | 22:A:815:CLA:HBB1 | 1.39 | 1.04 |
| 19:2:32:TYR:CD2 | 19:2:35:ALA:CB | 2.34 | 1.04 |
| 6:F:223:THR:OG1 | 6:F:227:ARG:NH2 | 1.91 | 1.03 |
| 22:7:620:CLA:CGA | 18:6:250:CYS:O | 2.06 | 1.03 |
| 17:5:203:GLN:NE2 | 30:5:620:LUT:O3 | 1.91 | 1.03 |
| 1:A:198:LEU:HD23 | 1:A:322:MET:HE1 | 1.33 | 1.02 |
| 15:8:242:PHE:CE2 | 15:8:243:LEU:HG | 1.94 | 1.02 |
| 22:A:805:CLA:C4 | 22:A:812:CLA:CBB | 2.37 | 1.01 |
| 6:F:223:THR:CB | 6:F:227:ARG:HH22 | 1.74 | 1.01 |
| 19:2:222:GLU:CG | 20:9:127:TYR:CE2 | 2.45 | 1.00 |
| 2:B:159:GLN:NE2 | 19:2:224:THR:HG21 | 1.77 | 1.00 |
| 22:B:831:CLA:HBC3 | 25:F:305:BCR:H362 | 1.43 | 1.00 |
| 22:A:815:CLA:H2 | 22:A:817:CLA:HMB2 | 1.43 | 0.99 |
| 2:B:159:GLN:HE21 | 19:2:224:THR:CG2 | 1.73 | 0.99 |
| 22:A:805:CLA:H43 | 22:A:812:CLA:HBB1 | 1.45 | 0.99 |
| 22:B:803:CLA:HMB1 | 22:B:803:CLA:HBB1 | 1.44 | 0.98 |
| 6:F:223:THR:CB | 6:F:227:ARG:NH2 | 2.27 | 0.98 |
| 2:B:416:LYS:HZ1 | 6:F:226:PRO:CG | 1.64 | 0.97 |
| 16:4:207:ASP:CB | 16:4:209:LYS:HE2 | 1.95 | 0.97 |
| 22:A:802:CLA:C19 | 22:A:842:CLA:H41 | 1.94 | 0.97 |
| 16:4:207:ASP:HB3 | 16:4:209:LYS:CE | 1.93 | 0.96 |
| 11:L:183:ALA:O | 11:L:187:VAL:HG23 | 1.66 | 0.96 |
| 1:A:198:LEU:CD2 | 1:A:322:MET:HE1 | 1.86 | 0.95 |
| 19:2:222:GLU:HG3 | 20:9:127:TYR:CE2 | 2.02 | 0.95 |
| 22:4:604:CLA:CHC | 25:4:621:BCR:H393 | 1.96 | 0.95 |
| 16:4:257:TRP:HD1 | 22:4:616:CLA:CBB | 1.65 | 0.94 |
| 1:A:212:ALA:HB3 | 22:A:815:CLA:HBB2 | 1.47 | 0.94 |
| 1:A:198:LEU:HD23 | 1:A:322:MET:HE3 | 1.39 | 0.94 |
| 22:7:620:CLA:H91 | 29:6:607:CHL:H42 | 1.47 | 0.93 |
| 16:4:257:TRP:NE1 | 22:4:616:CLA:CBB | 2.31 | 0.93 |
| 22:4:604:CLA:CHC | 25:4:621:BCR:C39 | 2.46 | 0.93 |
| 20:9:120:GLY:O | 20:9:124:ILE:HG12 | 1.68 | 0.93 |
| 18:6:257:PRO:HB2 | 22:6:616:CLA:CAB | 1.99 | 0.92 |
| 22:7:620:CLA:H111 | 29:6:607:CHL:H41 | 1.52 | 0.92 |
| 19:2:189:HIS:ND1 | 22:2:613:CLA:HAA1 | 1.84 | 0.92 |
| 19:2:222:GLU:HG2 | 20:9:127:TYR:CE2 | 2.05 | 0.91 |
| 24:6:619:LHG:H111 | 24:6:619:LHG:C27 | 1.99 | 0.91 |
| 22:B:812:CLA:CBB | 22:B:820:CLA:H72 | 2.00 | 0.91 |
| 19:2:214:LEU:O | 19:2:218:PRO:HD3 | 1.70 | 0.90 |
| 22:A:805:CLA:H41 | 22:A:812:CLA:HBB1 | 1.51 | 0.90 |
| 24:6:619:LHG:H111 | 24:6:619:LHG:H272 | 1.52 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:7:207:GLN:NE2 | 30:7:621:LUT:O3 | 2.04 | 0.90 |
| 11:L:186:TYR:C | 11:L:188:CYS:H | 1.72 | 0.89 |
| 18:6:257:PRO:CB | 22:6:616:CLA:HAB | 2.01 | 0.89 |
| 19:2:212:ALA:O | 19:2:216:VAL:HG23 | 1.74 | 0.88 |
| 6:F:224:VAL:HG12 | 6:F:226:PRO:CD | 2.05 | 0.87 |
| 16:4:257:TRP:CG | 22:4:616:CLA:CBB | 2.57 | 0.87 |
| 29:4:618:CHL:HBB2 | 25:4:621:BCR:H10C | 1.54 | 0.87 |
| 22:A:815:CLA:H122 | 22:3:607:CLA:HMC2 | 1.56 | 0.87 |
| 1:A:212:ALA:CB | 22:A:815:CLA:HBB2 | 2.04 | 0.86 |
| 19:2:219:MET:HE2 | 22:9:609:CLA:CMA | 2.07 | 0.85 |
| 1:A:198:LEU:HD23 | 1:A:322:MET:HE2 | 1.59 | 0.85 |
| 6:F:223:THR:CG2 | 6:F:227:ARG:HH22 | 1.89 | 0.84 |
| 29:1:607:CHL:HMB1 | 29:1:607:CHL:HBB1 | 1.60 | 0.83 |
| 22:4:604:CLA:C4B | 25:4:621:BCR:H393 | 2.07 | 0.83 |
| 22:6:601:CLA:C3B | 24:6:619:LHG:H282 | 2.07 | 0.83 |
| 6:F:224:VAL:HG12 | 6:F:226:PRO:HD2 | 1.58 | 0.83 |
| 16:4:111:VAL:HG11 | 30:4:619:LUT:H12 | 1.59 | 0.83 |
| 6:F:226:PRO:O | 6:F:227:ARG:HB2 | 1.76 | 0.82 |
| 13:3:194:GLY:O | 13:3:198:PHE:HB2 | 1.79 | 0.82 |
| 29:4:618:CHL:CBB | 25:4:621:BCR:H10C | 2.09 | 0.82 |
| 6:F:225:SER:N | 6:F:226:PRO:HD2 | 1.94 | 0.82 |
| 13:3:156:GLN:O | 13:3:160:LEU:HB2 | 1.79 | 0.82 |
| 22:6:601:CLA:H2 | 24:6:619:LHG:H152 | 1.62 | 0.82 |
| 20:9:83:GLY:O | 20:9:87:GLN:HG3 | 1.81 | 0.81 |
| 22:B:820:CLA:HBB1 | 22:B:820:CLA:CHC | 2.08 | 0.81 |
| 25:F:305:BCR:H331 | 25:F:305:BCR:C8 | 2.11 | 0.81 |
| 22:7:620:CLA:C9 | 29:6:607:CHL:H42 | 2.10 | 0.80 |
| 19:2:207:THR:O | 19:2:211:VAL:HG13 | 1.81 | 0.80 |
| 22:B:825:CLA:H72 | 22:B:841:CLA:H191 | 1.62 | 0.80 |
| 17:5:203:GLN:HE22 | 30:5:620:LUT:HO3 | 1.28 | 0.80 |
| 2:B:315:SER:OG | 22:B:841:CLA:O1A | 2.00 | 0.80 |
| 6:F:224:VAL:HG12 | 6:F:225:SER:H | 1.46 | 0.80 |
| 20:9:62:ARG:HD2 | 20:9:66:TYR:CE2 | 2.17 | 0.80 |
| 22:A:805:CLA:CBB | 22:A:807:CLA:CAD | 2.60 | 0.79 |
| 6:F:224:VAL:CG1 | 6:F:226:PRO:HD2 | 2.12 | 0.79 |
| 22:A:802:CLA:CGA | 22:A:802:CLA:H3A | 2.11 | 0.79 |
| 22:6:601:CLA:C4B | 24:6:619:LHG:H282 | 2.11 | 0.79 |
| 6:F:224:VAL:CB | 6:F:226:PRO:HD2 | 2.14 | 0.78 |
| 1:A:212:ALA:CB | 22:A:815:CLA:CBB | 2.62 | 0.77 |
| 1:A:707:LEU:HD13 | 25:F:305:BCR:H321 | 1.65 | 0.77 |
| 19:2:203:VAL:HG13 | 19:2:206:GLU:OE1 | 1.85 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:719:ILE:HG23 | 22:B:827:CLA:HBB1 | 1.66 | 0.76 |
| 17:5:171:PRO:HD2 | 30:5:620:LUT:H23 | 1.66 | 0.76 |
| 19:2:32:TYR:CE2 | 19:2:35:ALA:CA | 2.68 | 0.76 |
| 1:A:212:ALA:HB1 | 22:A:815:CLA:CBB | 2.16 | 0.76 |
| 12:Z:176:LYS:O | 12:Z:180:ASN:ND2 | 2.18 | 0.75 |
| 6:F:223:THR:HG21 | 6:F:227:ARG:NH2 | 2.02 | 0.75 |
| 11:L:55:LEU:HD23 | 11:L:56:GLU:N | 2.02 | 0.75 |
| 29:4:606:CHL:HAA1 | 25:4:621:BCR:H23C | 1.70 | 0.74 |
| 22:2:601:CLA:HBB2 | 22:2:602:CLA:HHD | 1.67 | 0.74 |
| 19:2:214:LEU:O | 19:2:217:LEU:HB3 | 1.87 | 0.73 |
| 22:3:610:CLA:HBB1 | 30:3:621:LUT:H32 | 1.69 | 0.73 |
| 16:4:208:ILE:CG1 | 22:4:610:CLA:HMA2 | 2.18 | 0.73 |
| 22:A:832:CLA:HED2 | 11:L:55:LEU:HD11 | 1.71 | 0.73 |
| 6:F:225:SER:N | 6:F:226:PRO:CD | 2.51 | 0.73 |
| 22:A:805:CLA:HBB2 | 22:A:807:CLA:CAD | 2.19 | 0.73 |
| 29:4:618:CHL:HAB | 25:4:621:BCR:C10 | 2.19 | 0.73 |
| 22:A:835:CLA:H42 | 25:L:201:BCR:C36 | 2.18 | 0.73 |
| 22:B:820:CLA:O1A | 22:B:820:CLA:H3A | 1.89 | 0.73 |
| 1:A:310:HIS:CE1 | 25:K:4001:BCR:H363 | 2.24 | 0.72 |
| 19:2:219:MET:HE2 | 22:9:609:CLA:HMA2 | 1.71 | 0.72 |
| 19:2:215:CYS:O | 19:2:218:PRO:HD2 | 1.88 | 0.72 |
| 16:4:208:ILE:CG2 | 16:4:212:LYS:HE3 | 2.20 | 0.72 |
| 16:4:156:LEU:HD12 | 25:4:621:BCR:C15 | 2.20 | 0.72 |
| 6:F:224:VAL:HG12 | 6:F:225:SER:N | 2.03 | 0.72 |
| 18:6:82:VAL:HG11 | 30:6:621:LUT:H12 | 1.71 | 0.72 |
| 1:A:198:LEU:HD21 | 1:A:322:MET:CE | 2.19 | 0.71 |
| 14:7:97:LEU:HD23 | 22:7:620:CLA:H2A | 1.71 | 0.71 |
| 22:A:832:CLA:HAA2 | 11:L:57:THR:HG23 | 1.72 | 0.71 |
| 16:4:208:ILE:HG12 | 22:4:610:CLA:HMA2 | 1.71 | 0.71 |
| 6:F:223:THR:HG21 | 6:F:227:ARG:HH22 | 1.54 | 0.71 |
| 22:A:806:CLA:H61 | 25:A:849:BCR:HC8 | 1.73 | 0.71 |
| 22:B:825:CLA:H52 | 22:B:841:CLA:H201 | 1.72 | 0.71 |
| 22:B:818:CLA:HAB | 22:B:818:CLA:H8 | 1.71 | 0.71 |
| 19:2:219:MET:CE | 22:9:609:CLA:CMA | 2.68 | 0.71 |
| 14:7:134:LYS:HG3 | 22:7:608:CLA:HBB1 | 1.73 | 0.71 |
| 22:A:835:CLA:O2D | 22:A:835:CLA:H2A | 1.91 | 0.70 |
| 22:B:806:CLA:HBB | 22:B:829:CLA:HAB | 1.71 | 0.70 |
| 22:A:806:CLA:H11 | 22:A:807:CLA:HBB1 | 1.71 | 0.70 |
| 22:A:835:CLA:H42 | 25:L:201:BCR:H363 | 1.74 | 0.70 |
| 2:B:487:PHE:O | 2:B:491:GLN:HB2 | 1.91 | 0.70 |
| 13:3:159:GLU:OE2 | 13:3:162:ARG:NH2 | 2.23 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:2:189:HIS:CG | 22:2:613:CLA:HAA2 | 2.19 | 0.70 |
| 19:2:219:MET:CE | 22:9:609:CLA:HMA2 | 2.22 | 0.70 |
| 29:4:618:CHL:CAB | 25:4:621:BCR:H10C | 2.20 | 0.70 |
| 19:2:222:GLU:HG2 | 20:9:127:TYR:CD2 | 2.27 | 0.69 |
| 22:A:802:CLA:H122 | 25:A:852:BCR:H23C | 1.75 | 0.69 |
| 6:F:224:VAL:C | 6:F:226:PRO:HD2 | 2.13 | 0.69 |
| 22:3:609:CLA:HBB1 | 22:3:617:CLA:HBB1 | 1.75 | 0.69 |
| 2:B:276:HIS:HE1 | 22:B:816:CLA:C1A | 2.05 | 0.69 |
| 6:F:224:VAL:HG12 | 6:F:226:PRO:HD3 | 1.75 | 0.69 |
| 19:2:206:GLU:O | 19:2:210:THR:HG23 | 1.92 | 0.69 |
| 22:A:835:CLA:C4 | 25:L:201:BCR:H363 | 2.22 | 0.69 |
| 16:4:203:TRP:O | 16:4:204:SER:HB2 | 1.90 | 0.69 |
| 22:A:802:CLA:H121 | 22:A:802:CLA:H91 | 1.74 | 0.69 |
| 22:A:835:CLA:HHC | 22:A:835:CLA:HBB1 | 1.74 | 0.69 |
| 2:B:545:SER:HA | 6:F:224:VAL:HG11 | 1.75 | 0.69 |
| 14:7:132:GLU:HG2 | 22:7:609:CLA:C1B | 2.23 | 0.69 |
| 1:A:169:MET:HG3 | 25:A:848:BCR:H322 | 1.75 | 0.68 |
| 22:B:812:CLA:CBB | 22:B:820:CLA:H102 | 2.24 | 0.68 |
| 2:B:290:HIS:O | 22:B:820:CLA:HED1 | 1.93 | 0.68 |
| 6:F:223:THR:CG2 | 6:F:227:ARG:NH2 | 2.54 | 0.68 |
| 19:2:216:VAL:O | 19:2:220:ILE:HG13 | 1.92 | 0.68 |
| 24:6:619:LHG:H111 | 24:6:619:LHG:C28 | 2.23 | 0.68 |
| 1:A:540:ALA:HB1 | 22:A:839:CLA:HMB3 | 1.74 | 0.68 |
| 22:A:843:CLA:H143 | 25:L:201:BCR:H17C | 1.74 | 0.68 |
| 1:A:297:HIS:HB2 | 22:A:819:CLA:C1B | 2.24 | 0.68 |
| 19:2:208:ALA:O | 19:2:211:VAL:HG22 | 1.95 | 0.67 |
| 22:A:832:CLA:HBB1 | 24:A:847:LHG:H141 | 1.76 | 0.67 |
| 24:6:619:LHG:H111 | 24:6:619:LHG:H281 | 1.77 | 0.67 |
| 22:6:613:CLA:H52 | 24:6:619:LHG:H182 | 1.77 | 0.67 |
| 22:A:805:CLA:HBB2 | 22:A:807:CLA:C3D | 2.25 | 0.67 |
| 29:4:608:CHL:HMA1 | 25:4:621:BCR:C36 | 2.25 | 0.66 |
| 1:A:458:HIS:HE1 | 22:A:835:CLA:C1A | 2.08 | 0.66 |
| 22:B:825:CLA:HMA1 | 25:B:847:BCR:H14C | 1.75 | 0.66 |
| 22:A:805:CLA:HBB1 | 22:A:805:CLA:CHC | 2.19 | 0.66 |
| 6:F:224:VAL:CG1 | 6:F:226:PRO:CD | 2.71 | 0.66 |
| 6:F:226:PRO:O | 6:F:227:ARG:CB | 2.43 | 0.66 |
| 2:B:416:LYS:CE | 6:F:226:PRO:HG2 | 2.26 | 0.66 |
| 16:4:208:ILE:CD1 | 22:4:610:CLA:HMA2 | 2.26 | 0.66 |
| 6:F:224:VAL:HB | 6:F:226:PRO:HD2 | 1.77 | 0.66 |
| 19:2:219:MET:HE2 | 22:9:609:CLA:HMA1 | 1.78 | 0.66 |
| 22:A:802:CLA:H191 | 22:A:842:CLA:C4 | 2.14 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:4:232:GLN:HE22 | 30:4:619:LUT:C3 | 2.08 | 0.65 |
| 29:4:608:CHL:HMA1 | 25:4:621:BCR:H362 | 1.76 | 0.65 |
| 22:1:602:CLA:HBB1 | 30:1:618:LUT:H32 | 1.79 | 0.65 |
| 16:4:159:TRP:CH2 | 25:4:621:BCR:H331 | 2.32 | 0.65 |
| 17:5:245:LEU:HD11 | 25:5:625:BCR:H352 | 1.78 | 0.65 |
| 16:4:207:ASP:HB2 | 16:4:209:LYS:HG2 | 1.78 | 0.65 |
| 22:7:620:CLA:H111 | 29:6:607:CHL:C4 | 2.26 | 0.65 |
| 22:A:802:CLA:H192 | 22:A:842:CLA:C4 | 2.15 | 0.65 |
| 16:4:208:ILE:HD11 | 22:4:610:CLA:HMA2 | 1.77 | 0.65 |
| 18:6:251:PHE:HB2 | 25:6:625:BCR:H282 | 1.77 | 0.65 |
| 13:3:238:THR:HG21 | 13:3:245:ASN:HD21 | 1.61 | 0.65 |
| 22:A:805:CLA:H41 | 22:A:812:CLA:CBB | 2.18 | 0.65 |
| 29:4:606:CHL:CBA | 25:4:621:BCR:H21C | 2.27 | 0.64 |
| 20:9:206:LEU:O | 20:9:209:THR:HG22 | 1.97 | 0.64 |
| 1:A:470:ASP:HB3 | 22:A:835:CLA:HED3 | 1.78 | 0.64 |
| 25:F:305:BCR:H383 | 25:F:305:BCR:H23C | 1.79 | 0.64 |
| 1:A:605:ILE:HD12 | 21:A:801:CL0:H53 | 1.79 | 0.64 |
| 22:A:809:CLA:HBB2 | 22:A:829:CLA:H203 | 1.80 | 0.64 |
| 14:7:132:GLU:HG2 | 22:7:609:CLA:NB | 2.12 | 0.64 |
| 16:4:208:ILE:HD11 | 22:4:610:CLA:H2A | 1.78 | 0.64 |
| 1:A:458:HIS:CE1 | 22:A:835:CLA:C1A | 2.81 | 0.64 |
| 2:B:690:ASN:O | 4:D:76:ARG:NH2 | 2.26 | 0.64 |
| 22:5:609:CLA:HBA1 | 22:5:621:CLA:HMD2 | 1.79 | 0.64 |
| 22:A:815:CLA:HBB1 | 22:A:815:CLA:CHC | 2.20 | 0.64 |
| 1:A:467:ARG:HH22 | 11:L:105:PRO:HB3 | 1.61 | 0.64 |
| 2:B:458:PRO:HG3 | 2:B:518:PHE:HB2 | 1.79 | 0.63 |
| 2:B:416:LYS:HZ3 | 6:F:226:PRO:CB | 2.11 | 0.63 |
| 12:Z:110:ALA:HB1 | 12:Z:127:LEU:HD12 | 1.80 | 0.63 |
| 29:4:618:CHL:HAB | 25:4:621:BCR:H10C | 1.79 | 0.63 |
| 2:B:92:ILE:HB | 2:B:113:PRO:HB2 | 1.79 | 0.63 |
| 16:4:263:ARG:HD2 | 22:4:616:CLA:HMA2 | 1.79 | 0.63 |
| 22:4:611:CLA:HAB | 25:6:623:BCR:H312 | 1.80 | 0.63 |
| 1:A:454:GLY:HA3 | 22:A:835:CLA:CBB | 2.27 | 0.63 |
| 1:A:706:LYS:HG2 | 22:B:831:CLA:HMA2 | 1.80 | 0.63 |
| 22:A:815:CLA:HBA2 | 22:A:817:CLA:HMB3 | 1.80 | 0.63 |
| 24:6:619:LHG:H272 | 24:6:619:LHG:C11 | 2.28 | 0.63 |
| 20:9:59:ASP:HB3 | 20:9:62:ARG:HB3 | 1.79 | 0.63 |
| 1:A:327:GLU:HG2 | 1:A:339:VAL:HG22 | 1.81 | 0.63 |
| 22:6:612:CLA:HMA2 | 22:6:612:CLA:H2 | 1.81 | 0.63 |
| 19:2:219:MET:HE3 | 22:9:609:CLA:H3A | 1.80 | 0.63 |
| 2:B:416:LYS:HZ1 | 6:F:226:PRO:HG2 | 1.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:831:CLA:HMD3 | 22:B:841:CLA:H92 | 1.81 | 0.63 |
| 18:6:252:LEU:HB2 | 22:6:622:CLA:HMA2 | 1.80 | 0.63 |
| 22:A:802:CLA:C1D | 2:B:583:TRP:HE1 | 2.11 | 0.62 |
| 22:A:805:CLA:CBB | 22:A:807:CLA:OBD | 2.46 | 0.62 |
| 16:4:159:TRP:CH2 | 25:4:621:BCR:C33 | 2.82 | 0.62 |
| 1:A:709:VAL:HG11 | 22:A:841:CLA:HMB3 | 1.80 | 0.62 |
| 1:A:198:LEU:HD21 | 1:A:322:MET:HE3 | 1.73 | 0.62 |
| 9:J:24:GLY:O | 9:J:28:GLU:HG2 | 1.99 | 0.62 |
| 1:A:572:ARG:NH1 | 24:A:846:LHG:O10 | 2.32 | 0.62 |
| 9:J:28:GLU:OE1 | 9:J:28:GLU:HA | 2.00 | 0.62 |
| 16:4:248:LEU:HD21 | 22:4:614:CLA:HMC3 | 1.82 | 0.62 |
| 22:6:616:CLA:CBB | 22:6:622:CLA:HMD3 | 2.30 | 0.62 |
| 22:B:819:CLA:HMB2 | 22:B:824:CLA:HMA3 | 1.81 | 0.62 |
| 18:6:76:ARG:NE | 18:6:176:GLU:OE2 | 2.29 | 0.62 |
| 22:A:802:CLA:H203 | 22:A:831:CLA:H191 | 1.81 | 0.62 |
| 25:B:801:BCR:H381 | 22:F:301:CLA:HMC2 | 1.82 | 0.62 |
| 22:B:823:CLA:HBA1 | 25:B:846:BCR:H16C | 1.82 | 0.62 |
| 20:9:119:MET:O | 20:9:123:GLU:HG2 | 1.99 | 0.61 |
| 22:A:803:CLA:H122 | 25:B:848:BCR:H12C | 1.82 | 0.61 |
| 12:Z:158:PHE:CZ | 22:Z:608:CLA:NC | 2.68 | 0.61 |
| 16:4:208:ILE:HG21 | 16:4:212:LYS:HE3 | 1.82 | 0.61 |
| 19:2:189:HIS:CE1 | 22:2:613:CLA:CAA | 2.56 | 0.61 |
| 22:A:833:CLA:OBD | 11:L:57:THR:CG2 | 2.29 | 0.61 |
| 22:B:837:CLA:H151 | 25:F:305:BCR:H21C | 1.83 | 0.61 |
| 22:7:610:CLA:HBB1 | 30:7:621:LUT:H32 | 1.83 | 0.61 |
| 29:4:606:CHL:HAA1 | 25:4:621:BCR:H21C | 1.82 | 0.61 |
| 17:5:199:ALA:O | 17:5:203:GLN:HG3 | 2.00 | 0.61 |
| 1:A:450:PHE:O | 22:A:835:CLA:HBB2 | 2.01 | 0.61 |
| 1:A:423:TYR:CE1 | 4:D:105:ILE:HG13 | 2.36 | 0.60 |
| 1:A:433:HIS:HB3 | 11:L:55:LEU:CD1 | 2.31 | 0.60 |
| 22:B:841:CLA:HMB3 | 22:1:603:CLA:H92 | 1.82 | 0.60 |
| 2:B:276:HIS:CE1 | 22:B:816:CLA:NA | 2.68 | 0.60 |
| 22:B:839:CLA:H142 | 25:L:201:BCR:H21C | 1.83 | 0.60 |
| 12:1:160:PRO:HD2 | 30:1:617:LUT:H23 | 1.83 | 0.60 |
| 22:B:812:CLA:H12 | 20:9:56:LEU:HD21 | 1.84 | 0.60 |
| 22:A:811:CLA:HBB2 | 22:A:814:CLA:HMA3 | 1.83 | 0.60 |
| 15:8:136:LYS:HE2 | 22:8:608:CLA:HMC3 | 1.82 | 0.60 |
| 16:4:207:ASP:O | 16:4:208:ILE:HG22 | 2.01 | 0.60 |
| 1:A:212:ALA:HB1 | 22:A:815:CLA:HBB1 | 1.83 | 0.60 |
| 14:7:207:GLN:HE22 | 30:7:621:LUT:C3 | 2.14 | 0.60 |
| 1:A:204:GLY:O | 1:A:208:LEU:HB2 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:B:841:CLA:HBB1 | 22:B:841:CLA:CHC | 2.16 | 0.60 |
| 11:L:187:VAL:HG12 | 11:L:187:VAL:O | 2.00 | 0.60 |
| 14:7:128:MET:O | 14:7:132:GLU:HB2 | 2.02 | 0.60 |
| 22:A:816:CLA:H71 | 25:3:719:BCR:H12C | 1.83 | 0.59 |
| 19:2:32:TYR:CZ | 19:2:35:ALA:HA | 2.38 | 0.59 |
| 19:2:203:VAL:O | 19:2:207:THR:HG23 | 2.00 | 0.59 |
| 19:2:218:PRO:CG | 22:2:601:CLA:HMA2 | 2.32 | 0.59 |
| 20:9:53:PRO:HD2 | 30:9:617:LUT:H23 | 1.84 | 0.59 |
| 22:A:805:CLA:HMA2 | 22:A:812:CLA:HMD2 | 1.84 | 0.59 |
| 16:4:209:LYS:N | 16:4:209:LYS:HD3 | 2.17 | 0.59 |
| 1:A:458:HIS:HE1 | 22:A:835:CLA:CHA | 2.14 | 0.59 |
| 22:A:802:CLA:HAA2 | 22:A:802:CLA:HBD | 1.85 | 0.59 |
| 1:A:706:LYS:HE3 | 6:F:216:LEU:HD22 | 1.84 | 0.59 |
| 22:B:815:CLA:HBB1 | 25:B:843:BCR:H382 | 1.85 | 0.59 |
| 13:3:159:GLU:OE2 | 13:3:162:ARG:NE | 2.35 | 0.59 |
| 13:3:250:LEU:HD21 | 22:3:614:CLA:HMC3 | 1.83 | 0.59 |
| 19:2:203:VAL:O | 19:2:203:VAL:HG12 | 2.02 | 0.59 |
| 12:Z:158:PHE:HZ | 22:Z:608:CLA:NC | 2.00 | 0.59 |
| 16:4:200:PRO:HD2 | 30:4:619:LUT:H23 | 1.84 | 0.59 |
| 17:5:219:LEU:HD21 | 22:5:614:CLA:HMC3 | 1.85 | 0.59 |
| 18:6:54:PRO:HD2 | 30:6:624:LUT:H23 | 1.84 | 0.59 |
| 22:1:610:CLA:HBB1 | 30:1:617:LUT:H32 | 1.85 | 0.58 |
| 14:7:97:LEU:HD23 | 22:7:620:CLA:C2A | 2.33 | 0.58 |
| 25:4:621:BCR:H331 | 25:4:621:BCR:C8 | 2.32 | 0.58 |
| 19:2:32:TYR:CZ | 19:2:35:ALA:CA | 2.86 | 0.58 |
| 2:B:374:THR:HG22 | 22:B:827:CLA:HAB | 1.85 | 0.58 |
| 16:4:208:ILE:HG23 | 16:4:212:LYS:HE3 | 1.83 | 0.58 |
| 22:A:805:CLA:CBB | 22:A:812:CLA:H142 | 2.33 | 0.58 |
| 14:7:97:LEU:CD2 | 22:7:620:CLA:H2A | 2.34 | 0.58 |
| 22:8:604:CLA:HBB1 | 25:8:619:BCR:H393 | 1.85 | 0.58 |
| 1:A:130:ASP:OD2 | 6:F:93:GLN:NE2 | 2.37 | 0.58 |
| 22:4:613:CLA:H2 | 22:4:614:CLA:HMD1 | 1.86 | 0.58 |
| 18:6:75:SER:HB2 | 18:6:180:GLY:HA3 | 1.85 | 0.58 |
| 22:B:837:CLA:H162 | 25:F:305:BCR:H383 | 1.86 | 0.58 |
| 15:8:172:PRO:HA | 12:Z:62:LEU:HD22 | 1.86 | 0.58 |
| 22:8:613:CLA:H2 | 22:8:614:CLA:HMD1 | 1.85 | 0.58 |
| 15:8:41:ASP:OD1 | 15:8:46:GLN:NE2 | 2.36 | 0.58 |
| 15:8:224:HIS:CD2 | 22:8:614:CLA:NC | 2.71 | 0.58 |
| 29:4:606:CHL:HBA2 | 25:4:621:BCR:H19C | 1.86 | 0.58 |
| 22:A:815:CLA:H111 | 22:3:607:CLA:CBB | 2.33 | 0.58 |
| 22:B:838:CLA:HBA2 | 22:B:841:CLA:H203 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:L:186:TYR:C | 11:L:188:CYS:N | 2.41 | 0.58 |
| 22:A:802:CLA:HBB1 | 22:A:802:CLA:HMB1 | 1.86 | 0.57 |
| 22:7:620:CLA:HBB1 | 22:7:620:CLA:H93 | 1.86 | 0.57 |
| 16:4:213:LEU:HD22 | 22:4:611:CLA:HED2 | 1.85 | 0.57 |
| 22:B:826:CLA:H122 | 25:B:846:BCR:H373 | 1.86 | 0.57 |
| 22:B:832:CLA:H192 | 22:B:837:CLA:H121 | 1.86 | 0.57 |
| 22:B:839:CLA:HBB2 | 23:B:842:PQN:H141 | 1.84 | 0.57 |
| 22:B:840:CLA:H191 | 8:I:89:ALA:HA | 1.87 | 0.57 |
| 14:7:55:PRO:HD2 | 30:7:622:LUT:H23 | 1.86 | 0.57 |
| 19:2:189:HIS:CG | 22:2:613:CLA:CAA | 2.80 | 0.57 |
| 15:8:134:GLU:OE1 | 15:8:134:GLU:HA | 2.04 | 0.57 |
| 2:B:547:LEU:O | 2:B:565:ARG:NH2 | 2.38 | 0.57 |
| 1:A:45:THR:HG23 | 5:E:78:GLN:HE21 | 1.67 | 0.57 |
| 29:5:607:CHL:H42 | 25:5:625:BCR:H383 | 1.85 | 0.57 |
| 19:2:218:PRO:HG2 | 22:2:601:CLA:HMA2 | 1.85 | 0.57 |
| 1:A:125:GLU:OE1 | 6:F:107:THR:OG1 | 2.22 | 0.57 |
| 1:A:736:ILE:HG21 | 22:A:829:CLA:HMC2 | 1.87 | 0.57 |
| 22:A:805:CLA:HAA1 | 22:A:805:CLA:HBD | 1.86 | 0.57 |
| 2:B:152:PHE:CE1 | 19:2:220:ILE:HD13 | 2.40 | 0.57 |
| 2:B:546:LYS:HD2 | 5:E:51:TYR:HA | 1.87 | 0.57 |
| 16:4:207:ASP:CB | 16:4:209:LYS:HG2 | 2.34 | 0.57 |
| 22:6:602:CLA:H61 | 30:6:624:LUT:H28 | 1.86 | 0.57 |
| 20:9:205:HIS:ND1 | 20:9:208:GLU:OE2 | 2.35 | 0.57 |
| 22:A:820:CLA:HAB | 22:A:820:CLA:H8 | 1.86 | 0.56 |
| 15:8:242:PHE:CD2 | 15:8:243:LEU:HG | 2.39 | 0.56 |
| 22:A:802:CLA:H91 | 22:A:802:CLA:C12 | 2.35 | 0.56 |
| 22:A:823:CLA:HMD2 | 25:K:4001:BCR:H24C | 1.88 | 0.56 |
| 2:B:375:HIS:HE2 | 22:B:828:CLA:C1B | 2.18 | 0.56 |
| 12:Z:160:PRO:HD2 | 30:Z:617:LUT:H23 | 1.87 | 0.56 |
| 18:6:95:VAL:HG11 | 22:6:604:CLA:HED2 | 1.87 | 0.56 |
| 16:4:221:LEU:HD11 | 22:4:611:CLA:HAC1 | 1.88 | 0.56 |
| 16:4:106:PHE:CZ | 29:4:608:CHL:HED2 | 2.40 | 0.56 |
| 22:B:822:CLA:HHC | 22:B:841:CLA:HED1 | 1.88 | 0.56 |
| 15:8:198:LEU:HD23 | 30:8:617:LUT:H11 | 1.86 | 0.56 |
| 18:6:255:LEU:O | 22:6:622:CLA:HMA3 | 2.05 | 0.56 |
| 22:A:841:CLA:H2 | 22:B:832:CLA:H42 | 1.88 | 0.56 |
| 22:1:610:CLA:H52 | 30:1:617:LUT:H30 | 1.87 | 0.56 |
| 16:4:247:HIS:CD2 | 22:4:614:CLA:NC | 2.73 | 0.56 |
| 2:B:281:ILE:HD12 | 22:B:818:CLA:HBB1 | 1.88 | 0.56 |
| 25:F:305:BCR:H331 | 25:F:305:BCR:HC8 | 1.88 | 0.56 |
| 22:7:601:CLA:H171 | 22:7:613:CLA:HBC1 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:835:CLA:H2 | 11:L:99:PRO:HB2 | 1.87 | 0.56 |
| 2:B:276:HIS:CE1 | 22:B:816:CLA:C1A | 2.88 | 0.56 |
| 13:3:245:ASN:HD22 | 22:3:613:CLA:HED2 | 1.71 | 0.56 |
| 19:2:188:LEU:HD22 | 22:2:613:CLA:HED1 | 1.88 | 0.56 |
| 19:2:211:VAL:HG23 | 19:2:212:ALA:N | 2.20 | 0.56 |
| 22:A:802:CLA:H3A | 22:A:802:CLA:O2A | 2.06 | 0.55 |
| 4:D:140:ARG:HB3 | 4:D:148:GLN:HB3 | 1.88 | 0.55 |
| 19:2:217:LEU:O | 19:2:217:LEU:HD12 | 2.06 | 0.55 |
| 22:A:835:CLA:HHC | 22:A:835:CLA:CBB | 2.35 | 0.55 |
| 22:B:821:CLA:HMD2 | 25:B:843:BCR:HC7 | 1.88 | 0.55 |
| 6:F:223:THR:HB | 6:F:227:ARG:NH2 | 2.20 | 0.55 |
| 22:3:620:CLA:HMC2 | 22:3:620:CLA:H92 | 1.88 | 0.55 |
| 2:B:54:GLN:HE21 | 2:B:58:ILE:HG13 | 1.72 | 0.55 |
| 22:A:815:CLA:HHC | 22:A:815:CLA:CBB | 2.26 | 0.55 |
| 11:L:57:THR:HG22 | 11:L:58:PRO:HD2 | 1.89 | 0.55 |
| 2:B:437:LEU:HD12 | 22:B:833:CLA:HAB | 1.89 | 0.55 |
| 22:4:604:CLA:C1C | 25:4:621:BCR:C39 | 2.85 | 0.55 |
| 17:5:203:GLN:OE1 | 30:5:620:LUT:H42 | 2.07 | 0.55 |
| 18:6:216:THR:H | 18:6:219:SER:HB2 | 1.72 | 0.55 |
| 22:B:820:CLA:C1C | 22:B:820:CLA:H71 | 2.37 | 0.55 |
| 12:Z:137:ALA:HB2 | 22:Z:606:CLA:H52 | 1.88 | 0.55 |
| 20:9:81:VAL:HG11 | 30:9:616:LUT:H12 | 1.89 | 0.54 |
| 16:4:226:PHE:CZ | 30:4:620:LUT:H10 | 2.43 | 0.54 |
| 29:4:606:CHL:CAA | 25:4:621:BCR:H21C | 2.37 | 0.54 |
| 3:C:61:ASP:O | 5:E:86:ASN:ND2 | 2.38 | 0.54 |
| 22:6:616:CLA:HBB2 | 22:6:622:CLA:HMD3 | 1.88 | 0.54 |
| 22:A:802:CLA:CGA | 22:A:802:CLA:C3A | 2.85 | 0.54 |
| 22:B:813:CLA:H42 | 25:B:844:BCR:H21C | 1.90 | 0.54 |
| 6:F:224:VAL:CG1 | 6:F:225:SER:H | 2.18 | 0.54 |
| 25:F:305:BCR:H383 | 25:F:305:BCR:C23 | 2.36 | 0.54 |
| 16:4:232:GLN:HG2 | 22:4:613:CLA:ND | 2.22 | 0.54 |
| 22:5:617:CLA:HED3 | 24:6:619:LHG:H142 | 1.89 | 0.54 |
| 20:9:206:LEU:O | 20:9:206:LEU:HD23 | 2.07 | 0.54 |
| 22:B:830:CLA:HBB2 | 22:B:838:CLA:HMC2 | 1.90 | 0.54 |
| 22:A:807:CLA:H151 | 22:A:830:CLA:HBB2 | 1.90 | 0.54 |
| 22:A:811:CLA:H12 | 22:A:813:CLA:H43 | 1.90 | 0.54 |
| 25:F:305:BCR:C23 | 25:F:305:BCR:C38 | 2.85 | 0.54 |
| 22:4:611:CLA:HBC3 | 24:4:622:LHG:HC62 | 1.90 | 0.54 |
| 2:B:192:THR:HG21 | 2:B:279:LEU:HB2 | 1.89 | 0.54 |
| 16:4:81:PHE:CZ | 22:4:601:CLA:HAB | 2.42 | 0.54 |
| 25:5:622:BCR:HC32 | 24:6:619:LHG:O9 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:4:160:VAL:HG21 | 25:4:621:BCR:H16C | 1.89 | 0.54 |
| 22:5:617:CLA:HMB2 | 22:6:622:CLA:HBC3 | 1.88 | 0.54 |
| 22:1:603:CLA:HBC1 | 29:1:607:CHL:HBB2 | 1.90 | 0.53 |
| 18:6:156:TYR:HB3 | 22:6:610:CLA:HED2 | 1.90 | 0.53 |
| 1:A:265:PHE:HA | 22:K:4003:CLA:HBC3 | 1.91 | 0.53 |
| 1:A:399:GLY:HA3 | 1:A:603:LEU:HD11 | 1.90 | 0.53 |
| 18:6:199:LYS:HE2 | 18:6:203:ALA:HB1 | 1.91 | 0.53 |
| 29:5:608:CHL:H12 | 30:5:620:LUT:H383 | 1.89 | 0.53 |
| 19:2:205:PRO:O | 19:2:209:VAL:HG23 | 2.08 | 0.53 |
| 22:A:804:CLA:HBB2 | 22:A:812:CLA:H72 | 1.90 | 0.53 |
| 2:B:352:HIS:ND1 | 22:B:817:CLA:OBD | 2.40 | 0.53 |
| 12:1:158:PHE:CZ | 22:1:608:CLA:NC | 2.76 | 0.53 |
| 14:7:221:ASP:HB3 | 14:7:229:VAL:HG11 | 1.91 | 0.53 |
| 16:4:217:LYS:NZ | 22:4:611:CLA:O1D | 2.29 | 0.53 |
| 22:4:601:CLA:HBB1 | 24:4:622:LHG:H272 | 1.89 | 0.53 |
| 22:A:802:CLA:H91 | 25:A:852:BCR:C21 | 2.38 | 0.53 |
| 12:1:153:TYR:HE1 | 12:1:177:GLU:OE1 | 1.91 | 0.53 |
| 22:Z:610:CLA:H52 | 30:Z:617:LUT:H30 | 1.90 | 0.53 |
| 22:6:611:CLA:HBC3 | 24:6:619:LHG:HC62 | 1.91 | 0.53 |
| 19:2:32:TYR:CE2 | 19:2:35:ALA:HA | 2.43 | 0.53 |
| 22:9:613:CLA:H2 | 22:9:614:CLA:HMD1 | 1.90 | 0.53 |
| 2:B:41:GLU:HG2 | 2:B:166:LEU:HB2 | 1.90 | 0.53 |
| 22:3:612:CLA:HHC | 22:3:612:CLA:HBB1 | 1.90 | 0.53 |
| 1:A:684:MET:HB2 | 22:A:802:CLA:C1C | 2.39 | 0.53 |
| 2:B:423:LEU:HD13 | 2:B:533:LEU:HA | 1.91 | 0.53 |
| 22:4:610:CLA:HBB1 | 30:4:619:LUT:H32 | 1.91 | 0.53 |
| 17:5:247:ILE:HD11 | 25:5:625:BCR:H351 | 1.89 | 0.53 |
| 1:A:458:HIS:CE1 | 22:A:835:CLA:NA | 2.77 | 0.53 |
| 1:A:487:ILE:HD11 | 22:A:838:CLA:H2 | 1.91 | 0.53 |
| 1:A:501:ASN:HB2 | 22:A:837:CLA:HED2 | 1.89 | 0.53 |
| 22:A:854:CLA:HBC2 | 2:B:586:ASN:HB2 | 1.91 | 0.53 |
| 2:B:335:LEU:HD11 | 22:B:829:CLA:HBB1 | 1.90 | 0.53 |
| 6:F:179:LYS:HB2 | 6:F:182:ASP:HB2 | 1.90 | 0.53 |
| 24:8:620:LHG:H271 | 24:8:620:LHG:HC91 | 1.91 | 0.53 |
| 22:B:805:CLA:C4B | 22:B:829:CLA:HMB2 | 2.38 | 0.52 |
| 16:4:160:VAL:CG2 | 25:4:621:BCR:H16C | 2.39 | 0.52 |
| 25:4:621:BCR:C33 | 25:4:621:BCR:C8 | 2.85 | 0.52 |
| 17:5:133:GLU:OE1 | 17:5:133:GLU:HA | 2.08 | 0.52 |
| 17:5:197:TYR:CD2 | 30:5:624:LUT:H12 | 2.44 | 0.52 |
| 1:A:330:ARG:HE | 1:A:336:GLU:HA | 1.75 | 0.52 |
| 2:B:698:PRO:O | 3:C:81:TYR:OH | 2.19 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:3:228:MET:HG2 | 30:3:622:LUT:H12 | 1.90 | 0.52 |
| 12:Z:50:PRO:O | 12:Z:56:ASN:ND2 | 2.43 | 0.52 |
| 22:5:613:CLA:HHC | 22:5:613:CLA:HBB1 | 1.90 | 0.52 |
| 22:A:807:CLA:HBB | 22:A:831:CLA:HAB | 1.91 | 0.52 |
| 22:A:815:CLA:H111 | 22:3:607:CLA:HBB1 | 1.90 | 0.52 |
| 2:B:416:LYS:HA | 2:B:419:LEU:HD12 | 1.91 | 0.52 |
| 15:8:56:PRO:HD2 | 30:8:618:LUT:H23 | 1.91 | 0.52 |
| 15:8:203:PHE:CD2 | 30:8:618:LUT:H12 | 2.44 | 0.52 |
| 16:4:150:PHE:HB2 | 29:4:607:CHL:HBC1 | 1.90 | 0.52 |
| 25:5:622:BCR:C3 | 24:6:619:LHG:O9 | 2.58 | 0.52 |
| 2:B:54:GLN:HB2 | 22:B:805:CLA:HMB2 | 1.92 | 0.52 |
| 12:1:118:TRP:HE1 | 30:1:619:LUT:HO3 | 1.51 | 0.52 |
| 22:A:805:CLA:HBB1 | 22:A:807:CLA:OBD | 2.08 | 0.52 |
| 22:A:843:CLA:H202 | 11:L:96:LEU:HD21 | 1.90 | 0.52 |
| 22:B:831:CLA:HAC1 | 22:B:838:CLA:HBC3 | 1.92 | 0.52 |
| 6:F:189:VAL:HG13 | 22:F:301:CLA:H122 | 1.90 | 0.52 |
| 12:1:61:PRO:HD2 | 30:1:618:LUT:H23 | 1.92 | 0.52 |
| 22:A:802:CLA:C1B | 22:A:854:CLA:HAB | 2.40 | 0.52 |
| 12:1:74:PHE:HB3 | 22:1:602:CLA:HBB | 1.92 | 0.52 |
| 22:7:604:CLA:C1B | 25:7:623:BCR:H281 | 2.21 | 0.52 |
| 22:A:840:CLA:HBA2 | 24:A:847:LHG:H221 | 1.92 | 0.52 |
| 2:B:627:LEU:O | 2:B:733:ARG:NH2 | 2.40 | 0.52 |
| 22:B:840:CLA:HBB1 | 25:B:848:BCR:H363 | 1.90 | 0.52 |
| 20:9:175:GLN:OE1 | 30:9:616:LUT:H42 | 2.09 | 0.52 |
| 22:A:835:CLA:HAA1 | 22:A:835:CLA:HBD | 1.91 | 0.52 |
| 22:B:826:CLA:H13 | 25:B:847:BCR:H15C | 1.92 | 0.52 |
| 14:7:97:LEU:HD22 | 22:7:620:CLA:O1D | 2.10 | 0.52 |
| 8:I:83:THR:HG22 | 8:I:87:LEU:HD12 | 1.92 | 0.52 |
| 12:1:197:ALA:HB2 | 22:1:616:CLA:HED2 | 1.90 | 0.52 |
| 22:1:602:CLA:H72 | 30:1:618:LUT:H28 | 1.91 | 0.52 |
| 1:A:704:HIS:HE1 | 22:A:841:CLA:C4D | 2.23 | 0.52 |
| 2:B:524:ILE:HG12 | 2:B:591:VAL:HG12 | 1.91 | 0.52 |
| 22:B:831:CLA:CBC | 25:F:305:BCR:H362 | 2.29 | 0.52 |
| 22:A:802:CLA:H192 | 22:A:842:CLA:H41 | 1.86 | 0.51 |
| 29:6:606:CHL:H51 | 29:6:608:CHL:HMB2 | 1.92 | 0.51 |
| 22:B:825:CLA:H92 | 22:B:836:CLA:H41 | 1.92 | 0.51 |
| 19:2:210:THR:O | 19:2:214:LEU:HG | 2.10 | 0.51 |
| 19:2:218:PRO:HG3 | 22:2:601:CLA:CMA | 2.41 | 0.51 |
| 22:A:802:CLA:HBC3 | 22:A:802:CLA:HHD | 1.93 | 0.51 |
| 22:3:617:CLA:HBA2 | 22:7:601:CLA:H72 | 1.91 | 0.51 |
| 22:7:606:CLA:HHC | 22:7:606:CLA:HBB1 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:805:CLA:HHC | 22:A:805:CLA:CBB | 2.26 | 0.51 |
| 22:1:611:CLA:HAB | 25:8:619:BCR:H312 | 1.92 | 0.51 |
| 18:6:255:LEU:HD13 | 22:6:622:CLA:HMB3 | 1.93 | 0.51 |
| 1:A:35:PHE:HB2 | 1:A:62:HIS:CD2 | 2.46 | 0.51 |
| 2:B:525:ALA:HB2 | 22:B:837:CLA:HMA1 | 1.93 | 0.51 |
| 6:F:186:ILE:HG12 | 9:J:10:THR:HG22 | 1.92 | 0.51 |
| 15:8:225:LEU:HD21 | 22:8:614:CLA:HMC3 | 1.93 | 0.51 |
| 1:A:147:LEU:HD11 | 22:A:830:CLA:H42 | 1.93 | 0.51 |
| 1:A:451:HIS:HA | 22:A:835:CLA:HAB | 1.93 | 0.51 |
| 22:A:809:CLA:H71 | 22:A:831:CLA:H171 | 1.93 | 0.51 |
| 22:A:829:CLA:H121 | 22:A:854:CLA:H203 | 1.92 | 0.51 |
| 2:B:358:PRO:HG3 | 22:B:818:CLA:HBA1 | 1.93 | 0.51 |
| 7:G:58:ARG:NH2 | 7:G:94:GLY:O | 2.44 | 0.51 |
| 12:Z:83:ARG:NH1 | 22:Z:608:CLA:OBD | 2.40 | 0.51 |
| 25:A:848:BCR:H362 | 25:A:849:BCR:H21C | 1.93 | 0.51 |
| 29:6:606:CHL:HHC | 29:6:606:CHL:HBB1 | 1.92 | 0.51 |
| 1:A:363:LEU:HD11 | 22:A:820:CLA:H71 | 1.93 | 0.50 |
| 17:5:80:TRP:CE2 | 29:5:608:CHL:HED2 | 2.46 | 0.50 |
| 17:5:226:ASN:HD22 | 17:5:227:ILE:H | 1.60 | 0.50 |
| 22:5:606:CLA:H71 | 29:5:608:CHL:HMB2 | 1.93 | 0.50 |
| 22:5:617:CLA:HMB2 | 22:6:622:CLA:CBC | 2.41 | 0.50 |
| 22:A:816:CLA:H101 | 25:3:719:BCR:H14C | 1.93 | 0.50 |
| 22:A:833:CLA:HMB1 | 22:A:843:CLA:HAA2 | 1.93 | 0.50 |
| 6:F:133:LEU:HD22 | 6:F:148:GLU:HB2 | 1.93 | 0.50 |
| 18:6:256:TRP:CG | 22:6:622:CLA:HED2 | 2.46 | 0.50 |
| 2:B:426:VAL:HG21 | 2:B:529:HIS:HD2 | 1.75 | 0.50 |
| 6:F:224:VAL:CG1 | 6:F:225:SER:N | 2.73 | 0.50 |
| 13:3:131:ILE:HG22 | 13:3:134:ALA:H | 1.76 | 0.50 |
| 22:3:606:CLA:HHC | 22:3:606:CLA:HBB1 | 1.94 | 0.50 |
| 29:6:606:CHL:HMB2 | 25:6:623:BCR:H373 | 1.91 | 0.50 |
| 22:A:802:CLA:CHB | 22:A:854:CLA:HAB | 2.42 | 0.50 |
| 22:B:820:CLA:CHB | 22:B:820:CLA:H12 | 2.41 | 0.50 |
| 1:A:481:PRO:HG3 | 1:A:533:PHE:HB2 | 1.92 | 0.50 |
| 25:B:801:BCR:H323 | 22:B:832:CLA:HBB1 | 1.93 | 0.50 |
| 3:C:2:ALA:N | 3:C:71:SER:O | 2.45 | 0.50 |
| 14:7:171:ASP:OD1 | 30:7:621:LUT:O23 | 2.29 | 0.50 |
| 17:5:32:ARG:NH2 | 17:5:52:ASP:O | 2.45 | 0.50 |
| 13:3:63:GLY:HA3 | 13:3:218:ILE:HG21 | 1.93 | 0.50 |
| 16:4:260:ASP:OD1 | 22:4:616:CLA:C4B | 2.51 | 0.50 |
| 22:A:841:CLA:HBC1 | 23:A:844:PQN:H201 | 1.93 | 0.50 |
| 22:4:604:CLA:C1C | 25:4:621:BCR:H391 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:412:MET:HG3 | 25:B:846:BCR:H402 | 1.93 | 0.50 |
| 22:B:805:CLA:HHC | 22:B:805:CLA:HBB1 | 1.94 | 0.50 |
| 3:C:4:ILE:HB | 3:C:68:TYR:HB2 | 1.93 | 0.50 |
| 10:K:35:ASN:ND2 | 22:K:4003:CLA:OBD | 2.45 | 0.50 |
| 13:3:164:GLN:OE1 | 13:3:167:ARG:NH2 | 2.43 | 0.50 |
| 15:8:154:LEU:HB2 | 22:Z:603:CLA:H2 | 1.93 | 0.50 |
| 16:4:157:PHE:HZ | 25:4:621:BCR:H373 | 1.76 | 0.50 |
| 1:A:18:ASP:OD2 | 1:A:71:ARG:NH2 | 2.41 | 0.50 |
| 22:A:835:CLA:H72 | 25:L:201:BCR:H14C | 1.93 | 0.50 |
| 4:D:125:THR:HG23 | 4:D:136:PRO:HG2 | 1.93 | 0.50 |
| 12:1:123:VAL:HG11 | 22:1:606:CLA:HMD1 | 1.93 | 0.50 |
| 13:3:141:TRP:NE1 | 22:3:606:CLA:OBD | 2.34 | 0.50 |
| 17:5:170:ASP:OD1 | 30:5:620:LUT:O23 | 2.27 | 0.50 |
| 17:5:245:LEU:HD13 | 18:6:224:VAL:HG21 | 1.92 | 0.50 |
| 22:2:610:CLA:HBB1 | 30:2:616:LUT:H32 | 1.93 | 0.50 |
| 2:B:340:ALA:HB2 | 25:B:847:BCR:H372 | 1.92 | 0.49 |
| 25:5:622:BCR:HC42 | 24:6:619:LHG:HC82 | 1.93 | 0.49 |
| 19:2:209:VAL:O | 19:2:213:VAL:CG2 | 2.44 | 0.49 |
| 3:C:34:CYS:HA | 5:E:67:VAL:HG23 | 1.94 | 0.49 |
| 4:D:128:LEU:HA | 4:D:132:PHE:HD2 | 1.77 | 0.49 |
| 22:F:303:CLA:HHC | 22:F:303:CLA:HBB1 | 1.92 | 0.49 |
| 15:8:233:TYR:CD1 | 22:8:613:CLA:H12 | 2.47 | 0.49 |
| 16:4:159:TRP:HH2 | 25:4:621:BCR:H333 | 1.77 | 0.49 |
| 1:A:658:ILE:HG13 | 1:A:659:GLN:HG3 | 1.94 | 0.49 |
| 22:A:832:CLA:HBA2 | 24:A:847:LHG:HC92 | 1.94 | 0.49 |
| 12:1:142:GLU:HG3 | 22:1:609:CLA:C4B | 2.43 | 0.49 |
| 22:6:604:CLA:H171 | 22:6:610:CLA:HBC1 | 1.93 | 0.49 |
| 22:A:805:CLA:H43 | 22:A:812:CLA:CBB | 2.27 | 0.49 |
| 2:B:277:HIS:HB2 | 22:B:817:CLA:C1B | 2.42 | 0.49 |
| 13:3:102:ALA:HA | 13:3:231:TYR:HE2 | 1.76 | 0.49 |
| 19:2:219:MET:HE3 | 22:9:609:CLA:C3A | 2.42 | 0.49 |
| 22:B:812:CLA:HHC | 22:B:812:CLA:HBB1 | 1.94 | 0.49 |
| 22:5:606:CLA:HMB2 | 25:5:622:BCR:H373 | 1.94 | 0.49 |
| 25:3:717:BCR:HC31 | 22:7:601:CLA:HBC2 | 1.94 | 0.49 |
| 12:Z:142:GLU:HA | 12:Z:142:GLU:OE1 | 2.12 | 0.49 |
| 16:4:203:TRP:O | 16:4:204:SER:CB | 2.61 | 0.49 |
| 16:4:208:ILE:HA | 16:4:211:LEU:HB2 | 1.93 | 0.49 |
| 18:6:123:TRP:CE2 | 25:6:623:BCR:H10C | 2.48 | 0.49 |
| 19:2:156:LYS:HD3 | 22:2:612:CLA:HAA2 | 1.95 | 0.49 |
| 22:A:818:CLA:CHD | 22:A:819:CLA:HBB2 | 2.43 | 0.49 |
| 22:B:831:CLA:HMD3 | 22:B:841:CLA:C9 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:4:130:ALA:HB1 | 16:4:132:VAL:HG23 | 1.95 | 0.49 |
| 29:4:606:CHL:CGA | 25:4:621:BCR:H21C | 2.43 | 0.49 |
| 22:5:604:CLA:HMB3 | 30:5:624:LUT:H162 | 1.95 | 0.49 |
| 22:6:614:CLA:HED1 | 24:6:619:LHG:C22 | 2.43 | 0.49 |
| 22:A:835:CLA:HBB1 | 22:A:835:CLA:CHC | 2.40 | 0.49 |
| 22:B:807:CLA:H12 | 8:I:83:THR:HG21 | 1.95 | 0.49 |
| 6:F:123:LEU:HD21 | 9:J:38:VAL:HG11 | 1.94 | 0.49 |
| 22:1:613:CLA:H2 | 22:1:614:CLA:OBD | 2.13 | 0.49 |
| 14:7:47:LEU:HD11 | 14:7:65:LEU:HD21 | 1.93 | 0.49 |
| 15:8:115:SER:OG | 15:8:116:PHE:N | 2.46 | 0.49 |
| 19:2:206:GLU:O | 19:2:210:THR:CG2 | 2.60 | 0.49 |
| 25:A:856:BCR:HC22 | 9:J:31:ARG:HH11 | 1.78 | 0.49 |
| 22:B:820:CLA:C4B | 22:B:820:CLA:H62 | 2.42 | 0.49 |
| 20:9:201:TYR:O | 20:9:205:HIS:HB2 | 2.12 | 0.49 |
| 22:A:843:CLA:H121 | 22:B:839:CLA:H102 | 1.95 | 0.48 |
| 16:4:106:PHE:CE1 | 29:4:608:CHL:HED2 | 2.47 | 0.48 |
| 17:5:226:ASN:ND2 | 22:5:614:CLA:O1D | 2.44 | 0.48 |
| 19:2:32:TYR:HE2 | 19:2:35:ALA:CB | 2.07 | 0.48 |
| 1:A:212:ALA:O | 22:A:815:CLA:HMC3 | 2.13 | 0.48 |
| 1:A:216:HIS:HB2 | 22:A:815:CLA:C1C | 2.42 | 0.48 |
| 4:D:88:TRP:HB3 | 4:D:136:PRO:HB3 | 1.95 | 0.48 |
| 11:L:131:CYS:HB3 | 25:L:205:BCR:H19C | 1.95 | 0.48 |
| 22:A:843:CLA:HAB | 2:B:692:VAL:HG11 | 1.95 | 0.48 |
| 22:B:839:CLA:H151 | 11:L:127:ILE:HG21 | 1.95 | 0.48 |
| 12:1:137:ALA:HB2 | 22:1:606:CLA:H52 | 1.95 | 0.48 |
| 22:1:613:CLA:H101 | 24:1:620:LHG:H301 | 1.94 | 0.48 |
| 13:3:159:GLU:CD | 13:3:162:ARG:HH21 | 2.14 | 0.48 |
| 29:4:618:CHL:HAB | 25:4:621:BCR:C11 | 2.42 | 0.48 |
| 18:6:127:ARG:HH21 | 29:6:618:CHL:HMC | 1.78 | 0.48 |
| 19:2:32:TYR:CE2 | 19:2:35:ALA:HB1 | 2.35 | 0.48 |
| 1:A:122:VAL:HB | 22:B:833:CLA:HMD1 | 1.95 | 0.48 |
| 22:A:821:CLA:HBB1 | 25:K:4001:BCR:H14C | 1.95 | 0.48 |
| 2:B:214:LEU:O | 20:9:180:ARG:NH1 | 2.46 | 0.48 |
| 22:B:811:CLA:O2D | 20:9:62:ARG:NH2 | 2.46 | 0.48 |
| 14:7:160:LEU:HD23 | 14:7:161:GLU:HG3 | 1.94 | 0.48 |
| 16:4:111:VAL:HG11 | 30:4:619:LUT:H10 | 1.94 | 0.48 |
| 17:5:242:VAL:HG11 | 25:5:625:BCR:H353 | 1.94 | 0.48 |
| 4:D:97:GLU:H | 4:D:127:GLN:HE22 | 1.61 | 0.48 |
| 14:7:223:LEU:HD21 | 22:7:614:CLA:HMC3 | 1.94 | 0.48 |
| 18:6:256:TRP:O | 22:6:622:CLA:O2D | 2.30 | 0.48 |
| 1:A:219:HIS:CE1 | 22:A:816:CLA:ND | 2.82 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:815:CLA:C2 | 22:A:817:CLA:HMB2 | 2.28 | 0.48 |
| 20:9:56:LEU:HD13 | 22:9:602:CLA:H42 | 1.96 | 0.48 |
| 22:9:611:CLA:HBA2 | 22:9:612:CLA:HMD1 | 1.96 | 0.48 |
| 22:A:808:CLA:H41 | 22:A:808:CLA:H61 | 1.57 | 0.48 |
| 12:1:159:ASP:OD1 | 30:1:617:LUT:O23 | 2.29 | 0.48 |
| 22:8:610:CLA:H52 | 30:8:617:LUT:H30 | 1.95 | 0.48 |
| 16:4:98:GLN:NE2 | 16:4:191:PRO:O | 2.44 | 0.48 |
| 16:4:104:ALA:HB1 | 16:4:219:GLY:HA3 | 1.96 | 0.48 |
| 16:4:256:VAL:HG23 | 22:4:613:CLA:O1A | 2.14 | 0.48 |
| 2:B:43:LEU:HD22 | 4:D:186:PHE:HZ | 1.79 | 0.48 |
| 22:1:603:CLA:CBC | 29:1:607:CHL:HBB2 | 2.44 | 0.48 |
| 22:1:606:CLA:H61 | 22:1:606:CLA:H41 | 1.63 | 0.48 |
| 16:4:149:LEU:HD21 | 29:4:606:CHL:HMD3 | 1.96 | 0.48 |
| 29:5:607:CHL:HBB2 | 22:5:609:CLA:HAC2 | 1.95 | 0.48 |
| 1:A:75:SER:HB3 | 22:A:812:CLA:HHD | 1.95 | 0.47 |
| 22:B:814:CLA:HMA1 | 25:B:845:BCR:H402 | 1.96 | 0.47 |
| 12:1:188:PHE:CD2 | 30:1:618:LUT:H12 | 2.49 | 0.47 |
| 22:1:602:CLA:H52 | 30:1:618:LUT:H28 | 1.95 | 0.47 |
| 22:5:602:CLA:H102 | 22:5:603:CLA:HMB3 | 1.96 | 0.47 |
| 22:A:841:CLA:H92 | 25:B:801:BCR:H15C | 1.96 | 0.47 |
| 17:5:197:TYR:CE2 | 30:5:624:LUT:H10 | 2.48 | 0.47 |
| 22:5:613:CLA:H2 | 22:5:614:CLA:HMD1 | 1.97 | 0.47 |
| 1:A:422:ASN:HD21 | 1:A:427:LEU:HD23 | 1.79 | 0.47 |
| 23:A:844:PQN:H162 | 25:B:801:BCR:H382 | 1.95 | 0.47 |
| 22:B:812:CLA:H2 | 22:B:812:CLA:H61 | 1.72 | 0.47 |
| 4:D:62:THR:HB | 4:D:112:LEU:HD22 | 1.96 | 0.47 |
| 22:Z:606:CLA:H41 | 22:Z:606:CLA:H61 | 1.66 | 0.47 |
| 22:Z:613:CLA:H93 | 24:Z:620:LHG:H321 | 1.96 | 0.47 |
| 16:4:156:LEU:HD12 | 25:4:621:BCR:C14 | 2.44 | 0.47 |
| 22:5:617:CLA:CMB | 22:6:622:CLA:HBC1 | 2.45 | 0.47 |
| 1:A:353:LEU:HD11 | 22:A:831:CLA:HBB1 | 1.97 | 0.47 |
| 22:A:836:CLA:HHC | 22:A:836:CLA:HBB1 | 1.97 | 0.47 |
| 13:3:182:ALA:HA | 13:3:185:LYS:HE2 | 1.96 | 0.47 |
| 17:5:133:GLU:HG3 | 22:5:609:CLA:C4B | 2.43 | 0.47 |
| 2:B:325:ASP:O | 2:B:329:ASN:ND2 | 2.47 | 0.47 |
| 22:B:832:CLA:H152 | 6:F:157:LEU:HD22 | 1.96 | 0.47 |
| 7:G:52:VAL:HG11 | 12:1:140:ALA:HA | 1.96 | 0.47 |
| 22:1:610:CLA:H13 | 30:1:617:LUT:H403 | 1.96 | 0.47 |
| 12:Z:61:PRO:HD2 | 30:Z:618:LUT:H23 | 1.96 | 0.47 |
| 17:5:133:GLU:HG3 | 22:5:609:CLA:NB | 2.29 | 0.47 |
| 17:5:202:LEU:HG | 22:5:613:CLA:HAC2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:9:123:GLU:HG3 | 22:9:609:CLA:C4B | 2.44 | 0.47 |
| 22:A:808:CLA:HMB3 | 22:A:809:CLA:HBB | 1.96 | 0.47 |
| 22:A:835:CLA:C4 | 25:L:201:BCR:C36 | 2.86 | 0.47 |
| 22:B:820:CLA:HHC | 22:B:820:CLA:CBB | 2.16 | 0.47 |
| 19:2:211:VAL:CG2 | 19:2:212:ALA:N | 2.77 | 0.47 |
| 22:2:611:CLA:H41 | 22:2:611:CLA:H61 | 1.66 | 0.47 |
| 22:B:841:CLA:HHC | 22:B:841:CLA:CBB | 2.23 | 0.47 |
| 13:3:95:ALA:HB1 | 13:3:221:GLY:HA3 | 1.97 | 0.47 |
| 30:9:616:LUT:H35 | 30:9:616:LUT:H401 | 1.80 | 0.47 |
| 1:A:131:VAL:HG12 | 1:A:139:GLN:HG2 | 1.96 | 0.47 |
| 1:A:304:LEU:HD21 | 22:A:828:CLA:H192 | 1.97 | 0.47 |
| 2:B:464:ILE:HD11 | 22:B:836:CLA:H2 | 1.97 | 0.47 |
| 22:B:823:CLA:HAB | 22:B:830:CLA:HMD2 | 1.97 | 0.47 |
| 19:2:218:PRO:CG | 22:2:601:CLA:CMA | 2.93 | 0.47 |
| 1:A:297:HIS:HB2 | 22:A:819:CLA:CHB | 2.45 | 0.47 |
| 22:A:842:CLA:HAC1 | 23:A:844:PQN:H172 | 1.97 | 0.47 |
| 2:B:550:ASP:OD2 | 4:D:175:ILE:HD11 | 2.15 | 0.47 |
| 14:7:134:LYS:HB3 | 22:7:608:CLA:HMC3 | 1.96 | 0.47 |
| 22:5:602:CLA:H122 | 30:5:624:LUT:H371 | 1.97 | 0.47 |
| 18:6:162:ALA:HB2 | 22:6:610:CLA:HBD | 1.97 | 0.47 |
| 22:A:811:CLA:H111 | 22:A:811:CLA:H152 | 1.76 | 0.47 |
| 25:F:305:BCR:C8 | 25:F:305:BCR:C33 | 2.85 | 0.47 |
| 12:Z:40:LEU:HD12 | 29:Z:601:CHL:HMA3 | 1.97 | 0.47 |
| 16:4:159:TRP:CH2 | 25:4:621:BCR:H333 | 2.49 | 0.47 |
| 22:A:802:CLA:HED3 | 25:B:801:BCR:H401 | 1.96 | 0.46 |
| 2:B:66:LEU:HD11 | 25:B:845:BCR:H271 | 1.97 | 0.46 |
| 2:B:549:PRO:HD2 | 3:C:62:PHE:CZ | 2.51 | 0.46 |
| 17:5:78:ALA:HB1 | 17:5:190:GLY:HA3 | 1.97 | 0.46 |
| 22:5:610:CLA:CBB | 30:5:620:LUT:H32 | 2.45 | 0.46 |
| 22:6:601:CLA:HBB1 | 24:6:619:LHG:H261 | 1.97 | 0.46 |
| 22:A:842:CLA:H102 | 22:A:842:CLA:H61 | 1.56 | 0.46 |
| 13:3:177:PHE:CE2 | 29:3:608:CHL:HBB2 | 2.50 | 0.46 |
| 22:7:611:CLA:HHC | 22:7:611:CLA:HBB1 | 1.96 | 0.46 |
| 15:8:81:MET:HB2 | 22:8:610:CLA:HMC3 | 1.96 | 0.46 |
| 16:4:215:GLU:HB2 | 22:4:610:CLA:C1B | 2.46 | 0.46 |
| 22:4:604:CLA:C1C | 25:4:621:BCR:H393 | 2.45 | 0.46 |
| 18:6:100:ALA:O | 18:6:104:VAL:HB | 2.16 | 0.46 |
| 22:A:814:CLA:HMB3 | 22:A:814:CLA:H112 | 1.96 | 0.46 |
| 22:A:854:CLA:HBB1 | 2:B:526:LEU:HD21 | 1.97 | 0.46 |
| 25:B:846:BCR:H15C | 25:B:846:BCR:H351 | 1.84 | 0.46 |
| 16:4:204:SER:OG | 22:4:610:CLA:HAA1 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:4:232:GLN:NE2 | 30:4:619:LUT:H42 | 2.30 | 0.46 |
| 18:6:33:LEU:HD21 | 22:6:601:CLA:HMA3 | 1.97 | 0.46 |
| 19:2:49:TYR:HB2 | 22:2:602:CLA:HMD1 | 1.96 | 0.46 |
| 20:9:62:ARG:HD2 | 20:9:66:TYR:CZ | 2.50 | 0.46 |
| 2:B:290:HIS:C | 22:B:820:CLA:HED1 | 2.36 | 0.46 |
| 17:5:247:ILE:HD11 | 25:5:625:BCR:H15C | 1.98 | 0.46 |
| 18:6:256:TRP:HB3 | 22:6:622:CLA:HED1 | 1.98 | 0.46 |
| 29:6:606:CHL:HAA1 | 25:6:623:BCR:H21C | 1.97 | 0.46 |
| 20:9:206:LEU:HD23 | 20:9:206:LEU:C | 2.36 | 0.46 |
| 1:A:198:LEU:HD22 | 22:A:826:CLA:HMD3 | 1.98 | 0.46 |
| 2:B:177:ASN:HD22 | 2:B:294:THR:HG23 | 1.81 | 0.46 |
| 12:1:57:TYR:HB2 | 22:1:602:CLA:HMD1 | 1.98 | 0.46 |
| 12:1:217:ASN:HD21 | 15:8:121:SER:HB2 | 1.80 | 0.46 |
| 16:4:81:PHE:CE1 | 22:4:601:CLA:HAB | 2.51 | 0.46 |
| 17:5:86:ALA:HB2 | 30:5:620:LUT:H401 | 1.97 | 0.46 |
| 17:5:89:LEU:HD22 | 22:5:612:CLA:HBB2 | 1.98 | 0.46 |
| 1:A:320:HIS:HB3 | 1:A:325:ILE:HD11 | 1.98 | 0.46 |
| 2:B:545:SER:HA | 6:F:224:VAL:CG1 | 2.44 | 0.46 |
| 14:7:146:ALA:HB1 | 14:7:155:GLU:H | 1.81 | 0.46 |
| 15:8:153:PHE:HB2 | 15:8:157:GLU:HB3 | 1.97 | 0.46 |
| 16:4:61:TRP:O | 22:4:601:CLA:ND | 2.49 | 0.46 |
| 16:4:255:THR:H | 16:4:258:GLN:HB2 | 1.79 | 0.46 |
| 22:A:815:CLA:CBA | 22:A:817:CLA:HMB3 | 2.46 | 0.46 |
| 17:5:142:ASN:ND2 | 18:6:35:GLY:O | 2.48 | 0.46 |
| 25:5:625:BCR:H351 | 25:5:625:BCR:H15C | 1.66 | 0.46 |
| 25:G:205:BCR:H20C | 25:G:205:BCR:H361 | 1.82 | 0.46 |
| 16:4:106:PHE:CE2 | 29:4:608:CHL:HED2 | 2.51 | 0.46 |
| 29:4:618:CHL:CAB | 25:4:621:BCR:C10 | 2.85 | 0.46 |
| 22:6:616:CLA:HBC3 | 22:6:622:CLA:HMC3 | 1.97 | 0.46 |
| 2:B:276:HIS:HE1 | 22:B:816:CLA:NA | 2.12 | 0.46 |
| 13:3:159:GLU:OE2 | 13:3:162:ARG:CZ | 2.64 | 0.46 |
| 12:Z:153:TYR:HB3 | 22:Z:610:CLA:HED2 | 1.97 | 0.46 |
| 22:A:841:CLA:HHC | 22:A:841:CLA:HBB1 | 1.98 | 0.46 |
| 2:B:204:ARG:NH2 | 2:B:252:GLY:O | 2.49 | 0.46 |
| 13:3:92:VAL:HG21 | 13:3:191:ALA:HB1 | 1.98 | 0.46 |
| 15:8:55:ASP:OD1 | 30:8:618:LUT:O23 | 2.33 | 0.46 |
| 12:Z:142:GLU:HG3 | 22:Z:609:CLA:C4B | 2.46 | 0.46 |
| 22:A:804:CLA:HHC | 22:A:804:CLA:HBB1 | 1.97 | 0.45 |
| 3:C:79:LEU:O | 4:D:77:LYS:NZ | 2.46 | 0.45 |
| 22:Z:602:CLA:H41 | 22:Z:602:CLA:H61 | 1.60 | 0.45 |
| 22:Z:608:CLA:HBB1 | 22:Z:608:CLA:H151 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:5:172:PHE:HD2 | 30:5:620:LUT:H222 | 1.81 | 0.45 |
| 18:6:256:TRP:HB3 | 22:6:622:CLA:CED | 2.47 | 0.45 |
| 1:A:589:TRP:CD1 | 22:A:831:CLA:HMD1 | 2.51 | 0.45 |
| 22:A:816:CLA:H41 | 22:A:816:CLA:H62 | 1.76 | 0.45 |
| 22:A:829:CLA:HBA2 | 22:A:829:CLA:H3A | 1.70 | 0.45 |
| 22:A:835:CLA:HMC2 | 22:B:803:CLA:H101 | 1.98 | 0.45 |
| 22:B:812:CLA:H143 | 22:B:812:CLA:H111 | 1.84 | 0.45 |
| 16:4:232:GLN:NE2 | 30:4:619:LUT:O3 | 2.45 | 0.45 |
| 18:6:69:GLU:HG2 | 18:6:132:LEU:HD12 | 1.97 | 0.45 |
| 18:6:223:VAL:HB | 22:6:616:CLA:C1C | 2.46 | 0.45 |
| 22:A:815:CLA:HBD | 22:A:815:CLA:HAA1 | 1.98 | 0.45 |
| 22:6:614:CLA:HED1 | 24:6:619:LHG:H221 | 1.97 | 0.45 |
| 22:9:602:CLA:CBB | 30:9:617:LUT:H32 | 2.46 | 0.45 |
| 22:A:841:CLA:HED2 | 2:B:421:SER:HB3 | 1.97 | 0.45 |
| 12:1:50:PRO:O | 12:1:56:ASN:ND2 | 2.50 | 0.45 |
| 25:7:623:BCR:H342 | 22:8:614:CLA:H62 | 1.99 | 0.45 |
| 16:4:111:VAL:HG22 | 16:4:229:PHE:HE2 | 1.81 | 0.45 |
| 20:9:116:PHE:HD1 | 22:9:609:CLA:HBB2 | 1.82 | 0.45 |
| 1:A:219:HIS:HE1 | 22:A:816:CLA:C4D | 2.30 | 0.45 |
| 1:A:277:THR:HA | 22:A:818:CLA:HED1 | 1.98 | 0.45 |
| 22:A:807:CLA:HMD1 | 22:A:812:CLA:H141 | 1.98 | 0.45 |
| 2:B:426:VAL:HG21 | 2:B:529:HIS:CD2 | 2.51 | 0.45 |
| 2:B:588:ILE:HA | 2:B:591:VAL:HG22 | 1.97 | 0.45 |
| 22:B:816:CLA:CHD | 22:B:817:CLA:HBB2 | 2.47 | 0.45 |
| 12:1:209:HIS:CD2 | 22:1:614:CLA:NC | 2.84 | 0.45 |
| 22:3:607:CLA:H142 | 22:3:617:CLA:HBB2 | 1.98 | 0.45 |
| 18:6:205:LEU:HD22 | 30:6:621:LUT:H163 | 1.98 | 0.45 |
| 29:7:607:CHL:H61 | 29:7:607:CHL:H41 | 1.78 | 0.45 |
| 16:4:208:ILE:HD11 | 22:4:610:CLA:C2A | 2.46 | 0.45 |
| 1:A:356:ASN:O | 1:A:360:PHE:HB2 | 2.17 | 0.45 |
| 22:A:802:CLA:HAA2 | 22:A:802:CLA:CBD | 2.46 | 0.45 |
| 22:A:816:CLA:H111 | 13:3:232:GLY:HA3 | 1.99 | 0.45 |
| 15:8:132:PHE:CE2 | 25:8:619:BCR:H10C | 2.52 | 0.45 |
| 15:8:143:LYS:HB2 | 15:8:146:SER:HB2 | 1.99 | 0.45 |
| 15:8:190:LEU:HA | 15:8:193:VAL:HG12 | 1.99 | 0.45 |
| 22:8:610:CLA:H91 | 22:8:610:CLA:H111 | 1.83 | 0.45 |
| 16:4:163:ARG:HE | 16:4:174:ALA:HB1 | 1.82 | 0.45 |
| 17:5:133:GLU:HG3 | 22:5:609:CLA:C1B | 2.47 | 0.45 |
| 1:A:226:LYS:HD3 | 1:A:253:LEU:HD23 | 1.98 | 0.45 |
| 22:A:806:CLA:HBA1 | 22:A:806:CLA:H3A | 1.78 | 0.45 |
| 22:A:829:CLA:H52 | 22:A:829:CLA:H8 | 1.75 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:175:ARG:HB2 | 22:B:813:CLA:HBC2 | 1.99 | 0.45 |
| 5:E:55:GLN:HE21 | 6:F:222:ILE:HB | 1.82 | 0.45 |
| 15:8:155:GLY:HA3 | 12:Z:74:PHE:CZ | 2.52 | 0.45 |
| 20:9:171:GLY:O | 20:9:175:GLN:HB3 | 2.17 | 0.45 |
| 1:A:54:ALA:HB2 | 24:A:846:LHG:HC82 | 1.99 | 0.45 |
| 22:B:820:CLA:H3A | 22:B:820:CLA:CGA | 2.47 | 0.45 |
| 25:B:844:BCR:H351 | 25:B:844:BCR:H15C | 1.76 | 0.45 |
| 22:8:606:CLA:HHC | 22:8:606:CLA:HBB1 | 1.99 | 0.45 |
| 22:A:842:CLA:H41 | 22:A:842:CLA:H62 | 1.62 | 0.45 |
| 25:3:717:BCR:H341 | 25:3:717:BCR:H11C | 1.71 | 0.45 |
| 22:8:602:CLA:H52 | 30:8:618:LUT:H28 | 1.99 | 0.45 |
| 16:4:244:LEU:HD22 | 30:4:619:LUT:H163 | 1.98 | 0.45 |
| 25:6:625:BCR:H11C | 25:6:625:BCR:H341 | 1.73 | 0.45 |
| 25:A:856:BCR:H391 | 9:J:12:PRO:HB2 | 1.98 | 0.44 |
| 2:B:194:HIS:HE1 | 22:B:814:CLA:C1A | 2.30 | 0.44 |
| 22:8:613:CLA:HMB3 | 30:8:617:LUT:H162 | 2.00 | 0.44 |
| 30:5:620:LUT:H15 | 30:5:620:LUT:H201 | 1.84 | 0.44 |
| 22:A:822:CLA:HMB2 | 22:A:826:CLA:HMA3 | 1.98 | 0.44 |
| 11:L:74:ALA:HB2 | 22:L:203:CLA:HMD1 | 1.98 | 0.44 |
| 15:8:175:PRO:HD2 | 30:8:617:LUT:H23 | 1.99 | 0.44 |
| 30:4:619:LUT:H401 | 30:4:619:LUT:H35 | 1.77 | 0.44 |
| 22:6:604:CLA:H41 | 22:6:604:CLA:H62 | 1.79 | 0.44 |
| 29:9:607:CHL:HBB1 | 28:9:620:LMG:H121 | 1.99 | 0.44 |
| 22:A:841:CLA:H121 | 22:F:303:CLA:HAC1 | 1.99 | 0.44 |
| 22:7:620:CLA:O2A | 18:6:250:CYS:O | 2.34 | 0.44 |
| 30:8:617:LUT:H401 | 30:8:617:LUT:H35 | 1.83 | 0.44 |
| 29:4:606:CHL:H51 | 29:4:608:CHL:HBB | 1.99 | 0.44 |
| 17:5:122:LEU:HD11 | 22:6:616:CLA:HBA2 | 1.99 | 0.44 |
| 19:2:38:PRO:HG2 | 19:2:52:ASP:HB3 | 1.98 | 0.44 |
| 1:A:425:ASN:OD1 | 1:A:426:LEU:N | 2.48 | 0.44 |
| 1:A:540:ALA:HB2 | 22:A:839:CLA:HMA1 | 1.99 | 0.44 |
| 22:A:834:CLA:HBB2 | 11:L:103:LEU:HD12 | 2.00 | 0.44 |
| 2:B:671:TYR:OH | 22:B:803:CLA:OBD | 2.28 | 0.44 |
| 13:3:78:SER:OG | 13:3:82:ILE:O | 2.34 | 0.44 |
| 13:3:184:PHE:CZ | 29:3:608:CHL:HBB1 | 2.53 | 0.44 |
| 22:3:610:CLA:H141 | 22:3:610:CLA:H162 | 1.86 | 0.44 |
| 25:7:623:BCR:H15C | 25:7:623:BCR:H351 | 1.81 | 0.44 |
| 22:5:606:CLA:HBA2 | 25:5:622:BCR:H19C | 1.99 | 0.44 |
| 22:5:617:CLA:CED | 24:6:619:LHG:H142 | 2.47 | 0.44 |
| 22:A:813:CLA:H41 | 22:A:813:CLA:H62 | 1.83 | 0.44 |
| 25:A:848:BCR:H11C | 25:A:848:BCR:H341 | 1.87 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:19:ARG:HG2 | 4:D:159:GLU:HG2 | 2.00 | 0.44 |
| 25:3:718:BCR:H20C | 25:3:718:BCR:H361 | 1.85 | 0.44 |
| 22:8:612:CLA:H41 | 22:8:612:CLA:H61 | 1.62 | 0.44 |
| 29:4:606:CHL:H3A | 25:4:621:BCR:C21 | 2.48 | 0.44 |
| 29:4:608:CHL:HMA1 | 25:4:621:BCR:H361 | 2.00 | 0.44 |
| 22:A:809:CLA:HAB | 25:J:3003:BCR:H352 | 2.00 | 0.44 |
| 22:A:825:CLA:H2 | 25:A:850:BCR:H363 | 2.00 | 0.44 |
| 22:B:807:CLA:O1A | 8:I:83:THR:OG1 | 2.32 | 0.44 |
| 22:7:601:CLA:H62 | 22:7:601:CLA:H41 | 1.76 | 0.44 |
| 1:A:150:ALA:HB2 | 1:A:378:PRO:HD2 | 2.00 | 0.44 |
| 1:A:715:PRO:HB3 | 22:F:301:CLA:HMC3 | 1.99 | 0.44 |
| 25:A:850:BCR:H24C | 25:A:850:BCR:H371 | 1.81 | 0.44 |
| 25:A:856:BCR:H333 | 22:J:3002:CLA:HMD3 | 2.00 | 0.44 |
| 2:B:545:SER:C | 6:F:224:VAL:HG13 | 2.38 | 0.44 |
| 22:B:814:CLA:HHB | 25:B:845:BCR:H23C | 2.00 | 0.44 |
| 29:1:601:CHL:HMD2 | 25:8:619:BCR:HC21 | 1.99 | 0.44 |
| 16:4:142:TYR:HB3 | 29:4:606:CHL:HMD3 | 2.00 | 0.44 |
| 22:5:612:CLA:H41 | 22:5:612:CLA:H62 | 1.71 | 0.44 |
| 18:6:125:GLU:HG3 | 22:6:609:CLA:NB | 2.32 | 0.44 |
| 1:A:711:PRO:HA | 6:F:171:LEU:HD11 | 2.00 | 0.44 |
| 22:A:834:CLA:H61 | 22:A:834:CLA:H41 | 1.76 | 0.44 |
| 22:B:819:CLA:H102 | 22:B:823:CLA:H43 | 1.99 | 0.44 |
| 22:B:820:CLA:CGA | 22:B:820:CLA:C3A | 2.96 | 0.44 |
| 7:G:89:THR:HG21 | 7:G:96:ASN:HA | 2.00 | 0.44 |
| 15:8:138:TRP:CE3 | 22:8:609:CLA:HMA1 | 2.52 | 0.44 |
| 22:Z:613:CLA:H2 | 22:Z:614:CLA:OBD | 2.17 | 0.44 |
| 16:4:208:ILE:HG12 | 16:4:212:LYS:HG3 | 2.00 | 0.44 |
| 17:5:109:LEU:HB2 | 17:5:114:THR:HA | 2.00 | 0.44 |
| 1:A:59:PHE:CD2 | 22:A:806:CLA:HMC2 | 2.53 | 0.44 |
| 1:A:121:ILE:HG12 | 1:A:122:VAL:HG13 | 2.00 | 0.44 |
| 22:B:818:CLA:H3A | 22:B:818:CLA:HBA2 | 1.68 | 0.44 |
| 22:3:613:CLA:H2 | 22:3:614:CLA:HMD1 | 2.00 | 0.44 |
| 22:6:604:CLA:H61 | 25:6:623:BCR:H402 | 1.99 | 0.44 |
| 19:2:174:GLN:OE1 | 22:2:613:CLA:ND | 2.51 | 0.44 |
| 1:A:685:PHE:HA | 23:A:844:PQN:H9 | 2.00 | 0.43 |
| 22:A:815:CLA:H102 | 22:A:817:CLA:C4B | 2.47 | 0.43 |
| 25:A:851:BCR:H15C | 25:A:851:BCR:H351 | 1.84 | 0.43 |
| 22:B:813:CLA:H203 | 22:B:828:CLA:H2 | 2.00 | 0.43 |
| 22:1:610:CLA:H93 | 22:1:610:CLA:H61 | 1.91 | 0.43 |
| 20:9:123:GLU:HG3 | 22:9:609:CLA:NB | 2.32 | 0.43 |
| 22:A:822:CLA:H111 | 22:A:822:CLA:H152 | 1.74 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:A:823:CLA:H11 | 25:K:4001:BCR:H271 | 2.00 | 0.43 |
| 22:A:831:CLA:H142 | 22:A:831:CLA:H111 | 1.84 | 0.43 |
| 22:B:806:CLA:H72 | 22:B:806:CLA:H111 | 1.66 | 0.43 |
| 22:1:602:CLA:H92 | 22:1:602:CLA:H61 | 1.89 | 0.43 |
| 22:1:604:CLA:H62 | 22:1:604:CLA:H41 | 1.73 | 0.43 |
| 22:2:610:CLA:H92 | 22:2:610:CLA:H62 | 1.86 | 0.43 |
| 30:2:617:LUT:H11 | 30:2:617:LUT:H191 | 1.91 | 0.43 |
| 30:2:617:LUT:H31 | 30:2:617:LUT:H391 | 1.91 | 0.43 |
| 20:9:191:LEU:HD21 | 22:9:614:CLA:HMC3 | 1.99 | 0.43 |
| 22:A:841:CLA:HBB1 | 22:A:841:CLA:H111 | 2.00 | 0.43 |
| 7:G:91:ASP:OD2 | 7:G:92:PRO:HD2 | 2.18 | 0.43 |
| 15:8:54:PHE:HB3 | 22:8:602:CLA:C3D | 2.48 | 0.43 |
| 30:5:620:LUT:C8 | 30:5:620:LUT:H181 | 2.48 | 0.43 |
| 20:9:62:ARG:CD | 20:9:66:TYR:CE2 | 2.96 | 0.43 |
| 1:A:294:THR:HG23 | 22:A:820:CLA:HMA3 | 2.01 | 0.43 |
| 1:A:458:HIS:CE1 | 22:A:835:CLA:CHA | 3.00 | 0.43 |
| 22:A:805:CLA:HMA2 | 22:A:812:CLA:CMD | 2.48 | 0.43 |
| 22:B:833:CLA:HBA1 | 9:J:36:PRO:HG2 | 2.00 | 0.43 |
| 25:G:205:BCR:H11C | 25:G:205:BCR:H341 | 1.90 | 0.43 |
| 13:3:73:LEU:HG | 22:3:602:CLA:HAA2 | 2.00 | 0.43 |
| 13:3:97:TRP:CE2 | 29:3:608:CHL:HED2 | 2.53 | 0.43 |
| 14:7:130:TRP:CZ2 | 25:7:623:BCR:HC8 | 2.53 | 0.43 |
| 22:7:620:CLA:CBA | 18:6:250:CYS:O | 2.65 | 0.43 |
| 15:8:122:LEU:HD11 | 22:8:606:CLA:C2D | 2.49 | 0.43 |
| 21:A:801:CL0:H15 | 21:A:801:CL0:H2 | 1.99 | 0.43 |
| 17:5:159:ASN:HB3 | 17:5:165:PRO:HA | 2.01 | 0.43 |
| 17:5:171:PRO:HD2 | 30:5:620:LUT:C23 | 2.41 | 0.43 |
| 30:2:617:LUT:H35 | 30:2:617:LUT:H401 | 1.64 | 0.43 |
| 1:A:329:HIS:HA | 22:A:845:CLA:HBC2 | 2.01 | 0.43 |
| 22:A:839:CLA:H62 | 22:A:839:CLA:H41 | 1.79 | 0.43 |
| 2:B:43:LEU:HD22 | 4:D:186:PHE:CZ | 2.54 | 0.43 |
| 2:B:178:HIS:CG | 22:B:813:CLA:HMC2 | 2.53 | 0.43 |
| 27:B:850:DGD:HA62 | 27:B:850:DGD:HA92 | 1.78 | 0.43 |
| 3:C:41:SER:HB2 | 4:D:168:ALA:H | 1.83 | 0.43 |
| 25:F:305:BCR:HC8 | 25:F:305:BCR:C33 | 2.48 | 0.43 |
| 15:8:48:LEU:HD21 | 15:8:70:GLN:HG3 | 1.99 | 0.43 |
| 15:8:132:PHE:CD2 | 25:8:619:BCR:H12C | 2.53 | 0.43 |
| 17:5:110:PRO:HG3 | 22:5:604:CLA:HBD | 2.01 | 0.43 |
| 1:A:29:TRP:CZ3 | 22:A:805:CLA:H92 | 2.54 | 0.43 |
| 1:A:32:PRO:HB2 | 1:A:48:TRP:HH2 | 1.84 | 0.43 |
| 22:A:823:CLA:HBA2 | 22:A:823:CLA:H3A | 1.60 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:3:249:HIS:CD2 | 22:3:614:CLA:NC | 2.87 | 0.43 |
| 22:3:603:CLA:H2 | 22:3:603:CLA:H61 | 1.68 | 0.43 |
| 15:8:240:LEU:HD12 | 15:8:242:PHE:CZ | 2.54 | 0.43 |
| 22:4:602:CLA:CBB | 30:4:620:LUT:H32 | 2.48 | 0.43 |
| 17:5:60:LEU:HD13 | 22:5:602:CLA:H42 | 2.00 | 0.43 |
| 1:A:112:LYS:HA | 1:A:113:PRO:HD3 | 1.91 | 0.43 |
| 22:A:825:CLA:H12 | 25:A:850:BCR:H14C | 2.01 | 0.43 |
| 25:A:849:BCR:H371 | 25:A:849:BCR:H24C | 1.86 | 0.43 |
| 7:G:45:PHE:HA | 7:G:48:ILE:HG22 | 2.01 | 0.43 |
| 11:L:57:THR:HG22 | 11:L:58:PRO:CD | 2.48 | 0.43 |
| 15:8:242:PHE:CE2 | 15:8:243:LEU:CG | 2.85 | 0.43 |
| 22:Z:613:CLA:HMB1 | 22:Z:613:CLA:H18 | 1.99 | 0.43 |
| 22:6:601:CLA:HBB1 | 24:6:619:LHG:C26 | 2.48 | 0.43 |
| 20:9:97:TRP:CD1 | 20:9:98:GLU:HG3 | 2.53 | 0.43 |
| 22:9:610:CLA:CBB | 30:9:616:LUT:H32 | 2.49 | 0.43 |
| 6:F:139:LEU:HD13 | 22:F:304:CLA:HED3 | 2.00 | 0.43 |
| 25:7:624:BCR:H15C | 25:7:624:BCR:H351 | 1.82 | 0.43 |
| 6:F:137:PRO:HG3 | 25:F:305:BCR:H281 | 1.99 | 0.43 |
| 6:F:158:TYR:HA | 6:F:202:TRP:HZ2 | 1.84 | 0.43 |
| 12:1:55:GLY:H | 12:1:175:LEU:HD23 | 1.83 | 0.43 |
| 24:1:620:LHG:H132 | 24:1:620:LHG:H101 | 1.85 | 0.43 |
| 16:4:111:VAL:CG1 | 30:4:619:LUT:H12 | 2.39 | 0.43 |
| 17:5:228:LEU:HG | 22:5:614:CLA:HED1 | 2.01 | 0.43 |
| 1:A:433:HIS:HB3 | 11:L:55:LEU:HD11 | 2.01 | 0.42 |
| 1:A:480:GLN:HA | 1:A:481:PRO:HD3 | 1.91 | 0.42 |
| 1:A:740:TRP:HB2 | 22:A:829:CLA:HBB1 | 2.00 | 0.42 |
| 22:A:805:CLA:H42 | 22:A:812:CLA:CBB | 2.28 | 0.42 |
| 22:A:811:CLA:HAA1 | 13:3:82:ILE:HD12 | 2.01 | 0.42 |
| 11:L:80:ALA:HB3 | 11:L:83:LEU:HD23 | 2.00 | 0.42 |
| 30:7:622:LUT:H35 | 30:7:622:LUT:H401 | 1.88 | 0.42 |
| 22:8:610:CLA:HBB1 | 22:8:610:CLA:H51 | 2.01 | 0.42 |
| 12:Z:188:PHE:CD2 | 30:Z:618:LUT:H12 | 2.54 | 0.42 |
| 25:4:621:BCR:H15C | 25:4:621:BCR:H351 | 1.75 | 0.42 |
| 18:6:163:PRO:HD2 | 30:6:621:LUT:H23 | 2.01 | 0.42 |
| 29:3:608:CHL:HMB3 | 25:3:717:BCR:H362 | 2.01 | 0.42 |
| 22:8:610:CLA:H92 | 22:8:610:CLA:H61 | 1.83 | 0.42 |
| 30:Z:619:LUT:H15 | 30:Z:619:LUT:H201 | 1.78 | 0.42 |
| 22:6:610:CLA:CBB | 30:6:621:LUT:H32 | 2.49 | 0.42 |
| 22:A:803:CLA:HMB1 | 22:A:803:CLA:HBB1 | 2.01 | 0.42 |
| 22:A:805:CLA:CBB | 22:A:812:CLA:C14 | 2.96 | 0.42 |
| 22:A:831:CLA:H41 | 22:A:831:CLA:H61 | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:A:849:BCR:H15C | 25:A:849:BCR:H351 | 1.83 | 0.42 |
| 25:A:851:BCR:H20C | 25:A:851:BCR:H361 | 1.90 | 0.42 |
| 25:A:856:BCR:H361 | 25:A:856:BCR:H20C | 1.83 | 0.42 |
| 11:L:55:LEU:HD23 | 11:L:55:LEU:C | 2.39 | 0.42 |
| 12:1:139:ALA:HA | 22:1:609:CLA:HAB | 2.00 | 0.42 |
| 14:7:82:GLY:O | 14:7:86:ILE:HG12 | 2.19 | 0.42 |
| 22:8:610:CLA:CBB | 30:8:617:LUT:H32 | 2.49 | 0.42 |
| 25:4:621:BCR:C33 | 25:4:621:BCR:HC8 | 2.50 | 0.42 |
| 18:6:242:LYS:HB2 | 25:6:625:BCR:H343 | 2.01 | 0.42 |
| 22:A:833:CLA:H143 | 22:A:833:CLA:H111 | 1.88 | 0.42 |
| 22:1:602:CLA:H61 | 22:1:602:CLA:H41 | 1.57 | 0.42 |
| 22:7:612:CLA:H41 | 22:7:612:CLA:H62 | 1.85 | 0.42 |
| 15:8:83:GLY:O | 15:8:87:ILE:HG12 | 2.19 | 0.42 |
| 22:4:610:CLA:CBB | 30:4:619:LUT:H32 | 2.49 | 0.42 |
| 17:5:218:HIS:CD2 | 22:5:614:CLA:NC | 2.86 | 0.42 |
| 22:5:602:CLA:CBB | 30:5:624:LUT:H32 | 2.49 | 0.42 |
| 20:9:169:PHE:CZ | 30:9:617:LUT:H10 | 2.54 | 0.42 |
| 1:A:465:LEU:HD13 | 2:B:96:HIS:O | 2.20 | 0.42 |
| 25:B:801:BCR:H11C | 25:B:801:BCR:H341 | 1.81 | 0.42 |
| 22:B:805:CLA:H162 | 22:B:805:CLA:H193 | 1.82 | 0.42 |
| 22:3:603:CLA:H141 | 22:3:603:CLA:H162 | 1.83 | 0.42 |
| 22:3:604:CLA:HMC1 | 25:3:718:BCR:H19C | 2.01 | 0.42 |
| 22:Z:604:CLA:H62 | 22:Z:604:CLA:H41 | 1.71 | 0.42 |
| 24:4:622:LHG:HC91 | 25:6:623:BCR:HC41 | 2.01 | 0.42 |
| 17:5:172:PHE:CD2 | 30:5:620:LUT:H222 | 2.54 | 0.42 |
| 22:6:609:CLA:HBA1 | 22:6:609:CLA:H3A | 1.85 | 0.42 |
| 20:9:52:ASP:OD1 | 30:9:617:LUT:O23 | 2.35 | 0.42 |
| 1:A:220:VAL:HG13 | 1:A:240:PRO:HB3 | 2.01 | 0.42 |
| 1:A:397:ILE:HG21 | 22:A:830:CLA:HHC | 2.01 | 0.42 |
| 1:A:429:ARG:HG2 | 1:A:432:ARG:HH22 | 1.85 | 0.42 |
| 22:A:818:CLA:H62 | 22:A:818:CLA:H41 | 1.59 | 0.42 |
| 22:A:842:CLA:C4D | 22:A:842:CLA:H12 | 2.49 | 0.42 |
| 2:B:610:PHE:O | 2:B:614:SER:HB3 | 2.19 | 0.42 |
| 2:B:722:TYR:HB2 | 22:B:802:CLA:HED2 | 2.01 | 0.42 |
| 30:3:621:LUT:H35 | 30:3:621:LUT:H401 | 1.91 | 0.42 |
| 30:8:618:LUT:H201 | 30:8:618:LUT:H15 | 1.79 | 0.42 |
| 19:2:219:MET:HE3 | 22:9:609:CLA:CMA | 2.49 | 0.42 |
| 1:A:646:LEU:HD13 | 2:B:652:LEU:HD21 | 2.02 | 0.42 |
| 22:A:835:CLA:HBC3 | 22:B:803:CLA:H143 | 2.01 | 0.42 |
| 2:B:118:THR:OG1 | 22:B:827:CLA:O1A | 2.36 | 0.42 |
| 22:B:825:CLA:H193 | 22:B:825:CLA:H161 | 1.91 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:B:829:CLA:H92 | 22:B:829:CLA:H61 | 1.91 | 0.42 |
| 12:Z:78:GLU:HG2 | 12:Z:178:ILE:HD11 | 2.00 | 0.42 |
| 30:Z:618:LUT:H15 | 30:Z:618:LUT:H201 | 1.87 | 0.42 |
| 30:4:620:LUT:H35 | 30:4:620:LUT:H401 | 1.82 | 0.42 |
| 25:4:621:BCR:C23 | 25:4:621:BCR:H383 | 2.49 | 0.42 |
| 25:5:625:BCR:H11C | 25:5:625:BCR:H341 | 1.73 | 0.42 |
| 1:A:60:ASP:OD2 | 1:A:350:HIS:NE2 | 2.51 | 0.42 |
| 2:B:71:TRP:CE2 | 8:I:71:PRO:HG2 | 2.55 | 0.42 |
| 2:B:416:LYS:HZ1 | 6:F:226:PRO:HG3 | 1.42 | 0.42 |
| 2:B:518:PHE:CE1 | 2:B:522:HIS:CE1 | 3.07 | 0.42 |
| 22:B:832:CLA:H61 | 25:F:305:BCR:H312 | 2.02 | 0.42 |
| 25:B:848:BCR:H15C | 25:B:848:BCR:H351 | 1.85 | 0.42 |
| 6:F:182:ASP:HA | 6:F:185:ILE:HG22 | 2.01 | 0.42 |
| 30:1:617:LUT:H35 | 30:1:617:LUT:H401 | 1.88 | 0.42 |
| 22:Z:602:CLA:H72 | 22:Z:602:CLA:H111 | 1.89 | 0.42 |
| 1:A:396:TRP:HB3 | 22:A:829:CLA:HMC3 | 2.01 | 0.42 |
| 1:A:426:LEU:HD13 | 22:A:825:CLA:C1C | 2.49 | 0.42 |
| 2:B:375:HIS:HB2 | 22:B:827:CLA:C1B | 2.50 | 0.42 |
| 12:1:158:PHE:HZ | 22:1:608:CLA:NC | 2.17 | 0.42 |
| 22:4:612:CLA:H52 | 22:4:612:CLA:H11 | 1.77 | 0.42 |
| 30:5:620:LUT:H11 | 30:5:620:LUT:H191 | 1.96 | 0.42 |
| 20:9:49:ASN:HB2 | 22:9:602:CLA:HMD1 | 2.00 | 0.42 |
| 1:A:349:TRP:HB3 | 22:A:806:CLA:HAC1 | 2.00 | 0.42 |
| 1:A:709:VAL:O | 22:F:301:CLA:HMD3 | 2.19 | 0.42 |
| 22:B:830:CLA:CBB | 22:B:841:CLA:H142 | 2.50 | 0.42 |
| 25:B:843:BCR:H15C | 25:B:843:BCR:H351 | 1.86 | 0.42 |
| 25:L:205:BCR:H11C | 25:L:205:BCR:H341 | 1.90 | 0.42 |
| 22:A:815:CLA:H62 | 22:A:815:CLA:H41 | 1.88 | 0.41 |
| 22:B:815:CLA:H11 | 22:B:815:CLA:H51 | 1.80 | 0.41 |
| 22:3:604:CLA:H11 | 22:5:616:CLA:HED2 | 2.01 | 0.41 |
| 22:3:610:CLA:H142 | 22:3:610:CLA:H111 | 1.86 | 0.41 |
| 22:5:609:CLA:H3A | 22:5:609:CLA:HBA2 | 1.65 | 0.41 |
| 1:A:166:GLY:HA2 | 25:A:848:BCR:HC22 | 2.02 | 0.41 |
| 22:A:827:CLA:H52 | 22:A:836:CLA:HBB2 | 2.01 | 0.41 |
| 2:B:86:ARG:HA | 2:B:87:PRO:HD3 | 1.88 | 0.41 |
| 2:B:194:HIS:HB2 | 22:B:814:CLA:CHC | 2.50 | 0.41 |
| 2:B:300:HIS:HB3 | 2:B:305:ILE:HD11 | 2.02 | 0.41 |
| 2:B:463:TRP:NE1 | 22:F:304:CLA:HAA2 | 2.35 | 0.41 |
| 2:B:610:PHE:O | 2:B:614:SER:CB | 2.68 | 0.41 |
| 25:B:846:BCR:H24C | 25:B:846:BCR:H371 | 1.83 | 0.41 |
| 25:K:4004:BCR:H351 | 25:K:4004:BCR:H15C | 1.78 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:3:604:CLA:HBA1 | 22:3:606:CLA:C1D | 2.50 | 0.41 |
| 15:8:88:LEU:O | 15:8:92:LEU:N | 2.43 | 0.41 |
| 15:8:174:ASP:OD1 | 30:8:617:LUT:O23 | 2.29 | 0.41 |
| 22:4:611:CLA:H61 | 22:4:611:CLA:H41 | 1.60 | 0.41 |
| 22:6:612:CLA:H41 | 22:6:612:CLA:H62 | 1.82 | 0.41 |
| 1:A:683:LEU:HB2 | 22:A:802:CLA:HMC3 | 2.02 | 0.41 |
| 22:A:832:CLA:CED | 11:L:55:LEU:HD11 | 2.47 | 0.41 |
| 13:3:216:LYS:HD3 | 22:3:612:CLA:HAA2 | 2.01 | 0.41 |
| 22:7:610:CLA:CBB | 30:7:621:LUT:H32 | 2.48 | 0.41 |
| 22:Z:611:CLA:H203 | 22:Z:611:CLA:H161 | 1.92 | 0.41 |
| 19:2:219:MET:O | 19:2:219:MET:SD | 2.79 | 0.41 |
| 1:A:216:HIS:CD2 | 1:A:216:HIS:C | 2.94 | 0.41 |
| 1:A:536:HIS:CG | 22:A:839:CLA:HED2 | 2.55 | 0.41 |
| 22:A:840:CLA:H161 | 22:A:840:CLA:H121 | 1.69 | 0.41 |
| 2:B:176:LEU:HD23 | 2:B:176:LEU:HA | 1.92 | 0.41 |
| 13:3:68:ASP:OD1 | 30:3:622:LUT:O23 | 2.38 | 0.41 |
| 13:3:246:LEU:HD21 | 30:3:621:LUT:H163 | 2.02 | 0.41 |
| 22:A:802:CLA:C3 | 22:A:802:CLA:HMA1 | 2.51 | 0.41 |
| 22:A:820:CLA:HBA2 | 22:A:820:CLA:H3A | 1.91 | 0.41 |
| 25:J:3003:BCR:H15C | 25:J:3003:BCR:H351 | 1.84 | 0.41 |
| 30:3:621:LUT:H15 | 30:3:621:LUT:H201 | 1.90 | 0.41 |
| 15:8:212:ALA:HB2 | 22:8:616:CLA:HED2 | 2.01 | 0.41 |
| 12:Z:173:LEU:HD23 | 12:Z:176:LYS:HD2 | 2.02 | 0.41 |
| 22:Z:613:CLA:H141 | 25:4:621:BCR:H322 | 2.01 | 0.41 |
| 16:4:232:GLN:HE22 | 30:4:619:LUT:C4 | 2.33 | 0.41 |
| 22:4:601:CLA:H112 | 22:4:601:CLA:H72 | 1.74 | 0.41 |
| 30:4:620:LUT:H15 | 30:4:620:LUT:H201 | 1.89 | 0.41 |
| 1:A:408:HIS:HE1 | 22:A:831:CLA:NA | 2.19 | 0.41 |
| 22:A:816:CLA:H92 | 22:A:816:CLA:H61 | 1.84 | 0.41 |
| 22:A:841:CLA:H62 | 22:A:841:CLA:H102 | 1.89 | 0.41 |
| 22:A:843:CLA:H13 | 22:A:843:CLA:H101 | 1.89 | 0.41 |
| 22:B:840:CLA:HHD | 22:B:840:CLA:HAC1 | 1.91 | 0.41 |
| 25:I:172:BCR:H15C | 25:I:172:BCR:H351 | 1.87 | 0.41 |
| 22:1:610:CLA:CBB | 30:1:617:LUT:H32 | 2.51 | 0.41 |
| 25:3:719:BCR:H20C | 25:3:719:BCR:H361 | 1.90 | 0.41 |
| 15:8:88:LEU:HD11 | 30:8:617:LUT:H10 | 2.03 | 0.41 |
| 22:6:610:CLA:H92 | 22:6:610:CLA:H61 | 1.83 | 0.41 |
| 1:A:121:ILE:HG23 | 1:A:122:VAL:HG22 | 2.03 | 0.41 |
| 1:A:474:ASP:O | 1:A:478:GLN:NE2 | 2.54 | 0.41 |
| 22:1:614:CLA:H91 | 22:1:614:CLA:H112 | 1.86 | 0.41 |
| 22:8:602:CLA:HBB1 | 22:8:602:CLA:H51 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:Z:619:LUT:H391 | 30:Z:619:LUT:H31 | 1.76 | 0.41 |
| 1:A:162:THR:HG23 | 22:A:815:CLA:O1A | 2.20 | 0.41 |
| 22:A:835:CLA:C5 | 22:A:835:CLA:H92 | 2.50 | 0.41 |
| 2:B:685:LYS:HE3 | 11:L:54:MET:SD | 2.61 | 0.41 |
| 22:B:841:CLA:H161 | 22:B:841:CLA:H192 | 1.73 | 0.41 |
| 25:K:4001:BCR:H361 | 25:K:4001:BCR:H20C | 1.81 | 0.41 |
| 22:3:603:CLA:H92 | 22:3:603:CLA:H62 | 1.89 | 0.41 |
| 29:3:608:CHL:HMB2 | 25:3:718:BCR:HC7 | 2.02 | 0.41 |
| 25:8:619:BCR:H15C | 25:8:619:BCR:H351 | 1.81 | 0.41 |
| 1:A:547:VAL:HG11 | 22:A:840:CLA:HMB3 | 2.02 | 0.41 |
| 21:A:801:CL0:H41 | 21:A:801:CL0:H49 | 1.95 | 0.41 |
| 22:A:824:CLA:H3A | 22:A:824:CLA:HBA2 | 1.77 | 0.41 |
| 22:A:834:CLA:H52 | 22:A:834:CLA:H11 | 1.85 | 0.41 |
| 25:A:851:BCR:H11C | 25:A:851:BCR:H341 | 1.85 | 0.41 |
| 2:B:32:PHE:HD2 | 22:B:805:CLA:HMC2 | 1.85 | 0.41 |
| 2:B:181:SER:HB3 | 2:B:289:GLY:HA3 | 2.03 | 0.41 |
| 22:B:813:CLA:H151 | 22:B:828:CLA:HMD2 | 2.03 | 0.41 |
| 22:B:815:CLA:H91 | 25:B:843:BCR:H23C | 2.03 | 0.41 |
| 22:B:835:CLA:H3A | 22:B:835:CLA:HBA2 | 1.71 | 0.41 |
| 22:B:835:CLA:HMB1 | 25:B:847:BCR:HC31 | 2.03 | 0.41 |
| 22:B:840:CLA:H193 | 22:B:840:CLA:H161 | 1.96 | 0.41 |
| 25:B:843:BCR:H362 | 25:G:205:BCR:H312 | 2.03 | 0.41 |
| 6:F:223:THR:HB | 6:F:227:ARG:HH21 | 1.86 | 0.41 |
| 12:1:64:LEU:HD13 | 22:1:602:CLA:H42 | 2.03 | 0.41 |
| 12:1:67:GLU:HA | 12:1:68:PRO:HD3 | 1.85 | 0.41 |
| 12:1:84:TRP:CE2 | 22:1:608:CLA:HED2 | 2.56 | 0.41 |
| 12:1:189:LEU:HD21 | 22:1:602:CLA:H18 | 2.02 | 0.41 |
| 25:3:718:BCR:H15C | 25:3:718:BCR:H351 | 1.83 | 0.41 |
| 25:3:718:BCR:H322 | 22:5:601:CLA:H101 | 2.02 | 0.41 |
| 22:7:602:CLA:H121 | 22:7:602:CLA:H161 | 1.85 | 0.41 |
| 22:7:613:CLA:HHD | 22:7:616:CLA:OBD | 2.21 | 0.41 |
| 12:Z:161:LEU:HD12 | 30:Z:617:LUT:H222 | 2.02 | 0.41 |
| 22:Z:613:CLA:H92 | 22:Z:613:CLA:HMC2 | 2.03 | 0.41 |
| 29:6:607:CHL:H41 | 29:6:607:CHL:H62 | 1.76 | 0.41 |
| 20:9:157:LYS:O | 20:9:161:ASN:HB2 | 2.21 | 0.41 |
| 22:A:802:CLA:H152 | 22:A:842:CLA:CBB | 2.51 | 0.41 |
| 25:A:849:BCR:H272 | 25:3:719:BCR:H352 | 2.03 | 0.41 |
| 22:B:802:CLA:H142 | 22:B:802:CLA:H111 | 1.93 | 0.41 |
| 22:B:834:CLA:H161 | 22:B:834:CLA:H122 | 1.76 | 0.41 |
| 14:7:77:ARG:NE | 14:7:190:GLU:OE2 | 2.50 | 0.41 |
| 14:7:231:PHE:O | 14:7:237:SER:OG | 2.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:Z:614:CLA:H142 | 22:Z:614:CLA:H112 | 1.86 | 0.41 |
| 18:6:127:ARG:NH2 | 29:6:618:CHL:HMC | 2.36 | 0.41 |
| 25:6:623:BCR:H24C | 25:6:623:BCR:H371 | 1.90 | 0.41 |
| 22:A:841:CLA:H2 | 22:A:841:CLA:H61 | 1.86 | 0.40 |
| 2:B:152:PHE:CZ | 19:2:220:ILE:HD13 | 2.56 | 0.40 |
| 2:B:320:HIS:CD2 | 22:B:823:CLA:ND | 2.89 | 0.40 |
| 22:B:808:CLA:H102 | 22:B:808:CLA:H62 | 1.84 | 0.40 |
| 22:B:809:CLA:H91 | 22:B:809:CLA:H111 | 1.94 | 0.40 |
| 4:D:74:LEU:HD22 | 4:D:78:ALA:HB2 | 2.03 | 0.40 |
| 22:1:608:CLA:HBB1 | 22:1:608:CLA:H121 | 2.02 | 0.40 |
| 22:1:608:CLA:HMA1 | 30:1:619:LUT:H203 | 2.02 | 0.40 |
| 30:3:622:LUT:H15 | 30:3:622:LUT:H201 | 1.88 | 0.40 |
| 22:8:601:CLA:H122 | 22:8:614:CLA:HBA2 | 2.04 | 0.40 |
| 22:8:609:CLA:H3A | 22:8:609:CLA:HBA1 | 1.83 | 0.40 |
| 18:6:149:LEU:HA | 18:6:150:PRO:HD3 | 1.90 | 0.40 |
| 22:6:601:CLA:H151 | 22:6:601:CLA:H112 | 1.78 | 0.40 |
| 25:6:623:BCR:H15C | 25:6:623:BCR:H351 | 1.89 | 0.40 |
| 1:A:316:TRP:CD1 | 10:K:87:VAL:HG21 | 2.56 | 0.40 |
| 1:A:677:PHE:CD2 | 25:A:852:BCR:H363 | 2.57 | 0.40 |
| 25:A:848:BCR:H402 | 25:3:719:BCR:HC7 | 2.03 | 0.40 |
| 2:B:16:ASP:HB3 | 2:B:21:ARG:HB2 | 2.03 | 0.40 |
| 25:B:846:BCR:H20C | 25:B:846:BCR:H361 | 1.97 | 0.40 |
| 25:3:719:BCR:H11C | 25:3:719:BCR:H341 | 1.96 | 0.40 |
| 30:7:621:LUT:H15 | 30:7:621:LUT:H201 | 1.96 | 0.40 |
| 22:A:802:CLA:H42 | 22:A:802:CLA:HHB | 2.02 | 0.40 |
| 25:A:850:BCR:H20C | 25:A:850:BCR:H361 | 1.84 | 0.40 |
| 25:A:856:BCR:H11C | 25:A:856:BCR:H341 | 1.88 | 0.40 |
| 2:B:194:HIS:HE1 | 22:B:814:CLA:NA | 2.16 | 0.40 |
| 5:E:62:VAL:HG22 | 5:E:71:VAL:HG22 | 2.04 | 0.40 |
| 25:7:623:BCR:H11C | 25:7:623:BCR:H341 | 1.92 | 0.40 |
| 22:Z:610:CLA:CBB | 30:Z:617:LUT:H32 | 2.52 | 0.40 |
| 22:Z:611:CLA:H72 | 22:Z:611:CLA:H111 | 1.93 | 0.40 |
| 16:4:156:LEU:CD1 | 25:4:621:BCR:C35 | 2.99 | 0.40 |
| 22:5:606:CLA:HBB1 | 29:5:607:CHL:CMC | 2.51 | 0.40 |
| 30:6:624:LUT:H201 | 30:6:624:LUT:H15 | 1.84 | 0.40 |
| 30:2:616:LUT:H401 | 30:2:616:LUT:H35 | 1.76 | 0.40 |
| 22:9:603:CLA:HBB1 | 22:9:603:CLA:HHC | 2.04 | 0.40 |
| 25:A:850:BCR:H11C | 25:A:850:BCR:H341 | 1.84 | 0.40 |
| 2:B:157:HIS:HE1 | 22:B:811:CLA:C1A | 2.34 | 0.40 |
| 2:B:390:HIS:HA | 2:B:393:ILE:HD12 | 2.03 | 0.40 |
| 2:B:601:THR:HG21 | 2:B:610:PHE:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:66:ILE:HB | 4:D:105:ILE:HB | 2.03 | 0.40 |
| 25:3:717:BCR:H15C | 25:3:717:BCR:H351 | 1.87 | 0.40 |
| 14:7:198:MET:SD | 22:7:602:CLA:HBB1 | 2.62 | 0.40 |
| 22:7:606:CLA:HMB1 | 22:7:609:CLA:HBC2 | 2.03 | 0.40 |
| 22:Z:602:CLA:H52 | 30:Z:618:LUT:H28 | 2.02 | 0.40 |
| 22:Z:612:CLA:H11 | 22:Z:612:CLA:H51 | 1.81 | 0.40 |
| 16:4:160:VAL:HG13 | 29:4:608:CHL:NB | 2.37 | 0.40 |
| 22:4:601:CLA:H111 | 22:4:601:CLA:H142 | 1.78 | 0.40 |
| 22:5:617:CLA:CMB | 22:6:622:CLA:CBC | 3.00 | 0.40 |
| 30:2:616:LUT:H11 | 30:2:616:LUT:H191 | 1.97 | 0.40 |
| 1:A:428:ASP:O | 1:A:432:ARG:HB2 | 2.21 | 0.40 |
| 22:A:843:CLA:H62 | 22:A:843:CLA:H41 | 1.68 | 0.40 |
| 2:B:157:HIS:HE1 | 22:B:811:CLA:NA | 2.18 | 0.40 |
| 25:F:305:BCR:H11C | 25:F:305:BCR:H341 | 1.76 | 0.40 |
| 7:G:32:LEU:HB3 | 7:G:33:ASP:H | 1.60 | 0.40 |
| 7:G:91:ASP:OD2 | 7:G:92:PRO:N | 2.55 | 0.40 |
| 12:1:42:GLY:HA3 | 15:8:146:SER:OG | 2.21 | 0.40 |
| 12:1:138:MET:O | 12:1:142:GLU:HG2 | 2.22 | 0.40 |
| 13:3:156:GLN:O | 13:3:160:LEU:CB | 2.61 | 0.40 |
| 22:3:603:CLA:HHC | 22:3:603:CLA:HBB1 | 2.02 | 0.40 |
| 22:7:613:CLA:H122 | 22:7:613:CLA:H162 | 1.81 | 0.40 |
| 16:4:247:HIS:CD2 | 22:4:614:CLA:C1C | 3.04 | 0.40 |
| 18:6:192:MET:HG3 | 22:6:613:CLA:HAC2 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1 | A | 734/751 (98%) | 713 (97%) | 20 (3%) | 1 (0%) | 51 82 |
| 2 | B | 730/755 (97%) | 708 (97%) | 22 (3%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | C | 78/81 (96%) | 74 (95%) | 4 (5%) | 0 | 100 | 100 |
| 4 | D | 142/161 (88%) | 135 (95%) | 7 (5%) | 0 | 100 | 100 |
| 5 | E | 59/73 (81%) | 55 (93%) | 4 (7%) | 0 | 100 | 100 |
| 6 | F | 163/165 (99%) | 155 (95%) | 8 (5%) | 0 | 100 | 100 |
| 7 | G | 64/94 (68%) | 64 (100%) | 0 | 0 | 100 | 100 |
| 8 | I | 35/106 (33%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 9 | J | 37/41 (90%) | 35 (95%) | 2 (5%) | 0 | 100 | 100 |
| 10 | K | 41/87 (47%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 114/156 (73%) | 108 (95%) | 5 (4%) | 1 (1%) | 17 | 48 |
| 12 | 1 | 192/194 (99%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 12 | Z | 188/194 (97%) | 181 (96%) | 7 (4%) | 0 | 100 | 100 |
| 13 | 3 | 200/268 (75%) | 191 (96%) | 9 (4%) | 0 | 100 | 100 |
| 14 | 7 | 210/215 (98%) | 200 (95%) | 10 (5%) | 0 | 100 | 100 |
| 15 | 8 | 215/217 (99%) | 206 (96%) | 9 (4%) | 0 | 100 | 100 |
| 16 | 4 | 199/236 (84%) | 187 (94%) | 11 (6%) | 1 (0%) | 29 | 61 |
| 17 | 5 | 219/229 (96%) | 201 (92%) | 18 (8%) | 0 | 100 | 100 |
| 18 | 6 | 227/232 (98%) | 216 (95%) | 11 (5%) | 0 | 100 | 100 |
| 19 | 2 | 107/221 (48%) | 107 (100%) | 0 | 0 | 100 | 100 |
| 20 | 9 | 144/189 (76%) | 136 (94%) | 8 (6%) | 0 | 100 | 100 |
| All | All | 4098/4665 (88%) | 3933 (96%) | 162 (4%) | 3 (0%) | 54 | 82 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | L | 187 | VAL |
| 16 | 4 | 208 | ILE |
| 1 | A | 122 | VAL |

5.3.2 Protein sidechains [i](#)

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 | 599/610 (98%) | 593 (99%) | 6 (1%) | 76 | 92 |
| 2 | B | 596/617 (97%) | 595 (100%) | 1 (0%) | 93 | 98 |
| 3 | C | 69/70 (99%) | 69 (100%) | 0 | 100 | 100 |
| 4 | D | 121/129 (94%) | 119 (98%) | 2 (2%) | 60 | 86 |
| 5 | E | 52/62 (84%) | 52 (100%) | 0 | 100 | 100 |
| 6 | F | 127/127 (100%) | 126 (99%) | 1 (1%) | 81 | 94 |
| 7 | G | 48/69 (70%) | 47 (98%) | 1 (2%) | 53 | 81 |
| 8 | I | 31/76 (41%) | 31 (100%) | 0 | 100 | 100 |
| 9 | J | 35/37 (95%) | 35 (100%) | 0 | 100 | 100 |
| 10 | K | 30/60 (50%) | 29 (97%) | 1 (3%) | 38 | 72 |
| 11 | L | 85/119 (71%) | 84 (99%) | 1 (1%) | 71 | 91 |
| 12 | 1 | 137/137 (100%) | 136 (99%) | 1 (1%) | 84 | 95 |
| 12 | Z | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 13 | 3 | 155/209 (74%) | 154 (99%) | 1 (1%) | 86 | 96 |
| 14 | 7 | 164/164 (100%) | 163 (99%) | 1 (1%) | 86 | 96 |
| 15 | 8 | 163/163 (100%) | 162 (99%) | 1 (1%) | 86 | 96 |
| 16 | 4 | 159/185 (86%) | 158 (99%) | 1 (1%) | 86 | 96 |
| 17 | 5 | 181/184 (98%) | 178 (98%) | 3 (2%) | 60 | 86 |
| 18 | 6 | 183/185 (99%) | 182 (100%) | 1 (0%) | 88 | 96 |
| 19 | 2 | 70/178 (39%) | 68 (97%) | 2 (3%) | 42 | 76 |
| 20 | 9 | 118/143 (82%) | 118 (100%) | 0 | 100 | 100 |
| All | All | 3260/3661 (89%) | 3236 (99%) | 24 (1%) | 84 | 95 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 17 | VAL |
| 1 | A | 205 | LEU |
| 1 | A | 206 | LEU |
| 1 | A | 372 | TYR |
| 1 | A | 584 | CYS |
| 1 | A | 657 | VAL |
| 2 | B | 479 | LEU |
| 4 | D | 59 | ASN |
| 4 | D | 139 | TYR |
| 6 | F | 168 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 118 | ASN |
| 10 | K | 35 | ASN |
| 11 | L | 54 | MET |
| 12 | 1 | 221 | ASN |
| 13 | 3 | 160 | LEU |
| 14 | 7 | 177 | ARG |
| 15 | 8 | 51 | ASN |
| 16 | 4 | 263 | ARG |
| 17 | 5 | 117 | ASN |
| 17 | 5 | 202 | LEU |
| 17 | 5 | 226 | ASN |
| 18 | 6 | 60 | ASN |
| 19 | 2 | 32 | TYR |
| 19 | 2 | 219 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 193 | ASN |
| 2 | B | 54 | GLN |
| 2 | B | 159 | GLN |
| 2 | B | 276 | HIS |
| 3 | C | 38 | GLN |
| 4 | D | 59 | ASN |
| 4 | D | 127 | GLN |
| 5 | E | 55 | GLN |
| 5 | E | 78 | GLN |
| 7 | G | 118 | ASN |
| 13 | 3 | 156 | GLN |
| 13 | 3 | 234 | GLN |
| 13 | 3 | 245 | ASN |
| 14 | 7 | 207 | GLN |
| 16 | 4 | 175 | ASN |
| 17 | 5 | 142 | ASN |
| 17 | 5 | 203 | GLN |
| 18 | 6 | 60 | ASN |
| 18 | 6 | 130 | GLN |
| 20 | 9 | 87 | 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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

313 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | 3 | 607 | 13 | 60,68,73 | 2.13 | 18 (30%) | 70,107,113 | 2.82 | 28 (40%) |
| 25 | BCR | G | 205 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.50 | 7 (12%) |
| 22 | CLA | G | 204 | 7 | 46,54,73 | 2.46 | 17 (36%) | 53,90,113 | 3.13 | 24 (45%) |
| 22 | CLA | A | 825 | 1 | 55,63,73 | 2.18 | 15 (27%) | 64,101,113 | 2.90 | 26 (40%) |
| 22 | CLA | 3 | 609 | 13 | 50,58,73 | 2.32 | 17 (34%) | 58,95,113 | 3.03 | 26 (44%) |
| 22 | CLA | 1 | 613 | - | 65,73,73 | 2.00 | 17 (26%) | 76,113,113 | 2.61 | 25 (32%) |
| 22 | CLA | B | 806 | 2 | 65,73,73 | 2.01 | 15 (23%) | 76,113,113 | 2.73 | 29 (38%) |
| 22 | CLA | 7 | 610 | 14 | 60,68,73 | 2.09 | 14 (23%) | 70,107,113 | 2.86 | 28 (40%) |
| 25 | BCR | 6 | 623 | - | 41,41,41 | 0.65 | 0 | 56,56,56 | 1.98 | 18 (32%) |
| 25 | BCR | K | 4001 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 2.00 | 15 (26%) |
| 29 | CHL | 1 | 601 | 12 | 53,61,74 | 2.20 | 18 (33%) | 57,98,114 | 3.36 | 27 (47%) |
| 22 | CLA | 7 | 611 | 24 | 41,49,73 | 2.50 | 19 (46%) | 47,84,113 | 3.41 | 26 (55%) |
| 22 | CLA | 4 | 614 | 16 | 45,53,73 | 2.44 | 17 (37%) | 52,89,113 | 3.14 | 25 (48%) |
| 22 | CLA | 1 | 602 | 12 | 65,73,73 | 1.99 | 15 (23%) | 76,113,113 | 2.67 | 28 (36%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | A | 832 | 1 | 50,58,73 | 2.27 | 16 (32%) | 58,95,113 | 3.00 | 27 (46%) |
| 25 | BCR | J | 3003 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.74 | 13 (23%) |
| 24 | LHG | Z | 620 | 22 | 42,42,48 | 0.99 | 2 (4%) | 45,48,54 | 1.06 | 2 (4%) |
| 22 | CLA | 4 | 611 | 24 | 55,63,73 | 2.25 | 18 (32%) | 64,101,113 | 2.83 | 28 (43%) |
| 24 | LHG | 4 | 623 | - | 31,31,48 | 1.14 | 2 (6%) | 34,37,54 | 1.14 | 3 (8%) |
| 25 | BCR | B | 847 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 1.71 | 14 (25%) |
| 22 | CLA | 3 | 613 | 13 | 55,63,73 | 2.18 | 17 (30%) | 64,101,113 | 2.77 | 24 (37%) |
| 29 | CHL | 6 | 607 | - | 56,64,74 | 2.14 | 18 (32%) | 61,102,114 | 3.10 | 29 (47%) |
| 22 | CLA | 5 | 616 | 17 | 46,54,73 | 2.40 | 18 (39%) | 53,90,113 | 3.07 | 26 (49%) |
| 22 | CLA | A | 835 | 1 | 65,73,73 | 2.09 | 17 (26%) | 76,113,113 | 2.75 | 26 (34%) |
| 22 | CLA | Z | 604 | - | 57,65,73 | 2.18 | 17 (29%) | 66,103,113 | 2.82 | 26 (39%) |
| 22 | CLA | A | 809 | 1 | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.80 | 29 (38%) |
| 22 | CLA | Z | 606 | - | 52,60,73 | 2.31 | 18 (34%) | 60,97,113 | 3.05 | 28 (46%) |
| 22 | CLA | 4 | 613 | 16 | 56,64,73 | 2.18 | 15 (26%) | 65,102,113 | 2.89 | 28 (43%) |
| 22 | CLA | 5 | 606 | - | 55,63,73 | 2.24 | 17 (30%) | 64,101,113 | 2.92 | 26 (40%) |
| 25 | BCR | L | 201 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.73 | 12 (21%) |
| 22 | CLA | 2 | 603 | 19 | 46,54,73 | 2.43 | 16 (34%) | 53,90,113 | 3.24 | 25 (47%) |
| 22 | CLA | 5 | 611 | 24 | 55,63,73 | 2.24 | 17 (30%) | 64,101,113 | 2.91 | 27 (42%) |
| 24 | LHG | 6 | 619 | 22 | 48,48,48 | 0.94 | 2 (4%) | 51,54,54 | 0.98 | 2 (3%) |
| 22 | CLA | A | 823 | 1 | 49,57,73 | 2.33 | 17 (34%) | 55,93,113 | 3.14 | 23 (41%) |
| 22 | CLA | 3 | 612 | 13 | 46,54,73 | 2.39 | 17 (36%) | 53,90,113 | 3.26 | 24 (45%) |
| 22 | CLA | A | 824 | 1 | 51,59,73 | 2.27 | 18 (35%) | 59,96,113 | 3.07 | 25 (42%) |
| 22 | CLA | 2 | 612 | 19 | 52,60,73 | 2.30 | 16 (30%) | 60,97,113 | 3.01 | 26 (43%) |
| 22 | CLA | B | 812 | 2 | 65,73,73 | 2.02 | 18 (27%) | 76,113,113 | 2.72 | 26 (34%) |
| 24 | LHG | 5 | 623 | 22 | 36,36,48 | 1.07 | 2 (5%) | 39,42,54 | 1.10 | 3 (7%) |
| 22 | CLA | 4 | 612 | 16 | 52,60,73 | 2.25 | 18 (34%) | 60,97,113 | 3.10 | 27 (45%) |
| 30 | LUT | 8 | 618 | - | 42,43,43 | 0.79 | 0 | 51,60,60 | 1.56 | 11 (21%) |
| 22 | CLA | 3 | 602 | 13 | 60,68,73 | 2.15 | 18 (30%) | 70,107,113 | 2.87 | 31 (44%) |
| 30 | LUT | 7 | 622 | - | 42,43,43 | 0.75 | 0 | 51,60,60 | 1.49 | 10 (19%) |
| 25 | BCR | 7 | 623 | - | 41,41,41 | 0.78 | 1 (2%) | 56,56,56 | 1.93 | 15 (26%) |
| 29 | CHL | 6 | 608 | - | 51,59,74 | 2.21 | 17 (33%) | 55,96,114 | 3.41 | 26 (47%) |
| 30 | LUT | 6 | 621 | - | 42,43,43 | 0.73 | 0 | 51,60,60 | 1.62 | 11 (21%) |
| 22 | CLA | B | 828 | 2 | 65,73,73 | 2.01 | 16 (24%) | 76,113,113 | 2.58 | 27 (35%) |
| 22 | CLA | B | 837 | 2 | 65,73,73 | 1.97 | 16 (24%) | 76,113,113 | 2.83 | 28 (36%) |
| 22 | CLA | A | 804 | 1 | 65,73,73 | 1.96 | 16 (24%) | 76,113,113 | 2.81 | 30 (39%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | BCR | B | 846 | - | 41,41,41 | 0.76 | 0 | 56,56,56 | 2.01 | 15 (26%) |
| 22 | CLA | A | 810 | 1 | 65,73,73 | 1.98 | 17 (26%) | 76,113,113 | 2.74 | 30 (39%) |
| 25 | BCR | 5 | 622 | - | 41,41,41 | 0.66 | 0 | 56,56,56 | 1.87 | 15 (26%) |
| 29 | CHL | 5 | 618 | 17 | 43,51,74 | 2.40 | 17 (39%) | 45,86,114 | 3.62 | 22 (48%) |
| 22 | CLA | 9 | 603 | 20 | 46,54,73 | 2.42 | 17 (36%) | 53,90,113 | 3.29 | 26 (49%) |
| 29 | CHL | 5 | 607 | - | 51,59,74 | 2.25 | 17 (33%) | 55,96,114 | 3.29 | 25 (45%) |
| 22 | CLA | J | 3002 | 9 | 42,50,73 | 2.46 | 15 (35%) | 48,85,113 | 3.32 | 24 (50%) |
| 22 | CLA | B | 808 | 2 | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.72 | 27 (35%) |
| 22 | CLA | A | 842 | 1 | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.80 | 27 (35%) |
| 22 | CLA | A | 821 | 1 | 45,53,73 | 2.41 | 16 (35%) | 52,89,113 | 3.12 | 25 (48%) |
| 25 | BCR | B | 801 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.97 | 14 (25%) |
| 22 | CLA | 5 | 613 | 17 | 56,64,73 | 2.17 | 16 (28%) | 65,102,113 | 2.79 | 24 (36%) |
| 22 | CLA | B | 833 | 2 | 58,66,73 | 2.15 | 16 (27%) | 67,104,113 | 2.95 | 28 (41%) |
| 25 | BCR | B | 848 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.53 | 10 (17%) |
| 21 | CL0 | A | 801 | 1 | 65,73,73 | 1.93 | 15 (23%) | 76,113,113 | 2.81 | 30 (39%) |
| 22 | CLA | 4 | 610 | 16 | 60,68,73 | 2.11 | 16 (26%) | 70,107,113 | 2.81 | 30 (42%) |
| 25 | BCR | K | 4004 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.74 | 14 (25%) |
| 22 | CLA | 9 | 609 | - | 50,58,73 | 2.32 | 16 (32%) | 58,95,113 | 3.06 | 27 (46%) |
| 29 | CHL | 9 | 607 | - | 51,59,74 | 2.30 | 17 (33%) | 55,96,114 | 3.17 | 24 (43%) |
| 22 | CLA | A | 803 | - | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.88 | 29 (38%) |
| 22 | CLA | B | 823 | 2 | 60,68,73 | 2.11 | 16 (26%) | 70,107,113 | 2.68 | 28 (40%) |
| 22 | CLA | 7 | 601 | 14 | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.77 | 26 (34%) |
| 22 | CLA | 7 | 603 | 14 | 46,54,73 | 2.40 | 17 (36%) | 53,90,113 | 3.28 | 24 (45%) |
| 29 | CHL | 8 | 607 | - | 56,64,74 | 2.12 | 17 (30%) | 61,102,114 | 3.10 | 24 (39%) |
| 22 | CLA | B | 824 | - | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.65 | 28 (36%) |
| 26 | SF4 | C | 101 | 3 | 0,12,12 | - | - | - | - | - |
| 22 | CLA | B | 852 | - | 65,73,73 | 2.07 | 17 (26%) | 76,113,113 | 2.60 | 27 (35%) |
| 22 | CLA | 6 | 602 | 18 | 65,73,73 | 2.02 | 14 (21%) | 76,113,113 | 2.74 | 26 (34%) |
| 30 | LUT | 5 | 620 | - | 42,43,43 | 0.78 | 0 | 51,60,60 | 1.72 | 14 (27%) |
| 30 | LUT | 2 | 617 | - | 42,43,43 | 0.72 | 0 | 51,60,60 | 1.79 | 12 (23%) |
| 22 | CLA | 9 | 614 | 20 | 45,53,73 | 2.49 | 16 (35%) | 52,89,113 | 3.23 | 27 (51%) |
| 22 | CLA | A | 802 | - | 65,73,73 | 2.09 | 17 (26%) | 76,113,113 | 2.72 | 29 (38%) |
| 22 | CLA | B | 830 | 2 | 50,58,73 | 2.28 | 16 (32%) | 58,95,113 | 3.14 | 27 (46%) |
| 22 | CLA | 5 | 604 | 17 | 50,58,73 | 2.33 | 15 (30%) | 58,95,113 | 2.98 | 27 (46%) |
| 22 | CLA | 8 | 614 | 15 | 55,63,73 | 2.23 | 17 (30%) | 64,101,113 | 2.86 | 29 (45%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | A | 819 | 1 | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.70 | 27 (35%) |
| 22 | CLA | B | 826 | 2 | 65,73,73 | 1.98 | 15 (23%) | 76,113,113 | 2.75 | 29 (38%) |
| 22 | CLA | 7 | 616 | 14 | 46,54,73 | 2.46 | 18 (39%) | 53,90,113 | 3.24 | 24 (45%) |
| 29 | CHL | 5 | 608 | - | 51,59,74 | 2.20 | 16 (31%) | 55,96,114 | 3.17 | 25 (45%) |
| 30 | LUT | 4 | 620 | - | 42,43,43 | 0.73 | 0 | 51,60,60 | 1.50 | 10 (19%) |
| 22 | CLA | 9 | 610 | 20 | 60,68,73 | 2.15 | 16 (26%) | 70,107,113 | 2.84 | 27 (38%) |
| 22 | CLA | 6 | 617 | 18 | 46,54,73 | 2.41 | 17 (36%) | 53,90,113 | 3.13 | 25 (47%) |
| 22 | CLA | 4 | 602 | 16 | 60,68,73 | 2.11 | 17 (28%) | 70,107,113 | 2.79 | 27 (38%) |
| 22 | CLA | 3 | 606 | - | 42,50,73 | 2.45 | 15 (35%) | 48,85,113 | 3.28 | 23 (47%) |
| 22 | CLA | 7 | 608 | - | 50,58,73 | 2.28 | 16 (32%) | 58,95,113 | 3.12 | 25 (43%) |
| 25 | BCR | 6 | 625 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 2.05 | 16 (28%) |
| 22 | CLA | 8 | 603 | 15 | 45,53,73 | 2.41 | 18 (40%) | 52,89,113 | 3.21 | 24 (46%) |
| 22 | CLA | B | 816 | 2 | 55,63,73 | 2.15 | 15 (27%) | 64,101,113 | 3.07 | 26 (40%) |
| 22 | CLA | A | 808 | 1 | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.80 | 28 (36%) |
| 22 | CLA | 2 | 613 | 19 | 50,58,73 | 2.39 | 16 (32%) | 58,95,113 | 3.10 | 30 (51%) |
| 22 | CLA | 8 | 616 | 15 | 46,54,73 | 2.41 | 17 (36%) | 53,90,113 | 3.01 | 24 (45%) |
| 22 | CLA | 3 | 610 | 13 | 65,73,73 | 1.99 | 15 (23%) | 76,113,113 | 2.81 | 31 (40%) |
| 22 | CLA | B | 811 | 2 | 54,62,73 | 2.14 | 16 (29%) | 67,100,113 | 3.03 | 32 (47%) |
| 22 | CLA | A | 806 | 1 | 65,73,73 | 2.01 | 15 (23%) | 76,113,113 | 2.72 | 25 (32%) |
| 25 | BCR | A | 848 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.76 | 15 (26%) |
| 22 | CLA | A | 854 | - | 65,73,73 | 2.02 | 15 (23%) | 76,113,113 | 2.81 | 28 (36%) |
| 22 | CLA | 9 | 612 | - | 52,60,73 | 2.32 | 16 (30%) | 60,97,113 | 3.00 | 27 (45%) |
| 25 | BCR | 4 | 621 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 2.00 | 18 (32%) |
| 22 | CLA | 8 | 611 | 24 | 46,54,73 | 2.42 | 17 (36%) | 53,90,113 | 3.13 | 26 (49%) |
| 29 | CHL | 7 | 607 | - | 54,62,74 | 2.20 | 17 (31%) | 58,99,114 | 3.03 | 23 (39%) |
| 22 | CLA | 7 | 606 | - | 42,50,73 | 2.41 | 15 (35%) | 48,85,113 | 3.48 | 24 (50%) |
| 30 | LUT | 9 | 617 | - | 42,43,43 | 0.75 | 0 | 51,60,60 | 1.60 | 13 (25%) |
| 22 | CLA | F | 303 | - | 45,53,73 | 2.42 | 17 (37%) | 52,89,113 | 3.21 | 22 (42%) |
| 22 | CLA | A | 817 | - | 57,65,73 | 2.15 | 17 (29%) | 66,103,113 | 2.94 | 26 (39%) |
| 22 | CLA | A | 818 | 1 | 65,73,73 | 1.96 | 15 (23%) | 76,113,113 | 2.85 | 26 (34%) |
| 22 | CLA | 1 | 603 | 12 | 65,73,73 | 2.01 | 16 (24%) | 76,113,113 | 2.76 | 27 (35%) |
| 25 | BCR | B | 845 | - | 41,41,41 | 0.73 | 0 | 56,56,56 | 1.84 | 15 (26%) |
| 22 | CLA | 5 | 602 | 17 | 65,73,73 | 2.00 | 15 (23%) | 76,113,113 | 2.77 | 26 (34%) |
| 22 | CLA | 8 | 609 | 15 | 46,54,73 | 2.42 | 16 (34%) | 53,90,113 | 3.04 | 26 (49%) |
| 22 | CLA | Z | 611 | 24 | 65,73,73 | 2.07 | 17 (26%) | 76,113,113 | 2.65 | 26 (34%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | 5 | 621 | - | 46,54,73 | 2.44 | 18 (39%) | 53,90,113 | 2.96 | 25 (47%) |
| 22 | CLA | 6 | 609 | 18 | 50,58,73 | 2.33 | 17 (34%) | 58,95,113 | 3.04 | 26 (44%) |
| 22 | CLA | 2 | 609 | 19 | 50,58,73 | 2.40 | 17 (34%) | 58,95,113 | 3.05 | 29 (50%) |
| 29 | CHL | 4 | 618 | 16 | 43,51,74 | 2.38 | 17 (39%) | 45,86,114 | 3.57 | 22 (48%) |
| 22 | CLA | 7 | 614 | 14 | 43,51,73 | 2.43 | 16 (37%) | 49,86,113 | 3.35 | 26 (53%) |
| 22 | CLA | A | 822 | - | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.57 | 26 (34%) |
| 22 | CLA | 2 | 610 | 19 | 60,68,73 | 2.18 | 16 (26%) | 70,107,113 | 2.86 | 27 (38%) |
| 29 | CHL | 3 | 608 | - | 66,74,74 | 1.89 | 16 (24%) | 73,114,114 | 2.86 | 24 (32%) |
| 24 | LHG | 1 | 620 | 22 | 42,42,48 | 0.99 | 2 (4%) | 45,48,54 | 1.10 | 3 (6%) |
| 22 | CLA | 8 | 606 | - | 42,50,73 | 2.46 | 17 (40%) | 48,85,113 | 3.25 | 22 (45%) |
| 30 | LUT | 3 | 621 | - | 42,43,43 | 0.77 | 0 | 51,60,60 | 1.52 | 13 (25%) |
| 22 | CLA | B | 840 | 2 | 65,73,73 | 2.06 | 16 (24%) | 76,113,113 | 2.82 | 25 (32%) |
| 25 | BCR | 5 | 625 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 2.25 | 15 (26%) |
| 22 | CLA | Z | 603 | 12 | 57,65,73 | 2.19 | 16 (28%) | 66,103,113 | 2.94 | 31 (46%) |
| 25 | BCR | A | 852 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.89 | 13 (23%) |
| 25 | BCR | 8 | 619 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.83 | 15 (26%) |
| 24 | LHG | A | 855 | - | 29,29,48 | 1.20 | 2 (6%) | 32,35,54 | 1.17 | 3 (9%) |
| 30 | LUT | 9 | 616 | - | 42,43,43 | 0.73 | 0 | 51,60,60 | 1.52 | 11 (21%) |
| 22 | CLA | 9 | 604 | 20 | 50,58,73 | 2.39 | 17 (34%) | 58,95,113 | 3.07 | 27 (46%) |
| 25 | BCR | A | 849 | - | 41,41,41 | 0.78 | 0 | 56,56,56 | 1.80 | 17 (30%) |
| 22 | CLA | 6 | 603 | 18 | 46,54,73 | 2.38 | 16 (34%) | 53,90,113 | 3.23 | 26 (49%) |
| 22 | CLA | A | 820 | 1 | 65,73,73 | 2.01 | 17 (26%) | 76,113,113 | 2.79 | 29 (38%) |
| 22 | CLA | 5 | 617 | 17 | 46,54,73 | 2.36 | 17 (36%) | 53,90,113 | 4.43 | 25 (47%) |
| 22 | CLA | A | 830 | 1 | 65,73,73 | 1.95 | 16 (24%) | 76,113,113 | 2.63 | 26 (34%) |
| 22 | CLA | A | 816 | 1 | 65,73,73 | 2.08 | 17 (26%) | 76,113,113 | 2.68 | 26 (34%) |
| 22 | CLA | B | 841 | 24 | 65,73,73 | 2.09 | 17 (26%) | 76,113,113 | 2.78 | 28 (36%) |
| 22 | CLA | 7 | 613 | 14 | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.65 | 23 (30%) |
| 22 | CLA | A | 826 | - | 65,73,73 | 1.99 | 17 (26%) | 76,113,113 | 2.71 | 26 (34%) |
| 23 | PQN | B | 842 | - | 34,34,34 | 1.56 | 2 (5%) | 42,45,45 | 0.94 | 2 (4%) |
| 22 | CLA | A | 827 | - | 65,73,73 | 2.02 | 15 (23%) | 76,113,113 | 2.70 | 27 (35%) |
| 22 | CLA | 1 | 611 | 24 | 65,73,73 | 2.06 | 17 (26%) | 76,113,113 | 2.65 | 25 (32%) |
| 22 | CLA | B | 815 | 2 | 57,65,73 | 2.14 | 15 (26%) | 66,103,113 | 2.92 | 27 (40%) |
| 22 | CLA | B | 832 | 2 | 65,73,73 | 1.97 | 15 (23%) | 76,113,113 | 2.76 | 27 (35%) |
| 22 | CLA | A | 807 | 1 | 65,73,73 | 2.03 | 17 (26%) | 76,113,113 | 2.74 | 25 (32%) |
| 30 | LUT | 8 | 617 | - | 42,43,43 | 0.77 | 0 | 51,60,60 | 1.70 | 13 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | 3 | 603 | 13 | 65,73,73 | 1.98 | 17 (26%) | 76,113,113 | 2.69 | 26 (34%) |
| 28 | LMG | J | 3001 | - | 35,35,55 | 0.94 | 2 (5%) | 43,43,63 | 1.23 | 5 (11%) |
| 22 | CLA | B | 825 | - | 65,73,73 | 2.01 | 16 (24%) | 76,113,113 | 2.65 | 28 (36%) |
| 22 | CLA | Z | 609 | 12 | 65,73,73 | 2.07 | 16 (24%) | 76,113,113 | 2.67 | 27 (35%) |
| 22 | CLA | A | 836 | 1 | 50,58,73 | 2.33 | 18 (36%) | 58,95,113 | 3.05 | 29 (50%) |
| 22 | CLA | A | 811 | 1 | 65,73,73 | 2.00 | 15 (23%) | 76,113,113 | 2.73 | 28 (36%) |
| 22 | CLA | A | 833 | 1 | 65,73,73 | 2.05 | 16 (24%) | 76,113,113 | 2.67 | 27 (35%) |
| 22 | CLA | 3 | 614 | 13 | 45,53,73 | 2.49 | 16 (35%) | 52,89,113 | 3.25 | 24 (46%) |
| 22 | CLA | 9 | 601 | 20 | 46,54,73 | 2.47 | 16 (34%) | 53,90,113 | 3.14 | 24 (45%) |
| 22 | CLA | 8 | 610 | 15 | 60,68,73 | 2.10 | 16 (26%) | 70,107,113 | 2.85 | 31 (44%) |
| 22 | CLA | A | 831 | 1 | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.77 | 29 (38%) |
| 24 | LHG | B | 851 | 22 | 22,22,48 | 1.15 | 2 (9%) | 25,28,54 | 1.24 | 2 (8%) |
| 29 | CHL | 9 | 606 | - | 42,50,74 | 2.38 | 16 (38%) | 44,85,114 | 3.67 | 23 (52%) |
| 22 | CLA | Z | 608 | - | 65,73,73 | 2.04 | 17 (26%) | 76,113,113 | 2.69 | 26 (34%) |
| 23 | PQN | A | 844 | - | 34,34,34 | 1.52 | 2 (5%) | 42,45,45 | 1.04 | 2 (4%) |
| 22 | CLA | 4 | 609 | 16 | 50,58,73 | 2.30 | 16 (32%) | 58,95,113 | 3.04 | 28 (48%) |
| 29 | CHL | 4 | 607 | - | 51,59,74 | 2.26 | 16 (31%) | 55,96,114 | 3.33 | 25 (45%) |
| 22 | CLA | B | 818 | 2 | 60,68,73 | 2.09 | 16 (26%) | 70,107,113 | 2.79 | 32 (45%) |
| 22 | CLA | 6 | 604 | - | 65,73,73 | 2.05 | 18 (27%) | 76,113,113 | 2.64 | 27 (35%) |
| 22 | CLA | 7 | 612 | 14 | 52,60,73 | 2.25 | 16 (30%) | 60,97,113 | 3.06 | 26 (43%) |
| 22 | CLA | 4 | 604 | - | 50,58,73 | 2.34 | 16 (32%) | 58,95,113 | 3.03 | 27 (46%) |
| 22 | CLA | 7 | 604 | - | 56,64,73 | 2.16 | 17 (30%) | 65,102,113 | 3.03 | 26 (40%) |
| 24 | LHG | A | 846 | - | 48,48,48 | 0.91 | 2 (4%) | 51,54,54 | 1.01 | 3 (5%) |
| 22 | CLA | 1 | 612 | 12 | 52,60,73 | 2.26 | 16 (30%) | 60,97,113 | 2.99 | 28 (46%) |
| 22 | CLA | 1 | 608 | - | 65,73,73 | 2.01 | 16 (24%) | 76,113,113 | 2.71 | 27 (35%) |
| 22 | CLA | B | 820 | 2 | 56,64,73 | 2.24 | 16 (28%) | 65,102,113 | 2.92 | 27 (41%) |
| 22 | CLA | 8 | 604 | - | 46,54,73 | 2.39 | 17 (36%) | 53,90,113 | 3.10 | 24 (45%) |
| 22 | CLA | 2 | 614 | - | 45,53,73 | 2.51 | 16 (35%) | 52,89,113 | 3.21 | 24 (46%) |
| 30 | LUT | 1 | 617 | - | 42,43,43 | 0.75 | 0 | 51,60,60 | 1.69 | 13 (25%) |
| 22 | CLA | Z | 610 | 12 | 60,68,73 | 2.09 | 15 (25%) | 70,107,113 | 2.92 | 28 (40%) |
| 22 | CLA | B | 822 | 2 | 59,67,73 | 2.12 | 17 (28%) | 68,105,113 | 2.86 | 28 (41%) |
| 24 | LHG | 7 | 625 | 22 | 36,36,48 | 1.02 | 2 (5%) | 39,42,54 | 1.13 | 3 (7%) |
| 22 | CLA | 5 | 603 | 17 | 46,54,73 | 2.38 | 17 (36%) | 53,90,113 | 3.18 | 26 (49%) |
| 22 | CLA | 9 | 611 | - | 55,63,73 | 2.27 | 16 (29%) | 64,101,113 | 2.87 | 27 (42%) |
| 25 | BCR | A | 856 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.77 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | K | 4003 | 10 | 46,54,73 | 2.43 | 15 (32%) | 53,90,113 | 3.16 | 23 (43%) |
| 22 | CLA | 6 | 610 | - | 60,68,73 | 2.14 | 16 (26%) | 70,107,113 | 2.82 | 30 (42%) |
| 22 | CLA | 5 | 612 | 17 | 52,60,73 | 2.26 | 17 (32%) | 60,97,113 | 3.02 | 27 (45%) |
| 22 | CLA | Z | 612 | 12 | 52,60,73 | 2.27 | 17 (32%) | 60,97,113 | 3.07 | 26 (43%) |
| 30 | LUT | 1 | 618 | - | 42,43,43 | 0.74 | 0 | 51,60,60 | 1.58 | 12 (23%) |
| 22 | CLA | B | 813 | 2 | 65,73,73 | 2.00 | 16 (24%) | 76,113,113 | 2.73 | 30 (39%) |
| 26 | SF4 | A | 853 | 2,1 | 0,12,12 | - | - | - | | |
| 22 | CLA | B | 807 | 2 | 65,73,73 | 2.04 | 16 (24%) | 76,113,113 | 2.74 | 27 (35%) |
| 28 | LMG | 9 | 620 | - | 44,44,55 | 0.85 | 2 (4%) | 52,52,63 | 1.23 | 2 (3%) |
| 22 | CLA | 2 | 601 | 19 | 46,54,73 | 2.45 | 16 (34%) | 53,90,113 | 3.14 | 25 (47%) |
| 22 | CLA | 4 | 601 | 16 | 61,69,73 | 2.08 | 16 (26%) | 71,108,113 | 2.80 | 27 (38%) |
| 25 | BCR | B | 843 | - | 41,41,41 | 0.72 | 0 | 56,56,56 | 1.56 | 8 (14%) |
| 29 | CHL | 4 | 608 | - | 51,59,74 | 2.17 | 16 (31%) | 55,96,114 | 3.26 | 24 (43%) |
| 25 | BCR | 7 | 624 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.75 | 12 (21%) |
| 22 | CLA | A | 845 | 24 | 52,60,73 | 2.29 | 16 (30%) | 60,97,113 | 3.07 | 23 (38%) |
| 29 | CHL | 4 | 606 | - | 56,64,74 | 2.12 | 17 (30%) | 61,102,114 | 3.05 | 24 (39%) |
| 22 | CLA | 3 | 611 | - | 41,49,73 | 2.55 | 16 (39%) | 47,84,113 | 3.30 | 25 (53%) |
| 22 | CLA | 8 | 601 | 15 | 65,73,73 | 2.03 | 18 (27%) | 76,113,113 | 2.69 | 28 (36%) |
| 30 | LUT | Z | 617 | - | 42,43,43 | 0.77 | 0 | 51,60,60 | 1.69 | 15 (29%) |
| 27 | DGD | B | 850 | - | 67,67,67 | 0.80 | 2 (2%) | 81,81,81 | 1.03 | 4 (4%) |
| 30 | LUT | 4 | 619 | - | 42,43,43 | 0.71 | 0 | 51,60,60 | 1.67 | 11 (21%) |
| 22 | CLA | B | 831 | 2 | 49,57,73 | 2.29 | 15 (30%) | 55,93,113 | 3.11 | 22 (40%) |
| 24 | LHG | A | 847 | 22 | 37,37,48 | 1.06 | 2 (5%) | 40,43,54 | 1.26 | 4 (10%) |
| 22 | CLA | 6 | 614 | 18 | 45,53,73 | 2.44 | 16 (35%) | 52,89,113 | 3.31 | 26 (50%) |
| 22 | CLA | B | 803 | - | 65,73,73 | 1.93 | 17 (26%) | 76,113,113 | 2.59 | 26 (34%) |
| 22 | CLA | Z | 616 | 12 | 46,54,73 | 2.44 | 17 (36%) | 53,90,113 | 3.09 | 24 (45%) |
| 22 | CLA | B | 810 | 2 | 65,73,73 | 2.05 | 17 (26%) | 76,113,113 | 2.74 | 25 (32%) |
| 22 | CLA | B | 838 | 2 | 47,55,73 | 2.35 | 17 (36%) | 54,91,113 | 3.15 | 24 (44%) |
| 22 | CLA | B | 827 | 2 | 65,73,73 | 2.00 | 17 (26%) | 76,113,113 | 2.70 | 28 (36%) |
| 22 | CLA | A | 814 | 1 | 65,73,73 | 2.00 | 17 (26%) | 76,113,113 | 2.78 | 26 (34%) |
| 22 | CLA | F | 301 | - | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.78 | 29 (38%) |
| 30 | LUT | Z | 618 | - | 42,43,43 | 0.71 | 0 | 51,60,60 | 1.58 | 12 (23%) |
| 29 | CHL | Z | 601 | 12 | 53,61,74 | 2.26 | 17 (32%) | 57,98,114 | 3.26 | 22 (38%) |
| 22 | CLA | Z | 602 | 12 | 65,73,73 | 2.00 | 18 (27%) | 76,113,113 | 2.73 | 28 (36%) |
| 22 | CLA | A | 812 | 1 | 65,73,73 | 1.99 | 18 (27%) | 76,113,113 | 2.85 | 25 (32%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | BCR | 3 | 719 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 1.64 | 13 (23%) |
| 22 | CLA | 4 | 616 | 16 | 41,49,73 | 2.56 | 15 (36%) | 47,84,113 | 3.46 | 25 (53%) |
| 22 | CLA | 1 | 609 | 12 | 65,73,73 | 2.05 | 17 (26%) | 76,113,113 | 2.73 | 26 (34%) |
| 22 | CLA | 9 | 613 | - | 50,58,73 | 2.35 | 17 (34%) | 58,95,113 | 3.00 | 27 (46%) |
| 22 | CLA | 3 | 620 | - | 56,64,73 | 2.19 | 17 (30%) | 65,102,113 | 2.88 | 26 (40%) |
| 30 | LUT | 6 | 624 | - | 42,43,43 | 0.72 | 0 | 51,60,60 | 1.44 | 8 (15%) |
| 22 | CLA | 6 | 611 | 24 | 55,63,73 | 2.24 | 18 (32%) | 64,101,113 | 2.82 | 26 (40%) |
| 25 | BCR | B | 844 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.75 | 11 (19%) |
| 22 | CLA | B | 834 | 2 | 65,73,73 | 2.07 | 15 (23%) | 76,113,113 | 2.72 | 30 (39%) |
| 22 | CLA | 3 | 617 | 13 | 46,54,73 | 2.41 | 16 (34%) | 53,90,113 | 3.14 | 25 (47%) |
| 25 | BCR | A | 851 | - | 41,41,41 | 0.81 | 2 (4%) | 56,56,56 | 1.83 | 12 (21%) |
| 22 | CLA | A | 828 | 1 | 65,73,73 | 1.98 | 17 (26%) | 76,113,113 | 2.83 | 23 (30%) |
| 22 | CLA | A | 840 | 1 | 65,73,73 | 1.98 | 18 (27%) | 76,113,113 | 2.83 | 27 (35%) |
| 22 | CLA | A | 805 | 1 | 55,63,73 | 2.22 | 17 (30%) | 64,101,113 | 2.94 | 26 (40%) |
| 25 | BCR | I | 172 | - | 41,41,41 | 0.67 | 0 | 56,56,56 | 1.97 | 15 (26%) |
| 22 | CLA | B | 817 | 2 | 59,67,73 | 2.09 | 16 (27%) | 68,105,113 | 2.83 | 26 (38%) |
| 22 | CLA | A | 839 | 1 | 65,73,73 | 2.00 | 16 (24%) | 76,113,113 | 2.77 | 27 (35%) |
| 22 | CLA | 7 | 620 | - | 60,68,73 | 2.15 | 16 (26%) | 70,107,113 | 2.79 | 28 (40%) |
| 22 | CLA | A | 829 | 1 | 65,73,73 | 1.96 | 16 (24%) | 76,113,113 | 2.73 | 29 (38%) |
| 22 | CLA | 5 | 614 | 17 | 45,53,73 | 2.45 | 16 (35%) | 52,89,113 | 3.30 | 26 (50%) |
| 22 | CLA | 8 | 613 | 15 | 65,73,73 | 2.03 | 16 (24%) | 76,113,113 | 2.60 | 25 (32%) |
| 22 | CLA | 6 | 612 | 18 | 52,60,73 | 2.26 | 17 (32%) | 60,97,113 | 3.00 | 25 (41%) |
| 22 | CLA | Z | 614 | 12 | 65,73,73 | 2.07 | 16 (24%) | 76,113,113 | 2.71 | 28 (36%) |
| 24 | LHG | 4 | 622 | 22 | 48,48,48 | 0.96 | 2 (4%) | 51,54,54 | 1.09 | 3 (5%) |
| 22 | CLA | K | 4002 | - | 45,53,73 | 2.49 | 17 (37%) | 52,89,113 | 3.18 | 26 (50%) |
| 22 | CLA | 8 | 612 | 15 | 52,60,73 | 2.26 | 16 (30%) | 60,97,113 | 3.00 | 29 (48%) |
| 22 | CLA | Z | 613 | - | 65,73,73 | 2.04 | 15 (23%) | 76,113,113 | 2.63 | 27 (35%) |
| 22 | CLA | 1 | 616 | 12 | 46,54,73 | 2.42 | 17 (36%) | 53,90,113 | 3.01 | 25 (47%) |
| 22 | CLA | A | 813 | 1 | 54,62,73 | 2.22 | 16 (29%) | 62,99,113 | 2.95 | 26 (41%) |
| 30 | LUT | 5 | 624 | - | 42,43,43 | 0.77 | 0 | 51,60,60 | 1.54 | 11 (21%) |
| 22 | CLA | G | 203 | 7 | 50,58,73 | 2.33 | 17 (34%) | 58,95,113 | 3.19 | 28 (48%) |
| 22 | CLA | B | 804 | 2 | 45,53,73 | 2.40 | 16 (35%) | 52,89,113 | 3.29 | 27 (51%) |
| 22 | CLA | 3 | 604 | - | 65,73,73 | 2.01 | 15 (23%) | 76,113,113 | 2.67 | 25 (32%) |
| 22 | CLA | L | 203 | 11 | 65,73,73 | 1.97 | 18 (27%) | 76,113,113 | 2.77 | 26 (34%) |
| 25 | BCR | A | 850 | - | 41,41,41 | 0.70 | 0 | 56,56,56 | 1.90 | 12 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | 6 | 601 | 18 | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.75 | 27 (35%) |
| 22 | CLA | 7 | 602 | 14 | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.80 | 28 (36%) |
| 22 | CLA | 6 | 616 | 18 | 46,54,73 | 2.45 | 17 (36%) | 53,90,113 | 3.19 | 28 (52%) |
| 29 | CHL | Z | 607 | - | 48,56,74 | 2.34 | 18 (37%) | 51,92,114 | 3.20 | 23 (45%) |
| 22 | CLA | 2 | 602 | 19 | 45,53,73 | 2.49 | 16 (35%) | 52,89,113 | 3.19 | 24 (46%) |
| 29 | CHL | 1 | 607 | - | 48,56,74 | 2.34 | 18 (37%) | 51,92,114 | 3.13 | 20 (39%) |
| 29 | CHL | 6 | 606 | - | 56,64,74 | 2.16 | 17 (30%) | 61,102,114 | 3.15 | 25 (40%) |
| 22 | CLA | 2 | 607 | - | 50,58,73 | 2.39 | 16 (32%) | 58,95,113 | 3.07 | 27 (46%) |
| 22 | CLA | 5 | 609 | 17 | 50,58,73 | 2.32 | 17 (34%) | 58,95,113 | 3.10 | 27 (46%) |
| 22 | CLA | B | 821 | 2 | 46,54,73 | 2.41 | 17 (36%) | 53,90,113 | 3.14 | 23 (43%) |
| 22 | CLA | L | 204 | - | 50,58,73 | 2.36 | 16 (32%) | 58,95,113 | 3.08 | 25 (43%) |
| 22 | CLA | A | 834 | 1 | 65,73,73 | 2.02 | 17 (26%) | 76,113,113 | 2.79 | 29 (38%) |
| 22 | CLA | B | 814 | 2 | 60,68,73 | 2.09 | 16 (26%) | 70,107,113 | 2.76 | 29 (41%) |
| 22 | CLA | 1 | 610 | 12 | 60,68,73 | 2.10 | 15 (25%) | 70,107,113 | 2.90 | 31 (44%) |
| 22 | CLA | 6 | 622 | 18 | 45,53,73 | 2.42 | 17 (37%) | 52,89,113 | 3.20 | 25 (48%) |
| 22 | CLA | 5 | 610 | 17 | 60,68,73 | 2.11 | 16 (26%) | 70,107,113 | 2.85 | 30 (42%) |
| 22 | CLA | B | 805 | 2 | 65,73,73 | 1.99 | 16 (24%) | 76,113,113 | 2.79 | 26 (34%) |
| 22 | CLA | 8 | 608 | - | 50,58,73 | 2.25 | 16 (32%) | 58,95,113 | 3.14 | 25 (43%) |
| 25 | BCR | 3 | 718 | - | 41,41,41 | 0.74 | 0 | 56,56,56 | 1.90 | 17 (30%) |
| 22 | CLA | 1 | 604 | - | 57,65,73 | 2.18 | 17 (29%) | 66,103,113 | 2.82 | 29 (43%) |
| 22 | CLA | 1 | 606 | - | 52,60,73 | 2.28 | 17 (32%) | 60,97,113 | 2.99 | 27 (45%) |
| 22 | CLA | 8 | 602 | 15 | 62,70,73 | 2.02 | 15 (24%) | 72,109,113 | 2.87 | 28 (38%) |
| 25 | BCR | F | 305 | - | 41,41,41 | 0.69 | 0 | 56,56,56 | 1.88 | 13 (23%) |
| 22 | CLA | B | 829 | 2 | 65,73,73 | 2.05 | 17 (26%) | 76,113,113 | 2.86 | 30 (39%) |
| 22 | CLA | 2 | 611 | - | 55,63,73 | 2.27 | 16 (29%) | 64,101,113 | 2.88 | 28 (43%) |
| 26 | SF4 | C | 102 | 3 | 0,12,12 | - | - | - | - | - |
| 24 | LHG | 8 | 620 | 22 | 36,36,48 | 1.02 | 2 (5%) | 39,42,54 | 1.14 | 5 (12%) |
| 22 | CLA | B | 836 | 2 | 60,68,73 | 2.13 | 17 (28%) | 70,107,113 | 2.89 | 29 (41%) |
| 22 | CLA | 1 | 614 | 12 | 65,73,73 | 2.05 | 17 (26%) | 76,113,113 | 2.77 | 25 (32%) |
| 22 | CLA | A | 841 | 1 | 65,73,73 | 2.01 | 17 (26%) | 76,113,113 | 2.79 | 28 (36%) |
| 29 | CHL | 6 | 618 | 18 | 43,51,74 | 2.36 | 15 (34%) | 45,86,114 | 3.52 | 23 (51%) |
| 30 | LUT | 7 | 621 | - | 42,43,43 | 0.73 | 0 | 51,60,60 | 1.53 | 10 (19%) |
| 22 | CLA | 7 | 609 | 14 | 50,58,73 | 2.32 | 16 (32%) | 58,95,113 | 3.11 | 27 (46%) |
| 22 | CLA | B | 802 | 2 | 65,73,73 | 1.92 | 17 (26%) | 76,113,113 | 2.84 | 27 (35%) |
| 25 | BCR | L | 205 | - | 41,41,41 | 0.71 | 0 | 56,56,56 | 1.60 | 12 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 30 | LUT | 3 | 622 | - | 42,43,43 | 0.80 | 0 | 51,60,60 | 1.67 | 10 (19%) |
| 22 | CLA | A | 838 | 1 | 51,59,73 | 2.28 | 16 (31%) | 59,96,113 | 3.13 | 30 (50%) |
| 22 | CLA | F | 304 | 6 | 65,73,73 | 2.06 | 18 (27%) | 76,113,113 | 2.72 | 25 (32%) |
| 22 | CLA | B | 835 | - | 45,53,73 | 2.45 | 17 (37%) | 52,89,113 | 3.08 | 25 (48%) |
| 22 | CLA | 5 | 601 | 17 | 65,73,73 | 2.06 | 17 (26%) | 76,113,113 | 2.72 | 29 (38%) |
| 22 | CLA | B | 809 | 2 | 65,73,73 | 1.97 | 14 (21%) | 76,113,113 | 2.67 | 28 (36%) |
| 22 | CLA | B | 819 | - | 65,73,73 | 2.02 | 16 (24%) | 76,113,113 | 2.58 | 27 (35%) |
| 22 | CLA | 9 | 602 | 20 | 60,68,73 | 2.12 | 15 (25%) | 70,107,113 | 2.83 | 28 (40%) |
| 25 | BCR | 3 | 717 | - | 41,41,41 | 0.75 | 0 | 56,56,56 | 1.87 | 16 (28%) |
| 22 | CLA | 4 | 603 | 16 | 46,54,73 | 2.38 | 16 (34%) | 53,90,113 | 3.18 | 25 (47%) |
| 22 | CLA | A | 837 | 1 | 45,53,73 | 2.49 | 17 (37%) | 52,89,113 | 3.08 | 26 (50%) |
| 30 | LUT | 2 | 616 | - | 42,43,43 | 0.75 | 0 | 51,60,60 | 1.72 | 15 (29%) |
| 22 | CLA | B | 839 | - | 65,73,73 | 2.05 | 18 (27%) | 76,113,113 | 2.66 | 26 (34%) |
| 22 | CLA | 2 | 606 | - | 41,49,73 | 2.58 | 16 (39%) | 47,84,113 | 3.36 | 26 (55%) |
| 30 | LUT | Z | 619 | - | 42,43,43 | 0.71 | 0 | 51,60,60 | 1.76 | 12 (23%) |
| 30 | LUT | 1 | 619 | - | 42,43,43 | 0.76 | 0 | 51,60,60 | 1.83 | 14 (27%) |
| 22 | CLA | A | 815 | 1 | 60,68,73 | 2.17 | 17 (28%) | 70,107,113 | 2.88 | 27 (38%) |
| 22 | CLA | A | 843 | - | 65,73,73 | 2.01 | 18 (27%) | 76,113,113 | 2.61 | 27 (35%) |
| 22 | CLA | 6 | 613 | - | 56,64,73 | 2.22 | 17 (30%) | 65,102,113 | 2.84 | 27 (41%) |

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 |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22 | CLA | 3 | 607 | 13 | 1/1/14/20 | 15/31/109/115 | - |
| 25 | BCR | G | 205 | - | - | 2/29/63/63 | 0/2/2/2 |
| 22 | CLA | G | 204 | 7 | 1/1/11/20 | 5/15/93/115 | - |
| 22 | CLA | A | 825 | 1 | - | 7/25/103/115 | - |
| 22 | CLA | 3 | 609 | 13 | 1/1/12/20 | 5/19/97/115 | - |
| 22 | CLA | 1 | 613 | - | 1/1/15/20 | 7/37/115/115 | - |
| 22 | CLA | B | 806 | 2 | 1/1/15/20 | 13/37/115/115 | - |
| 22 | CLA | 7 | 610 | 14 | 1/1/14/20 | 6/31/109/115 | - |
| 25 | BCR | 6 | 623 | - | - | 9/29/63/63 | 0/2/2/2 |
| 25 | BCR | K | 4001 | - | - | 5/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 29 | CHL | 1 | 601 | 12 | 3/3/17/26 | 11/24/122/137 | - |
| 22 | CLA | 7 | 611 | 24 | 1/1/10/20 | 2/8/86/115 | - |
| 22 | CLA | 4 | 614 | 16 | 1/1/11/20 | 2/13/91/115 | - |
| 22 | CLA | 1 | 602 | 12 | 1/1/15/20 | 13/37/115/115 | - |
| 22 | CLA | A | 832 | 1 | 1/1/12/20 | 2/19/97/115 | - |
| 25 | BCR | J | 3003 | - | - | 8/29/63/63 | 0/2/2/2 |
| 24 | LHG | Z | 620 | 22 | - | 15/47/47/53 | - |
| 22 | CLA | 4 | 611 | 24 | 1/1/13/20 | 8/25/103/115 | - |
| 24 | LHG | 4 | 623 | - | - | 9/36/36/53 | - |
| 25 | BCR | B | 847 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | CLA | 3 | 613 | 13 | - | 14/25/103/115 | - |
| 29 | CHL | 6 | 607 | - | 2/2/18/26 | 12/27/125/137 | - |
| 22 | CLA | 5 | 616 | 17 | 1/1/11/20 | 7/15/93/115 | - |
| 22 | CLA | A | 835 | 1 | 1/1/15/20 | 4/37/115/115 | - |
| 22 | CLA | Z | 604 | - | 1/1/13/20 | 9/28/106/115 | - |
| 22 | CLA | A | 809 | 1 | 1/1/15/20 | 17/37/115/115 | - |
| 22 | CLA | Z | 606 | - | 1/1/12/20 | 4/22/100/115 | - |
| 22 | CLA | 4 | 613 | 16 | - | 10/27/105/115 | - |
| 22 | CLA | 5 | 606 | - | 1/1/13/20 | 5/25/103/115 | - |
| 25 | BCR | L | 201 | - | - | 8/29/63/63 | 0/2/2/2 |
| 22 | CLA | 2 | 603 | 19 | 1/1/11/20 | 6/15/93/115 | - |
| 22 | CLA | 5 | 611 | 24 | 1/1/13/20 | 7/25/103/115 | - |
| 24 | LHG | 6 | 619 | 22 | - | 11/53/53/53 | - |
| 22 | CLA | A | 823 | 1 | - | 10/18/96/115 | - |
| 22 | CLA | 3 | 612 | 13 | 1/1/11/20 | 2/15/93/115 | - |
| 22 | CLA | A | 824 | 1 | 1/1/12/20 | 8/21/99/115 | - |
| 22 | CLA | 2 | 612 | 19 | 1/1/12/20 | 5/22/100/115 | - |
| 22 | CLA | B | 812 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | LHG | 5 | 623 | 22 | - | 10/41/41/53 | - |
| 22 | CLA | 4 | 612 | 16 | 1/1/12/20 | 3/22/100/115 | - |
| 30 | LUT | 8 | 618 | - | - | 4/29/67/67 | 0/2/2/2 |
| 22 | CLA | 3 | 602 | 13 | 1/1/14/20 | 8/31/109/115 | - |
| 30 | LUT | 7 | 622 | - | - | 3/29/67/67 | 0/2/2/2 |
| 25 | BCR | 7 | 623 | - | - | 7/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 29 | CHL | 6 | 608 | - | 3/3/17/26 | 4/21/119/137 | - |
| 30 | LUT | 6 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | B | 828 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 837 | 2 | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | A | 804 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 25 | BCR | B | 846 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | A | 810 | 1 | - | 11/37/115/115 | - |
| 25 | BCR | 5 | 622 | - | - | 7/29/63/63 | 0/2/2/2 |
| 29 | CHL | 5 | 618 | 17 | 3/3/15/26 | 4/12/110/137 | - |
| 22 | CLA | 9 | 603 | 20 | 1/1/11/20 | 1/15/93/115 | - |
| 29 | CHL | 5 | 607 | - | 3/3/17/26 | 10/21/119/137 | - |
| 22 | CLA | J | 3002 | 9 | 1/1/10/20 | 3/10/88/115 | - |
| 22 | CLA | B | 808 | 2 | 1/1/15/20 | 10/37/115/115 | - |
| 22 | CLA | A | 842 | 1 | 1/1/15/20 | 16/37/115/115 | - |
| 22 | CLA | A | 821 | 1 | 1/1/11/20 | 2/13/91/115 | - |
| 25 | BCR | B | 801 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | 5 | 613 | 17 | 1/1/13/20 | 8/27/105/115 | - |
| 22 | CLA | B | 833 | 2 | 1/1/13/20 | 8/29/107/115 | - |
| 25 | BCR | B | 848 | - | - | 3/29/63/63 | 0/2/2/2 |
| 21 | CL0 | A | 801 | 1 | 2/2/20/25 | 6/37/135/135 | - |
| 22 | CLA | 4 | 610 | 16 | 1/1/14/20 | 9/31/109/115 | - |
| 25 | BCR | K | 4004 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | 9 | 609 | - | 1/1/12/20 | 0/19/97/115 | - |
| 29 | CHL | 9 | 607 | - | 3/3/17/26 | 7/21/119/137 | - |
| 22 | CLA | A | 803 | - | 1/1/15/20 | 4/37/115/115 | - |
| 22 | CLA | B | 823 | 2 | 1/1/14/20 | 8/31/109/115 | - |
| 22 | CLA | 7 | 601 | 14 | 1/1/15/20 | 16/37/115/115 | - |
| 22 | CLA | 7 | 603 | 14 | 1/1/11/20 | 2/15/93/115 | - |
| 29 | CHL | 8 | 607 | - | 3/3/18/26 | 11/27/125/137 | - |
| 22 | CLA | B | 824 | - | 1/1/15/20 | 9/37/115/115 | - |
| 26 | SF4 | C | 101 | 3 | - | - | 0/6/5/5 |
| 22 | CLA | B | 852 | - | 1/1/15/20 | 5/37/115/115 | - |
| 22 | CLA | 6 | 602 | 18 | 1/1/15/20 | 13/37/115/115 | - |
| 30 | LUT | 5 | 620 | - | - | 0/29/67/67 | 0/2/2/2 |
| 30 | LUT | 2 | 617 | - | - | 3/29/67/67 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | 9 | 614 | 20 | - | 4/13/91/115 | - |
| 22 | CLA | A | 802 | - | 1/1/15/20 | 5/37/115/115 | - |
| 22 | CLA | B | 830 | 2 | - | 3/19/97/115 | - |
| 22 | CLA | 5 | 604 | 17 | - | 5/19/97/115 | - |
| 22 | CLA | 8 | 614 | 15 | 1/1/13/20 | 6/25/103/115 | - |
| 22 | CLA | A | 819 | 1 | 1/1/15/20 | 12/37/115/115 | - |
| 22 | CLA | B | 826 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | 7 | 616 | 14 | 1/1/11/20 | 5/15/93/115 | - |
| 29 | CHL | 5 | 608 | - | 3/3/17/26 | 8/21/119/137 | - |
| 30 | LUT | 4 | 620 | - | - | 3/29/67/67 | 0/2/2/2 |
| 22 | CLA | 9 | 610 | 20 | - | 4/31/109/115 | - |
| 22 | CLA | 6 | 617 | 18 | 1/1/11/20 | 3/15/93/115 | - |
| 22 | CLA | 4 | 602 | 16 | - | 12/31/109/115 | - |
| 22 | CLA | 3 | 606 | - | 1/1/10/20 | 0/10/88/115 | - |
| 22 | CLA | 7 | 608 | - | - | 3/19/97/115 | - |
| 25 | BCR | 6 | 625 | - | - | 9/29/63/63 | 0/2/2/2 |
| 22 | CLA | 8 | 603 | 15 | 1/1/11/20 | 2/13/91/115 | - |
| 22 | CLA | B | 816 | 2 | 1/1/13/20 | 8/25/103/115 | - |
| 22 | CLA | A | 808 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 22 | CLA | 2 | 613 | 19 | - | 3/19/97/115 | - |
| 22 | CLA | 8 | 616 | 15 | 1/1/11/20 | 2/15/93/115 | - |
| 22 | CLA | 3 | 610 | 13 | 1/1/15/20 | 14/37/115/115 | - |
| 22 | CLA | B | 811 | 2 | 1/1/13/20 | 5/25/101/115 | - |
| 22 | CLA | A | 806 | 1 | 1/1/15/20 | 16/37/115/115 | - |
| 25 | BCR | A | 848 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | CLA | A | 854 | - | 1/1/15/20 | 12/37/115/115 | - |
| 22 | CLA | 9 | 612 | - | 1/1/12/20 | 4/22/100/115 | - |
| 25 | BCR | 4 | 621 | - | - | 3/29/63/63 | 0/2/2/2 |
| 22 | CLA | 8 | 611 | 24 | 1/1/11/20 | 3/15/93/115 | - |
| 29 | CHL | 7 | 607 | - | 3/3/17/26 | 9/25/123/137 | - |
| 22 | CLA | 7 | 606 | - | 1/1/10/20 | 7/10/88/115 | - |
| 30 | LUT | 9 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | F | 303 | - | 1/1/11/20 | 4/13/91/115 | - |
| 22 | CLA | A | 817 | - | 1/1/13/20 | 6/28/106/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | A | 818 | 1 | - | 14/37/115/115 | - |
| 22 | CLA | 1 | 603 | 12 | 1/1/15/20 | 8/37/115/115 | - |
| 25 | BCR | B | 845 | - | - | 10/29/63/63 | 0/2/2/2 |
| 22 | CLA | 5 | 602 | 17 | - | 10/37/115/115 | - |
| 22 | CLA | 8 | 609 | 15 | 1/1/11/20 | 3/15/93/115 | - |
| 22 | CLA | Z | 611 | 24 | 1/1/15/20 | 16/37/115/115 | - |
| 22 | CLA | 5 | 621 | - | 1/1/11/20 | 3/15/93/115 | - |
| 22 | CLA | 6 | 609 | 18 | 1/1/12/20 | 4/19/97/115 | - |
| 22 | CLA | 2 | 609 | 19 | 1/1/12/20 | 4/19/97/115 | - |
| 29 | CHL | 4 | 618 | 16 | 3/3/15/26 | 4/12/110/137 | - |
| 22 | CLA | 7 | 614 | 14 | 1/1/10/20 | 2/11/89/115 | - |
| 22 | CLA | A | 822 | - | 1/1/15/20 | 13/37/115/115 | - |
| 22 | CLA | 2 | 610 | 19 | - | 11/31/109/115 | - |
| 29 | CHL | 3 | 608 | - | 3/3/20/26 | 22/39/137/137 | - |
| 24 | LHG | 1 | 620 | 22 | - | 14/47/47/53 | - |
| 22 | CLA | 8 | 606 | - | 1/1/10/20 | 4/10/88/115 | - |
| 30 | LUT | 3 | 621 | - | - | 5/29/67/67 | 0/2/2/2 |
| 22 | CLA | B | 840 | 2 | - | 6/37/115/115 | - |
| 25 | BCR | 5 | 625 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | CLA | Z | 603 | 12 | 1/1/13/20 | 9/28/106/115 | - |
| 25 | BCR | A | 852 | - | - | 7/29/63/63 | 0/2/2/2 |
| 25 | BCR | 8 | 619 | - | - | 6/29/63/63 | 0/2/2/2 |
| 24 | LHG | A | 855 | - | - | 10/34/34/53 | - |
| 30 | LUT | 9 | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | 9 | 604 | 20 | - | 6/19/97/115 | - |
| 25 | BCR | A | 849 | - | - | 3/29/63/63 | 0/2/2/2 |
| 22 | CLA | 6 | 603 | 18 | 1/1/11/20 | 1/15/93/115 | - |
| 22 | CLA | A | 820 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 22 | CLA | 5 | 617 | 17 | 1/1/11/20 | 4/15/93/115 | - |
| 22 | CLA | A | 830 | 1 | 1/1/15/20 | 8/37/115/115 | - |
| 22 | CLA | A | 816 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 22 | CLA | B | 841 | 24 | 1/1/15/20 | 5/37/115/115 | - |
| 22 | CLA | 7 | 613 | 14 | - | 10/37/115/115 | - |
| 22 | CLA | A | 826 | - | 1/1/15/20 | 16/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 23 | PQN | B | 842 | - | - | 4/23/43/43 | 0/2/2/2 |
| 22 | CLA | A | 827 | - | 1/1/15/20 | 6/37/115/115 | - |
| 22 | CLA | 1 | 611 | 24 | 1/1/15/20 | 10/37/115/115 | - |
| 22 | CLA | B | 815 | 2 | 1/1/13/20 | 6/28/106/115 | - |
| 22 | CLA | B | 832 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | A | 807 | 1 | 1/1/15/20 | 18/37/115/115 | - |
| 30 | LUT | 8 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | 3 | 603 | 13 | 1/1/15/20 | 7/37/115/115 | - |
| 28 | LMG | J | 3001 | - | - | 12/30/50/70 | 0/1/1/1 |
| 22 | CLA | B | 825 | - | 1/1/15/20 | 7/37/115/115 | - |
| 22 | CLA | Z | 609 | 12 | 1/1/15/20 | 4/37/115/115 | - |
| 22 | CLA | A | 836 | 1 | - | 2/19/97/115 | - |
| 22 | CLA | A | 811 | 1 | 1/1/15/20 | 8/37/115/115 | - |
| 22 | CLA | A | 833 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 22 | CLA | 3 | 614 | 13 | - | 2/13/91/115 | - |
| 22 | CLA | 9 | 601 | 20 | 1/1/11/20 | 6/15/93/115 | - |
| 22 | CLA | 8 | 610 | 15 | 1/1/14/20 | 12/31/109/115 | - |
| 22 | CLA | A | 831 | 1 | 1/1/15/20 | 14/37/115/115 | - |
| 24 | LHG | B | 851 | 22 | - | 12/26/26/53 | - |
| 29 | CHL | 9 | 606 | - | 3/3/15/26 | 4/10/108/137 | - |
| 22 | CLA | Z | 608 | - | 1/1/15/20 | 17/37/115/115 | - |
| 23 | PQN | A | 844 | - | - | 12/23/43/43 | 0/2/2/2 |
| 22 | CLA | 4 | 609 | 16 | 1/1/12/20 | 7/19/97/115 | - |
| 29 | CHL | 4 | 607 | - | 3/3/17/26 | 7/21/119/137 | - |
| 22 | CLA | B | 818 | 2 | 1/1/14/20 | 12/31/109/115 | - |
| 22 | CLA | 6 | 604 | - | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | 7 | 612 | 14 | 1/1/12/20 | 7/22/100/115 | - |
| 22 | CLA | 4 | 604 | - | - | 4/19/97/115 | - |
| 22 | CLA | 7 | 604 | - | 1/1/13/20 | 9/27/105/115 | - |
| 24 | LHG | A | 846 | - | - | 16/53/53/53 | - |
| 22 | CLA | 1 | 612 | 12 | 1/1/12/20 | 8/22/100/115 | - |
| 22 | CLA | 1 | 608 | - | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | B | 820 | 2 | 1/1/13/20 | 6/27/105/115 | - |
| 22 | CLA | 8 | 604 | - | 1/1/11/20 | 3/15/93/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22 | CLA | 2 | 614 | - | - | 2/13/91/115 | - |
| 30 | LUT | 1 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | Z | 610 | 12 | 1/1/14/20 | 14/31/109/115 | - |
| 22 | CLA | B | 822 | 2 | - | 8/30/108/115 | - |
| 24 | LHG | 7 | 625 | 22 | - | 10/41/41/53 | - |
| 22 | CLA | 5 | 603 | 17 | 1/1/11/20 | 1/15/93/115 | - |
| 22 | CLA | 9 | 611 | - | 1/1/13/20 | 10/25/103/115 | - |
| 25 | BCR | A | 856 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | CLA | K | 4003 | 10 | 1/1/11/20 | 3/15/93/115 | - |
| 22 | CLA | 6 | 610 | - | 1/1/14/20 | 9/31/109/115 | - |
| 22 | CLA | 5 | 612 | 17 | 1/1/12/20 | 3/22/100/115 | - |
| 22 | CLA | Z | 612 | 12 | 1/1/12/20 | 6/22/100/115 | - |
| 30 | LUT | 1 | 618 | - | - | 3/29/67/67 | 0/2/2/2 |
| 22 | CLA | B | 813 | 2 | 1/1/15/20 | 13/37/115/115 | - |
| 26 | SF4 | A | 853 | 2,1 | - | - | 0/6/5/5 |
| 22 | CLA | B | 807 | 2 | 1/1/15/20 | 11/37/115/115 | - |
| 28 | LMG | 9 | 620 | - | - | 16/39/59/70 | 0/1/1/1 |
| 22 | CLA | 2 | 601 | 19 | 1/1/11/20 | 7/15/93/115 | - |
| 22 | CLA | 4 | 601 | 16 | 1/1/14/20 | 11/33/111/115 | - |
| 25 | BCR | B | 843 | - | - | 10/29/63/63 | 0/2/2/2 |
| 29 | CHL | 4 | 608 | - | 3/3/17/26 | 6/21/119/137 | - |
| 25 | BCR | 7 | 624 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | CLA | A | 845 | 24 | 1/1/12/20 | 15/22/100/115 | - |
| 22 | CLA | 3 | 611 | - | 1/1/10/20 | 2/8/86/115 | - |
| 22 | CLA | 8 | 601 | 15 | 1/1/15/20 | 13/37/115/115 | - |
| 29 | CHL | 4 | 606 | - | 3/3/18/26 | 3/27/125/137 | - |
| 30 | LUT | Z | 617 | - | - | 4/29/67/67 | 0/2/2/2 |
| 27 | DGD | B | 850 | - | - | 17/55/95/95 | 0/2/2/2 |
| 30 | LUT | 4 | 619 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | B | 831 | 2 | 1/1/11/20 | 5/18/96/115 | - |
| 24 | LHG | A | 847 | 22 | - | 14/42/42/53 | - |
| 22 | CLA | 6 | 614 | 18 | 1/1/11/20 | 4/13/91/115 | - |
| 22 | CLA | B | 803 | - | 1/1/15/20 | 6/37/115/115 | - |
| 22 | CLA | Z | 616 | 12 | 1/1/11/20 | 4/15/93/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|-----------|---------------|---------|
| 22 | CLA | B | 810 | 2 | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | B | 838 | 2 | 1/1/11/20 | 4/16/94/115 | - |
| 22 | CLA | B | 827 | 2 | 1/1/15/20 | 16/37/115/115 | - |
| 22 | CLA | A | 814 | 1 | 1/1/15/20 | 15/37/115/115 | - |
| 22 | CLA | F | 301 | - | 1/1/15/20 | 10/37/115/115 | - |
| 30 | LUT | Z | 618 | - | - | 4/29/67/67 | 0/2/2/2 |
| 29 | CHL | Z | 601 | 12 | 3/3/17/26 | 11/24/122/137 | - |
| 22 | CLA | Z | 602 | 12 | - | 10/37/115/115 | - |
| 22 | CLA | A | 812 | 1 | 1/1/15/20 | 13/37/115/115 | - |
| 25 | BCR | 3 | 719 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | CLA | 4 | 616 | 16 | 1/1/10/20 | 0/8/86/115 | - |
| 22 | CLA | 1 | 609 | 12 | 1/1/15/20 | 7/37/115/115 | - |
| 22 | CLA | 9 | 613 | - | 1/1/12/20 | 8/19/97/115 | - |
| 22 | CLA | 3 | 620 | - | 1/1/13/20 | 8/27/105/115 | - |
| 30 | LUT | 6 | 624 | - | - | 3/29/67/67 | 0/2/2/2 |
| 22 | CLA | 6 | 611 | 24 | 1/1/13/20 | 7/25/103/115 | - |
| 25 | BCR | B | 844 | - | - | 7/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 834 | 2 | 1/1/15/20 | 13/37/115/115 | - |
| 22 | CLA | 3 | 617 | 13 | 1/1/11/20 | 3/15/93/115 | - |
| 25 | BCR | A | 851 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | CLA | A | 828 | 1 | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | A | 840 | 1 | 1/1/15/20 | 8/37/115/115 | - |
| 22 | CLA | A | 805 | 1 | 1/1/13/20 | 8/25/103/115 | - |
| 25 | BCR | I | 172 | - | - | 6/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 817 | 2 | 1/1/13/20 | 12/30/108/115 | - |
| 22 | CLA | A | 839 | 1 | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | 7 | 620 | - | 1/1/14/20 | 8/31/109/115 | - |
| 22 | CLA | A | 829 | 1 | 1/1/15/20 | 19/37/115/115 | - |
| 22 | CLA | 5 | 614 | 17 | - | 1/13/91/115 | - |
| 22 | CLA | 8 | 613 | 15 | - | 12/37/115/115 | - |
| 22 | CLA | 6 | 612 | 18 | 1/1/12/20 | 5/22/100/115 | - |
| 22 | CLA | Z | 614 | 12 | 1/1/15/20 | 9/37/115/115 | - |
| 24 | LHG | 4 | 622 | 22 | - | 19/53/53/53 | - |
| 22 | CLA | K | 4002 | - | - | 6/13/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | 8 | 612 | 15 | 1/1/12/20 | 6/22/100/115 | - |
| 22 | CLA | Z | 613 | - | 1/1/15/20 | 11/37/115/115 | - |
| 22 | CLA | 1 | 616 | 12 | 1/1/11/20 | 3/15/93/115 | - |
| 22 | CLA | A | 813 | 1 | 1/1/12/20 | 7/24/102/115 | - |
| 30 | LUT | 5 | 624 | - | - | 3/29/67/67 | 0/2/2/2 |
| 22 | CLA | G | 203 | 7 | 1/1/12/20 | 3/19/97/115 | - |
| 22 | CLA | B | 804 | 2 | 1/1/11/20 | 4/13/91/115 | - |
| 22 | CLA | 3 | 604 | - | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | L | 203 | 11 | - | 10/37/115/115 | - |
| 25 | BCR | A | 850 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | CLA | 6 | 601 | 18 | 1/1/15/20 | 14/37/115/115 | - |
| 22 | CLA | 7 | 602 | 14 | 1/1/15/20 | 12/37/115/115 | - |
| 22 | CLA | 6 | 616 | 18 | 1/1/11/20 | 2/15/93/115 | - |
| 29 | CHL | Z | 607 | - | 3/3/16/26 | 4/18/116/137 | - |
| 22 | CLA | 2 | 602 | 19 | - | 4/13/91/115 | - |
| 29 | CHL | 1 | 607 | - | 3/3/16/26 | 7/18/116/137 | - |
| 29 | CHL | 6 | 606 | - | 3/3/18/26 | 8/27/125/137 | - |
| 22 | CLA | 2 | 607 | - | - | 5/19/97/115 | - |
| 22 | CLA | 5 | 609 | 17 | 1/1/12/20 | 4/19/97/115 | - |
| 22 | CLA | B | 821 | 2 | - | 4/15/93/115 | - |
| 22 | CLA | L | 204 | - | - | 5/19/97/115 | - |
| 22 | CLA | A | 834 | 1 | 1/1/15/20 | 10/37/115/115 | - |
| 22 | CLA | B | 814 | 2 | 1/1/14/20 | 11/31/109/115 | - |
| 22 | CLA | 1 | 610 | 12 | 1/1/14/20 | 12/31/109/115 | - |
| 22 | CLA | 6 | 622 | 18 | 1/1/11/20 | 3/13/91/115 | - |
| 22 | CLA | 5 | 610 | 17 | 1/1/14/20 | 7/31/109/115 | - |
| 22 | CLA | B | 805 | 2 | 1/1/15/20 | 14/37/115/115 | - |
| 22 | CLA | 8 | 608 | - | 1/1/12/20 | 1/19/97/115 | - |
| 25 | BCR | 3 | 718 | - | - | 4/29/63/63 | 0/2/2/2 |
| 22 | CLA | 1 | 604 | - | 1/1/13/20 | 8/28/106/115 | - |
| 22 | CLA | 1 | 606 | - | 1/1/12/20 | 5/22/100/115 | - |
| 22 | CLA | 8 | 602 | 15 | 1/1/14/20 | 10/34/112/115 | - |
| 25 | BCR | F | 305 | - | - | 2/29/63/63 | 0/2/2/2 |
| 22 | CLA | B | 829 | 2 | 1/1/15/20 | 9/37/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 22 | CLA | 2 | 611 | - | - | 7/25/103/115 | - |
| 26 | SF4 | C | 102 | 3 | - | - | 0/6/5/5 |
| 24 | LHG | 8 | 620 | 22 | - | 14/41/41/53 | - |
| 22 | CLA | B | 836 | 2 | 1/1/14/20 | 5/31/109/115 | - |
| 22 | CLA | 1 | 614 | 12 | 1/1/15/20 | 13/37/115/115 | - |
| 22 | CLA | A | 841 | 1 | 1/1/15/20 | 9/37/115/115 | - |
| 29 | CHL | 6 | 618 | 18 | 3/3/15/26 | 6/12/110/137 | - |
| 30 | LUT | 7 | 621 | - | - | 3/29/67/67 | 0/2/2/2 |
| 22 | CLA | 7 | 609 | 14 | 1/1/12/20 | 5/19/97/115 | - |
| 22 | CLA | B | 802 | 2 | 1/1/15/20 | 9/37/115/115 | - |
| 25 | BCR | L | 205 | - | - | 9/29/63/63 | 0/2/2/2 |
| 30 | LUT | 3 | 622 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | A | 838 | 1 | 1/1/12/20 | 5/21/99/115 | - |
| 22 | CLA | F | 304 | 6 | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 835 | - | 1/1/11/20 | 5/13/91/115 | - |
| 22 | CLA | 5 | 601 | 17 | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | B | 809 | 2 | 1/1/15/20 | 12/37/115/115 | - |
| 22 | CLA | B | 819 | - | 1/1/15/20 | 9/37/115/115 | - |
| 22 | CLA | 9 | 602 | 20 | 1/1/14/20 | 9/31/109/115 | - |
| 25 | BCR | 3 | 717 | - | - | 5/29/63/63 | 0/2/2/2 |
| 22 | CLA | 4 | 603 | 16 | 1/1/11/20 | 2/15/93/115 | - |
| 22 | CLA | A | 837 | 1 | 1/1/11/20 | 9/13/91/115 | - |
| 30 | LUT | 2 | 616 | - | - | 0/29/67/67 | 0/2/2/2 |
| 22 | CLA | B | 839 | - | 1/1/15/20 | 7/37/115/115 | - |
| 22 | CLA | 2 | 606 | - | 1/1/10/20 | 1/8/86/115 | - |
| 30 | LUT | Z | 619 | - | - | 4/29/67/67 | 0/2/2/2 |
| 30 | LUT | 1 | 619 | - | - | 2/29/67/67 | 0/2/2/2 |
| 22 | CLA | A | 815 | 1 | 1/1/14/20 | 11/31/109/115 | - |
| 22 | CLA | A | 843 | - | 1/1/15/20 | 17/37/115/115 | - |
| 22 | CLA | 6 | 613 | - | 1/1/13/20 | 4/27/105/115 | - |

All (3969) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 23 | B | 842 | PQN | C3-C2 | 7.50 | 1.48 | 1.35 |
| 23 | A | 844 | PQN | C3-C2 | 7.35 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | B | 836 | CLA | C3B-C2B | 6.40 | 1.49 | 1.40 |
| 22 | 3 | 602 | CLA | C3B-C2B | 6.31 | 1.49 | 1.40 |
| 22 | 5 | 621 | CLA | C3B-C2B | 6.19 | 1.49 | 1.40 |
| 22 | B | 829 | CLA | C3B-C2B | 6.15 | 1.48 | 1.40 |
| 22 | 8 | 616 | CLA | C3B-C2B | 6.11 | 1.48 | 1.40 |
| 22 | B | 840 | CLA | C3C-C2C | 6.11 | 1.49 | 1.36 |
| 22 | 4 | 616 | CLA | C3B-C2B | 6.03 | 1.48 | 1.40 |
| 22 | 2 | 614 | CLA | C3B-C2B | 6.02 | 1.48 | 1.40 |
| 22 | 9 | 611 | CLA | C3B-C2B | 6.01 | 1.48 | 1.40 |
| 22 | B | 841 | CLA | C3B-C2B | 6.01 | 1.48 | 1.40 |
| 29 | Z | 601 | CHL | C3B-C2B | 6.01 | 1.48 | 1.40 |
| 22 | 2 | 610 | CLA | C3B-C2B | 5.99 | 1.48 | 1.40 |
| 22 | 6 | 616 | CLA | C3B-C2B | 5.98 | 1.48 | 1.40 |
| 29 | 1 | 607 | CHL | C3B-C2B | 5.97 | 1.48 | 1.40 |
| 22 | 7 | 601 | CLA | C3B-C2B | 5.97 | 1.48 | 1.40 |
| 22 | 9 | 601 | CLA | C3B-C2B | 5.96 | 1.48 | 1.40 |
| 22 | 2 | 606 | CLA | C3B-C2B | 5.96 | 1.48 | 1.40 |
| 22 | B | 852 | CLA | C3B-C2B | 5.96 | 1.48 | 1.40 |
| 22 | 2 | 613 | CLA | C3B-C2B | 5.95 | 1.48 | 1.40 |
| 22 | 2 | 609 | CLA | C3B-C2B | 5.95 | 1.48 | 1.40 |
| 22 | 8 | 614 | CLA | C3B-C2B | 5.93 | 1.48 | 1.40 |
| 22 | A | 815 | CLA | C3B-C2B | 5.92 | 1.48 | 1.40 |
| 29 | 4 | 618 | CHL | C3B-C2B | 5.92 | 1.48 | 1.40 |
| 22 | 2 | 607 | CLA | C3B-C2B | 5.91 | 1.48 | 1.40 |
| 22 | A | 806 | CLA | C3B-C2B | 5.91 | 1.48 | 1.40 |
| 22 | 7 | 620 | CLA | C3B-C2B | 5.90 | 1.48 | 1.40 |
| 22 | G | 203 | CLA | C3B-C2B | 5.90 | 1.48 | 1.40 |
| 22 | 4 | 611 | CLA | C3B-C2B | 5.90 | 1.48 | 1.40 |
| 22 | Z | 616 | CLA | C3B-C2B | 5.89 | 1.48 | 1.40 |
| 22 | B | 820 | CLA | C3B-C2B | 5.89 | 1.48 | 1.40 |
| 22 | Z | 613 | CLA | C3B-C2B | 5.88 | 1.48 | 1.40 |
| 22 | 2 | 601 | CLA | C3B-C2B | 5.88 | 1.48 | 1.40 |
| 29 | 7 | 607 | CHL | C3B-C2B | 5.88 | 1.48 | 1.40 |
| 29 | Z | 607 | CHL | C3B-C2B | 5.87 | 1.48 | 1.40 |
| 22 | B | 804 | CLA | C3B-C2B | 5.86 | 1.48 | 1.40 |
| 22 | 9 | 612 | CLA | C3B-C2B | 5.86 | 1.48 | 1.40 |
| 22 | 3 | 611 | CLA | C3B-C2B | 5.86 | 1.48 | 1.40 |
| 22 | 1 | 616 | CLA | C3B-C2B | 5.85 | 1.48 | 1.40 |
| 29 | 6 | 618 | CHL | C3B-C2B | 5.84 | 1.48 | 1.40 |
| 29 | 5 | 618 | CHL | C3B-C2B | 5.84 | 1.48 | 1.40 |
| 22 | B | 825 | CLA | C3B-C2B | 5.83 | 1.48 | 1.40 |
| 22 | K | 4003 | CLA | C3B-C2B | 5.83 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | A | 835 | CLA | C3B-C2B | 5.83 | 1.48 | 1.40 |
| 29 | 1 | 601 | CHL | C3B-C2B | 5.83 | 1.48 | 1.40 |
| 22 | 5 | 603 | CLA | C3B-C2B | 5.82 | 1.48 | 1.40 |
| 22 | B | 821 | CLA | C3B-C2B | 5.82 | 1.48 | 1.40 |
| 22 | 2 | 611 | CLA | C3B-C2B | 5.82 | 1.48 | 1.40 |
| 22 | B | 834 | CLA | C3B-C2B | 5.80 | 1.48 | 1.40 |
| 22 | A | 803 | CLA | C3B-C2B | 5.80 | 1.48 | 1.40 |
| 22 | B | 839 | CLA | C3B-C2B | 5.80 | 1.48 | 1.40 |
| 22 | G | 204 | CLA | C3B-C2B | 5.79 | 1.48 | 1.40 |
| 22 | J | 3002 | CLA | C3B-C2B | 5.79 | 1.48 | 1.40 |
| 22 | A | 802 | CLA | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 22 | K | 4002 | CLA | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 29 | 4 | 607 | CHL | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 22 | 3 | 614 | CLA | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 22 | 6 | 617 | CLA | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 22 | 4 | 614 | CLA | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 29 | 9 | 607 | CHL | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 22 | B | 810 | CLA | C3B-C2B | 5.78 | 1.48 | 1.40 |
| 22 | 2 | 602 | CLA | C3B-C2B | 5.77 | 1.48 | 1.40 |
| 22 | Z | 608 | CLA | C3B-C2B | 5.77 | 1.48 | 1.40 |
| 22 | 6 | 622 | CLA | C3B-C2B | 5.76 | 1.48 | 1.40 |
| 22 | 5 | 617 | CLA | C3B-C2B | 5.75 | 1.48 | 1.40 |
| 22 | Z | 614 | CLA | C3B-C2B | 5.75 | 1.48 | 1.40 |
| 22 | Z | 611 | CLA | C3B-C2B | 5.75 | 1.48 | 1.40 |
| 22 | 8 | 601 | CLA | C3B-C2B | 5.75 | 1.48 | 1.40 |
| 22 | 1 | 614 | CLA | C3B-C2B | 5.75 | 1.48 | 1.40 |
| 22 | A | 816 | CLA | C3B-C2B | 5.74 | 1.48 | 1.40 |
| 22 | 2 | 603 | CLA | C3B-C2B | 5.74 | 1.48 | 1.40 |
| 22 | 5 | 616 | CLA | C3B-C2B | 5.73 | 1.48 | 1.40 |
| 22 | 9 | 613 | CLA | C3B-C2B | 5.73 | 1.48 | 1.40 |
| 22 | 8 | 611 | CLA | C3B-C2B | 5.73 | 1.48 | 1.40 |
| 22 | 4 | 601 | CLA | C3B-C2B | 5.73 | 1.48 | 1.40 |
| 22 | 5 | 601 | CLA | C3B-C2B | 5.72 | 1.48 | 1.40 |
| 22 | 9 | 614 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | 7 | 616 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | A | 836 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | 9 | 604 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | 8 | 608 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | L | 204 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | 6 | 613 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 22 | F | 303 | CLA | C3B-C2B | 5.71 | 1.48 | 1.40 |
| 29 | 8 | 607 | CHL | C3B-C2B | 5.71 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 5 | 614 | CLA | C3B-C2B | 5.70 | 1.48 | 1.40 |
| 22 | A | 833 | CLA | C3B-C2B | 5.70 | 1.48 | 1.40 |
| 22 | 5 | 611 | CLA | C3B-C2B | 5.69 | 1.48 | 1.40 |
| 22 | 8 | 612 | CLA | C3B-C2B | 5.69 | 1.48 | 1.40 |
| 22 | 4 | 612 | CLA | C3B-C2B | 5.69 | 1.48 | 1.40 |
| 22 | 5 | 612 | CLA | C3B-C2B | 5.69 | 1.48 | 1.40 |
| 29 | 9 | 606 | CHL | C3B-C2B | 5.68 | 1.48 | 1.40 |
| 22 | Z | 612 | CLA | C3B-C2B | 5.68 | 1.48 | 1.40 |
| 22 | A | 805 | CLA | C3B-C2B | 5.68 | 1.48 | 1.40 |
| 22 | B | 808 | CLA | C3B-C2B | 5.67 | 1.48 | 1.40 |
| 22 | A | 807 | CLA | C3B-C2B | 5.67 | 1.48 | 1.40 |
| 22 | A | 824 | CLA | C3B-C2B | 5.67 | 1.48 | 1.40 |
| 22 | 1 | 608 | CLA | C3B-C2B | 5.66 | 1.48 | 1.40 |
| 22 | 7 | 606 | CLA | C3B-C2B | 5.66 | 1.48 | 1.40 |
| 22 | 6 | 611 | CLA | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 22 | 7 | 614 | CLA | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 22 | Z | 609 | CLA | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 22 | 5 | 610 | CLA | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 22 | 8 | 613 | CLA | C3B-C2B | 5.65 | 1.48 | 1.40 |
| 22 | B | 835 | CLA | C3B-C2B | 5.64 | 1.48 | 1.40 |
| 22 | F | 301 | CLA | C3B-C2B | 5.64 | 1.48 | 1.40 |
| 22 | Z | 603 | CLA | C3B-C2B | 5.64 | 1.48 | 1.40 |
| 29 | 6 | 606 | CHL | C3B-C2B | 5.63 | 1.48 | 1.40 |
| 22 | 7 | 610 | CLA | CHC-C1C | 5.63 | 1.49 | 1.35 |
| 22 | B | 833 | CLA | C3B-C2B | 5.62 | 1.48 | 1.40 |
| 22 | 6 | 612 | CLA | C3B-C2B | 5.62 | 1.48 | 1.40 |
| 22 | B | 816 | CLA | C3B-C2B | 5.62 | 1.48 | 1.40 |
| 22 | 9 | 610 | CLA | C3B-C2B | 5.61 | 1.48 | 1.40 |
| 22 | 6 | 610 | CLA | C3B-C2B | 5.61 | 1.48 | 1.40 |
| 22 | 1 | 611 | CLA | C3B-C2B | 5.61 | 1.48 | 1.40 |
| 22 | 8 | 609 | CLA | C3B-C2B | 5.61 | 1.48 | 1.40 |
| 22 | A | 809 | CLA | C3B-C2B | 5.61 | 1.48 | 1.40 |
| 22 | A | 814 | CLA | C3B-C2B | 5.60 | 1.48 | 1.40 |
| 22 | A | 813 | CLA | C3B-C2B | 5.60 | 1.48 | 1.40 |
| 22 | A | 834 | CLA | C3B-C2B | 5.60 | 1.48 | 1.40 |
| 22 | 6 | 602 | CLA | C3B-C2B | 5.60 | 1.48 | 1.40 |
| 22 | A | 827 | CLA | C3B-C2B | 5.59 | 1.48 | 1.40 |
| 22 | 2 | 612 | CLA | C3B-C2B | 5.59 | 1.48 | 1.40 |
| 22 | B | 838 | CLA | C3B-C2B | 5.58 | 1.48 | 1.40 |
| 22 | F | 304 | CLA | C3B-C2B | 5.58 | 1.48 | 1.40 |
| 22 | 7 | 611 | CLA | C3B-C2B | 5.58 | 1.48 | 1.40 |
| 22 | Z | 610 | CLA | C3B-C2B | 5.58 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 1 | 609 | CLA | C3B-C2B | 5.57 | 1.48 | 1.40 |
| 22 | 9 | 603 | CLA | C3B-C2B | 5.57 | 1.48 | 1.40 |
| 22 | 3 | 609 | CLA | C3B-C2B | 5.57 | 1.48 | 1.40 |
| 22 | A | 817 | CLA | C1D-ND | 5.56 | 1.44 | 1.37 |
| 22 | 8 | 610 | CLA | C3B-C2B | 5.56 | 1.48 | 1.40 |
| 22 | B | 807 | CLA | C3B-C2B | 5.56 | 1.48 | 1.40 |
| 22 | 6 | 609 | CLA | C3B-C2B | 5.56 | 1.48 | 1.40 |
| 22 | 5 | 606 | CLA | C3B-C2B | 5.55 | 1.48 | 1.40 |
| 22 | B | 812 | CLA | C3B-C2B | 5.55 | 1.48 | 1.40 |
| 22 | 6 | 603 | CLA | C3B-C2B | 5.55 | 1.48 | 1.40 |
| 22 | 3 | 607 | CLA | C3B-C2B | 5.54 | 1.48 | 1.40 |
| 22 | 3 | 612 | CLA | C3B-C2B | 5.54 | 1.48 | 1.40 |
| 22 | A | 845 | CLA | C3B-C2B | 5.54 | 1.48 | 1.40 |
| 22 | 7 | 603 | CLA | C3B-C2B | 5.54 | 1.48 | 1.40 |
| 22 | B | 805 | CLA | C3B-C2B | 5.53 | 1.48 | 1.40 |
| 22 | A | 811 | CLA | C3B-C2B | 5.53 | 1.48 | 1.40 |
| 22 | 3 | 620 | CLA | C3B-C2B | 5.53 | 1.48 | 1.40 |
| 29 | 6 | 607 | CHL | C3B-C2B | 5.53 | 1.48 | 1.40 |
| 22 | A | 821 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | A | 808 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | A | 819 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | A | 812 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | Z | 606 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | 3 | 617 | CLA | C3B-C2B | 5.52 | 1.48 | 1.40 |
| 22 | 6 | 601 | CLA | C3B-C2B | 5.51 | 1.48 | 1.40 |
| 22 | B | 826 | CLA | C3B-C2B | 5.51 | 1.48 | 1.40 |
| 22 | A | 823 | CLA | C3B-C2B | 5.51 | 1.48 | 1.40 |
| 22 | 8 | 606 | CLA | C3B-C2B | 5.50 | 1.48 | 1.40 |
| 22 | 1 | 612 | CLA | C3B-C2B | 5.50 | 1.48 | 1.40 |
| 29 | 5 | 607 | CHL | C3B-C2B | 5.50 | 1.48 | 1.40 |
| 22 | A | 828 | CLA | C3B-C2B | 5.50 | 1.48 | 1.40 |
| 22 | A | 839 | CLA | C3B-C2B | 5.50 | 1.48 | 1.40 |
| 22 | A | 843 | CLA | C3B-C2B | 5.49 | 1.48 | 1.40 |
| 22 | A | 854 | CLA | C3B-C2B | 5.49 | 1.48 | 1.40 |
| 22 | 8 | 602 | CLA | C3B-C2B | 5.49 | 1.48 | 1.40 |
| 22 | B | 806 | CLA | C3B-C2B | 5.49 | 1.48 | 1.40 |
| 22 | B | 824 | CLA | C3B-C2B | 5.48 | 1.48 | 1.40 |
| 22 | L | 204 | CLA | C3C-C2C | 5.48 | 1.48 | 1.36 |
| 22 | 2 | 609 | CLA | C1D-ND | 5.48 | 1.44 | 1.37 |
| 22 | B | 815 | CLA | C3B-C2B | 5.48 | 1.48 | 1.40 |
| 22 | 5 | 609 | CLA | C3B-C2B | 5.47 | 1.48 | 1.40 |
| 22 | 1 | 610 | CLA | C3B-C2B | 5.47 | 1.48 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 7 | 609 | CLA | C3C-C2C | 5.47 | 1.48 | 1.36 |
| 22 | A | 854 | CLA | CHC-C1C | 5.47 | 1.49 | 1.35 |
| 22 | A | 816 | CLA | C3C-C2C | 5.47 | 1.48 | 1.36 |
| 22 | 6 | 614 | CLA | C3B-C2B | 5.46 | 1.48 | 1.40 |
| 22 | 1 | 610 | CLA | CHC-C1C | 5.46 | 1.49 | 1.35 |
| 29 | 4 | 608 | CHL | C3B-C2B | 5.46 | 1.47 | 1.40 |
| 22 | 7 | 608 | CLA | C3B-C2B | 5.46 | 1.47 | 1.40 |
| 22 | 1 | 613 | CLA | C3B-C2B | 5.46 | 1.47 | 1.40 |
| 22 | A | 842 | CLA | C3B-C2B | 5.46 | 1.47 | 1.40 |
| 22 | A | 802 | CLA | C3C-C2C | 5.45 | 1.48 | 1.36 |
| 22 | B | 828 | CLA | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 22 | 4 | 602 | CLA | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 22 | B | 813 | CLA | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 22 | 8 | 603 | CLA | C3B-C2B | 5.45 | 1.47 | 1.40 |
| 22 | 7 | 613 | CLA | C3B-C2B | 5.44 | 1.47 | 1.40 |
| 22 | B | 840 | CLA | C3B-C2B | 5.44 | 1.47 | 1.40 |
| 22 | Z | 611 | CLA | C3C-C2C | 5.44 | 1.48 | 1.36 |
| 22 | 1 | 606 | CLA | C3B-C2B | 5.43 | 1.47 | 1.40 |
| 22 | Z | 606 | CLA | C1D-ND | 5.43 | 1.44 | 1.37 |
| 22 | Z | 614 | CLA | C3C-C2C | 5.43 | 1.48 | 1.36 |
| 22 | 3 | 613 | CLA | C3B-C2B | 5.43 | 1.47 | 1.40 |
| 22 | 2 | 606 | CLA | C3C-C2C | 5.43 | 1.48 | 1.36 |
| 22 | 7 | 612 | CLA | C3B-C2B | 5.43 | 1.47 | 1.40 |
| 22 | A | 825 | CLA | C3B-C2B | 5.43 | 1.47 | 1.40 |
| 22 | 3 | 607 | CLA | C3C-C2C | 5.42 | 1.48 | 1.36 |
| 22 | 6 | 614 | CLA | C3C-C2C | 5.42 | 1.48 | 1.36 |
| 22 | 7 | 602 | CLA | C3B-C2B | 5.42 | 1.47 | 1.40 |
| 22 | 6 | 609 | CLA | C3C-C2C | 5.42 | 1.48 | 1.36 |
| 22 | A | 835 | CLA | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 22 | A | 845 | CLA | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 22 | 9 | 609 | CLA | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 22 | B | 827 | CLA | C3C-C2C | 5.41 | 1.48 | 1.36 |
| 22 | A | 837 | CLA | C3B-C2B | 5.40 | 1.47 | 1.40 |
| 22 | 1 | 614 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 22 | 9 | 602 | CLA | C3B-C2B | 5.40 | 1.47 | 1.40 |
| 22 | 1 | 611 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 22 | 4 | 616 | CLA | C1D-ND | 5.40 | 1.44 | 1.37 |
| 22 | 2 | 606 | CLA | C1D-ND | 5.40 | 1.44 | 1.37 |
| 22 | B | 825 | CLA | C3C-C2C | 5.40 | 1.48 | 1.36 |
| 22 | A | 820 | CLA | C3B-C2B | 5.39 | 1.47 | 1.40 |
| 22 | 8 | 614 | CLA | C3C-C2C | 5.39 | 1.48 | 1.36 |
| 22 | A | 832 | CLA | C3B-C2B | 5.39 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | A | 840 | CLA | C3B-C2B | 5.39 | 1.47 | 1.40 |
| 22 | 7 | 609 | CLA | C3B-C2B | 5.39 | 1.47 | 1.40 |
| 22 | A | 830 | CLA | C3B-C2B | 5.38 | 1.47 | 1.40 |
| 22 | B | 822 | CLA | C3B-C2B | 5.38 | 1.47 | 1.40 |
| 22 | 6 | 604 | CLA | C3B-C2B | 5.38 | 1.47 | 1.40 |
| 29 | 5 | 608 | CHL | C3B-C2B | 5.38 | 1.47 | 1.40 |
| 22 | A | 822 | CLA | C3C-C2C | 5.38 | 1.48 | 1.36 |
| 22 | 2 | 607 | CLA | C3C-C2C | 5.38 | 1.48 | 1.36 |
| 22 | 9 | 604 | CLA | C1D-ND | 5.37 | 1.44 | 1.37 |
| 22 | 7 | 601 | CLA | C3C-C2C | 5.37 | 1.48 | 1.36 |
| 22 | Z | 610 | CLA | CHC-C1C | 5.37 | 1.48 | 1.35 |
| 22 | 4 | 610 | CLA | C3C-C2C | 5.36 | 1.48 | 1.36 |
| 22 | 3 | 614 | CLA | C1D-ND | 5.36 | 1.44 | 1.37 |
| 22 | 3 | 610 | CLA | C3B-C2B | 5.36 | 1.47 | 1.40 |
| 22 | 2 | 611 | CLA | C3C-C2C | 5.36 | 1.48 | 1.36 |
| 22 | Z | 604 | CLA | C3B-C2B | 5.36 | 1.47 | 1.40 |
| 22 | 1 | 603 | CLA | C3B-C2B | 5.36 | 1.47 | 1.40 |
| 22 | 2 | 611 | CLA | C1D-ND | 5.35 | 1.44 | 1.37 |
| 22 | 2 | 609 | CLA | C3C-C2C | 5.35 | 1.48 | 1.36 |
| 22 | 7 | 616 | CLA | C1D-ND | 5.35 | 1.44 | 1.37 |
| 22 | 4 | 603 | CLA | C3B-C2B | 5.35 | 1.47 | 1.40 |
| 22 | 5 | 613 | CLA | C3B-C2B | 5.35 | 1.47 | 1.40 |
| 22 | A | 838 | CLA | C3B-C2B | 5.35 | 1.47 | 1.40 |
| 22 | B | 835 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 22 | K | 4002 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 22 | 9 | 603 | CLA | C1D-ND | 5.34 | 1.44 | 1.37 |
| 22 | 5 | 611 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 22 | A | 823 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 22 | 2 | 601 | CLA | C1D-ND | 5.34 | 1.44 | 1.37 |
| 22 | 5 | 601 | CLA | C3C-C2C | 5.34 | 1.48 | 1.36 |
| 22 | 3 | 610 | CLA | CHC-C1C | 5.33 | 1.48 | 1.35 |
| 22 | 2 | 602 | CLA | C1D-ND | 5.33 | 1.44 | 1.37 |
| 22 | 9 | 601 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 22 | B | 841 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 22 | 5 | 606 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 22 | A | 828 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 22 | 9 | 604 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 22 | J | 3002 | CLA | C3C-C2C | 5.33 | 1.48 | 1.36 |
| 22 | A | 805 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |
| 22 | B | 852 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |
| 22 | 2 | 607 | CLA | C1D-ND | 5.32 | 1.44 | 1.37 |
| 22 | B | 821 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 29 | Z | 601 | CHL | C2C-C3C | 5.32 | 1.48 | 1.36 |
| 22 | 5 | 602 | CLA | C3B-C2B | 5.32 | 1.47 | 1.40 |
| 22 | B | 814 | CLA | C3B-C2B | 5.32 | 1.47 | 1.40 |
| 22 | A | 815 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |
| 22 | B | 820 | CLA | C3C-C2C | 5.32 | 1.48 | 1.36 |
| 22 | A | 845 | CLA | C1D-ND | 5.32 | 1.44 | 1.37 |
| 22 | 4 | 613 | CLA | C3B-C2B | 5.32 | 1.47 | 1.40 |
| 22 | 9 | 614 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | 7 | 620 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | 9 | 611 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | 8 | 604 | CLA | C3B-C2B | 5.31 | 1.47 | 1.40 |
| 29 | 1 | 601 | CHL | C2C-C3C | 5.31 | 1.48 | 1.36 |
| 22 | A | 834 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | 2 | 603 | CLA | C1D-ND | 5.31 | 1.44 | 1.37 |
| 22 | 8 | 611 | CLA | C1D-ND | 5.31 | 1.44 | 1.37 |
| 22 | 7 | 602 | CLA | CHC-C1C | 5.31 | 1.48 | 1.35 |
| 22 | B | 830 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | 2 | 610 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | B | 838 | CLA | C3C-C2C | 5.31 | 1.48 | 1.36 |
| 22 | K | 4003 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 22 | 7 | 602 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 22 | 2 | 614 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 22 | 5 | 611 | CLA | C1D-ND | 5.30 | 1.44 | 1.37 |
| 22 | 3 | 606 | CLA | C3B-C2B | 5.30 | 1.47 | 1.40 |
| 29 | 7 | 607 | CHL | C2C-C3C | 5.30 | 1.48 | 1.36 |
| 29 | 9 | 607 | CHL | C2C-C3C | 5.30 | 1.48 | 1.36 |
| 22 | A | 810 | CLA | C3B-C2B | 5.30 | 1.47 | 1.40 |
| 22 | B | 831 | CLA | CHC-C1C | 5.30 | 1.48 | 1.35 |
| 22 | 7 | 620 | CLA | C1D-ND | 5.30 | 1.44 | 1.37 |
| 22 | 4 | 601 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 22 | A | 827 | CLA | C3C-C2C | 5.30 | 1.48 | 1.36 |
| 22 | 8 | 606 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 22 | 6 | 604 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 22 | 2 | 610 | CLA | C1D-ND | 5.29 | 1.44 | 1.37 |
| 22 | A | 841 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 22 | A | 841 | CLA | C3B-C2B | 5.29 | 1.47 | 1.40 |
| 22 | B | 802 | CLA | C3B-C2B | 5.29 | 1.47 | 1.40 |
| 22 | 9 | 601 | CLA | C1D-ND | 5.29 | 1.44 | 1.37 |
| 22 | A | 820 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 22 | G | 204 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 22 | 2 | 612 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |
| 22 | 2 | 602 | CLA | C3C-C2C | 5.29 | 1.48 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | A | 831 | CLA | C3B-C2B | 5.29 | 1.47 | 1.40 |
| 22 | 1 | 609 | CLA | C1D-ND | 5.28 | 1.44 | 1.37 |
| 22 | G | 203 | CLA | C3C-C2C | 5.28 | 1.48 | 1.36 |
| 22 | Z | 609 | CLA | C1D-ND | 5.28 | 1.44 | 1.37 |
| 22 | 5 | 604 | CLA | C1D-ND | 5.28 | 1.44 | 1.37 |
| 22 | B | 810 | CLA | C3C-C2C | 5.28 | 1.47 | 1.36 |
| 22 | 4 | 611 | CLA | C3C-C2C | 5.28 | 1.47 | 1.36 |
| 22 | A | 819 | CLA | C3C-C2C | 5.28 | 1.47 | 1.36 |
| 22 | B | 825 | CLA | CHC-C1C | 5.28 | 1.48 | 1.35 |
| 22 | 5 | 617 | CLA | C3C-C2C | 5.27 | 1.47 | 1.36 |
| 22 | B | 811 | CLA | C3C-C2C | 5.27 | 1.47 | 1.36 |
| 22 | A | 813 | CLA | C3C-C2C | 5.27 | 1.47 | 1.36 |
| 29 | 5 | 618 | CHL | C2C-C3C | 5.27 | 1.48 | 1.36 |
| 22 | Z | 611 | CLA | C1D-ND | 5.27 | 1.44 | 1.37 |
| 22 | 2 | 613 | CLA | C1D-ND | 5.27 | 1.44 | 1.37 |
| 22 | B | 819 | CLA | C3C-C2C | 5.27 | 1.47 | 1.36 |
| 22 | 9 | 612 | CLA | C1D-ND | 5.27 | 1.44 | 1.37 |
| 22 | A | 838 | CLA | C3C-C2C | 5.27 | 1.47 | 1.36 |
| 22 | 7 | 604 | CLA | C1D-ND | 5.26 | 1.44 | 1.37 |
| 22 | A | 809 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | A | 839 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | A | 829 | CLA | C3B-C2B | 5.26 | 1.47 | 1.40 |
| 22 | 5 | 609 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | L | 203 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | 8 | 609 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | 1 | 604 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | 9 | 612 | CLA | C3C-C2C | 5.26 | 1.47 | 1.36 |
| 22 | B | 834 | CLA | C1D-ND | 5.26 | 1.44 | 1.37 |
| 22 | A | 827 | CLA | CHC-C1C | 5.26 | 1.48 | 1.35 |
| 22 | A | 854 | CLA | C3C-C2C | 5.25 | 1.47 | 1.36 |
| 22 | A | 818 | CLA | C3B-C2B | 5.25 | 1.47 | 1.40 |
| 22 | B | 818 | CLA | C3B-C2B | 5.25 | 1.47 | 1.40 |
| 22 | 3 | 611 | CLA | C3C-C2C | 5.25 | 1.47 | 1.36 |
| 22 | 2 | 601 | CLA | O2D-CGD | 5.25 | 1.46 | 1.33 |
| 22 | A | 815 | CLA | CHC-C1C | 5.25 | 1.48 | 1.35 |
| 22 | 2 | 609 | CLA | O2D-CGD | 5.25 | 1.46 | 1.33 |
| 22 | A | 824 | CLA | C3C-C2C | 5.25 | 1.47 | 1.36 |
| 22 | Z | 603 | CLA | C3C-C2C | 5.25 | 1.47 | 1.36 |
| 22 | 4 | 603 | CLA | C3C-C2C | 5.25 | 1.47 | 1.36 |
| 22 | 2 | 614 | CLA | C1D-ND | 5.24 | 1.44 | 1.37 |
| 22 | A | 816 | CLA | C1D-ND | 5.24 | 1.44 | 1.37 |
| 22 | 2 | 607 | CLA | O2D-CGD | 5.24 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | 4 | 614 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | 4 | 616 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | 2 | 613 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | Z | 612 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | 2 | 601 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | 7 | 608 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | 7 | 614 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | B | 834 | CLA | C3C-C2C | 5.24 | 1.47 | 1.36 |
| 22 | 3 | 606 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | 3 | 612 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | Z | 608 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | F | 304 | CLA | C1D-ND | 5.23 | 1.44 | 1.37 |
| 22 | B | 822 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | Z | 616 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | K | 4002 | CLA | C1D-ND | 5.23 | 1.44 | 1.37 |
| 29 | 6 | 607 | CHL | C2C-C3C | 5.23 | 1.47 | 1.36 |
| 22 | 5 | 621 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | 3 | 604 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | Z | 604 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | B | 832 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | 5 | 614 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | 6 | 601 | CLA | C3C-C2C | 5.23 | 1.47 | 1.36 |
| 22 | 9 | 611 | CLA | O2D-CGD | 5.22 | 1.45 | 1.33 |
| 22 | 9 | 609 | CLA | C3B-C2B | 5.22 | 1.47 | 1.40 |
| 22 | 9 | 614 | CLA | C1D-ND | 5.22 | 1.44 | 1.37 |
| 22 | 4 | 610 | CLA | C3B-C2B | 5.22 | 1.47 | 1.40 |
| 22 | A | 807 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | 2 | 603 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | B | 826 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | B | 831 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | B | 839 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | 7 | 614 | CLA | C1D-ND | 5.22 | 1.44 | 1.37 |
| 22 | 5 | 616 | CLA | C1D-ND | 5.22 | 1.44 | 1.37 |
| 22 | 8 | 616 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | Z | 606 | CLA | C3C-C2C | 5.22 | 1.47 | 1.36 |
| 22 | B | 807 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | F | 304 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | 1 | 608 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | 9 | 603 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | 6 | 613 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | B | 829 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | A | 831 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 4 | 604 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | A | 837 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | F | 301 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | 5 | 604 | CLA | C3B-C2B | 5.21 | 1.47 | 1.40 |
| 22 | 5 | 603 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | 4 | 602 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | 2 | 614 | CLA | O2D-CGD | 5.21 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | O2D-CGD | 5.21 | 1.45 | 1.33 |
| 22 | A | 804 | CLA | C3B-C2B | 5.21 | 1.47 | 1.40 |
| 22 | B | 838 | CLA | CHC-C1C | 5.21 | 1.48 | 1.35 |
| 22 | 1 | 616 | CLA | C3C-C2C | 5.21 | 1.47 | 1.36 |
| 22 | A | 836 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 29 | 4 | 606 | CHL | C3B-C2B | 5.20 | 1.47 | 1.40 |
| 22 | 6 | 611 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 6 | 617 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 4 | 611 | CLA | C1D-ND | 5.20 | 1.44 | 1.37 |
| 22 | 9 | 602 | CLA | C1D-ND | 5.20 | 1.44 | 1.37 |
| 22 | 3 | 614 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 9 | 611 | CLA | C1D-ND | 5.20 | 1.44 | 1.37 |
| 22 | 1 | 612 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 8 | 604 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 6 | 602 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | A | 821 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 1 | 606 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 3 | 603 | CLA | C3B-C2B | 5.20 | 1.47 | 1.40 |
| 22 | Z | 609 | CLA | C3C-C2C | 5.20 | 1.47 | 1.36 |
| 22 | 1 | 603 | CLA | C1D-ND | 5.20 | 1.44 | 1.37 |
| 22 | 1 | 603 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | B | 803 | CLA | C3B-C2B | 5.19 | 1.47 | 1.40 |
| 22 | 1 | 602 | CLA | C3B-C2B | 5.19 | 1.47 | 1.40 |
| 22 | 8 | 603 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | A | 826 | CLA | C1D-ND | 5.19 | 1.44 | 1.37 |
| 22 | 5 | 602 | CLA | CHC-C1C | 5.19 | 1.48 | 1.35 |
| 22 | 9 | 609 | CLA | C1D-ND | 5.19 | 1.44 | 1.37 |
| 22 | 9 | 610 | CLA | C1D-ND | 5.19 | 1.44 | 1.37 |
| 22 | A | 804 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | 2 | 612 | CLA | O2D-CGD | 5.19 | 1.45 | 1.33 |
| 22 | 7 | 606 | CLA | C1D-ND | 5.19 | 1.44 | 1.37 |
| 22 | 7 | 603 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | Z | 608 | CLA | C1D-ND | 5.19 | 1.44 | 1.37 |
| 22 | 6 | 602 | CLA | CHC-C1C | 5.19 | 1.48 | 1.35 |
| 22 | 7 | 606 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 3 | 611 | CLA | C1D-ND | 5.19 | 1.44 | 1.37 |
| 22 | 9 | 610 | CLA | C3C-C2C | 5.19 | 1.47 | 1.36 |
| 22 | 6 | 603 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 22 | 4 | 612 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 22 | 5 | 612 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 22 | 8 | 601 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 22 | G | 204 | CLA | C1D-ND | 5.18 | 1.44 | 1.37 |
| 22 | 9 | 613 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 22 | 3 | 606 | CLA | O2D-CGD | 5.18 | 1.45 | 1.33 |
| 22 | Z | 614 | CLA | O2D-CGD | 5.18 | 1.45 | 1.33 |
| 22 | A | 833 | CLA | C3C-C2C | 5.18 | 1.47 | 1.36 |
| 22 | Z | 616 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | 7 | 609 | CLA | O2D-CGD | 5.17 | 1.45 | 1.33 |
| 22 | 3 | 609 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | F | 303 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | 7 | 604 | CLA | C3B-C2B | 5.17 | 1.47 | 1.40 |
| 22 | 8 | 606 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | 5 | 603 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | A | 842 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | A | 826 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | B | 830 | CLA | C3B-C2B | 5.17 | 1.47 | 1.40 |
| 22 | 6 | 622 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | B | 852 | CLA | O2D-CGD | 5.17 | 1.45 | 1.33 |
| 22 | 5 | 616 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | 2 | 612 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | F | 303 | CLA | O2D-CGD | 5.17 | 1.45 | 1.33 |
| 22 | 3 | 620 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | B | 837 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | A | 816 | CLA | CHC-C1C | 5.17 | 1.48 | 1.35 |
| 22 | A | 810 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | 4 | 613 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | B | 830 | CLA | CHC-C1C | 5.17 | 1.48 | 1.35 |
| 22 | B | 808 | CLA | C3C-C2C | 5.17 | 1.47 | 1.36 |
| 22 | 3 | 620 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 22 | 2 | 602 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 22 | B | 805 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 22 | B | 806 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 22 | 2 | 606 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 22 | Z | 604 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 22 | 4 | 609 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 22 | B | 815 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 22 | 6 | 610 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | A | 828 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 22 | 8 | 610 | CLA | C3C-C2C | 5.16 | 1.47 | 1.36 |
| 22 | Z | 602 | CLA | C3B-C2B | 5.16 | 1.47 | 1.40 |
| 22 | 9 | 610 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 22 | A | 805 | CLA | CHC-C1C | 5.16 | 1.48 | 1.35 |
| 22 | 7 | 611 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 22 | J | 3002 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 22 | 9 | 612 | CLA | O2D-CGD | 5.16 | 1.45 | 1.33 |
| 22 | A | 817 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 22 | 4 | 616 | CLA | O2D-CGD | 5.15 | 1.45 | 1.33 |
| 22 | B | 810 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 22 | B | 829 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 22 | Z | 614 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 22 | A | 818 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 22 | 7 | 603 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 22 | 1 | 602 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 29 | 4 | 608 | CHL | CHC-C1C | 5.15 | 1.48 | 1.35 |
| 22 | B | 833 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 22 | 2 | 603 | CLA | O2D-CGD | 5.15 | 1.45 | 1.33 |
| 22 | 6 | 611 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 22 | B | 828 | CLA | C3C-C2C | 5.15 | 1.47 | 1.36 |
| 22 | 4 | 609 | CLA | C3B-C2B | 5.15 | 1.47 | 1.40 |
| 29 | 9 | 606 | CHL | O2D-CGD | 5.15 | 1.45 | 1.33 |
| 22 | 9 | 603 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 22 | Z | 613 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 22 | G | 203 | CLA | C1D-ND | 5.14 | 1.44 | 1.37 |
| 22 | 5 | 610 | CLA | CHC-C1C | 5.14 | 1.48 | 1.35 |
| 22 | B | 823 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 22 | 1 | 602 | CLA | CHC-C1C | 5.14 | 1.48 | 1.35 |
| 22 | B | 832 | CLA | C3B-C2B | 5.14 | 1.47 | 1.40 |
| 22 | A | 809 | CLA | CHC-C1C | 5.14 | 1.48 | 1.35 |
| 22 | B | 841 | CLA | CHC-C1C | 5.14 | 1.48 | 1.35 |
| 22 | B | 827 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 22 | 5 | 604 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 22 | 3 | 617 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 22 | 5 | 604 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |
| 22 | A | 835 | CLA | C1D-ND | 5.14 | 1.44 | 1.37 |
| 29 | 6 | 618 | CHL | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 22 | G | 204 | CLA | O2D-CGD | 5.14 | 1.45 | 1.33 |
| 22 | 8 | 608 | CLA | C1D-ND | 5.14 | 1.44 | 1.37 |
| 29 | Z | 607 | CHL | C2C-C3C | 5.14 | 1.47 | 1.36 |
| 22 | B | 823 | CLA | C3C-C2C | 5.14 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | 2 | 610 | CLA | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 22 | B | 831 | CLA | C3B-C2B | 5.13 | 1.47 | 1.40 |
| 22 | 2 | 611 | CLA | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 22 | 7 | 616 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 22 | 6 | 614 | CLA | C1D-ND | 5.13 | 1.44 | 1.37 |
| 22 | B | 814 | CLA | C3C-C2C | 5.13 | 1.47 | 1.36 |
| 22 | 8 | 613 | CLA | C1D-ND | 5.13 | 1.44 | 1.37 |
| 22 | 9 | 610 | CLA | CHC-C1C | 5.13 | 1.48 | 1.35 |
| 22 | 4 | 604 | CLA | O2D-CGD | 5.13 | 1.45 | 1.33 |
| 29 | 6 | 606 | CHL | CHC-C1C | 5.12 | 1.48 | 1.35 |
| 22 | 3 | 606 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 22 | 5 | 606 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 22 | 5 | 610 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 22 | A | 812 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 22 | 7 | 616 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | A | 845 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | L | 204 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 29 | 9 | 607 | CHL | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | K | 4003 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | A | 802 | CLA | CHC-C1C | 5.12 | 1.48 | 1.35 |
| 22 | 1 | 604 | CLA | C3B-C2B | 5.12 | 1.47 | 1.40 |
| 22 | 9 | 601 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | 6 | 613 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 22 | 6 | 612 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 22 | A | 836 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | A | 808 | CLA | C3C-C2C | 5.12 | 1.47 | 1.36 |
| 29 | 5 | 607 | CHL | C2C-C3C | 5.12 | 1.47 | 1.36 |
| 22 | 6 | 603 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | B | 805 | CLA | CHC-C1C | 5.12 | 1.48 | 1.35 |
| 22 | 5 | 612 | CLA | O2D-CGD | 5.12 | 1.45 | 1.33 |
| 22 | L | 203 | CLA | C3B-C2B | 5.12 | 1.47 | 1.40 |
| 22 | B | 823 | CLA | C3B-C2B | 5.11 | 1.47 | 1.40 |
| 29 | 4 | 606 | CHL | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | 1 | 604 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | 7 | 611 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 22 | 8 | 602 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 22 | 4 | 604 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 22 | 2 | 614 | CLA | CHC-C1C | 5.11 | 1.48 | 1.35 |
| 22 | Z | 606 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | B | 829 | CLA | CHC-C1C | 5.11 | 1.48 | 1.35 |
| 22 | 9 | 602 | CLA | CHC-C1C | 5.11 | 1.48 | 1.35 |
| 22 | Z | 612 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | Z | 613 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | 4 | 603 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | A | 819 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | 4 | 604 | CLA | C3B-C2B | 5.11 | 1.47 | 1.40 |
| 22 | A | 802 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | A | 835 | CLA | CHC-C1C | 5.11 | 1.48 | 1.35 |
| 22 | 1 | 608 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 22 | 8 | 603 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 22 | 4 | 609 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 22 | B | 804 | CLA | C3C-C2C | 5.11 | 1.47 | 1.36 |
| 22 | 7 | 608 | CLA | CHC-C1C | 5.11 | 1.48 | 1.35 |
| 22 | 6 | 610 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 22 | F | 304 | CLA | O2D-CGD | 5.11 | 1.45 | 1.33 |
| 22 | 1 | 606 | CLA | CHC-C1C | 5.11 | 1.48 | 1.35 |
| 29 | 6 | 608 | CHL | C3B-C2B | 5.11 | 1.47 | 1.40 |
| 22 | B | 816 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 22 | K | 4003 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 22 | 7 | 610 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 22 | 9 | 614 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 22 | 3 | 613 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 22 | 5 | 603 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 22 | 1 | 609 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 22 | 7 | 612 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 22 | 4 | 603 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 22 | A | 843 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 22 | 7 | 604 | CLA | O2D-CGD | 5.10 | 1.45 | 1.33 |
| 22 | A | 832 | CLA | C3C-C2C | 5.10 | 1.47 | 1.36 |
| 22 | A | 841 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | A | 837 | CLA | CHC-C1C | 5.09 | 1.48 | 1.35 |
| 22 | 9 | 609 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | 3 | 613 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | 1 | 606 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | 1 | 606 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 22 | 1 | 613 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 22 | B | 812 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 22 | B | 827 | CLA | C3B-C2B | 5.09 | 1.47 | 1.40 |
| 22 | 3 | 604 | CLA | C3B-C2B | 5.09 | 1.47 | 1.40 |
| 22 | 9 | 602 | CLA | C3C-C2C | 5.09 | 1.47 | 1.36 |
| 22 | B | 816 | CLA | CHC-C1C | 5.09 | 1.48 | 1.35 |
| 22 | 6 | 614 | CLA | CHC-C1C | 5.09 | 1.48 | 1.35 |
| 22 | 4 | 602 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | 2 | 613 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 807 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 22 | L | 203 | CLA | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | 9 | 613 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 29 | Z | 607 | CHL | O2D-CGD | 5.09 | 1.45 | 1.33 |
| 22 | B | 820 | CLA | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 22 | 5 | 609 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 22 | B | 818 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 22 | 6 | 604 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 22 | 6 | 616 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 22 | Z | 611 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 29 | 4 | 607 | CHL | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 22 | B | 806 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 22 | 6 | 613 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 21 | A | 801 | CL0 | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 22 | B | 837 | CLA | C3B-C2B | 5.08 | 1.47 | 1.40 |
| 29 | 1 | 607 | CHL | C2C-C3C | 5.08 | 1.47 | 1.36 |
| 22 | A | 828 | CLA | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 22 | 1 | 612 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 22 | F | 301 | CLA | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 22 | 8 | 614 | CLA | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 29 | 5 | 608 | CHL | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 22 | 2 | 607 | CLA | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 22 | A | 833 | CLA | CHC-C1C | 5.08 | 1.48 | 1.35 |
| 22 | B | 819 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 22 | A | 833 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 22 | 7 | 613 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 22 | 7 | 610 | CLA | C3C-C2C | 5.08 | 1.47 | 1.36 |
| 22 | 5 | 621 | CLA | O2D-CGD | 5.08 | 1.45 | 1.33 |
| 22 | B | 807 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 29 | 7 | 607 | CHL | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | 5 | 606 | CLA | CHC-C1C | 5.07 | 1.48 | 1.35 |
| 22 | 8 | 612 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | B | 839 | CLA | C1D-ND | 5.07 | 1.44 | 1.37 |
| 22 | A | 829 | CLA | CHC-C1C | 5.07 | 1.48 | 1.35 |
| 22 | 3 | 612 | CLA | C1D-ND | 5.07 | 1.44 | 1.37 |
| 22 | G | 203 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | 4 | 614 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | F | 301 | CLA | C1D-ND | 5.07 | 1.44 | 1.37 |
| 22 | 5 | 613 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | 9 | 604 | CLA | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | A | 840 | CLA | C3C-C2C | 5.07 | 1.47 | 1.36 |
| 22 | 2 | 610 | CLA | CHC-C1C | 5.07 | 1.48 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 29 | 6 | 606 | CHL | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 29 | 5 | 618 | CHL | O2D-CGD | 5.07 | 1.45 | 1.33 |
| 22 | Z | 602 | CLA | CHC-C1C | 5.07 | 1.48 | 1.35 |
| 29 | 4 | 618 | CHL | C2C-C3C | 5.06 | 1.47 | 1.36 |
| 22 | 8 | 613 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 22 | K | 4002 | CLA | CHC-C1C | 5.06 | 1.47 | 1.35 |
| 22 | A | 815 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 22 | 3 | 614 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 22 | 4 | 614 | CLA | CHC-C1C | 5.06 | 1.47 | 1.35 |
| 22 | 3 | 612 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 22 | 6 | 612 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 22 | 1 | 614 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 22 | 3 | 609 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 22 | A | 803 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 22 | 4 | 613 | CLA | C3C-C2C | 5.06 | 1.47 | 1.36 |
| 22 | 5 | 606 | CLA | O2D-CGD | 5.06 | 1.45 | 1.33 |
| 29 | 6 | 618 | CHL | C2C-C3C | 5.06 | 1.47 | 1.36 |
| 22 | 8 | 602 | CLA | CHC-C1C | 5.06 | 1.47 | 1.35 |
| 22 | 6 | 610 | CLA | CHC-C1C | 5.06 | 1.47 | 1.35 |
| 22 | 9 | 611 | CLA | CHC-C1C | 5.05 | 1.47 | 1.35 |
| 22 | Z | 613 | CLA | CHC-C1C | 5.05 | 1.47 | 1.35 |
| 29 | 8 | 607 | CHL | C2C-C3C | 5.05 | 1.47 | 1.36 |
| 22 | B | 817 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 22 | 5 | 611 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | A | 837 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 22 | 3 | 602 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 22 | B | 820 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | 3 | 611 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | Z | 603 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 22 | A | 813 | CLA | CHC-C1C | 5.05 | 1.47 | 1.35 |
| 22 | 4 | 610 | CLA | CHC-C1C | 5.05 | 1.47 | 1.35 |
| 22 | A | 815 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | B | 822 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | Z | 602 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 22 | B | 813 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 22 | 8 | 604 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | 4 | 609 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 22 | A | 825 | CLA | C3C-C2C | 5.05 | 1.47 | 1.36 |
| 22 | A | 817 | CLA | O2D-CGD | 5.05 | 1.45 | 1.33 |
| 22 | A | 822 | CLA | CHC-C1C | 5.04 | 1.47 | 1.35 |
| 22 | 6 | 616 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 22 | B | 819 | CLA | CHC-C1C | 5.04 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | A | 838 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 22 | 8 | 610 | CLA | CHC-C1C | 5.04 | 1.47 | 1.35 |
| 22 | Z | 604 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 22 | 1 | 610 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 22 | B | 821 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 22 | 1 | 614 | CLA | CHC-C1C | 5.04 | 1.47 | 1.35 |
| 22 | 8 | 616 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 22 | B | 837 | CLA | CHC-C1C | 5.04 | 1.47 | 1.35 |
| 22 | A | 811 | CLA | C3C-C2C | 5.04 | 1.47 | 1.36 |
| 22 | B | 805 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 22 | 7 | 611 | CLA | O2D-CGD | 5.04 | 1.45 | 1.33 |
| 22 | 8 | 606 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | 4 | 612 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | 3 | 607 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | Z | 614 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | B | 833 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 22 | 1 | 616 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 22 | 8 | 611 | CLA | C3C-C2C | 5.03 | 1.47 | 1.36 |
| 22 | 7 | 609 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | 3 | 617 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | 6 | 603 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 22 | A | 811 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | A | 823 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 29 | 1 | 607 | CHL | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | 1 | 604 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | 9 | 614 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | 1 | 611 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 29 | 6 | 606 | CHL | C2C-C3C | 5.03 | 1.47 | 1.36 |
| 22 | 3 | 617 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 22 | B | 839 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 29 | 4 | 608 | CHL | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | A | 819 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | J | 3002 | CLA | O2D-CGD | 5.03 | 1.45 | 1.33 |
| 22 | 1 | 611 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 22 | B | 814 | CLA | CHC-C1C | 5.03 | 1.47 | 1.35 |
| 22 | A | 824 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | A | 830 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 22 | 8 | 612 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 29 | 4 | 618 | CHL | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 8 | 611 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 7 | 612 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 7 | 620 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 804 | CLA | CHC-C1C | 5.02 | 1.47 | 1.35 |
| 22 | 5 | 601 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 3 | 620 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 7 | 602 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 22 | 3 | 603 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 6 | 617 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | L | 204 | CLA | CHC-C1C | 5.02 | 1.47 | 1.35 |
| 22 | Z | 616 | CLA | CHC-C1C | 5.02 | 1.47 | 1.35 |
| 22 | 1 | 614 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 6 | 611 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 2 | 606 | CLA | CHC-C1C | 5.02 | 1.47 | 1.35 |
| 22 | B | 811 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | B | 836 | CLA | C3C-C2C | 5.02 | 1.47 | 1.36 |
| 22 | 6 | 609 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 22 | 1 | 616 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 9 | 602 | CLA | O2D-CGD | 5.02 | 1.45 | 1.33 |
| 22 | 4 | 604 | CLA | CHC-C1C | 5.02 | 1.47 | 1.35 |
| 22 | B | 835 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 29 | 8 | 607 | CHL | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | B | 852 | CLA | CHC-C1C | 5.01 | 1.47 | 1.35 |
| 22 | A | 832 | CLA | CHC-C1C | 5.01 | 1.47 | 1.35 |
| 22 | 9 | 613 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | B | 827 | CLA | CHC-C1C | 5.01 | 1.47 | 1.35 |
| 22 | B | 821 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 29 | Z | 601 | CHL | CHC-C1C | 5.01 | 1.47 | 1.35 |
| 22 | 6 | 616 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | 7 | 613 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 22 | 5 | 613 | CLA | C1D-ND | 5.01 | 1.43 | 1.37 |
| 22 | A | 826 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | 3 | 603 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 22 | A | 807 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | 8 | 601 | CLA | C1D-ND | 5.01 | 1.43 | 1.37 |
| 22 | Z | 606 | CLA | CHC-C1C | 5.01 | 1.47 | 1.35 |
| 29 | 4 | 607 | CHL | C2C-C3C | 5.01 | 1.47 | 1.36 |
| 22 | F | 303 | CLA | C3C-C2C | 5.01 | 1.47 | 1.36 |
| 22 | B | 841 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | 1 | 613 | CLA | O2D-CGD | 5.01 | 1.45 | 1.33 |
| 22 | B | 822 | CLA | C1D-ND | 5.00 | 1.43 | 1.37 |
| 29 | 4 | 607 | CHL | CHC-C1C | 5.00 | 1.47 | 1.35 |
| 22 | 6 | 604 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 22 | A | 816 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 22 | B | 840 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | Z | 603 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 29 | 6 | 608 | CHL | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 22 | 6 | 604 | CLA | CHC-C1C | 5.00 | 1.47 | 1.35 |
| 22 | B | 809 | CLA | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 22 | B | 824 | CLA | C3C-C2C | 5.00 | 1.47 | 1.36 |
| 22 | B | 824 | CLA | CHC-C1C | 5.00 | 1.47 | 1.35 |
| 22 | Z | 611 | CLA | CHC-C1C | 5.00 | 1.47 | 1.35 |
| 22 | B | 806 | CLA | CHC-C1C | 5.00 | 1.47 | 1.35 |
| 22 | A | 836 | CLA | C1D-ND | 5.00 | 1.43 | 1.37 |
| 22 | 8 | 610 | CLA | O2D-CGD | 5.00 | 1.45 | 1.33 |
| 22 | A | 821 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | 7 | 602 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | B | 835 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 22 | Z | 616 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | 4 | 602 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 22 | Z | 609 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | 5 | 614 | CLA | C1D-ND | 4.99 | 1.43 | 1.37 |
| 22 | A | 820 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | A | 825 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | A | 814 | CLA | C3C-C2C | 4.99 | 1.47 | 1.36 |
| 22 | B | 838 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | K | 4002 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | 6 | 613 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 29 | 9 | 607 | CHL | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 22 | 8 | 608 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | 5 | 614 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | 4 | 611 | CLA | O2D-CGD | 4.99 | 1.45 | 1.33 |
| 22 | A | 808 | CLA | C1D-ND | 4.99 | 1.43 | 1.37 |
| 22 | B | 821 | CLA | CHC-C1C | 4.99 | 1.47 | 1.35 |
| 22 | B | 811 | CLA | C1D-ND | 4.99 | 1.43 | 1.37 |
| 22 | 5 | 613 | CLA | C3C-C2C | 4.98 | 1.47 | 1.36 |
| 29 | 9 | 606 | CHL | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 22 | B | 840 | CLA | C1D-ND | 4.98 | 1.43 | 1.37 |
| 22 | Z | 602 | CLA | C1D-ND | 4.98 | 1.43 | 1.37 |
| 22 | A | 830 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | B | 812 | CLA | C1D-ND | 4.98 | 1.43 | 1.37 |
| 22 | 3 | 603 | CLA | C1D-ND | 4.98 | 1.43 | 1.37 |
| 29 | 1 | 607 | CHL | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 22 | B | 817 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | B | 813 | CLA | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 22 | 6 | 609 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | 6 | 622 | CLA | CHC-C1C | 4.98 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | A | 839 | CLA | C1D-ND | 4.98 | 1.43 | 1.37 |
| 22 | 4 | 610 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | 2 | 602 | CLA | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 22 | B | 828 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | 1 | 608 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | 8 | 614 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | 6 | 610 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | B | 817 | CLA | C1D-ND | 4.98 | 1.43 | 1.37 |
| 22 | B | 832 | CLA | CHC-C1C | 4.98 | 1.47 | 1.35 |
| 22 | 8 | 603 | CLA | O2D-CGD | 4.98 | 1.45 | 1.33 |
| 22 | 7 | 612 | CLA | C1D-ND | 4.97 | 1.43 | 1.37 |
| 22 | G | 204 | CLA | CHC-C1C | 4.97 | 1.47 | 1.35 |
| 22 | B | 812 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | B | 810 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | 8 | 616 | CLA | CHC-C1C | 4.97 | 1.47 | 1.35 |
| 22 | 7 | 620 | CLA | CHC-C1C | 4.97 | 1.47 | 1.35 |
| 22 | 3 | 602 | CLA | C3C-C2C | 4.97 | 1.47 | 1.36 |
| 22 | A | 825 | CLA | C1D-ND | 4.97 | 1.43 | 1.37 |
| 22 | B | 818 | CLA | C1D-ND | 4.97 | 1.43 | 1.37 |
| 22 | 3 | 604 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | 7 | 603 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | Z | 608 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | 7 | 614 | CLA | CHC-C1C | 4.97 | 1.47 | 1.35 |
| 22 | A | 835 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | A | 840 | CLA | C1D-ND | 4.97 | 1.43 | 1.37 |
| 22 | A | 812 | CLA | O2D-CGD | 4.97 | 1.45 | 1.33 |
| 22 | 4 | 613 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 22 | A | 823 | CLA | C1D-ND | 4.96 | 1.43 | 1.37 |
| 22 | Z | 610 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 22 | Z | 602 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 22 | A | 834 | CLA | C1D-ND | 4.96 | 1.43 | 1.37 |
| 22 | B | 815 | CLA | C1D-ND | 4.96 | 1.43 | 1.37 |
| 22 | 6 | 617 | CLA | C1D-ND | 4.96 | 1.43 | 1.37 |
| 22 | 7 | 608 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 22 | 7 | 610 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 22 | A | 829 | CLA | O2D-CGD | 4.96 | 1.45 | 1.33 |
| 22 | 5 | 601 | CLA | C1D-ND | 4.96 | 1.43 | 1.37 |
| 22 | 5 | 602 | CLA | C3C-C2C | 4.96 | 1.47 | 1.36 |
| 22 | 7 | 616 | CLA | CHC-C1C | 4.96 | 1.47 | 1.35 |
| 22 | 9 | 601 | CLA | CHC-C1C | 4.96 | 1.47 | 1.35 |
| 22 | 4 | 613 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | B | 820 | CLA | C1D-ND | 4.95 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 3 | 614 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | 5 | 612 | CLA | C1D-ND | 4.95 | 1.43 | 1.37 |
| 22 | 7 | 604 | CLA | C3C-C2C | 4.95 | 1.47 | 1.36 |
| 22 | 3 | 611 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | 5 | 601 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | Z | 608 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | A | 811 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 22 | B | 822 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | 5 | 621 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | 5 | 602 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 22 | 3 | 602 | CLA | CHC-C1C | 4.95 | 1.47 | 1.35 |
| 22 | B | 837 | CLA | C1D-ND | 4.95 | 1.43 | 1.37 |
| 22 | 6 | 622 | CLA | O2D-CGD | 4.95 | 1.45 | 1.33 |
| 22 | 3 | 602 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | 8 | 601 | CLA | CHC-C1C | 4.94 | 1.47 | 1.35 |
| 22 | 9 | 604 | CLA | CHC-C1C | 4.94 | 1.47 | 1.35 |
| 22 | B | 834 | CLA | CHC-C1C | 4.94 | 1.47 | 1.35 |
| 22 | 2 | 611 | CLA | CHC-C1C | 4.94 | 1.47 | 1.35 |
| 22 | 4 | 612 | CLA | C1D-ND | 4.94 | 1.43 | 1.37 |
| 22 | B | 841 | CLA | C1D-ND | 4.94 | 1.43 | 1.37 |
| 22 | 6 | 611 | CLA | CHC-C1C | 4.94 | 1.47 | 1.35 |
| 29 | Z | 601 | CHL | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | B | 831 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | A | 843 | CLA | C3C-C2C | 4.94 | 1.47 | 1.36 |
| 22 | B | 818 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | B | 834 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | A | 832 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | A | 837 | CLA | O2D-CGD | 4.94 | 1.45 | 1.33 |
| 22 | B | 809 | CLA | C3B-C2B | 4.94 | 1.47 | 1.40 |
| 22 | 5 | 614 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 29 | 4 | 618 | CHL | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | 5 | 610 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 22 | 5 | 617 | CLA | O2D-CGD | 4.93 | 1.45 | 1.33 |
| 22 | L | 204 | CLA | C1D-ND | 4.93 | 1.43 | 1.37 |
| 22 | 8 | 609 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | A | 802 | CLA | C1D-ND | 4.93 | 1.43 | 1.37 |
| 22 | B | 833 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | B | 823 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | 2 | 609 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | 8 | 608 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | 5 | 617 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | 8 | 613 | CLA | C3C-C2C | 4.93 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | K | 4003 | CLA | CHC-C1C | 4.93 | 1.47 | 1.35 |
| 22 | 1 | 612 | CLA | C1D-ND | 4.92 | 1.43 | 1.37 |
| 29 | 1 | 601 | CHL | CHC-C1C | 4.92 | 1.47 | 1.35 |
| 22 | 8 | 601 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 22 | 1 | 616 | CLA | CHC-C1C | 4.92 | 1.47 | 1.35 |
| 22 | B | 816 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 22 | B | 817 | CLA | C3B-C2B | 4.92 | 1.47 | 1.40 |
| 22 | 1 | 602 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 22 | 6 | 612 | CLA | CHC-C1C | 4.92 | 1.47 | 1.35 |
| 22 | Z | 612 | CLA | C1D-ND | 4.92 | 1.43 | 1.37 |
| 22 | 6 | 602 | CLA | C1D-ND | 4.92 | 1.43 | 1.37 |
| 22 | B | 811 | CLA | CHC-C1C | 4.92 | 1.47 | 1.35 |
| 22 | 6 | 602 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 22 | 1 | 604 | CLA | C1D-ND | 4.92 | 1.43 | 1.37 |
| 22 | 3 | 610 | CLA | C3C-C2C | 4.92 | 1.47 | 1.36 |
| 22 | A | 806 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 29 | 3 | 608 | CHL | C2C-C3C | 4.92 | 1.47 | 1.36 |
| 22 | B | 833 | CLA | O2D-CGD | 4.92 | 1.45 | 1.33 |
| 22 | B | 852 | CLA | C1D-ND | 4.91 | 1.43 | 1.37 |
| 22 | A | 839 | CLA | CHC-C1C | 4.91 | 1.47 | 1.35 |
| 22 | B | 808 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | 3 | 610 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | 6 | 601 | CLA | C1D-ND | 4.91 | 1.43 | 1.37 |
| 22 | 8 | 609 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | B | 806 | CLA | C1D-ND | 4.91 | 1.43 | 1.37 |
| 22 | 5 | 611 | CLA | CHC-C1C | 4.91 | 1.47 | 1.35 |
| 22 | A | 833 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 29 | 5 | 607 | CHL | CHC-C1C | 4.91 | 1.47 | 1.35 |
| 22 | A | 805 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | A | 827 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 29 | 7 | 607 | CHL | CHC-C1C | 4.91 | 1.47 | 1.35 |
| 22 | 1 | 609 | CLA | O2D-CGD | 4.91 | 1.45 | 1.33 |
| 22 | 7 | 603 | CLA | CHC-C1C | 4.91 | 1.47 | 1.35 |
| 22 | A | 818 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |
| 22 | A | 823 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |
| 22 | 2 | 613 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |
| 22 | A | 822 | CLA | O2D-CGD | 4.90 | 1.45 | 1.33 |
| 22 | 2 | 601 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |
| 22 | 8 | 602 | CLA | C1D-ND | 4.90 | 1.43 | 1.37 |
| 22 | 5 | 604 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |
| 22 | A | 806 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |
| 22 | B | 810 | CLA | CHC-C1C | 4.90 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | B | 839 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | A | 841 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | 6 | 617 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 29 | 6 | 608 | CHL | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 29 | 4 | 606 | CHL | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | A | 834 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 22 | 3 | 609 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 29 | 6 | 607 | CHL | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | A | 829 | CLA | C3C-C2C | 4.89 | 1.47 | 1.36 |
| 22 | 3 | 606 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | A | 808 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 29 | 6 | 618 | CHL | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | 7 | 606 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 22 | 8 | 606 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | 8 | 604 | CLA | C1D-ND | 4.89 | 1.43 | 1.37 |
| 22 | A | 818 | CLA | O2D-CGD | 4.89 | 1.45 | 1.33 |
| 22 | 4 | 614 | CLA | C1D-ND | 4.89 | 1.43 | 1.37 |
| 22 | B | 815 | CLA | CHC-C1C | 4.89 | 1.47 | 1.35 |
| 22 | A | 841 | CLA | C1D-ND | 4.88 | 1.43 | 1.37 |
| 22 | 6 | 601 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 22 | 8 | 613 | CLA | CHC-C1C | 4.88 | 1.47 | 1.35 |
| 22 | A | 803 | CLA | C1D-ND | 4.88 | 1.43 | 1.37 |
| 22 | A | 842 | CLA | C1D-ND | 4.88 | 1.43 | 1.37 |
| 22 | J | 3002 | CLA | CHC-C1C | 4.88 | 1.47 | 1.35 |
| 22 | 3 | 617 | CLA | CHC-C1C | 4.88 | 1.47 | 1.35 |
| 21 | A | 801 | CL0 | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 22 | 8 | 602 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 22 | B | 809 | CLA | O2D-CGD | 4.88 | 1.45 | 1.33 |
| 22 | 3 | 620 | CLA | CHC-C1C | 4.88 | 1.47 | 1.35 |
| 22 | 3 | 607 | CLA | C1D-ND | 4.88 | 1.43 | 1.37 |
| 22 | G | 203 | CLA | CHC-C1C | 4.88 | 1.47 | 1.35 |
| 22 | 4 | 612 | CLA | CHC-C1C | 4.88 | 1.47 | 1.35 |
| 22 | L | 203 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | 1 | 613 | CLA | C1D-ND | 4.87 | 1.43 | 1.37 |
| 22 | 6 | 616 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | 3 | 604 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | B | 826 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | B | 826 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 22 | B | 812 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | 5 | 609 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 29 | 1 | 601 | CHL | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 22 | 4 | 601 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 835 | CLA | C1D-ND | 4.87 | 1.43 | 1.37 |
| 22 | B | 836 | CLA | C1D-ND | 4.87 | 1.43 | 1.37 |
| 22 | 4 | 601 | CLA | C1D-ND | 4.87 | 1.43 | 1.37 |
| 22 | Z | 604 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | 8 | 609 | CLA | C1D-ND | 4.87 | 1.43 | 1.37 |
| 22 | F | 303 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 22 | A | 809 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 22 | 9 | 612 | CLA | CHC-C1C | 4.87 | 1.47 | 1.35 |
| 29 | 4 | 606 | CHL | C2C-C3C | 4.87 | 1.47 | 1.36 |
| 29 | 3 | 608 | CHL | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 22 | A | 810 | CLA | O2D-CGD | 4.87 | 1.45 | 1.33 |
| 22 | 3 | 604 | CLA | C1D-ND | 4.86 | 1.43 | 1.37 |
| 22 | Z | 613 | CLA | C1D-ND | 4.86 | 1.43 | 1.37 |
| 22 | A | 810 | CLA | CHC-C1C | 4.86 | 1.47 | 1.35 |
| 29 | Z | 607 | CHL | CHC-C1C | 4.86 | 1.47 | 1.35 |
| 22 | B | 836 | CLA | O2D-CGD | 4.86 | 1.45 | 1.33 |
| 22 | 8 | 612 | CLA | CHC-C1C | 4.86 | 1.47 | 1.35 |
| 22 | B | 823 | CLA | C1D-ND | 4.86 | 1.43 | 1.37 |
| 22 | 9 | 609 | CLA | CHC-C1C | 4.86 | 1.47 | 1.35 |
| 22 | 1 | 610 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 22 | 1 | 602 | CLA | C1D-ND | 4.86 | 1.43 | 1.37 |
| 22 | B | 802 | CLA | C3C-C2C | 4.86 | 1.47 | 1.36 |
| 29 | 8 | 607 | CHL | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 21 | A | 801 | CL0 | C3B-C2B | 4.85 | 1.47 | 1.40 |
| 22 | 8 | 611 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 22 | A | 804 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 22 | A | 814 | CLA | C1D-ND | 4.85 | 1.43 | 1.37 |
| 22 | B | 829 | CLA | O2D-CGD | 4.85 | 1.45 | 1.33 |
| 22 | A | 830 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 22 | A | 808 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 22 | Z | 612 | CLA | CHC-C1C | 4.85 | 1.47 | 1.35 |
| 29 | 6 | 608 | CHL | C2C-C3C | 4.84 | 1.47 | 1.36 |
| 22 | 7 | 614 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 22 | B | 836 | CLA | CHC-C1C | 4.84 | 1.47 | 1.35 |
| 22 | 7 | 609 | CLA | C1D-ND | 4.84 | 1.43 | 1.37 |
| 22 | 5 | 609 | CLA | O2D-CGD | 4.84 | 1.45 | 1.33 |
| 22 | A | 818 | CLA | C1D-ND | 4.84 | 1.43 | 1.37 |
| 22 | A | 843 | CLA | C1D-ND | 4.84 | 1.43 | 1.37 |
| 22 | A | 817 | CLA | C3B-C2B | 4.84 | 1.47 | 1.40 |
| 22 | 9 | 613 | CLA | CHC-C1C | 4.84 | 1.47 | 1.35 |
| 29 | 3 | 608 | CHL | C3B-C2B | 4.83 | 1.47 | 1.40 |
| 22 | B | 803 | CLA | C3C-C2C | 4.83 | 1.47 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 8 | 612 | CLA | C1D-ND | 4.83 | 1.43 | 1.37 |
| 22 | A | 803 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | 1 | 603 | CLA | O2D-CGD | 4.83 | 1.45 | 1.33 |
| 22 | F | 304 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | A | 820 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | 1 | 611 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | 7 | 601 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | 2 | 612 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | 6 | 612 | CLA | C1D-ND | 4.83 | 1.43 | 1.37 |
| 22 | A | 845 | CLA | CHC-C1C | 4.83 | 1.47 | 1.35 |
| 22 | B | 803 | CLA | CHC-C1C | 4.82 | 1.47 | 1.35 |
| 22 | B | 830 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 22 | 7 | 601 | CLA | C1D-ND | 4.82 | 1.43 | 1.37 |
| 29 | 5 | 618 | CHL | CHC-C1C | 4.82 | 1.47 | 1.35 |
| 22 | 6 | 601 | CLA | CHC-C1C | 4.82 | 1.47 | 1.35 |
| 29 | 5 | 608 | CHL | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 22 | A | 842 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 22 | 5 | 616 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 22 | 7 | 601 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 22 | A | 831 | CLA | O2D-CGD | 4.82 | 1.45 | 1.33 |
| 22 | B | 814 | CLA | O2D-CGD | 4.81 | 1.44 | 1.33 |
| 22 | 4 | 611 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 22 | 4 | 602 | CLA | C1D-ND | 4.81 | 1.43 | 1.37 |
| 22 | A | 824 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 22 | 7 | 606 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 22 | F | 301 | CLA | O2D-CGD | 4.81 | 1.44 | 1.33 |
| 22 | A | 814 | CLA | CHC-C1C | 4.81 | 1.47 | 1.35 |
| 22 | A | 812 | CLA | C1D-ND | 4.81 | 1.43 | 1.37 |
| 22 | B | 813 | CLA | C3C-C2C | 4.80 | 1.46 | 1.36 |
| 22 | B | 814 | CLA | C1D-ND | 4.80 | 1.43 | 1.37 |
| 22 | B | 816 | CLA | C3C-C2C | 4.80 | 1.46 | 1.36 |
| 22 | B | 824 | CLA | O2D-CGD | 4.80 | 1.44 | 1.33 |
| 22 | A | 834 | CLA | CHC-C1C | 4.80 | 1.47 | 1.35 |
| 22 | A | 838 | CLA | O2D-CGD | 4.80 | 1.44 | 1.33 |
| 22 | A | 812 | CLA | CHC-C1C | 4.80 | 1.47 | 1.35 |
| 22 | 1 | 612 | CLA | CHC-C1C | 4.80 | 1.47 | 1.35 |
| 22 | Z | 610 | CLA | C3C-C2C | 4.80 | 1.46 | 1.36 |
| 22 | A | 811 | CLA | C1D-ND | 4.79 | 1.43 | 1.37 |
| 22 | A | 819 | CLA | C1D-ND | 4.79 | 1.43 | 1.37 |
| 22 | 3 | 613 | CLA | C1D-ND | 4.79 | 1.43 | 1.37 |
| 22 | 5 | 603 | CLA | CHC-C1C | 4.79 | 1.47 | 1.35 |
| 22 | 1 | 609 | CLA | CHC-C1C | 4.79 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | A | 824 | CLA | C1D-ND | 4.79 | 1.43 | 1.37 |
| 22 | B | 802 | CLA | O2D-CGD | 4.79 | 1.44 | 1.33 |
| 29 | 9 | 606 | CHL | C2C-C3C | 4.79 | 1.47 | 1.36 |
| 22 | 1 | 613 | CLA | CHC-C1C | 4.79 | 1.47 | 1.35 |
| 22 | 7 | 613 | CLA | C1D-ND | 4.79 | 1.43 | 1.37 |
| 22 | 4 | 613 | CLA | O2A-CGA | 4.78 | 1.47 | 1.33 |
| 22 | A | 806 | CLA | C3C-C2C | 4.78 | 1.46 | 1.36 |
| 22 | 1 | 608 | CLA | CHC-C1C | 4.78 | 1.47 | 1.35 |
| 22 | A | 840 | CLA | O2D-CGD | 4.78 | 1.44 | 1.33 |
| 22 | A | 843 | CLA | CHC-C1C | 4.78 | 1.47 | 1.35 |
| 22 | A | 813 | CLA | O2D-CGD | 4.77 | 1.44 | 1.33 |
| 22 | 7 | 612 | CLA | CHC-C1C | 4.77 | 1.47 | 1.35 |
| 29 | 4 | 608 | CHL | C2C-C3C | 4.77 | 1.47 | 1.36 |
| 22 | A | 827 | CLA | C1D-ND | 4.77 | 1.43 | 1.37 |
| 22 | 8 | 610 | CLA | C1D-ND | 4.77 | 1.43 | 1.37 |
| 22 | A | 809 | CLA | C1D-ND | 4.77 | 1.43 | 1.37 |
| 22 | 8 | 614 | CLA | C1D-ND | 4.77 | 1.43 | 1.37 |
| 22 | 7 | 610 | CLA | C3B-C2B | 4.77 | 1.47 | 1.40 |
| 22 | 6 | 609 | CLA | CHC-C1C | 4.77 | 1.47 | 1.35 |
| 29 | 5 | 607 | CHL | O2D-CGD | 4.77 | 1.44 | 1.33 |
| 22 | B | 832 | CLA | C1D-ND | 4.77 | 1.43 | 1.37 |
| 22 | A | 842 | CLA | CHC-C1C | 4.77 | 1.47 | 1.35 |
| 22 | 3 | 607 | CLA | CHC-C1C | 4.76 | 1.47 | 1.35 |
| 22 | A | 840 | CLA | CHC-C1C | 4.76 | 1.47 | 1.35 |
| 22 | 4 | 601 | CLA | O2D-CGD | 4.76 | 1.44 | 1.33 |
| 22 | 8 | 604 | CLA | CHC-C1C | 4.76 | 1.47 | 1.35 |
| 22 | 6 | 622 | CLA | C1D-ND | 4.76 | 1.43 | 1.37 |
| 22 | A | 807 | CLA | CHC-C1C | 4.75 | 1.47 | 1.35 |
| 22 | A | 813 | CLA | C1D-ND | 4.75 | 1.43 | 1.37 |
| 22 | 3 | 613 | CLA | CHC-C1C | 4.75 | 1.47 | 1.35 |
| 22 | A | 807 | CLA | C1D-ND | 4.75 | 1.43 | 1.37 |
| 22 | A | 829 | CLA | C1D-ND | 4.75 | 1.43 | 1.37 |
| 22 | B | 815 | CLA | O2D-CGD | 4.75 | 1.44 | 1.33 |
| 22 | 5 | 610 | CLA | C1D-ND | 4.74 | 1.43 | 1.37 |
| 22 | 6 | 603 | CLA | CHC-C1C | 4.74 | 1.47 | 1.35 |
| 22 | B | 808 | CLA | CHC-C1C | 4.74 | 1.47 | 1.35 |
| 22 | Z | 610 | CLA | C1D-ND | 4.74 | 1.43 | 1.37 |
| 22 | 9 | 603 | CLA | CHC-C1C | 4.74 | 1.47 | 1.35 |
| 22 | 2 | 603 | CLA | CHC-C1C | 4.74 | 1.47 | 1.35 |
| 22 | B | 804 | CLA | O2D-CGD | 4.73 | 1.44 | 1.33 |
| 22 | 5 | 602 | CLA | C1D-ND | 4.73 | 1.43 | 1.37 |
| 29 | 3 | 608 | CHL | CHC-C1C | 4.73 | 1.47 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 4 | 616 | CLA | CHC-C1C | 4.73 | 1.47 | 1.35 |
| 22 | A | 839 | CLA | O2D-CGD | 4.73 | 1.44 | 1.33 |
| 22 | Z | 603 | CLA | CHC-C1C | 4.73 | 1.47 | 1.35 |
| 22 | A | 804 | CLA | O2D-CGD | 4.73 | 1.44 | 1.33 |
| 22 | 5 | 613 | CLA | CHC-C1C | 4.72 | 1.47 | 1.35 |
| 22 | A | 805 | CLA | C1D-ND | 4.72 | 1.43 | 1.37 |
| 22 | 7 | 611 | CLA | CHC-C1C | 4.72 | 1.47 | 1.35 |
| 22 | A | 828 | CLA | O2D-CGD | 4.72 | 1.44 | 1.33 |
| 22 | 4 | 610 | CLA | C1D-ND | 4.72 | 1.43 | 1.37 |
| 22 | A | 821 | CLA | CHC-C1C | 4.72 | 1.47 | 1.35 |
| 22 | B | 802 | CLA | CHC-C1C | 4.72 | 1.47 | 1.35 |
| 22 | B | 831 | CLA | C1D-ND | 4.71 | 1.43 | 1.37 |
| 22 | A | 826 | CLA | CHC-C1C | 4.71 | 1.47 | 1.35 |
| 22 | A | 821 | CLA | C1D-ND | 4.71 | 1.43 | 1.37 |
| 22 | B | 819 | CLA | C1D-ND | 4.71 | 1.43 | 1.37 |
| 22 | 5 | 612 | CLA | CHC-C1C | 4.71 | 1.47 | 1.35 |
| 29 | 5 | 608 | CHL | C2C-C3C | 4.71 | 1.46 | 1.36 |
| 22 | Z | 609 | CLA | CHC-C1C | 4.71 | 1.47 | 1.35 |
| 22 | 8 | 603 | CLA | CHC-C1C | 4.70 | 1.47 | 1.35 |
| 22 | B | 838 | CLA | C1D-ND | 4.70 | 1.43 | 1.37 |
| 22 | A | 836 | CLA | CHC-C1C | 4.70 | 1.47 | 1.35 |
| 22 | A | 838 | CLA | CHC-C1C | 4.69 | 1.47 | 1.35 |
| 22 | B | 807 | CLA | CHC-C1C | 4.69 | 1.47 | 1.35 |
| 22 | B | 803 | CLA | O2D-CGD | 4.68 | 1.44 | 1.33 |
| 22 | 5 | 616 | CLA | CHC-C1C | 4.68 | 1.47 | 1.35 |
| 22 | A | 820 | CLA | C1D-ND | 4.67 | 1.43 | 1.37 |
| 22 | 7 | 613 | CLA | CHC-C1C | 4.67 | 1.46 | 1.35 |
| 22 | B | 837 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 21 | A | 801 | CL0 | C1D-ND | 4.66 | 1.43 | 1.37 |
| 22 | B | 832 | CLA | O2D-CGD | 4.66 | 1.44 | 1.33 |
| 22 | 4 | 609 | CLA | CHC-C1C | 4.66 | 1.46 | 1.35 |
| 22 | 3 | 603 | CLA | CHC-C1C | 4.66 | 1.46 | 1.35 |
| 22 | A | 803 | CLA | O2D-CGD | 4.65 | 1.44 | 1.33 |
| 22 | A | 817 | CLA | CHC-C1C | 4.65 | 1.46 | 1.35 |
| 22 | 1 | 603 | CLA | CHC-C1C | 4.64 | 1.46 | 1.35 |
| 22 | 8 | 608 | CLA | C3C-C2C | 4.64 | 1.46 | 1.36 |
| 22 | B | 804 | CLA | C1D-ND | 4.64 | 1.43 | 1.37 |
| 22 | 7 | 608 | CLA | C1D-ND | 4.64 | 1.43 | 1.37 |
| 22 | F | 304 | CLA | O2A-CGA | 4.63 | 1.46 | 1.33 |
| 22 | A | 831 | CLA | CHC-C1C | 4.63 | 1.46 | 1.35 |
| 22 | A | 806 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 22 | A | 825 | CLA | CHC-C1C | 4.63 | 1.46 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | B | 830 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 22 | A | 810 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 22 | B | 826 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 22 | 1 | 610 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 22 | A | 814 | CLA | O2D-CGD | 4.62 | 1.44 | 1.33 |
| 22 | A | 822 | CLA | C3B-C2B | 4.61 | 1.46 | 1.40 |
| 23 | B | 842 | PQN | C10-C5 | 4.61 | 1.48 | 1.40 |
| 22 | 7 | 604 | CLA | CHC-C1C | 4.61 | 1.46 | 1.35 |
| 22 | 5 | 613 | CLA | O2A-CGA | 4.61 | 1.46 | 1.33 |
| 22 | B | 841 | CLA | CHD-C1D | 4.61 | 1.47 | 1.38 |
| 22 | A | 831 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 22 | B | 813 | CLA | O2D-CGD | 4.61 | 1.44 | 1.33 |
| 22 | A | 854 | CLA | O2D-CGD | 4.60 | 1.44 | 1.33 |
| 22 | 4 | 603 | CLA | CHC-C1C | 4.60 | 1.46 | 1.35 |
| 22 | B | 809 | CLA | CHC-C1C | 4.60 | 1.46 | 1.35 |
| 22 | 8 | 616 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 22 | B | 828 | CLA | CHC-C1C | 4.59 | 1.46 | 1.35 |
| 22 | B | 824 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 29 | 5 | 607 | CHL | O2A-CGA | 4.59 | 1.46 | 1.33 |
| 22 | 1 | 604 | CLA | CHD-C1D | 4.59 | 1.47 | 1.38 |
| 22 | B | 818 | CLA | CHC-C1C | 4.58 | 1.46 | 1.35 |
| 22 | 5 | 621 | CLA | C1D-ND | 4.58 | 1.43 | 1.37 |
| 22 | A | 854 | CLA | C1D-ND | 4.58 | 1.43 | 1.37 |
| 22 | 3 | 609 | CLA | O2D-CGD | 4.56 | 1.44 | 1.33 |
| 22 | 9 | 604 | CLA | CHD-C1D | 4.56 | 1.47 | 1.38 |
| 22 | 3 | 612 | CLA | CHC-C1C | 4.55 | 1.46 | 1.35 |
| 22 | 6 | 614 | CLA | O2D-CGD | 4.55 | 1.44 | 1.33 |
| 22 | 5 | 617 | CLA | C1D-ND | 4.55 | 1.43 | 1.37 |
| 22 | A | 826 | CLA | C3B-C2B | 4.55 | 1.46 | 1.40 |
| 22 | 5 | 604 | CLA | CHD-C1D | 4.55 | 1.47 | 1.38 |
| 22 | 1 | 609 | CLA | O2A-CGA | 4.54 | 1.46 | 1.33 |
| 22 | B | 834 | CLA | CHD-C1D | 4.54 | 1.47 | 1.38 |
| 22 | K | 4002 | CLA | CHD-C1D | 4.54 | 1.47 | 1.38 |
| 22 | L | 203 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 22 | 3 | 610 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 29 | 6 | 606 | CHL | O2A-CGA | 4.53 | 1.46 | 1.33 |
| 22 | Z | 603 | CLA | CHD-C1D | 4.52 | 1.47 | 1.38 |
| 22 | Z | 603 | CLA | O2A-CGA | 4.52 | 1.46 | 1.33 |
| 22 | B | 808 | CLA | C1D-ND | 4.52 | 1.43 | 1.37 |
| 22 | B | 827 | CLA | C1D-ND | 4.51 | 1.43 | 1.37 |
| 22 | 4 | 604 | CLA | CHD-C1D | 4.51 | 1.47 | 1.38 |
| 22 | A | 802 | CLA | CHD-C1D | 4.51 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | B | 825 | CLA | C1D-ND | 4.51 | 1.43 | 1.37 |
| 22 | Z | 609 | CLA | CHD-C1D | 4.51 | 1.47 | 1.38 |
| 22 | 5 | 614 | CLA | O2A-CGA | 4.50 | 1.45 | 1.30 |
| 22 | 3 | 614 | CLA | O2A-CGA | 4.50 | 1.45 | 1.30 |
| 21 | A | 801 | CL0 | CHC-C1C | 4.50 | 1.46 | 1.35 |
| 23 | A | 844 | PQN | C10-C5 | 4.50 | 1.48 | 1.40 |
| 22 | A | 804 | CLA | C1D-ND | 4.50 | 1.43 | 1.37 |
| 22 | 7 | 616 | CLA | CHD-C1D | 4.50 | 1.47 | 1.38 |
| 22 | A | 821 | CLA | O2A-CGA | 4.50 | 1.45 | 1.30 |
| 22 | 4 | 603 | CLA | CHD-C1D | 4.50 | 1.47 | 1.38 |
| 22 | B | 819 | CLA | C3B-C2B | 4.50 | 1.46 | 1.40 |
| 22 | A | 822 | CLA | C1D-ND | 4.50 | 1.43 | 1.37 |
| 22 | B | 809 | CLA | C1D-ND | 4.50 | 1.43 | 1.37 |
| 22 | 2 | 614 | CLA | O2A-CGA | 4.49 | 1.45 | 1.30 |
| 22 | 2 | 602 | CLA | O2A-CGA | 4.49 | 1.45 | 1.30 |
| 22 | B | 817 | CLA | CHC-C1C | 4.49 | 1.46 | 1.35 |
| 22 | B | 825 | CLA | O2D-CGD | 4.49 | 1.44 | 1.33 |
| 22 | 9 | 614 | CLA | CHD-C1D | 4.49 | 1.47 | 1.38 |
| 22 | 9 | 614 | CLA | O2A-CGA | 4.49 | 1.45 | 1.30 |
| 22 | 1 | 603 | CLA | O2A-CGA | 4.49 | 1.46 | 1.33 |
| 22 | K | 4002 | CLA | O2A-CGA | 4.49 | 1.45 | 1.30 |
| 22 | B | 820 | CLA | CHD-C1D | 4.48 | 1.47 | 1.38 |
| 22 | 9 | 613 | CLA | O2A-CGA | 4.48 | 1.46 | 1.33 |
| 22 | B | 812 | CLA | O2A-CGA | 4.48 | 1.46 | 1.33 |
| 22 | A | 815 | CLA | CHD-C1D | 4.48 | 1.47 | 1.38 |
| 22 | 2 | 609 | CLA | CHD-C1D | 4.47 | 1.47 | 1.38 |
| 22 | 6 | 622 | CLA | O2A-CGA | 4.47 | 1.45 | 1.30 |
| 22 | 8 | 603 | CLA | O2A-CGA | 4.47 | 1.45 | 1.30 |
| 22 | B | 828 | CLA | O2A-CGA | 4.46 | 1.46 | 1.33 |
| 22 | A | 835 | CLA | CHD-C1D | 4.46 | 1.47 | 1.38 |
| 22 | 2 | 606 | CLA | CHD-C1D | 4.46 | 1.47 | 1.38 |
| 22 | 7 | 613 | CLA | O2A-CGA | 4.46 | 1.46 | 1.33 |
| 22 | A | 837 | CLA | CHD-C1D | 4.45 | 1.47 | 1.38 |
| 22 | 4 | 611 | CLA | CHD-C1D | 4.45 | 1.47 | 1.38 |
| 22 | 1 | 611 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 22 | A | 826 | CLA | CHD-C1D | 4.45 | 1.47 | 1.38 |
| 22 | 3 | 606 | CLA | CHD-C1D | 4.45 | 1.47 | 1.38 |
| 22 | B | 840 | CLA | CHC-C1C | 4.45 | 1.46 | 1.35 |
| 22 | 2 | 612 | CLA | CHD-C1D | 4.45 | 1.47 | 1.38 |
| 22 | B | 814 | CLA | O2A-CGA | 4.45 | 1.46 | 1.33 |
| 22 | A | 837 | CLA | O2A-CGA | 4.44 | 1.45 | 1.30 |
| 22 | 4 | 616 | CLA | CHD-C1D | 4.44 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | J | 3002 | CLA | CHD-C1D | 4.44 | 1.47 | 1.38 |
| 22 | 9 | 612 | CLA | CHD-C1D | 4.43 | 1.47 | 1.38 |
| 22 | 2 | 601 | CLA | CHD-C1D | 4.43 | 1.47 | 1.38 |
| 22 | 2 | 607 | CLA | CHD-C1D | 4.43 | 1.47 | 1.38 |
| 22 | B | 835 | CLA | O2A-CGA | 4.43 | 1.45 | 1.30 |
| 22 | G | 204 | CLA | CHD-C1D | 4.42 | 1.47 | 1.38 |
| 29 | 4 | 606 | CHL | O2A-CGA | 4.42 | 1.46 | 1.33 |
| 22 | 9 | 610 | CLA | O2A-CGA | 4.42 | 1.46 | 1.33 |
| 24 | 4 | 622 | LHG | O7-C7 | 4.41 | 1.46 | 1.34 |
| 22 | 2 | 613 | CLA | CHD-C1D | 4.41 | 1.47 | 1.38 |
| 22 | F | 303 | CLA | O2A-CGA | 4.41 | 1.45 | 1.30 |
| 22 | 1 | 603 | CLA | CHD-C1D | 4.41 | 1.47 | 1.38 |
| 22 | 3 | 611 | CLA | CHD-C1D | 4.41 | 1.46 | 1.38 |
| 22 | 6 | 616 | CLA | CHD-C1D | 4.40 | 1.46 | 1.38 |
| 22 | B | 802 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 22 | 6 | 613 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 22 | 9 | 601 | CLA | CHD-C1D | 4.40 | 1.46 | 1.38 |
| 22 | Z | 612 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 22 | 9 | 613 | CLA | CHD-C1D | 4.40 | 1.46 | 1.38 |
| 22 | A | 818 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 22 | A | 836 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 22 | 3 | 609 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 22 | 3 | 613 | CLA | O2A-CGA | 4.40 | 1.46 | 1.33 |
| 22 | 8 | 611 | CLA | CHD-C1D | 4.40 | 1.46 | 1.38 |
| 22 | B | 819 | CLA | CHD-C1D | 4.40 | 1.46 | 1.38 |
| 22 | 2 | 603 | CLA | CHD-C1D | 4.40 | 1.46 | 1.38 |
| 22 | K | 4003 | CLA | CHD-C1D | 4.39 | 1.46 | 1.38 |
| 22 | Z | 613 | CLA | O2A-CGA | 4.39 | 1.46 | 1.33 |
| 22 | 3 | 614 | CLA | CHD-C1D | 4.39 | 1.46 | 1.38 |
| 22 | 6 | 610 | CLA | CHD-C1D | 4.39 | 1.46 | 1.38 |
| 22 | 5 | 611 | CLA | CHD-C1D | 4.39 | 1.46 | 1.38 |
| 22 | 8 | 609 | CLA | CHD-C1D | 4.38 | 1.46 | 1.38 |
| 22 | B | 818 | CLA | CHD-C1D | 4.38 | 1.46 | 1.38 |
| 22 | 2 | 602 | CLA | CHD-C1D | 4.38 | 1.46 | 1.38 |
| 22 | A | 854 | CLA | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 22 | 3 | 617 | CLA | CHD-C1D | 4.37 | 1.46 | 1.38 |
| 22 | 6 | 613 | CLA | CHD-C1D | 4.37 | 1.46 | 1.38 |
| 22 | 2 | 611 | CLA | CHD-C1D | 4.37 | 1.46 | 1.38 |
| 22 | B | 815 | CLA | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 22 | 5 | 601 | CLA | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 22 | 2 | 607 | CLA | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 22 | 2 | 610 | CLA | CHD-C1D | 4.37 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 1 | 613 | CLA | O2A-CGA | 4.37 | 1.46 | 1.33 |
| 22 | B | 805 | CLA | C1D-ND | 4.36 | 1.43 | 1.37 |
| 22 | A | 838 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 22 | 9 | 603 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 22 | 7 | 614 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 22 | A | 810 | CLA | O2A-CGA | 4.36 | 1.46 | 1.33 |
| 22 | Z | 604 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 22 | 7 | 611 | CLA | CHD-C1D | 4.36 | 1.46 | 1.38 |
| 22 | 4 | 614 | CLA | O2A-CGA | 4.35 | 1.45 | 1.30 |
| 22 | Z | 609 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | 6 | 611 | CLA | CHD-C1D | 4.35 | 1.46 | 1.38 |
| 22 | 6 | 611 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | 8 | 612 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | 6 | 612 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | B | 836 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | A | 823 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | 2 | 612 | CLA | O2A-CGA | 4.35 | 1.46 | 1.33 |
| 22 | 8 | 613 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 22 | 1 | 611 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | 3 | 602 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | 8 | 606 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 29 | 7 | 607 | CHL | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | B | 817 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | 6 | 604 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | A | 840 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 22 | A | 838 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 22 | A | 825 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 22 | 5 | 614 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | 7 | 608 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 22 | Z | 611 | CLA | CHD-C1D | 4.34 | 1.46 | 1.38 |
| 22 | B | 807 | CLA | O2A-CGA | 4.34 | 1.46 | 1.33 |
| 22 | 3 | 604 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 22 | A | 822 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 22 | B | 822 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 22 | Z | 608 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 22 | 9 | 602 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 22 | A | 817 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 22 | 1 | 614 | CLA | CHD-C1D | 4.33 | 1.46 | 1.38 |
| 22 | 5 | 610 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 22 | 9 | 612 | CLA | O2A-CGA | 4.33 | 1.46 | 1.33 |
| 22 | 4 | 602 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 22 | 9 | 610 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 6 | 614 | CLA | O2A-CGA | 4.32 | 1.45 | 1.30 |
| 22 | 2 | 614 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 22 | A | 805 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 22 | 3 | 607 | CLA | CHD-C1D | 4.32 | 1.46 | 1.38 |
| 22 | B | 839 | CLA | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 29 | 1 | 607 | CHL | O2A-CGA | 4.32 | 1.46 | 1.33 |
| 22 | B | 824 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | B | 833 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | B | 811 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | 3 | 612 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | 6 | 614 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | A | 843 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | 7 | 612 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | 7 | 603 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | 4 | 609 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | Z | 614 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | Z | 606 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | 3 | 607 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | B | 811 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | 5 | 612 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | 6 | 601 | CLA | CHD-C1D | 4.31 | 1.46 | 1.38 |
| 22 | Z | 606 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | G | 203 | CLA | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 29 | 7 | 607 | CHL | O2A-CGA | 4.31 | 1.45 | 1.33 |
| 22 | 5 | 601 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 22 | A | 845 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 24 | A | 855 | LHG | O8-C23 | 4.30 | 1.45 | 1.33 |
| 29 | 1 | 601 | CHL | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 22 | 6 | 603 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 22 | 1 | 609 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 29 | 4 | 606 | CHL | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 22 | A | 833 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 22 | A | 807 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 22 | L | 203 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 29 | Z | 607 | CHL | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 22 | Z | 616 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 22 | Z | 608 | CLA | O2A-CGA | 4.30 | 1.45 | 1.33 |
| 22 | A | 825 | CLA | CHD-C1D | 4.30 | 1.46 | 1.38 |
| 22 | B | 840 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | B | 816 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | B | 833 | CLA | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 22 | 2 | 611 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 4 | 604 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | A | 832 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | 1 | 614 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | A | 832 | CLA | C1D-ND | 4.29 | 1.43 | 1.37 |
| 29 | 9 | 606 | CHL | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 22 | A | 808 | CLA | CHD-C1D | 4.29 | 1.46 | 1.38 |
| 22 | 1 | 604 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | 6 | 610 | CLA | O2A-CGA | 4.29 | 1.45 | 1.33 |
| 22 | 5 | 604 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | A | 813 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | 5 | 611 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | 5 | 606 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | B | 807 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 9 | 604 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | F | 304 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 5 | 609 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | A | 830 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 22 | B | 814 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 1 | 612 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 29 | 5 | 608 | CHL | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | B | 852 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 9 | 609 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | A | 816 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 6 | 617 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 29 | Z | 601 | CHL | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | 7 | 620 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 2 | 613 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | A | 817 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | A | 835 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | Z | 613 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 5 | 621 | CLA | CHD-C1D | 4.28 | 1.46 | 1.38 |
| 22 | 6 | 604 | CLA | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 29 | 4 | 607 | CHL | O2A-CGA | 4.28 | 1.45 | 1.33 |
| 22 | B | 804 | CLA | O2A-CGA | 4.28 | 1.45 | 1.30 |
| 22 | B | 828 | CLA | C1D-ND | 4.28 | 1.43 | 1.37 |
| 22 | 8 | 603 | CLA | CHD-C1D | 4.27 | 1.46 | 1.38 |
| 22 | B | 820 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 22 | 5 | 613 | CLA | CHD-C1D | 4.27 | 1.46 | 1.38 |
| 22 | 4 | 613 | CLA | CHD-C1D | 4.27 | 1.46 | 1.38 |
| 22 | L | 204 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 22 | 3 | 602 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 22 | A | 824 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 1 | 606 | CLA | O2A-CGA | 4.27 | 1.45 | 1.33 |
| 22 | 3 | 620 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 22 | 2 | 610 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 22 | B | 839 | CLA | CHD-C1D | 4.26 | 1.46 | 1.38 |
| 22 | 8 | 604 | CLA | CHD-C1D | 4.26 | 1.46 | 1.38 |
| 22 | B | 840 | CLA | CHD-C1D | 4.26 | 1.46 | 1.38 |
| 22 | 5 | 616 | CLA | CHD-C1D | 4.26 | 1.46 | 1.38 |
| 22 | 7 | 602 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 29 | 9 | 607 | CHL | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 22 | 4 | 612 | CLA | O2A-CGA | 4.26 | 1.45 | 1.33 |
| 22 | 1 | 610 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 22 | B | 830 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 24 | 6 | 619 | LHG | O8-C23 | 4.25 | 1.45 | 1.33 |
| 22 | 1 | 608 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 22 | 1 | 612 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 22 | 3 | 609 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 22 | 8 | 602 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 29 | 9 | 607 | CHL | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 22 | B | 852 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 22 | 5 | 602 | CLA | O2A-CGA | 4.25 | 1.45 | 1.33 |
| 22 | B | 823 | CLA | CHD-C1D | 4.25 | 1.46 | 1.38 |
| 22 | B | 819 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 22 | B | 817 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 22 | 8 | 608 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 22 | B | 836 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 22 | A | 845 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 22 | 7 | 620 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 22 | 9 | 611 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 22 | Z | 614 | CLA | O2A-CGA | 4.24 | 1.45 | 1.33 |
| 22 | 1 | 616 | CLA | CHD-C1D | 4.24 | 1.46 | 1.38 |
| 22 | A | 839 | CLA | CHD-C1D | 4.23 | 1.46 | 1.38 |
| 22 | B | 810 | CLA | CHD-C1D | 4.23 | 1.46 | 1.38 |
| 22 | A | 808 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 22 | B | 815 | CLA | CHD-C1D | 4.23 | 1.46 | 1.38 |
| 22 | 4 | 611 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 22 | 4 | 610 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 22 | 2 | 609 | CLA | O2A-CGA | 4.23 | 1.45 | 1.33 |
| 22 | 4 | 601 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 22 | 5 | 606 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 22 | B | 827 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 22 | A | 815 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 22 | 1 | 606 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 813 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 22 | 6 | 609 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 22 | B | 806 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 22 | B | 841 | CLA | O2A-CGA | 4.22 | 1.45 | 1.33 |
| 29 | 6 | 606 | CHL | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 22 | L | 204 | CLA | CHD-C1D | 4.22 | 1.46 | 1.38 |
| 24 | 1 | 620 | LHG | O8-C23 | 4.22 | 1.45 | 1.33 |
| 22 | A | 821 | CLA | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 22 | 8 | 610 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 22 | B | 835 | CLA | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 22 | 9 | 611 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 29 | 5 | 618 | CHL | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 22 | A | 816 | CLA | O2A-CGA | 4.21 | 1.45 | 1.33 |
| 29 | 6 | 608 | CHL | CHD-C1D | 4.21 | 1.46 | 1.38 |
| 22 | B | 831 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 22 | 3 | 620 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 22 | B | 810 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 22 | 6 | 612 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 22 | 8 | 601 | CLA | O2A-CGA | 4.20 | 1.45 | 1.33 |
| 22 | B | 841 | CLA | CHD-C4C | 4.20 | 1.48 | 1.39 |
| 22 | A | 807 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 22 | 8 | 614 | CLA | CHD-C1D | 4.20 | 1.46 | 1.38 |
| 22 | 5 | 612 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 22 | 6 | 609 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 24 | 4 | 622 | LHG | O8-C23 | 4.19 | 1.45 | 1.33 |
| 22 | B | 821 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 22 | 7 | 612 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 22 | 8 | 614 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 22 | 4 | 612 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 22 | 7 | 601 | CLA | O2A-CGA | 4.19 | 1.45 | 1.33 |
| 22 | B | 837 | CLA | CHD-C1D | 4.19 | 1.46 | 1.38 |
| 22 | 7 | 608 | CLA | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 22 | Z | 611 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | 5 | 609 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | 3 | 617 | CLA | O2A-CGA | 4.18 | 1.46 | 1.33 |
| 24 | 6 | 619 | LHG | O7-C7 | 4.18 | 1.46 | 1.34 |
| 22 | Z | 604 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | A | 815 | CLA | CHD-C4C | 4.18 | 1.48 | 1.39 |
| 22 | F | 301 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 22 | 1 | 602 | CLA | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | A | 802 | CLA | CHD-C4C | 4.18 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 29 | 4 | 608 | CHL | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 29 | 4 | 607 | CHL | CHD-C1D | 4.18 | 1.46 | 1.38 |
| 29 | 5 | 608 | CHL | O2A-CGA | 4.18 | 1.45 | 1.33 |
| 22 | 6 | 601 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 22 | A | 836 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 22 | A | 814 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 22 | A | 820 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 22 | A | 824 | CLA | CHD-C1D | 4.17 | 1.46 | 1.38 |
| 24 | 5 | 623 | LHG | O8-C23 | 4.17 | 1.45 | 1.33 |
| 22 | 7 | 604 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 22 | Z | 610 | CLA | O2A-CGA | 4.17 | 1.45 | 1.33 |
| 22 | A | 802 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | 6 | 614 | CLA | CHD-C4C | 4.16 | 1.48 | 1.39 |
| 29 | 6 | 608 | CHL | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | 3 | 603 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | B | 838 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | A | 822 | CLA | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 22 | 6 | 602 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | 9 | 614 | CLA | CHD-C4C | 4.16 | 1.48 | 1.39 |
| 22 | 9 | 602 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | B | 829 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 22 | B | 826 | CLA | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 29 | 6 | 607 | CHL | O2A-CGA | 4.16 | 1.45 | 1.33 |
| 29 | Z | 607 | CHL | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 22 | B | 809 | CLA | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 22 | 1 | 608 | CLA | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 22 | 4 | 609 | CLA | CHD-C1D | 4.16 | 1.46 | 1.38 |
| 22 | B | 834 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 22 | 4 | 602 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 22 | 8 | 616 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 22 | 9 | 609 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 22 | B | 822 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 22 | 4 | 614 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 22 | 7 | 613 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 22 | 7 | 609 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 22 | B | 818 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 22 | A | 806 | CLA | CHD-C1D | 4.15 | 1.46 | 1.38 |
| 22 | A | 805 | CLA | O2A-CGA | 4.15 | 1.45 | 1.33 |
| 22 | B | 806 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 29 | 3 | 608 | CHL | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 22 | B | 812 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | A | 813 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 3 | 610 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 22 | A | 832 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | A | 820 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | A | 834 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 29 | 4 | 618 | CHL | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | B | 805 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 22 | B | 802 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 22 | A | 842 | CLA | O2A-CGA | 4.14 | 1.45 | 1.33 |
| 22 | 8 | 613 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | B | 808 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | 7 | 604 | CLA | CHD-C1D | 4.14 | 1.46 | 1.38 |
| 22 | 9 | 604 | CLA | CHD-C4C | 4.13 | 1.48 | 1.39 |
| 22 | B | 809 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 22 | 8 | 601 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 22 | A | 817 | CLA | CHD-C4C | 4.13 | 1.48 | 1.39 |
| 24 | Z | 620 | LHG | O7-C7 | 4.13 | 1.46 | 1.34 |
| 22 | A | 829 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 22 | Z | 602 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 22 | 4 | 601 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 22 | 3 | 604 | CLA | O2A-CGA | 4.13 | 1.45 | 1.33 |
| 29 | 5 | 607 | CHL | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 22 | A | 835 | CLA | CHD-C4C | 4.13 | 1.48 | 1.39 |
| 22 | 8 | 612 | CLA | CHD-C1D | 4.13 | 1.46 | 1.38 |
| 22 | 7 | 610 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 22 | A | 833 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 22 | B | 824 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 22 | 5 | 602 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 24 | A | 847 | LHG | O7-C7 | 4.12 | 1.45 | 1.34 |
| 22 | 5 | 610 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 22 | 7 | 616 | CLA | C3D-C2D | 4.12 | 1.50 | 1.39 |
| 22 | 8 | 610 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 22 | G | 203 | CLA | CHD-C1D | 4.12 | 1.46 | 1.38 |
| 24 | A | 847 | LHG | O8-C23 | 4.12 | 1.45 | 1.33 |
| 22 | A | 831 | CLA | O2A-CGA | 4.12 | 1.45 | 1.33 |
| 22 | B | 820 | CLA | CHD-C4C | 4.12 | 1.48 | 1.39 |
| 29 | 4 | 608 | CHL | CHD-C1D | 4.11 | 1.46 | 1.38 |
| 22 | A | 826 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 29 | 8 | 607 | CHL | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 22 | 7 | 616 | CLA | CHD-C4C | 4.11 | 1.48 | 1.39 |
| 22 | A | 839 | CLA | O2A-CGA | 4.11 | 1.45 | 1.33 |
| 22 | 9 | 612 | CLA | CHD-C4C | 4.11 | 1.48 | 1.39 |
| 22 | F | 301 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | A | 841 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | B | 825 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | B | 830 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 22 | B | 808 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 22 | A | 811 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 24 | Z | 620 | LHG | O8-C23 | 4.10 | 1.45 | 1.33 |
| 22 | A | 819 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 24 | 1 | 620 | LHG | O7-C7 | 4.10 | 1.45 | 1.34 |
| 22 | B | 832 | CLA | O2A-CGA | 4.10 | 1.45 | 1.33 |
| 24 | A | 855 | LHG | O7-C7 | 4.10 | 1.45 | 1.34 |
| 22 | 4 | 610 | CLA | CHD-C1D | 4.10 | 1.46 | 1.38 |
| 22 | 6 | 617 | CLA | O2A-CGA | 4.10 | 1.46 | 1.33 |
| 22 | 1 | 613 | CLA | CHD-C1D | 4.09 | 1.46 | 1.38 |
| 22 | B | 823 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 22 | 5 | 604 | CLA | CHD-C4C | 4.09 | 1.48 | 1.39 |
| 22 | A | 843 | CLA | O2A-CGA | 4.09 | 1.45 | 1.33 |
| 24 | 4 | 623 | LHG | O8-C23 | 4.09 | 1.45 | 1.33 |
| 22 | A | 842 | CLA | CHD-C1D | 4.09 | 1.46 | 1.38 |
| 22 | 1 | 604 | CLA | CHD-C4C | 4.09 | 1.48 | 1.39 |
| 22 | 4 | 604 | CLA | CHD-C4C | 4.09 | 1.48 | 1.39 |
| 22 | 2 | 606 | CLA | CHD-C4C | 4.09 | 1.48 | 1.39 |
| 22 | 6 | 603 | CLA | O2A-CGA | 4.09 | 1.46 | 1.33 |
| 22 | B | 819 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 22 | A | 833 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 22 | A | 837 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 22 | 3 | 614 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 24 | B | 851 | LHG | O7-C7 | 4.08 | 1.45 | 1.34 |
| 22 | B | 828 | CLA | CHD-C1D | 4.08 | 1.46 | 1.38 |
| 22 | A | 814 | CLA | CHD-C1D | 4.08 | 1.46 | 1.38 |
| 22 | A | 828 | CLA | O2A-CGA | 4.08 | 1.45 | 1.33 |
| 22 | 5 | 614 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 22 | B | 803 | CLA | C1D-ND | 4.08 | 1.42 | 1.37 |
| 22 | 9 | 601 | CLA | O2A-CGA | 4.08 | 1.46 | 1.33 |
| 22 | 6 | 601 | CLA | CHD-C4C | 4.08 | 1.48 | 1.39 |
| 22 | 3 | 603 | CLA | CHD-C1D | 4.07 | 1.46 | 1.38 |
| 22 | Z | 612 | CLA | CHD-C1D | 4.07 | 1.46 | 1.38 |
| 22 | G | 204 | CLA | O2A-CGA | 4.07 | 1.46 | 1.33 |
| 22 | A | 854 | CLA | CHD-C1D | 4.07 | 1.46 | 1.38 |
| 22 | A | 819 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 22 | B | 834 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |
| 22 | B | 829 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 22 | 2 | 603 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | 2 | 609 | CLA | CHD-C4C | 4.06 | 1.48 | 1.39 |
| 22 | 7 | 610 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 24 | A | 846 | LHG | O7-C7 | 4.06 | 1.45 | 1.34 |
| 22 | A | 803 | CLA | CHD-C1D | 4.06 | 1.46 | 1.38 |
| 22 | 4 | 602 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 22 | A | 827 | CLA | CHD-C1D | 4.05 | 1.46 | 1.38 |
| 22 | 3 | 611 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 22 | 7 | 616 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 22 | 2 | 610 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 21 | A | 801 | CL0 | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 22 | B | 814 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 22 | 2 | 602 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 22 | A | 806 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 24 | 4 | 623 | LHG | O7-C7 | 4.05 | 1.45 | 1.34 |
| 22 | A | 854 | CLA | C3D-C2D | 4.05 | 1.50 | 1.39 |
| 22 | A | 805 | CLA | CHD-C4C | 4.05 | 1.48 | 1.39 |
| 22 | 5 | 617 | CLA | O2A-CGA | 4.05 | 1.45 | 1.33 |
| 22 | 6 | 602 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 24 | 5 | 623 | LHG | O7-C7 | 4.04 | 1.45 | 1.34 |
| 22 | 4 | 601 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 22 | Z | 616 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 22 | Z | 603 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 22 | 7 | 609 | CLA | CHD-C1D | 4.04 | 1.46 | 1.38 |
| 27 | B | 850 | DGD | O1G-C1A | 4.04 | 1.45 | 1.33 |
| 22 | 7 | 603 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 22 | 2 | 613 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 22 | 5 | 616 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 22 | B | 810 | CLA | CHD-C4C | 4.04 | 1.48 | 1.39 |
| 22 | 2 | 601 | CLA | O2A-CGA | 4.04 | 1.45 | 1.33 |
| 22 | 6 | 616 | CLA | CHD-C4C | 4.03 | 1.48 | 1.39 |
| 22 | B | 803 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 22 | 3 | 613 | CLA | CHD-C1D | 4.03 | 1.46 | 1.38 |
| 22 | K | 4002 | CLA | CHD-C4C | 4.03 | 1.48 | 1.39 |
| 22 | 7 | 602 | CLA | CHD-C1D | 4.03 | 1.46 | 1.38 |
| 29 | 1 | 601 | CHL | CHD-C1D | 4.03 | 1.46 | 1.38 |
| 22 | 2 | 611 | CLA | CHD-C4C | 4.03 | 1.48 | 1.39 |
| 22 | K | 4003 | CLA | O2A-CGA | 4.03 | 1.45 | 1.33 |
| 22 | 2 | 614 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | A | 834 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 22 | 8 | 611 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 22 | Z | 609 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | 5 | 603 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 6 | 622 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | B | 821 | CLA | O2A-CGA | 4.02 | 1.45 | 1.33 |
| 29 | 1 | 607 | CHL | OBD-CAD | 4.02 | 1.29 | 1.22 |
| 22 | 2 | 601 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | G | 204 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | L | 204 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | 1 | 609 | CLA | CHD-C4C | 4.02 | 1.48 | 1.39 |
| 22 | A | 804 | CLA | CHD-C1D | 4.02 | 1.46 | 1.38 |
| 22 | 8 | 616 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 22 | Z | 614 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 22 | 5 | 621 | CLA | O2A-CGA | 4.01 | 1.45 | 1.33 |
| 29 | 6 | 618 | CHL | CHD-C1D | 4.01 | 1.46 | 1.38 |
| 22 | 3 | 606 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 22 | A | 831 | CLA | CHD-C1D | 4.01 | 1.46 | 1.38 |
| 22 | Z | 606 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 22 | B | 839 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 22 | Z | 616 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 22 | 9 | 601 | CLA | CHD-C4C | 4.01 | 1.48 | 1.39 |
| 22 | 5 | 603 | CLA | O2A-CGA | 4.00 | 1.45 | 1.33 |
| 22 | 7 | 606 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 22 | 9 | 613 | CLA | CHD-C4C | 4.00 | 1.48 | 1.39 |
| 22 | 9 | 610 | CLA | CHD-C4C | 4.00 | 1.48 | 1.39 |
| 22 | Z | 602 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 22 | B | 832 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 22 | A | 823 | CLA | CHD-C1D | 4.00 | 1.46 | 1.38 |
| 22 | 8 | 604 | CLA | O2A-CGA | 3.99 | 1.45 | 1.33 |
| 22 | 5 | 606 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 22 | 1 | 614 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 22 | A | 809 | CLA | CHD-C1D | 3.99 | 1.46 | 1.38 |
| 22 | Z | 608 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 22 | 6 | 610 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 29 | Z | 601 | CHL | CHD-C1D | 3.99 | 1.46 | 1.38 |
| 22 | 6 | 616 | CLA | O2A-CGA | 3.99 | 1.45 | 1.33 |
| 22 | 6 | 617 | CLA | CHD-C4C | 3.99 | 1.48 | 1.39 |
| 22 | 2 | 603 | CLA | O2A-CGA | 3.99 | 1.45 | 1.33 |
| 22 | 8 | 609 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 22 | 5 | 610 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 22 | 1 | 616 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 22 | 9 | 603 | CLA | O2A-CGA | 3.98 | 1.45 | 1.33 |
| 22 | 8 | 606 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 24 | 7 | 625 | LHG | O8-C23 | 3.98 | 1.45 | 1.33 |
| 22 | 7 | 620 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 4 | 616 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 22 | 2 | 607 | CLA | CHD-C4C | 3.98 | 1.48 | 1.39 |
| 22 | 3 | 620 | CLA | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 22 | 1 | 602 | CLA | CHD-C1D | 3.97 | 1.46 | 1.38 |
| 24 | A | 846 | LHG | O8-C23 | 3.97 | 1.44 | 1.33 |
| 22 | A | 802 | CLA | C3D-C2D | 3.97 | 1.50 | 1.39 |
| 22 | 2 | 612 | CLA | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 22 | 4 | 603 | CLA | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 22 | Z | 604 | CLA | CHD-C4C | 3.97 | 1.48 | 1.39 |
| 29 | 8 | 607 | CHL | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 22 | A | 811 | CLA | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 22 | J | 3002 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 22 | 6 | 604 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 22 | 7 | 609 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 29 | 1 | 607 | CHL | CHD-C1D | 3.96 | 1.46 | 1.38 |
| 22 | B | 837 | CLA | O2A-CGA | 3.96 | 1.44 | 1.33 |
| 29 | Z | 601 | CHL | C1D-ND | -3.96 | 1.32 | 1.37 |
| 22 | A | 838 | CLA | CHD-C4C | 3.96 | 1.48 | 1.39 |
| 22 | 7 | 614 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 22 | 3 | 612 | CLA | O2A-CGA | 3.95 | 1.45 | 1.33 |
| 22 | A | 812 | CLA | CHD-C1D | 3.95 | 1.46 | 1.38 |
| 22 | B | 827 | CLA | CHD-C1D | 3.95 | 1.46 | 1.38 |
| 22 | B | 813 | CLA | O2A-CGA | 3.95 | 1.44 | 1.33 |
| 22 | 6 | 611 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 22 | B | 852 | CLA | C3D-C2D | 3.95 | 1.49 | 1.39 |
| 22 | 1 | 611 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 22 | 9 | 603 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 22 | 6 | 613 | CLA | CHD-C4C | 3.95 | 1.48 | 1.39 |
| 22 | A | 804 | CLA | O2A-CGA | 3.95 | 1.44 | 1.33 |
| 22 | A | 812 | CLA | O2A-CGA | 3.95 | 1.44 | 1.33 |
| 22 | A | 841 | CLA | CHD-C1D | 3.95 | 1.46 | 1.38 |
| 22 | A | 825 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 22 | 5 | 611 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 22 | A | 809 | CLA | O2A-CGA | 3.94 | 1.44 | 1.33 |
| 22 | A | 803 | CLA | O2A-CGA | 3.94 | 1.44 | 1.33 |
| 29 | Z | 607 | CHL | OBD-CAD | 3.94 | 1.29 | 1.22 |
| 22 | 5 | 609 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 22 | 9 | 602 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 22 | B | 826 | CLA | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 22 | 8 | 604 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 21 | A | 801 | CL0 | CHD-C1D | 3.94 | 1.46 | 1.38 |
| 22 | 1 | 603 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | B | 841 | CLA | C3D-C2D | 3.94 | 1.49 | 1.39 |
| 22 | 9 | 611 | CLA | CHD-C4C | 3.94 | 1.48 | 1.39 |
| 22 | G | 204 | CLA | OBD-CAD | 3.93 | 1.29 | 1.22 |
| 22 | F | 301 | CLA | CHD-C4C | 3.93 | 1.48 | 1.39 |
| 22 | K | 4003 | CLA | CHD-C4C | 3.93 | 1.48 | 1.39 |
| 22 | 8 | 609 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | 5 | 601 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | 3 | 610 | CLA | CHD-C1D | 3.92 | 1.46 | 1.38 |
| 22 | 4 | 610 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | 8 | 611 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | 6 | 622 | CLA | CHD-C1D | 3.92 | 1.46 | 1.38 |
| 22 | 3 | 602 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | G | 203 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | 8 | 601 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | B | 823 | CLA | C3D-C2D | 3.92 | 1.49 | 1.39 |
| 22 | 7 | 603 | CLA | CHD-C4C | 3.92 | 1.48 | 1.39 |
| 22 | 4 | 611 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | Z | 611 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | A | 822 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | 3 | 607 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | 6 | 603 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | B | 836 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | A | 830 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 22 | 3 | 604 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | A | 827 | CLA | O2A-CGA | 3.91 | 1.44 | 1.33 |
| 22 | A | 826 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | 5 | 617 | CLA | CHD-C4C | 3.91 | 1.48 | 1.39 |
| 22 | 4 | 603 | CLA | O2A-CGA | 3.91 | 1.45 | 1.33 |
| 22 | F | 303 | CLA | CHD-C1D | 3.90 | 1.46 | 1.38 |
| 22 | A | 816 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 22 | B | 823 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 22 | B | 838 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 22 | 4 | 613 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 22 | 8 | 614 | CLA | C3D-C2D | 3.90 | 1.49 | 1.39 |
| 22 | A | 839 | CLA | CHD-C4C | 3.90 | 1.48 | 1.39 |
| 22 | B | 807 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 22 | B | 818 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 22 | A | 806 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 22 | B | 833 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 22 | 3 | 610 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 22 | 9 | 609 | CLA | CHD-C4C | 3.89 | 1.48 | 1.39 |
| 24 | 8 | 620 | LHG | O7-C7 | 3.88 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | A | 835 | CLA | C3D-C2D | 3.88 | 1.49 | 1.39 |
| 22 | 6 | 609 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 22 | 3 | 617 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 24 | 8 | 620 | LHG | O8-C23 | 3.88 | 1.44 | 1.33 |
| 22 | A | 813 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 29 | 3 | 608 | CHL | CHD-C1D | 3.88 | 1.45 | 1.38 |
| 22 | 1 | 608 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 22 | 3 | 607 | CLA | C3D-C2D | 3.88 | 1.49 | 1.39 |
| 22 | B | 817 | CLA | CHD-C4C | 3.88 | 1.48 | 1.39 |
| 22 | A | 810 | CLA | CHD-C1D | 3.87 | 1.45 | 1.38 |
| 22 | B | 820 | CLA | C3D-C2D | 3.87 | 1.49 | 1.39 |
| 22 | A | 809 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 22 | B | 852 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 27 | B | 850 | DGD | O2G-C1B | 3.87 | 1.45 | 1.34 |
| 22 | 7 | 601 | CLA | CHD-C1D | 3.87 | 1.45 | 1.38 |
| 22 | 3 | 609 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 22 | A | 815 | CLA | C3D-C2D | 3.87 | 1.49 | 1.39 |
| 22 | 7 | 611 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 22 | B | 811 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 22 | B | 840 | CLA | CHD-C4C | 3.87 | 1.48 | 1.39 |
| 22 | 2 | 612 | CLA | C3D-C2D | 3.86 | 1.49 | 1.39 |
| 22 | 5 | 602 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | B | 812 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | 5 | 603 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | 5 | 616 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | B | 804 | CLA | CHD-C1D | 3.86 | 1.45 | 1.38 |
| 22 | Z | 612 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | 1 | 602 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | A | 807 | CLA | CHD-C4C | 3.86 | 1.48 | 1.39 |
| 22 | A | 841 | CLA | C3D-C2D | 3.85 | 1.49 | 1.39 |
| 22 | A | 843 | CLA | C3D-C2D | 3.85 | 1.49 | 1.39 |
| 22 | 2 | 611 | CLA | C3D-C2D | 3.85 | 1.49 | 1.39 |
| 22 | Z | 610 | CLA | CHD-C1D | 3.85 | 1.45 | 1.38 |
| 22 | A | 823 | CLA | CHD-C4C | 3.85 | 1.48 | 1.39 |
| 22 | 8 | 603 | CLA | CHD-C4C | 3.85 | 1.48 | 1.39 |
| 22 | 4 | 609 | CLA | CHD-C4C | 3.84 | 1.48 | 1.39 |
| 29 | 5 | 618 | CHL | CHD-C4C | 3.84 | 1.48 | 1.39 |
| 22 | 2 | 610 | CLA | C3D-C2D | 3.84 | 1.49 | 1.39 |
| 22 | 3 | 612 | CLA | CHD-C4C | 3.84 | 1.48 | 1.39 |
| 22 | 8 | 614 | CLA | CHD-C4C | 3.84 | 1.48 | 1.39 |
| 22 | 1 | 616 | CLA | CHD-C4C | 3.83 | 1.48 | 1.39 |
| 22 | B | 803 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 7 | 602 | CLA | CHD-C4C | 3.83 | 1.48 | 1.39 |
| 22 | 6 | 611 | CLA | C3D-C2D | 3.83 | 1.49 | 1.39 |
| 22 | F | 304 | CLA | CHD-C4C | 3.83 | 1.48 | 1.39 |
| 22 | B | 821 | CLA | CHD-C4C | 3.83 | 1.48 | 1.39 |
| 22 | 4 | 614 | CLA | CHD-C4C | 3.82 | 1.48 | 1.39 |
| 22 | A | 820 | CLA | CHD-C4C | 3.82 | 1.48 | 1.39 |
| 22 | B | 837 | CLA | CHD-C4C | 3.82 | 1.48 | 1.39 |
| 22 | 8 | 608 | CLA | CHD-C1D | 3.82 | 1.45 | 1.38 |
| 22 | 6 | 612 | CLA | CHD-C4C | 3.82 | 1.48 | 1.39 |
| 22 | 4 | 609 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 22 | 1 | 610 | CLA | CHD-C1D | 3.82 | 1.45 | 1.38 |
| 22 | A | 829 | CLA | CHD-C1D | 3.82 | 1.45 | 1.38 |
| 22 | A | 827 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 22 | B | 809 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 22 | 2 | 613 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 22 | 8 | 609 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 22 | 8 | 613 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 22 | A | 840 | CLA | CHD-C1D | 3.82 | 1.45 | 1.38 |
| 22 | 1 | 606 | CLA | CHD-C4C | 3.82 | 1.47 | 1.39 |
| 22 | 2 | 607 | CLA | C3D-C2D | 3.82 | 1.49 | 1.39 |
| 22 | 5 | 613 | CLA | CHD-C4C | 3.81 | 1.47 | 1.39 |
| 22 | A | 805 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 22 | 2 | 609 | CLA | C3D-C2D | 3.81 | 1.49 | 1.39 |
| 24 | 7 | 625 | LHG | O7-C7 | 3.80 | 1.45 | 1.34 |
| 22 | 5 | 601 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 22 | 5 | 609 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 22 | 9 | 604 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 22 | 9 | 614 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 22 | A | 836 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 22 | A | 836 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | B | 822 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | A | 840 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | A | 834 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | A | 832 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | 4 | 611 | CLA | C3D-C2D | 3.80 | 1.49 | 1.39 |
| 22 | 6 | 602 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | B | 832 | CLA | CHD-C4C | 3.80 | 1.47 | 1.39 |
| 22 | 1 | 610 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 22 | 5 | 604 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 22 | B | 835 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 22 | 2 | 606 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 22 | 8 | 610 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 831 | CLA | CHD-C1D | 3.79 | 1.45 | 1.38 |
| 22 | A | 816 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 22 | B | 830 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 22 | 7 | 601 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 22 | 1 | 614 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 22 | B | 806 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 22 | 7 | 612 | CLA | CHD-C4C | 3.79 | 1.47 | 1.39 |
| 22 | 9 | 612 | CLA | C3D-C2D | 3.79 | 1.49 | 1.39 |
| 22 | L | 203 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | L | 203 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 22 | 2 | 614 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 22 | A | 814 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | A | 819 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | 9 | 609 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 22 | A | 803 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | A | 821 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | B | 816 | CLA | CHD-C1D | 3.78 | 1.45 | 1.38 |
| 22 | 5 | 621 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | A | 825 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 22 | 4 | 610 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 22 | B | 829 | CLA | CHD-C4C | 3.78 | 1.47 | 1.39 |
| 22 | 5 | 614 | CLA | C3D-C2D | 3.78 | 1.49 | 1.39 |
| 22 | B | 807 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 22 | 8 | 613 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 22 | A | 818 | CLA | CHD-C1D | 3.77 | 1.45 | 1.38 |
| 22 | 9 | 601 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 22 | A | 804 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 22 | 9 | 610 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 22 | B | 838 | CLA | CHD-C1D | 3.77 | 1.45 | 1.38 |
| 22 | 1 | 611 | CLA | C3D-C2D | 3.77 | 1.49 | 1.39 |
| 22 | A | 842 | CLA | CHD-C4C | 3.77 | 1.47 | 1.39 |
| 22 | 9 | 604 | CLA | OBD-CAD | 3.76 | 1.29 | 1.22 |
| 22 | B | 815 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 22 | 6 | 610 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 22 | 8 | 606 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 22 | 4 | 604 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 22 | 3 | 611 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 22 | Z | 602 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 29 | 9 | 607 | CHL | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 22 | A | 845 | CLA | CHD-C4C | 3.76 | 1.47 | 1.39 |
| 22 | 2 | 602 | CLA | C3D-C2D | 3.76 | 1.49 | 1.39 |
| 22 | 6 | 601 | CLA | OBD-CAD | 3.76 | 1.29 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | L | 204 | CLA | OBD-CAD | 3.75 | 1.28 | 1.22 |
| 22 | Z | 609 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 22 | A | 843 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | 1 | 602 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 29 | 6 | 606 | CHL | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | 1 | 613 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | A | 812 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | 8 | 608 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | B | 809 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | B | 821 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 29 | 6 | 608 | CHL | C1D-ND | -3.75 | 1.33 | 1.37 |
| 22 | 7 | 610 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | 4 | 612 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 29 | 4 | 618 | CHL | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | 2 | 601 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 22 | B | 827 | CLA | CHD-C4C | 3.75 | 1.47 | 1.39 |
| 22 | Z | 614 | CLA | C3D-C2D | 3.75 | 1.49 | 1.39 |
| 22 | B | 835 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | 3 | 603 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 22 | B | 813 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 22 | 7 | 609 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | 1 | 610 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | G | 204 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | 1 | 616 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | 7 | 614 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | 3 | 613 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 22 | 7 | 604 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 22 | K | 4002 | CLA | C3D-C2D | 3.74 | 1.49 | 1.39 |
| 22 | 1 | 612 | CLA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 22 | Z | 610 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 22 | K | 4003 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 22 | 1 | 612 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 22 | 9 | 610 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 22 | 3 | 612 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 22 | 7 | 606 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 22 | A | 837 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 22 | F | 303 | CLA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 22 | Z | 606 | CLA | C3D-C2D | 3.73 | 1.49 | 1.39 |
| 22 | 8 | 602 | CLA | CHD-C1D | 3.73 | 1.45 | 1.38 |
| 29 | 9 | 607 | CHL | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 22 | A | 837 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 22 | 9 | 601 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | 2 | 610 | CLA | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 29 | Z | 601 | CHL | OBD-CAD | 3.73 | 1.28 | 1.22 |
| 22 | B | 803 | CLA | CHD-C1D | 3.73 | 1.45 | 1.38 |
| 22 | 6 | 609 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | 9 | 613 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | 6 | 616 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | Z | 611 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | 5 | 606 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 22 | B | 815 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | 2 | 611 | CLA | OBD-CAD | 3.72 | 1.28 | 1.22 |
| 22 | 8 | 611 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | A | 823 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | 9 | 611 | CLA | C3D-C2D | 3.72 | 1.49 | 1.39 |
| 22 | 2 | 606 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 22 | B | 811 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | A | 830 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | 6 | 601 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | 3 | 617 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | G | 203 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | A | 841 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 22 | 8 | 616 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 22 | 3 | 612 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 22 | 5 | 611 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | Z | 616 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | 2 | 613 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 22 | 4 | 612 | CLA | CHD-C4C | 3.71 | 1.47 | 1.39 |
| 22 | 2 | 614 | CLA | OBD-CAD | 3.71 | 1.28 | 1.22 |
| 22 | A | 830 | CLA | CHD-C1D | 3.71 | 1.45 | 1.38 |
| 22 | A | 839 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | 3 | 613 | CLA | C3D-C2D | 3.71 | 1.49 | 1.39 |
| 22 | A | 824 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 22 | 5 | 612 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 22 | A | 822 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 22 | B | 818 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 22 | 5 | 612 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 22 | 9 | 602 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 22 | B | 852 | CLA | OBD-CAD | 3.70 | 1.28 | 1.22 |
| 22 | A | 808 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 22 | A | 803 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 22 | A | 831 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 22 | B | 825 | CLA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 22 | 2 | 603 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22 | B | 805 | CLA | CHD-C1D | 3.70 | 1.45 | 1.38 |
| 22 | 3 | 606 | CLA | C3D-C2D | 3.70 | 1.49 | 1.39 |
| 22 | 9 | 611 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 22 | B | 834 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | Z | 613 | CLA | CHD-C4C | 3.69 | 1.47 | 1.39 |
| 22 | A | 811 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | B | 808 | CLA | CHD-C4C | 3.69 | 1.47 | 1.39 |
| 22 | 5 | 606 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | 3 | 604 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | 7 | 620 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 29 | 6 | 607 | CHL | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 22 | 5 | 613 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | B | 833 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | 4 | 613 | CLA | C3D-C2D | 3.69 | 1.49 | 1.39 |
| 22 | 8 | 604 | CLA | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 29 | 4 | 618 | CHL | OBD-CAD | 3.69 | 1.28 | 1.22 |
| 29 | 9 | 606 | CHL | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 22 | 3 | 603 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 22 | B | 805 | CLA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 22 | Z | 604 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 22 | B | 810 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 22 | 9 | 603 | CLA | C3D-C2D | 3.68 | 1.49 | 1.39 |
| 22 | 6 | 614 | CLA | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 29 | 4 | 606 | CHL | OBD-CAD | 3.68 | 1.28 | 1.22 |
| 29 | 9 | 606 | CHL | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 22 | B | 835 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 22 | A | 808 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 22 | A | 809 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 29 | 5 | 608 | CHL | CHD-C4C | 3.67 | 1.47 | 1.39 |
| 22 | 2 | 607 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 22 | 6 | 612 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 29 | 5 | 607 | CHL | CHD-C4C | 3.67 | 1.47 | 1.39 |
| 22 | A | 808 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 22 | B | 803 | CLA | CHD-C4C | 3.67 | 1.47 | 1.39 |
| 22 | 2 | 602 | CLA | OBD-CAD | 3.67 | 1.28 | 1.22 |
| 22 | L | 204 | CLA | C3D-C2D | 3.67 | 1.49 | 1.39 |
| 22 | B | 819 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 22 | 6 | 617 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 22 | 4 | 616 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 22 | 1 | 604 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 22 | 7 | 613 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 22 | 4 | 601 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | Z | 603 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 22 | Z | 610 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 22 | 6 | 604 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 22 | A | 831 | CLA | C3D-C2D | 3.66 | 1.49 | 1.39 |
| 29 | 7 | 607 | CHL | CHD-C4C | 3.66 | 1.47 | 1.39 |
| 22 | 4 | 604 | CLA | OBD-CAD | 3.66 | 1.28 | 1.22 |
| 22 | A | 810 | CLA | CHD-C4C | 3.65 | 1.47 | 1.39 |
| 22 | Z | 604 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 22 | 6 | 613 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 22 | B | 825 | CLA | CHD-C1D | 3.65 | 1.45 | 1.38 |
| 22 | B | 822 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 22 | 8 | 604 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 22 | 4 | 614 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 22 | B | 813 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 22 | 7 | 604 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 22 | 8 | 616 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 22 | Z | 602 | CLA | C3D-C2D | 3.65 | 1.49 | 1.39 |
| 29 | 5 | 618 | CHL | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 22 | 4 | 616 | CLA | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 29 | 6 | 606 | CHL | OBD-CAD | 3.65 | 1.28 | 1.22 |
| 22 | 3 | 614 | CLA | C3D-C2D | 3.64 | 1.49 | 1.39 |
| 22 | 3 | 613 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 22 | 8 | 603 | CLA | C3D-C2D | 3.64 | 1.49 | 1.39 |
| 22 | 6 | 602 | CLA | C3D-C2D | 3.64 | 1.49 | 1.39 |
| 22 | K | 4003 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 22 | 2 | 601 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 21 | A | 801 | CL0 | C3D-C2D | 3.64 | 1.49 | 1.39 |
| 22 | 7 | 608 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 22 | 6 | 616 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 22 | Z | 612 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 22 | 1 | 609 | CLA | C3D-C2D | 3.64 | 1.49 | 1.39 |
| 22 | 5 | 604 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 29 | 6 | 618 | CHL | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 22 | 9 | 609 | CLA | OBD-CAD | 3.64 | 1.28 | 1.22 |
| 22 | A | 811 | CLA | CHD-C4C | 3.64 | 1.47 | 1.39 |
| 22 | B | 839 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | B | 820 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 22 | Z | 612 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | 7 | 611 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | 6 | 604 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | B | 804 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | A | 807 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | 4 | 607 | CHL | CHD-C4C | 3.63 | 1.47 | 1.39 |
| 22 | 1 | 606 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | 7 | 612 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | Z | 613 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | 7 | 614 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 22 | F | 303 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | A | 832 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | B | 804 | CLA | CHD-C4C | 3.63 | 1.47 | 1.39 |
| 22 | A | 817 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 22 | 3 | 604 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 22 | 2 | 609 | CLA | OBD-CAD | 3.63 | 1.28 | 1.22 |
| 22 | A | 812 | CLA | C3D-C2D | 3.63 | 1.49 | 1.39 |
| 22 | 8 | 613 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | 9 | 613 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 29 | 4 | 607 | CHL | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | B | 823 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | 8 | 612 | CLA | C3D-C2D | 3.62 | 1.49 | 1.39 |
| 29 | 8 | 607 | CHL | C1D-ND | -3.62 | 1.33 | 1.37 |
| 22 | 2 | 603 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | B | 831 | CLA | CHD-C4C | 3.62 | 1.47 | 1.39 |
| 29 | 6 | 618 | CHL | CHD-C4C | 3.62 | 1.47 | 1.39 |
| 22 | 3 | 620 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | A | 823 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | A | 829 | CLA | C3D-C2D | 3.62 | 1.49 | 1.39 |
| 22 | 7 | 603 | CLA | C3D-C2D | 3.62 | 1.49 | 1.39 |
| 22 | A | 802 | CLA | OBD-CAD | 3.62 | 1.28 | 1.22 |
| 22 | L | 203 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | B | 834 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | Z | 611 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 29 | 5 | 607 | CHL | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | B | 828 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | A | 843 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | 3 | 609 | CLA | C3D-C2D | 3.61 | 1.49 | 1.39 |
| 22 | B | 824 | CLA | CHD-C4C | 3.61 | 1.47 | 1.39 |
| 22 | Z | 613 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | 5 | 602 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | B | 824 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | F | 304 | CLA | C3D-C2D | 3.61 | 1.49 | 1.39 |
| 22 | 2 | 612 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 29 | 7 | 607 | CHL | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | 8 | 612 | CLA | CHD-C4C | 3.61 | 1.47 | 1.39 |
| 22 | A | 828 | CLA | CHD-C1D | 3.61 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | 3 | 611 | CLA | OBD-CAD | 3.61 | 1.28 | 1.22 |
| 22 | 5 | 610 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | 6 | 603 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | 8 | 602 | CLA | CHD-C4C | 3.60 | 1.47 | 1.39 |
| 22 | B | 808 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | 1 | 603 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | 1 | 604 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | A | 826 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | 8 | 610 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | Z | 609 | CLA | OBD-CAD | 3.60 | 1.28 | 1.22 |
| 22 | A | 833 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | 5 | 616 | CLA | C3D-C2D | 3.60 | 1.49 | 1.39 |
| 22 | J | 3002 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 22 | 3 | 620 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 22 | 5 | 612 | CLA | OBD-CAD | 3.60 | 1.28 | 1.22 |
| 22 | 3 | 614 | CLA | OBD-CAD | 3.60 | 1.28 | 1.22 |
| 22 | B | 837 | CLA | C3D-C2D | 3.60 | 1.48 | 1.39 |
| 29 | 6 | 618 | CHL | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 22 | A | 854 | CLA | CHD-C4C | 3.59 | 1.47 | 1.39 |
| 22 | A | 815 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 22 | B | 824 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 22 | A | 835 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 22 | B | 804 | CLA | OBD-CAD | 3.59 | 1.28 | 1.22 |
| 22 | 6 | 622 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 22 | A | 845 | CLA | C3D-C2D | 3.59 | 1.48 | 1.39 |
| 22 | 3 | 602 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | 5 | 601 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 29 | 6 | 608 | CHL | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 22 | 5 | 617 | CLA | CHD-C1D | 3.58 | 1.45 | 1.38 |
| 22 | B | 832 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | 7 | 620 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 22 | 6 | 622 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 22 | 1 | 612 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 22 | A | 820 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | B | 805 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | A | 819 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | B | 827 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | B | 817 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | 5 | 617 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | 8 | 606 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |
| 22 | 4 | 603 | CLA | C3D-C2D | 3.58 | 1.48 | 1.39 |
| 22 | B | 825 | CLA | OBD-CAD | 3.58 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 22 | 1 | 609 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 29 | 4 | 608 | CHL | CHD-C4C | 3.57 | 1.47 | 1.39 |
| 22 | A | 807 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 22 | J | 3002 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 22 | B | 816 | CLA | CHD-C4C | 3.57 | 1.47 | 1.39 |
| 22 | 9 | 602 | CLA | OBD-CAD | 3.57 | 1.28 | 1.22 |
| 22 | B | 828 | CLA | C3D-C2D | 3.57 | 1.48 | 1.39 |
| 22 | B | 828 | CLA | CHD-C4C | 3.57 | 1.47 | 1.39 |
| 22 | A | 834 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | A | 845 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | B | 833 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | 1 | 606 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | 6 | 611 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | A | 805 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | B | 817 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | 5 | 621 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | 6 | 613 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 22 | 6 | 609 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | K | 4002 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | A | 818 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 22 | B | 808 | CLA | OBD-CAD | 3.56 | 1.28 | 1.22 |
| 22 | B | 812 | CLA | C3D-C2D | 3.56 | 1.48 | 1.39 |
| 22 | A | 818 | CLA | CHD-C4C | 3.56 | 1.47 | 1.39 |
| 22 | 7 | 612 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | A | 842 | CLA | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 22 | 1 | 613 | CLA | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 22 | A | 824 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | F | 304 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | B | 841 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | 3 | 617 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | B | 830 | CLA | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 22 | L | 203 | CLA | CHD-C1D | 3.55 | 1.45 | 1.38 |
| 22 | 7 | 613 | CLA | CHD-C4C | 3.55 | 1.47 | 1.39 |
| 22 | 9 | 612 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | B | 806 | CLA | C3D-C2D | 3.55 | 1.48 | 1.39 |
| 22 | 3 | 606 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | B | 814 | CLA | OBD-CAD | 3.55 | 1.28 | 1.22 |
| 22 | 4 | 613 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | 5 | 603 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 29 | Z | 601 | CHL | CHD-C4C | 3.54 | 1.47 | 1.39 |
| 29 | 6 | 607 | CHL | CHD-C4C | 3.54 | 1.47 | 1.39 |
| 22 | A | 821 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 836 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 22 | A | 813 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 22 | B | 813 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | 7 | 609 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | B | 840 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 22 | 8 | 602 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 22 | A | 826 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | Z | 602 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | A | 818 | CLA | OBD-CAD | 3.54 | 1.28 | 1.22 |
| 22 | 7 | 602 | CLA | C3D-C2D | 3.54 | 1.48 | 1.39 |
| 29 | 3 | 608 | CHL | C1D-ND | -3.54 | 1.33 | 1.37 |
| 22 | 7 | 601 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 22 | 4 | 601 | CLA | C3D-C2D | 3.53 | 1.48 | 1.39 |
| 22 | B | 831 | CLA | C3D-C2D | 3.53 | 1.48 | 1.39 |
| 22 | A | 838 | CLA | C3D-C2D | 3.53 | 1.48 | 1.39 |
| 22 | 6 | 602 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 29 | 1 | 601 | CHL | C1D-ND | -3.53 | 1.33 | 1.37 |
| 29 | 8 | 607 | CHL | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 29 | 5 | 618 | CHL | C1D-ND | -3.53 | 1.33 | 1.37 |
| 29 | 6 | 608 | CHL | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 22 | B | 826 | CLA | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 22 | 3 | 602 | CLA | OBD-CAD | 3.53 | 1.28 | 1.22 |
| 29 | 1 | 607 | CHL | CHD-C4C | 3.53 | 1.47 | 1.39 |
| 21 | A | 801 | CL0 | CHD-C4C | 3.52 | 1.47 | 1.39 |
| 22 | 4 | 610 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 22 | A | 830 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 22 | A | 840 | CLA | C3D-C2D | 3.52 | 1.48 | 1.39 |
| 29 | Z | 601 | CHL | C3D-C2D | 3.52 | 1.48 | 1.39 |
| 22 | 7 | 606 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 22 | 1 | 616 | CLA | OBD-CAD | 3.52 | 1.28 | 1.22 |
| 29 | 1 | 601 | CHL | CHD-C4C | 3.52 | 1.47 | 1.39 |
| 22 | 9 | 603 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | A | 830 | CLA | CHD-C4C | 3.51 | 1.47 | 1.39 |
| 22 | B | 812 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | 9 | 614 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | A | 829 | CLA | CHD-C4C | 3.51 | 1.47 | 1.39 |
| 22 | A | 813 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | 7 | 610 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 22 | Z | 608 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 22 | A | 810 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | 5 | 616 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | 4 | 602 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | 4 | 618 | CHL | C1D-ND | -3.51 | 1.33 | 1.37 |
| 22 | 5 | 611 | CLA | OBD-CAD | 3.51 | 1.28 | 1.22 |
| 22 | 7 | 601 | CLA | C3D-C2D | 3.51 | 1.48 | 1.39 |
| 22 | A | 811 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 22 | B | 802 | CLA | CHD-C1D | 3.50 | 1.45 | 1.38 |
| 29 | Z | 607 | CHL | CHD-C4C | 3.50 | 1.47 | 1.39 |
| 22 | Z | 606 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 22 | 4 | 614 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 22 | A | 831 | CLA | C1B-NB | -3.50 | 1.32 | 1.35 |
| 22 | B | 802 | CLA | OBD-CAD | 3.50 | 1.28 | 1.22 |
| 29 | 3 | 608 | CHL | CHD-C4C | 3.50 | 1.47 | 1.39 |
| 29 | 4 | 618 | CHL | C3D-C2D | 3.50 | 1.48 | 1.39 |
| 22 | B | 811 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 22 | A | 824 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 22 | A | 834 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 22 | B | 810 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 22 | 8 | 612 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 22 | 5 | 609 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 29 | 5 | 618 | CHL | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 22 | 8 | 616 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 22 | 6 | 617 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 22 | A | 806 | CLA | C3D-C2D | 3.49 | 1.48 | 1.39 |
| 22 | B | 829 | CLA | OBD-CAD | 3.49 | 1.28 | 1.22 |
| 22 | 7 | 604 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 22 | 3 | 607 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | A | 814 | CLA | C3D-C2D | 3.48 | 1.48 | 1.39 |
| 22 | B | 819 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | B | 809 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | B | 815 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | 4 | 602 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 29 | 6 | 618 | CHL | C1D-ND | -3.48 | 1.33 | 1.37 |
| 29 | 4 | 606 | CHL | CHD-C4C | 3.48 | 1.47 | 1.39 |
| 22 | 5 | 617 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | A | 833 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | B | 827 | CLA | OBD-CAD | 3.48 | 1.28 | 1.22 |
| 22 | 1 | 610 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 22 | 1 | 613 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 22 | 7 | 608 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 22 | A | 828 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 22 | B | 818 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 22 | A | 817 | CLA | C3D-C2D | 3.47 | 1.48 | 1.39 |
| 22 | 5 | 614 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A | 809 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 22 | 1 | 611 | CLA | OBD-CAD | 3.47 | 1.28 | 1.22 |
| 22 | A | 814 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 22 | G | 203 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 22 | 6 | 612 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 22 | B | 816 | CLA | C3D-C2D | 3.46 | 1.48 | 1.39 |
| 22 | 3 | 609 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 22 | 7 | 613 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 22 | A | 832 | CLA | OBD-CAD | 3.46 | 1.28 | 1.22 |
| 29 | 8 | 607 | CHL | CHD-C4C | 3.46 | 1.47 | 1.39 |
| 29 | Z | 607 | CHL | C1D-ND | -3.46 | 1.33 | 1.37 |
| 29 | 9 | 607 | CHL | C1D-ND | -3.46 | 1.33 | 1.37 |
| 22 | A | 827 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 22 | 8 | 608 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 22 | Z | 616 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 22 | B | 838 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 22 | B | 840 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 22 | B | 832 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 22 | 7 | 606 | CLA | C3D-C2D | 3.45 | 1.48 | 1.39 |
| 22 | A | 836 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 22 | B | 821 | CLA | OBD-CAD | 3.45 | 1.28 | 1.22 |
| 22 | B | 802 | CLA | CHD-C4C | 3.44 | 1.47 | 1.39 |
| 29 | 1 | 607 | CHL | C1D-ND | -3.44 | 1.33 | 1.37 |
| 22 | 7 | 611 | CLA | C3A-C2A | -3.44 | 1.51 | 1.54 |
| 22 | B | 822 | CLA | OBD-CAD | 3.44 | 1.28 | 1.22 |
| 22 | A | 842 | CLA | OBD-CAD | 3.44 | 1.28 | 1.22 |
| 22 | A | 804 | CLA | OBD-CAD | 3.44 | 1.28 | 1.22 |
| 22 | A | 810 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 22 | 8 | 601 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 29 | 5 | 608 | CHL | OBD-CAD | 3.44 | 1.28 | 1.22 |
| 22 | 1 | 608 | CLA | C3D-C2D | 3.44 | 1.48 | 1.39 |
| 29 | 5 | 608 | CHL | C1D-ND | -3.43 | 1.33 | 1.37 |
| 22 | 5 | 613 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 22 | A | 816 | CLA | OBD-CAD | 3.43 | 1.28 | 1.22 |
| 29 | 9 | 607 | CHL | C3D-C2D | 3.42 | 1.48 | 1.39 |
| 21 | A | 801 | CL0 | OBD-CAD | 3.42 | 1.28 | 1.22 |
| 29 | 4 | 607 | CHL | C1D-ND | -3.41 | 1.33 | 1.37 |
| 29 | 4 | 606 | CHL | C1D-ND | -3.41 | 1.33 | 1.37 |
| 22 | 8 | 611 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 22 | A | 806 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 22 | B | 831 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 22 | F | 303 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 5 | 602 | CLA | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 22 | 5 | 610 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 22 | A | 821 | CLA | OBD-CAD | 3.41 | 1.28 | 1.22 |
| 22 | B | 814 | CLA | C3D-C2D | 3.41 | 1.48 | 1.39 |
| 22 | A | 838 | CLA | OBD-CAD | 3.40 | 1.28 | 1.22 |
| 22 | Z | 614 | CLA | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 29 | 1 | 607 | CHL | C3D-C2D | 3.39 | 1.48 | 1.39 |
| 29 | 6 | 608 | CHL | C3D-C2D | 3.39 | 1.48 | 1.39 |
| 22 | A | 820 | CLA | OBD-CAD | 3.39 | 1.28 | 1.22 |
| 29 | 4 | 607 | CHL | C3D-C2D | 3.39 | 1.48 | 1.39 |
| 22 | B | 839 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 22 | 8 | 614 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 22 | 8 | 601 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 22 | 8 | 602 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 22 | 4 | 611 | CLA | OBD-CAD | 3.38 | 1.28 | 1.22 |
| 29 | 9 | 606 | CHL | C3D-C2D | 3.38 | 1.48 | 1.39 |
| 22 | B | 830 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 29 | 6 | 607 | CHL | C3D-C2D | 3.37 | 1.48 | 1.39 |
| 22 | A | 841 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 22 | A | 827 | CLA | OBD-CAD | 3.37 | 1.28 | 1.22 |
| 22 | B | 805 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 22 | 7 | 610 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 22 | 1 | 602 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 22 | Z | 603 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 22 | Z | 608 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 22 | 5 | 621 | CLA | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 22 | B | 807 | CLA | OBD-CAD | 3.36 | 1.28 | 1.22 |
| 22 | B | 802 | CLA | C3D-C2D | 3.36 | 1.48 | 1.39 |
| 22 | A | 812 | CLA | OBD-CAD | 3.35 | 1.28 | 1.22 |
| 22 | F | 301 | CLA | C3D-C2D | 3.35 | 1.48 | 1.39 |
| 22 | A | 828 | CLA | CHD-C4C | 3.35 | 1.46 | 1.39 |
| 29 | 5 | 607 | CHL | C3D-C2D | 3.34 | 1.48 | 1.39 |
| 22 | 7 | 603 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 22 | Z | 610 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 22 | 7 | 608 | CLA | OBD-CAD | 3.34 | 1.28 | 1.22 |
| 22 | 4 | 609 | CLA | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 22 | A | 840 | CLA | OBD-CAD | 3.33 | 1.28 | 1.22 |
| 22 | B | 826 | CLA | C3D-C2D | 3.32 | 1.48 | 1.39 |
| 22 | A | 825 | CLA | OBD-CAD | 3.32 | 1.28 | 1.22 |
| 22 | 3 | 610 | CLA | C3D-C2D | 3.31 | 1.48 | 1.39 |
| 29 | 3 | 608 | CHL | C1B-NB | -3.31 | 1.32 | 1.35 |
| 22 | 4 | 612 | CLA | OBD-CAD | 3.30 | 1.28 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | Z | 607 | CHL | C3D-C2D | 3.30 | 1.48 | 1.39 |
| 22 | A | 819 | CLA | OBD-CAD | 3.29 | 1.28 | 1.22 |
| 29 | 4 | 606 | CHL | C3D-C2D | 3.29 | 1.48 | 1.39 |
| 29 | 8 | 607 | CHL | C3D-C2D | 3.28 | 1.48 | 1.39 |
| 29 | 9 | 606 | CHL | C1D-ND | -3.28 | 1.33 | 1.37 |
| 22 | 6 | 614 | CLA | C3D-C2D | 3.28 | 1.48 | 1.39 |
| 22 | A | 831 | CLA | OBD-CAD | 3.28 | 1.28 | 1.22 |
| 29 | 6 | 606 | CHL | C3D-C2D | 3.28 | 1.48 | 1.39 |
| 29 | 6 | 607 | CHL | C1D-ND | -3.28 | 1.33 | 1.37 |
| 22 | B | 825 | CLA | C3D-C2D | 3.27 | 1.48 | 1.39 |
| 22 | B | 803 | CLA | OBD-CAD | 3.27 | 1.28 | 1.22 |
| 22 | B | 838 | CLA | OBD-CAD | 3.27 | 1.28 | 1.22 |
| 29 | 6 | 606 | CHL | C1D-ND | -3.27 | 1.33 | 1.37 |
| 29 | 5 | 607 | CHL | C1D-ND | -3.25 | 1.33 | 1.37 |
| 22 | 1 | 608 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 22 | 8 | 608 | CLA | OBD-CAD | 3.24 | 1.28 | 1.22 |
| 29 | 5 | 608 | CHL | C3D-C2D | 3.23 | 1.47 | 1.39 |
| 29 | 5 | 607 | CHL | MG-NA | -3.22 | 1.98 | 2.06 |
| 22 | 6 | 610 | CLA | OBD-CAD | 3.21 | 1.28 | 1.22 |
| 22 | B | 826 | CLA | OBD-CAD | 3.20 | 1.28 | 1.22 |
| 22 | 7 | 611 | CLA | OBD-CAD | 3.20 | 1.28 | 1.22 |
| 22 | 8 | 609 | CLA | OBD-CAD | 3.20 | 1.28 | 1.22 |
| 22 | F | 301 | CLA | OBD-CAD | 3.19 | 1.28 | 1.22 |
| 29 | 4 | 608 | CHL | C1D-ND | -3.19 | 1.33 | 1.37 |
| 29 | 7 | 607 | CHL | C3D-C2D | 3.18 | 1.47 | 1.39 |
| 29 | 7 | 607 | CHL | C1D-ND | -3.18 | 1.33 | 1.37 |
| 22 | A | 828 | CLA | OBD-CAD | 3.18 | 1.28 | 1.22 |
| 29 | 1 | 601 | CHL | OBD-CAD | 3.18 | 1.28 | 1.22 |
| 22 | 8 | 603 | CLA | OBD-CAD | 3.18 | 1.28 | 1.22 |
| 22 | A | 822 | CLA | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 22 | B | 829 | CLA | C3D-C2D | 3.17 | 1.47 | 1.39 |
| 22 | A | 829 | CLA | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 22 | 3 | 610 | CLA | OBD-CAD | 3.17 | 1.27 | 1.22 |
| 22 | 7 | 616 | CLA | OBD-CAD | 3.16 | 1.27 | 1.22 |
| 22 | B | 828 | CLA | C1B-NB | -3.15 | 1.32 | 1.35 |
| 29 | 1 | 601 | CHL | C3D-C2D | 3.15 | 1.47 | 1.39 |
| 22 | 1 | 614 | CLA | OBD-CAD | 3.14 | 1.27 | 1.22 |
| 29 | 4 | 608 | CHL | C3D-C2D | 3.13 | 1.47 | 1.39 |
| 22 | 7 | 602 | CLA | OBD-CAD | 3.13 | 1.27 | 1.22 |
| 29 | 3 | 608 | CHL | C3D-C2D | 3.11 | 1.47 | 1.39 |
| 22 | 4 | 603 | CLA | OBD-CAD | 3.10 | 1.27 | 1.22 |
| 22 | 3 | 603 | CLA | OBD-CAD | 3.10 | 1.27 | 1.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A | 839 | CLA | OBD-CAD | 3.09 | 1.27 | 1.22 |
| 22 | A | 803 | CLA | OBD-CAD | 3.07 | 1.27 | 1.22 |
| 22 | A | 803 | CLA | C1B-NB | -3.07 | 1.32 | 1.35 |
| 22 | 6 | 603 | CLA | OBD-CAD | 3.06 | 1.27 | 1.22 |
| 22 | A | 854 | CLA | OBD-CAD | 3.06 | 1.27 | 1.22 |
| 22 | B | 826 | CLA | C1B-NB | -3.03 | 1.32 | 1.35 |
| 29 | 4 | 608 | CHL | OBD-CAD | 3.02 | 1.27 | 1.22 |
| 22 | B | 809 | CLA | C1B-NB | -3.01 | 1.32 | 1.35 |
| 29 | 1 | 607 | CHL | MG-NA | -3.01 | 1.99 | 2.06 |
| 22 | 1 | 603 | CLA | OBD-CAD | 3.00 | 1.27 | 1.22 |
| 22 | 4 | 616 | CLA | C3A-C2A | -3.00 | 1.51 | 1.54 |
| 22 | A | 806 | CLA | C1B-NB | -2.98 | 1.32 | 1.35 |
| 22 | A | 837 | CLA | C1B-NB | -2.96 | 1.32 | 1.35 |
| 22 | A | 820 | CLA | C1B-NB | -2.93 | 1.32 | 1.35 |
| 22 | A | 804 | CLA | C3D-C2D | 2.93 | 1.47 | 1.39 |
| 29 | 4 | 607 | CHL | MG-NA | -2.93 | 1.99 | 2.06 |
| 22 | B | 806 | CLA | OBD-CAD | 2.93 | 1.27 | 1.22 |
| 29 | 3 | 608 | CHL | OBD-CAD | 2.92 | 1.27 | 1.22 |
| 22 | B | 837 | CLA | OBD-CAD | 2.91 | 1.27 | 1.22 |
| 22 | 3 | 611 | CLA | C3A-C2A | -2.90 | 1.51 | 1.54 |
| 22 | B | 831 | CLA | C1B-NB | -2.89 | 1.32 | 1.35 |
| 22 | B | 816 | CLA | OBD-CAD | 2.89 | 1.27 | 1.22 |
| 22 | B | 803 | CLA | C1B-NB | -2.87 | 1.32 | 1.35 |
| 29 | 8 | 607 | CHL | MG-NA | -2.87 | 1.99 | 2.06 |
| 29 | 4 | 618 | CHL | MG-NA | -2.87 | 1.99 | 2.06 |
| 22 | 8 | 610 | CLA | OBD-CAD | 2.86 | 1.27 | 1.22 |
| 29 | Z | 607 | CHL | MG-NA | -2.86 | 1.99 | 2.06 |
| 22 | A | 804 | CLA | C3D-C4D | -2.85 | 1.37 | 1.44 |
| 29 | 1 | 601 | CHL | C3D-C4D | -2.85 | 1.37 | 1.44 |
| 22 | 8 | 612 | CLA | C1B-NB | -2.83 | 1.32 | 1.35 |
| 22 | B | 805 | CLA | C1B-NB | -2.81 | 1.32 | 1.35 |
| 22 | A | 833 | CLA | C1B-NB | -2.81 | 1.32 | 1.35 |
| 29 | 4 | 606 | CHL | MG-NA | -2.81 | 1.99 | 2.06 |
| 29 | 9 | 607 | CHL | MG-NA | -2.81 | 1.99 | 2.06 |
| 22 | A | 822 | CLA | C1B-NB | -2.80 | 1.32 | 1.35 |
| 22 | A | 821 | CLA | C1B-NB | -2.80 | 1.32 | 1.35 |
| 22 | 7 | 606 | CLA | C1B-NB | -2.80 | 1.32 | 1.35 |
| 22 | Z | 610 | CLA | C1C-C2C | 2.78 | 1.50 | 1.44 |
| 22 | 5 | 603 | CLA | C4D-CHA | 2.76 | 1.48 | 1.38 |
| 29 | 6 | 607 | CHL | MG-NA | -2.76 | 1.99 | 2.06 |
| 29 | 5 | 608 | CHL | MG-NA | -2.76 | 1.99 | 2.06 |
| 22 | B | 818 | CLA | C1B-NB | -2.75 | 1.32 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 1 | 610 | CLA | C1C-C2C | 2.75 | 1.49 | 1.44 |
| 22 | 9 | 604 | CLA | C4C-C3C | 2.75 | 1.49 | 1.45 |
| 22 | B | 840 | CLA | C1C-NC | -2.75 | 1.33 | 1.37 |
| 22 | 4 | 611 | CLA | C4D-CHA | 2.75 | 1.48 | 1.38 |
| 22 | 2 | 609 | CLA | C4D-CHA | 2.75 | 1.48 | 1.38 |
| 22 | A | 837 | CLA | C4D-CHA | 2.75 | 1.48 | 1.38 |
| 22 | L | 204 | CLA | C4C-C3C | 2.75 | 1.49 | 1.45 |
| 22 | 8 | 611 | CLA | C4D-CHA | 2.74 | 1.48 | 1.38 |
| 22 | A | 830 | CLA | C1B-NB | -2.74 | 1.32 | 1.35 |
| 29 | 6 | 608 | CHL | MG-NA | -2.74 | 1.99 | 2.06 |
| 22 | A | 813 | CLA | C1B-NB | -2.74 | 1.32 | 1.35 |
| 22 | B | 836 | CLA | OBD-CAD | 2.74 | 1.27 | 1.22 |
| 29 | 3 | 608 | CHL | C3D-C4D | -2.73 | 1.38 | 1.44 |
| 22 | 7 | 610 | CLA | C4B-CHC | 2.73 | 1.48 | 1.41 |
| 22 | 9 | 601 | CLA | C4D-CHA | 2.73 | 1.48 | 1.38 |
| 29 | 5 | 618 | CHL | MG-NA | -2.73 | 1.99 | 2.06 |
| 29 | 9 | 606 | CHL | MG-NA | -2.72 | 1.99 | 2.06 |
| 22 | 8 | 601 | CLA | C4D-CHA | 2.72 | 1.48 | 1.38 |
| 22 | Z | 609 | CLA | C4D-CHA | 2.72 | 1.48 | 1.38 |
| 22 | K | 4002 | CLA | C4D-CHA | 2.72 | 1.48 | 1.38 |
| 22 | 9 | 611 | CLA | C4D-CHA | 2.71 | 1.48 | 1.38 |
| 22 | 4 | 609 | CLA | C4D-CHA | 2.71 | 1.48 | 1.38 |
| 22 | 7 | 611 | CLA | C4D-CHA | 2.71 | 1.48 | 1.38 |
| 22 | 3 | 603 | CLA | C4D-CHA | 2.71 | 1.48 | 1.38 |
| 22 | 4 | 610 | CLA | C1B-NB | -2.71 | 1.32 | 1.35 |
| 29 | 8 | 607 | CHL | C3D-C4D | -2.70 | 1.38 | 1.44 |
| 22 | 7 | 614 | CLA | C4D-CHA | 2.70 | 1.48 | 1.38 |
| 22 | 5 | 604 | CLA | C4C-C3C | 2.70 | 1.49 | 1.45 |
| 22 | F | 303 | CLA | C4D-CHA | 2.70 | 1.48 | 1.38 |
| 22 | 5 | 616 | CLA | C4D-CHA | 2.70 | 1.48 | 1.38 |
| 22 | B | 808 | CLA | C1B-NB | -2.69 | 1.32 | 1.35 |
| 22 | A | 854 | CLA | C1B-NB | -2.69 | 1.32 | 1.35 |
| 22 | 5 | 606 | CLA | C4D-CHA | 2.69 | 1.48 | 1.38 |
| 22 | B | 807 | CLA | C4D-CHA | 2.69 | 1.48 | 1.38 |
| 22 | 6 | 609 | CLA | C4D-CHA | 2.69 | 1.47 | 1.38 |
| 22 | 3 | 620 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 22 | 6 | 604 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 22 | Z | 603 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 22 | 5 | 604 | CLA | C4D-CHA | 2.68 | 1.47 | 1.38 |
| 22 | 3 | 611 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | B | 817 | CLA | C4B-NB | -2.67 | 1.32 | 1.35 |
| 22 | 5 | 611 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 835 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | B | 836 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | A | 843 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | Z | 616 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | B | 838 | CLA | C4B-CHC | 2.67 | 1.48 | 1.41 |
| 22 | F | 304 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | 5 | 603 | CLA | C3D-C4D | -2.67 | 1.38 | 1.44 |
| 22 | 6 | 603 | CLA | C4D-CHA | 2.67 | 1.47 | 1.38 |
| 22 | 7 | 616 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | 1 | 616 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | G | 204 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | 3 | 604 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 29 | 7 | 607 | CHL | MG-NA | -2.66 | 1.99 | 2.06 |
| 22 | A | 816 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | B | 834 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | 2 | 606 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | 8 | 609 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | B | 805 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | A | 836 | CLA | C4D-CHA | 2.66 | 1.47 | 1.38 |
| 22 | B | 827 | CLA | C1B-NB | -2.65 | 1.32 | 1.35 |
| 22 | 1 | 603 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | B | 852 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 7 | 620 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 5 | 601 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | A | 839 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 9 | 613 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 1 | 613 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 29 | 3 | 608 | CHL | MG-NA | -2.65 | 2.00 | 2.06 |
| 22 | B | 836 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 22 | 1 | 609 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | B | 811 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 8 | 616 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 9 | 614 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | B | 809 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | 3 | 606 | CLA | C4D-CHA | 2.65 | 1.47 | 1.38 |
| 22 | B | 806 | CLA | C3D-C4D | -2.65 | 1.38 | 1.44 |
| 22 | B | 823 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | 7 | 602 | CLA | C4B-CHC | 2.64 | 1.48 | 1.41 |
| 22 | B | 813 | CLA | C1B-NB | -2.64 | 1.32 | 1.35 |
| 29 | 4 | 607 | CHL | C3D-C4D | -2.64 | 1.38 | 1.44 |
| 22 | 5 | 614 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 29 | 6 | 606 | CHL | C3D-C4D | -2.64 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 2 | 613 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | 5 | 609 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | G | 203 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | B | 806 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | 9 | 602 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | 3 | 610 | CLA | C1C-C2C | 2.64 | 1.49 | 1.44 |
| 22 | Z | 613 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | 5 | 612 | CLA | C4D-CHA | 2.64 | 1.47 | 1.38 |
| 22 | 6 | 616 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | 9 | 609 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | B | 818 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | 6 | 616 | CLA | C1B-NB | -2.63 | 1.32 | 1.35 |
| 22 | B | 815 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | 6 | 611 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | A | 840 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 29 | 6 | 618 | CHL | MG-NA | -2.63 | 2.00 | 2.06 |
| 22 | 9 | 612 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | Z | 604 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | 2 | 601 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | 2 | 603 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | A | 845 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | B | 833 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | 3 | 614 | CLA | C4D-CHA | 2.63 | 1.47 | 1.38 |
| 22 | A | 831 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 22 | 3 | 607 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 21 | A | 801 | CL0 | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 29 | 6 | 606 | CHL | MG-NA | -2.62 | 2.00 | 2.06 |
| 29 | 6 | 606 | CHL | C2C-C1C | 2.62 | 1.50 | 1.44 |
| 22 | A | 826 | CLA | C4D-CHA | 2.62 | 1.47 | 1.38 |
| 22 | B | 805 | CLA | C4B-CHC | 2.62 | 1.48 | 1.41 |
| 22 | 1 | 610 | CLA | C4B-CHC | 2.62 | 1.48 | 1.41 |
| 22 | 8 | 614 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | Z | 608 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | B | 814 | CLA | C3D-C4D | -2.61 | 1.38 | 1.44 |
| 22 | J | 3002 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | 6 | 610 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | A | 830 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | A | 822 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | 3 | 610 | CLA | C4B-CHC | 2.61 | 1.48 | 1.41 |
| 22 | B | 817 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |
| 22 | 1 | 602 | CLA | C4B-CHC | 2.61 | 1.48 | 1.41 |
| 22 | A | 833 | CLA | C4D-CHA | 2.61 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 7 | 603 | CLA | C3D-C4D | -2.61 | 1.38 | 1.44 |
| 22 | B | 831 | CLA | C4B-CHC | 2.60 | 1.48 | 1.41 |
| 22 | Z | 614 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | A | 828 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 29 | 6 | 608 | CHL | C3D-C4D | -2.60 | 1.38 | 1.44 |
| 22 | B | 826 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | 4 | 603 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | A | 813 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | A | 832 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | A | 838 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | Z | 606 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | 5 | 621 | CLA | C4C-C3C | 2.60 | 1.49 | 1.45 |
| 29 | Z | 601 | CHL | MG-NA | -2.60 | 2.00 | 2.06 |
| 22 | 4 | 616 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | F | 301 | CLA | C3D-C4D | -2.60 | 1.38 | 1.44 |
| 22 | B | 839 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | 3 | 609 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | 5 | 621 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | A | 809 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | 6 | 622 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | B | 813 | CLA | C4D-CHA | 2.60 | 1.47 | 1.38 |
| 22 | 6 | 602 | CLA | C4B-CHC | 2.59 | 1.48 | 1.41 |
| 22 | 8 | 610 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 22 | 2 | 612 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 29 | 7 | 607 | CHL | C3D-C4D | -2.59 | 1.38 | 1.44 |
| 21 | A | 801 | CL0 | C1B-NB | -2.59 | 1.32 | 1.35 |
| 22 | 3 | 604 | CLA | C1B-NB | -2.59 | 1.32 | 1.35 |
| 22 | Z | 610 | CLA | C4B-CHC | 2.59 | 1.48 | 1.41 |
| 22 | A | 842 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 22 | 2 | 607 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 22 | A | 808 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 22 | 1 | 608 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 22 | A | 819 | CLA | C4D-CHA | 2.59 | 1.47 | 1.38 |
| 22 | B | 840 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 22 | A | 841 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 22 | A | 842 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 22 | B | 824 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 22 | B | 836 | CLA | C1B-NB | -2.58 | 1.32 | 1.35 |
| 29 | 4 | 606 | CHL | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 22 | B | 819 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 22 | B | 828 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 22 | 8 | 603 | CLA | C3D-C4D | -2.58 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A | 823 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 29 | 5 | 618 | CHL | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 22 | F | 301 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 22 | 4 | 610 | CLA | C4D-CHA | 2.58 | 1.47 | 1.38 |
| 29 | Z | 601 | CHL | C3D-C4D | -2.58 | 1.38 | 1.44 |
| 22 | A | 825 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | 2 | 602 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | 4 | 604 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | B | 823 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |
| 22 | 3 | 613 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | 1 | 606 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | A | 841 | CLA | C4B-CHC | 2.57 | 1.48 | 1.41 |
| 22 | 7 | 609 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | 5 | 610 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | A | 821 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | 2 | 612 | CLA | C4C-C3C | 2.57 | 1.49 | 1.45 |
| 22 | 6 | 612 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | 4 | 601 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | B | 825 | CLA | C1B-NB | -2.57 | 1.32 | 1.35 |
| 29 | 4 | 608 | CHL | C2C-C1C | 2.57 | 1.50 | 1.44 |
| 22 | B | 804 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | Z | 611 | CLA | C4D-CHA | 2.57 | 1.47 | 1.38 |
| 22 | A | 807 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | B | 837 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 4 | 612 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 8 | 606 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 9 | 603 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 7 | 612 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 5 | 602 | CLA | C4B-CHC | 2.56 | 1.48 | 1.41 |
| 22 | B | 819 | CLA | C1B-NB | -2.56 | 1.32 | 1.35 |
| 22 | 8 | 612 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 2 | 606 | CLA | C3A-C2A | -2.56 | 1.52 | 1.54 |
| 22 | A | 834 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 8 | 602 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 9 | 604 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | 3 | 617 | CLA | C4D-CHA | 2.56 | 1.47 | 1.38 |
| 22 | A | 809 | CLA | C1C-C2C | 2.56 | 1.49 | 1.44 |
| 22 | 7 | 604 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | L | 204 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | B | 829 | CLA | C3D-C4D | -2.55 | 1.38 | 1.44 |
| 22 | 6 | 617 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | B | 830 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 7 | 610 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | 7 | 613 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | Z | 612 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | 4 | 614 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | K | 4003 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | B | 820 | CLA | C3D-C4D | -2.55 | 1.38 | 1.44 |
| 22 | 1 | 604 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | B | 840 | CLA | C3D-C4D | -2.55 | 1.38 | 1.44 |
| 22 | 1 | 611 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 22 | 1 | 602 | CLA | C4D-CHA | 2.55 | 1.47 | 1.38 |
| 29 | 4 | 618 | CHL | C3D-C4D | -2.54 | 1.38 | 1.44 |
| 22 | 5 | 613 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 1 | 606 | CLA | C4B-CHC | 2.54 | 1.48 | 1.41 |
| 22 | B | 832 | CLA | C1B-NB | -2.54 | 1.32 | 1.35 |
| 22 | B | 835 | CLA | C1B-NB | -2.54 | 1.32 | 1.35 |
| 22 | A | 824 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 3 | 613 | CLA | C4C-C3C | 2.54 | 1.49 | 1.45 |
| 22 | Z | 610 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 2 | 611 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 8 | 613 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | B | 826 | CLA | C3D-C4D | -2.54 | 1.38 | 1.44 |
| 22 | B | 804 | CLA | C1B-NB | -2.54 | 1.32 | 1.35 |
| 22 | 2 | 614 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | A | 854 | CLA | C4B-CHC | 2.54 | 1.48 | 1.41 |
| 22 | B | 838 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 7 | 603 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 8 | 603 | CLA | C4D-CHA | 2.54 | 1.47 | 1.38 |
| 22 | 5 | 621 | CLA | C3D-C4D | -2.54 | 1.38 | 1.44 |
| 22 | 7 | 608 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 22 | 7 | 610 | CLA | C1C-C2C | 2.53 | 1.49 | 1.44 |
| 22 | 4 | 602 | CLA | C4C-C3C | 2.53 | 1.49 | 1.45 |
| 22 | F | 301 | CLA | C4B-CHC | 2.53 | 1.48 | 1.41 |
| 22 | 3 | 612 | CLA | C1B-NB | -2.53 | 1.32 | 1.35 |
| 22 | B | 839 | CLA | C3D-C4D | -2.53 | 1.38 | 1.44 |
| 22 | 2 | 610 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 22 | B | 829 | CLA | C1C-C2C | 2.53 | 1.49 | 1.44 |
| 22 | B | 824 | CLA | C1B-NB | -2.53 | 1.32 | 1.35 |
| 22 | B | 812 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 22 | B | 817 | CLA | C3D-C4D | -2.53 | 1.38 | 1.44 |
| 22 | 7 | 612 | CLA | C1B-NB | -2.53 | 1.33 | 1.35 |
| 22 | 6 | 601 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 22 | B | 821 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 4 | 603 | CLA | C3D-C4D | -2.53 | 1.38 | 1.44 |
| 22 | A | 803 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 22 | 8 | 601 | CLA | C4C-C3C | 2.53 | 1.49 | 1.45 |
| 22 | B | 803 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 22 | Z | 602 | CLA | C4D-CHA | 2.53 | 1.47 | 1.38 |
| 29 | 5 | 608 | CHL | C3D-C4D | -2.53 | 1.38 | 1.44 |
| 22 | 6 | 602 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 22 | 4 | 613 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 29 | 6 | 608 | CHL | C2C-C1C | 2.52 | 1.49 | 1.44 |
| 22 | A | 841 | CLA | C1B-NB | -2.52 | 1.33 | 1.35 |
| 22 | 9 | 610 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 22 | 2 | 603 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 22 | A | 828 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 22 | 2 | 613 | CLA | C4C-C3C | 2.52 | 1.49 | 1.45 |
| 22 | B | 822 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 22 | B | 803 | CLA | C1C-NC | -2.52 | 1.34 | 1.37 |
| 29 | 9 | 607 | CHL | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 22 | A | 814 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 22 | 1 | 612 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 22 | B | 816 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 22 | A | 819 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 22 | B | 816 | CLA | C3D-C4D | -2.52 | 1.38 | 1.44 |
| 22 | 3 | 612 | CLA | C4D-CHA | 2.52 | 1.47 | 1.38 |
| 29 | 9 | 607 | CHL | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 22 | A | 817 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | 8 | 604 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | B | 827 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | B | 802 | CLA | C1B-NB | -2.51 | 1.33 | 1.35 |
| 22 | A | 805 | CLA | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 22 | B | 831 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | 6 | 613 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 29 | 5 | 607 | CHL | C3D-C4D | -2.51 | 1.38 | 1.44 |
| 22 | Z | 602 | CLA | C4B-CHC | 2.51 | 1.48 | 1.41 |
| 22 | A | 818 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | 9 | 614 | CLA | C4C-C3C | 2.51 | 1.49 | 1.45 |
| 22 | 1 | 610 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | 3 | 610 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | 7 | 606 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | 1 | 614 | CLA | C4D-CHA | 2.51 | 1.47 | 1.38 |
| 22 | Z | 609 | CLA | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 22 | B | 830 | CLA | C3D-C4D | -2.50 | 1.38 | 1.44 |
| 22 | 7 | 601 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 8 | 610 | CLA | C1C-C2C | 2.50 | 1.49 | 1.44 |
| 29 | 4 | 608 | CHL | C3D-C4D | -2.50 | 1.38 | 1.44 |
| 22 | 7 | 608 | CLA | C4B-CHC | 2.50 | 1.47 | 1.41 |
| 22 | 7 | 608 | CLA | C3D-C4D | -2.50 | 1.38 | 1.44 |
| 22 | B | 812 | CLA | C4B-CHC | 2.50 | 1.47 | 1.41 |
| 29 | 9 | 606 | CHL | C3D-C4D | -2.50 | 1.38 | 1.44 |
| 22 | A | 810 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 22 | A | 829 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 22 | 4 | 611 | CLA | C4C-C3C | 2.50 | 1.49 | 1.45 |
| 22 | 8 | 608 | CLA | C4D-CHA | 2.50 | 1.47 | 1.38 |
| 22 | B | 810 | CLA | C4D-CHA | 2.49 | 1.47 | 1.38 |
| 22 | A | 806 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 29 | Z | 607 | CHL | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 22 | 9 | 601 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 22 | A | 820 | CLA | C4D-CHA | 2.49 | 1.47 | 1.38 |
| 22 | A | 840 | CLA | C1B-NB | -2.49 | 1.33 | 1.35 |
| 22 | 2 | 609 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 29 | 1 | 601 | CHL | MG-NA | -2.49 | 2.00 | 2.06 |
| 22 | 9 | 603 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 22 | A | 838 | CLA | C3D-C4D | -2.49 | 1.38 | 1.44 |
| 22 | 4 | 602 | CLA | C4D-CHA | 2.49 | 1.47 | 1.38 |
| 22 | A | 816 | CLA | C4C-C3C | 2.49 | 1.49 | 1.45 |
| 22 | 3 | 602 | CLA | C4D-CHA | 2.49 | 1.47 | 1.38 |
| 22 | 4 | 614 | CLA | C1C-C2C | 2.49 | 1.49 | 1.44 |
| 22 | 5 | 617 | CLA | C4D-CHA | 2.48 | 1.47 | 1.38 |
| 22 | A | 816 | CLA | C4B-CHC | 2.48 | 1.47 | 1.41 |
| 22 | A | 829 | CLA | C1C-C2C | 2.48 | 1.49 | 1.44 |
| 22 | B | 808 | CLA | C4D-CHA | 2.48 | 1.47 | 1.38 |
| 22 | 6 | 603 | CLA | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 22 | 3 | 611 | CLA | C4C-C3C | 2.48 | 1.49 | 1.45 |
| 22 | 4 | 616 | CLA | C4C-C3C | 2.48 | 1.49 | 1.45 |
| 22 | A | 806 | CLA | C4D-CHA | 2.48 | 1.47 | 1.38 |
| 29 | Z | 601 | CHL | C2C-C1C | 2.48 | 1.49 | 1.44 |
| 29 | 6 | 618 | CHL | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 29 | 6 | 607 | CHL | C3D-C4D | -2.48 | 1.38 | 1.44 |
| 22 | A | 815 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | 4 | 602 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | A | 822 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | A | 854 | CLA | C1C-C2C | 2.47 | 1.49 | 1.44 |
| 22 | A | 835 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | B | 841 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | B | 832 | CLA | C4D-CHA | 2.47 | 1.47 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 5 | 602 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | 2 | 607 | CLA | C4C-C3C | 2.47 | 1.49 | 1.45 |
| 22 | 5 | 603 | CLA | C1B-NB | -2.47 | 1.33 | 1.35 |
| 22 | A | 802 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | A | 827 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | B | 807 | CLA | C3D-C4D | -2.47 | 1.38 | 1.44 |
| 22 | 3 | 603 | CLA | C1B-NB | -2.46 | 1.33 | 1.35 |
| 22 | 2 | 610 | CLA | C4B-CHC | 2.46 | 1.47 | 1.41 |
| 22 | Z | 613 | CLA | C1C-C2C | 2.46 | 1.49 | 1.44 |
| 22 | 6 | 609 | CLA | C4C-C3C | 2.46 | 1.49 | 1.45 |
| 22 | 8 | 610 | CLA | C3D-C4D | -2.46 | 1.38 | 1.44 |
| 22 | 1 | 612 | CLA | C1B-NB | -2.46 | 1.33 | 1.35 |
| 22 | 5 | 621 | CLA | C1B-NB | -2.46 | 1.33 | 1.35 |
| 22 | B | 814 | CLA | C4D-CHA | 2.46 | 1.47 | 1.38 |
| 22 | 2 | 614 | CLA | C4C-C3C | 2.46 | 1.49 | 1.45 |
| 29 | 1 | 601 | CHL | C1B-NB | -2.46 | 1.33 | 1.35 |
| 22 | 7 | 604 | CLA | C1B-CHB | 2.46 | 1.47 | 1.41 |
| 22 | G | 204 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 22 | 2 | 606 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 22 | B | 825 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |
| 22 | 7 | 611 | CLA | C1B-NB | -2.45 | 1.33 | 1.35 |
| 22 | A | 854 | CLA | C4D-CHA | 2.45 | 1.47 | 1.38 |
| 29 | 6 | 606 | CHL | C4B-CHC | 2.45 | 1.47 | 1.41 |
| 22 | A | 807 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |
| 22 | 7 | 602 | CLA | C4D-CHA | 2.45 | 1.47 | 1.38 |
| 22 | A | 815 | CLA | C4B-CHC | 2.45 | 1.47 | 1.41 |
| 22 | A | 827 | CLA | C4B-CHC | 2.45 | 1.47 | 1.41 |
| 22 | B | 838 | CLA | C3D-C4D | -2.45 | 1.38 | 1.44 |
| 22 | B | 852 | CLA | C4C-C3C | 2.45 | 1.49 | 1.45 |
| 29 | 6 | 618 | CHL | C2C-C1C | 2.45 | 1.49 | 1.44 |
| 22 | A | 832 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 22 | A | 811 | CLA | C4D-CHA | 2.44 | 1.47 | 1.38 |
| 22 | A | 828 | CLA | C4B-CHC | 2.44 | 1.47 | 1.41 |
| 22 | B | 829 | CLA | C4D-CHA | 2.44 | 1.47 | 1.38 |
| 22 | 8 | 606 | CLA | C4B-CHC | 2.44 | 1.47 | 1.41 |
| 22 | 3 | 614 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 22 | A | 835 | CLA | C4D-CHA | 2.44 | 1.47 | 1.38 |
| 24 | B | 851 | LHG | O8-C23 | 2.44 | 1.45 | 1.33 |
| 22 | B | 816 | CLA | C1C-C2C | 2.44 | 1.49 | 1.44 |
| 22 | B | 828 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 22 | A | 840 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 29 | 4 | 606 | CHL | C2C-C1C | 2.44 | 1.49 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 6 | 614 | CLA | C4D-CHA | 2.44 | 1.47 | 1.38 |
| 22 | B | 840 | CLA | C1B-NB | -2.44 | 1.33 | 1.35 |
| 22 | 7 | 609 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 22 | 6 | 602 | CLA | C1C-C2C | 2.44 | 1.49 | 1.44 |
| 22 | 5 | 613 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 22 | 7 | 614 | CLA | C4C-C3C | 2.44 | 1.49 | 1.45 |
| 22 | A | 825 | CLA | C3D-C4D | -2.44 | 1.38 | 1.44 |
| 22 | A | 808 | CLA | C1C-C2C | 2.43 | 1.49 | 1.44 |
| 22 | Z | 603 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 22 | A | 826 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 22 | B | 806 | CLA | C1C-C2C | 2.43 | 1.49 | 1.44 |
| 22 | 9 | 611 | CLA | C4B-CHC | 2.43 | 1.47 | 1.41 |
| 22 | 6 | 614 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 22 | 5 | 603 | CLA | OBD-CAD | 2.43 | 1.26 | 1.22 |
| 22 | A | 820 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 22 | 5 | 602 | CLA | C4D-CHA | 2.43 | 1.47 | 1.38 |
| 21 | A | 801 | CL0 | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 22 | Z | 604 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 22 | B | 820 | CLA | C4D-CHA | 2.43 | 1.47 | 1.38 |
| 22 | B | 837 | CLA | C4B-CHC | 2.43 | 1.47 | 1.41 |
| 22 | 8 | 602 | CLA | C4B-CHC | 2.43 | 1.47 | 1.41 |
| 22 | 2 | 607 | CLA | C4B-CHC | 2.43 | 1.47 | 1.41 |
| 22 | 9 | 613 | CLA | C4C-C3C | 2.43 | 1.49 | 1.45 |
| 29 | 4 | 608 | CHL | MG-NA | -2.43 | 2.00 | 2.06 |
| 22 | A | 814 | CLA | C3D-C4D | -2.43 | 1.38 | 1.44 |
| 22 | 7 | 606 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | 7 | 616 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 22 | 5 | 614 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 22 | A | 809 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | A | 819 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | Z | 616 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 22 | 8 | 608 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | A | 817 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 22 | B | 852 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | A | 810 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 22 | 3 | 611 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | B | 829 | CLA | C1B-CHB | 2.42 | 1.47 | 1.41 |
| 22 | Z | 606 | CLA | C4B-CHC | 2.42 | 1.47 | 1.41 |
| 22 | 8 | 606 | CLA | C3D-C4D | -2.42 | 1.38 | 1.44 |
| 22 | L | 203 | CLA | C4D-CHA | 2.42 | 1.47 | 1.38 |
| 22 | 1 | 616 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |
| 22 | 2 | 611 | CLA | C4C-C3C | 2.42 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 811 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | 1 | 603 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | B | 839 | CLA | C1B-NB | -2.41 | 1.33 | 1.35 |
| 22 | B | 834 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 22 | 2 | 606 | CLA | C4B-CHC | 2.41 | 1.47 | 1.41 |
| 22 | 7 | 608 | CLA | C1C-C2C | 2.41 | 1.49 | 1.44 |
| 22 | A | 816 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | 6 | 611 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 22 | B | 838 | CLA | C1B-CHB | 2.41 | 1.47 | 1.41 |
| 22 | 6 | 622 | CLA | C4C-C3C | 2.41 | 1.49 | 1.45 |
| 22 | B | 829 | CLA | C4B-CHC | 2.41 | 1.47 | 1.41 |
| 22 | F | 301 | CLA | C1C-C2C | 2.41 | 1.49 | 1.44 |
| 22 | A | 821 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | B | 822 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | 9 | 611 | CLA | C1C-C2C | 2.41 | 1.49 | 1.44 |
| 22 | B | 824 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | 1 | 606 | CLA | C1B-NB | -2.41 | 1.33 | 1.35 |
| 22 | B | 816 | CLA | C4B-CHC | 2.41 | 1.47 | 1.41 |
| 22 | 1 | 608 | CLA | C3D-C4D | -2.41 | 1.38 | 1.44 |
| 22 | 8 | 614 | CLA | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 22 | 7 | 601 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 22 | 2 | 610 | CLA | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 22 | B | 825 | CLA | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 22 | A | 805 | CLA | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 22 | B | 834 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 29 | 5 | 608 | CHL | C4D-CHA | 2.40 | 1.46 | 1.38 |
| 22 | B | 819 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 22 | 3 | 609 | CLA | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 22 | 2 | 614 | CLA | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 22 | B | 802 | CLA | C4D-CHA | 2.40 | 1.46 | 1.38 |
| 22 | 7 | 616 | CLA | C1D-C2D | 2.40 | 1.50 | 1.45 |
| 22 | 5 | 621 | CLA | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 22 | A | 813 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 29 | 9 | 606 | CHL | C2C-C1C | 2.40 | 1.49 | 1.44 |
| 22 | 9 | 603 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 22 | Z | 614 | CLA | C4B-CHC | 2.40 | 1.47 | 1.41 |
| 22 | B | 841 | CLA | C4D-CHA | 2.40 | 1.46 | 1.38 |
| 22 | 3 | 617 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 22 | 2 | 602 | CLA | C4C-C3C | 2.40 | 1.49 | 1.45 |
| 22 | 1 | 612 | CLA | C3D-C4D | -2.40 | 1.38 | 1.44 |
| 22 | 8 | 609 | CLA | C1B-NB | -2.40 | 1.33 | 1.35 |
| 22 | A | 827 | CLA | C4D-CHA | 2.40 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 7 | 601 | CLA | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 22 | Z | 603 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 22 | A | 812 | CLA | C4D-CHA | 2.39 | 1.46 | 1.38 |
| 22 | B | 804 | CLA | C1C-C2C | 2.39 | 1.49 | 1.44 |
| 22 | A | 802 | CLA | C4D-CHA | 2.39 | 1.46 | 1.38 |
| 22 | 5 | 606 | CLA | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 22 | A | 824 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 22 | 8 | 609 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 22 | A | 808 | CLA | C1B-NB | -2.39 | 1.33 | 1.35 |
| 22 | A | 838 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 22 | A | 815 | CLA | C4D-CHA | 2.39 | 1.46 | 1.38 |
| 22 | 6 | 613 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 22 | 4 | 609 | CLA | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 22 | 9 | 602 | CLA | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 22 | B | 813 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 22 | 1 | 603 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 22 | 5 | 602 | CLA | C1C-C2C | 2.39 | 1.49 | 1.44 |
| 22 | 1 | 611 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 22 | B | 828 | CLA | C4C-C3C | 2.39 | 1.49 | 1.45 |
| 22 | B | 841 | CLA | C4B-CHC | 2.39 | 1.47 | 1.41 |
| 22 | 8 | 608 | CLA | C3D-C4D | -2.39 | 1.38 | 1.44 |
| 22 | A | 837 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 22 | J | 3002 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 22 | 4 | 601 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 22 | 9 | 612 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 29 | 1 | 607 | CHL | C4D-CHA | 2.38 | 1.46 | 1.38 |
| 22 | 1 | 606 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 22 | A | 835 | CLA | C4B-CHC | 2.38 | 1.47 | 1.41 |
| 22 | F | 303 | CLA | C1C-NC | -2.38 | 1.34 | 1.37 |
| 22 | 9 | 601 | CLA | C4B-CHC | 2.38 | 1.47 | 1.41 |
| 29 | Z | 601 | CHL | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 22 | 4 | 614 | CLA | C4B-CHC | 2.38 | 1.47 | 1.41 |
| 22 | A | 825 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 22 | B | 808 | CLA | C4C-C3C | 2.38 | 1.49 | 1.45 |
| 22 | A | 808 | CLA | C3D-C4D | -2.38 | 1.38 | 1.44 |
| 22 | 8 | 601 | CLA | C1C-C2C | 2.38 | 1.49 | 1.44 |
| 22 | 7 | 610 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 22 | 7 | 601 | CLA | C1B-NB | -2.37 | 1.33 | 1.35 |
| 22 | B | 830 | CLA | C4B-CHC | 2.37 | 1.47 | 1.41 |
| 22 | 4 | 613 | CLA | C4C-C3C | 2.37 | 1.49 | 1.45 |
| 22 | K | 4002 | CLA | C4B-CHC | 2.37 | 1.47 | 1.41 |
| 22 | 7 | 608 | CLA | C1B-NB | -2.37 | 1.33 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | B | 809 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 22 | A | 836 | CLA | C4C-C3C | 2.37 | 1.49 | 1.45 |
| 22 | A | 833 | CLA | C4B-CHC | 2.37 | 1.47 | 1.41 |
| 22 | 7 | 613 | CLA | C1B-NB | -2.37 | 1.33 | 1.35 |
| 22 | 3 | 610 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 22 | B | 822 | CLA | C4B-CHC | 2.37 | 1.47 | 1.41 |
| 22 | A | 804 | CLA | C1B-NB | -2.37 | 1.33 | 1.35 |
| 22 | 7 | 602 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 22 | 7 | 620 | CLA | C4B-CHC | 2.37 | 1.47 | 1.41 |
| 22 | 7 | 612 | CLA | C3D-C4D | -2.37 | 1.38 | 1.44 |
| 29 | 9 | 606 | CHL | C3A-C2A | -2.36 | 1.52 | 1.54 |
| 22 | B | 818 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 22 | A | 813 | CLA | C1C-C2C | 2.36 | 1.49 | 1.44 |
| 22 | 6 | 604 | CLA | C1C-C2C | 2.36 | 1.49 | 1.44 |
| 22 | A | 813 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | B | 832 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 22 | 3 | 620 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | Z | 616 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | B | 817 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | 1 | 604 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | A | 830 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | B | 820 | CLA | C1B-CHB | 2.36 | 1.47 | 1.41 |
| 22 | 4 | 603 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | A | 802 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | 1 | 614 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | 5 | 616 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | 3 | 613 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 22 | Z | 611 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | 6 | 604 | CLA | C1B-NB | -2.36 | 1.33 | 1.35 |
| 22 | 8 | 611 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | A | 804 | CLA | C1C-NC | -2.36 | 1.34 | 1.37 |
| 29 | 4 | 608 | CHL | C4D-CHA | 2.36 | 1.46 | 1.38 |
| 22 | 8 | 601 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | B | 826 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 22 | F | 303 | CLA | C4B-CHC | 2.36 | 1.47 | 1.41 |
| 29 | 5 | 608 | CHL | C2C-C1C | 2.36 | 1.49 | 1.44 |
| 22 | A | 836 | CLA | C1B-NB | -2.36 | 1.33 | 1.35 |
| 22 | 8 | 601 | CLA | C1B-NB | -2.36 | 1.33 | 1.35 |
| 22 | K | 4002 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | 2 | 606 | CLA | C1C-C2C | 2.36 | 1.49 | 1.44 |
| 22 | 5 | 613 | CLA | C1B-NB | -2.36 | 1.33 | 1.35 |
| 22 | A | 839 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 7 | 620 | CLA | C4C-C3C | 2.36 | 1.49 | 1.45 |
| 22 | A | 833 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 22 | 3 | 602 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 22 | 6 | 613 | CLA | C3D-C4D | -2.36 | 1.38 | 1.44 |
| 22 | 2 | 601 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | B | 828 | CLA | C1C-NC | -2.35 | 1.34 | 1.37 |
| 29 | Z | 601 | CHL | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 22 | B | 825 | CLA | C4D-CHA | 2.35 | 1.46 | 1.38 |
| 22 | 7 | 611 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | B | 819 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | B | 808 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | 6 | 610 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | A | 811 | CLA | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 22 | A | 812 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | Z | 608 | CLA | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 22 | Z | 604 | CLA | C1B-NB | -2.35 | 1.33 | 1.35 |
| 22 | 5 | 609 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | 7 | 606 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | 8 | 613 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | 9 | 612 | CLA | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 22 | A | 803 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | B | 811 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | A | 805 | CLA | C1C-C2C | 2.35 | 1.49 | 1.44 |
| 22 | 1 | 611 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | 8 | 604 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | L | 203 | CLA | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 29 | 5 | 618 | CHL | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | 7 | 609 | CLA | C3D-C4D | -2.35 | 1.38 | 1.44 |
| 22 | 3 | 606 | CLA | C4B-CHC | 2.35 | 1.47 | 1.41 |
| 22 | A | 815 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | 3 | 612 | CLA | C4C-C3C | 2.35 | 1.49 | 1.45 |
| 22 | 1 | 602 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | 3 | 603 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | Z | 602 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | 8 | 616 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | 2 | 610 | CLA | C1C-C2C | 2.34 | 1.49 | 1.44 |
| 22 | 2 | 610 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | A | 817 | CLA | C4C-C3C | 2.34 | 1.49 | 1.45 |
| 22 | A | 838 | CLA | C1C-NC | -2.34 | 1.34 | 1.37 |
| 22 | B | 807 | CLA | C4C-C3C | 2.34 | 1.49 | 1.45 |
| 22 | B | 810 | CLA | C4C-C3C | 2.34 | 1.49 | 1.45 |
| 22 | 4 | 604 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 7 | 613 | CLA | C4C-C3C | 2.34 | 1.49 | 1.45 |
| 22 | 3 | 606 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | B | 832 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 22 | B | 826 | CLA | C1C-NC | -2.34 | 1.34 | 1.37 |
| 22 | 6 | 622 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 22 | B | 810 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | 1 | 604 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | 6 | 613 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 22 | B | 821 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | 4 | 612 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 22 | A | 836 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 22 | 8 | 602 | CLA | C3D-C4D | -2.34 | 1.38 | 1.44 |
| 22 | A | 805 | CLA | C4D-CHA | 2.34 | 1.46 | 1.38 |
| 22 | 4 | 612 | CLA | C1B-NB | -2.34 | 1.33 | 1.35 |
| 22 | 5 | 610 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 22 | 8 | 616 | CLA | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 29 | 4 | 608 | CHL | C4B-CHC | 2.34 | 1.47 | 1.41 |
| 29 | 9 | 607 | CHL | C2C-C1C | 2.34 | 1.49 | 1.44 |
| 22 | 8 | 601 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 22 | 8 | 610 | CLA | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 22 | A | 810 | CLA | C1B-NB | -2.33 | 1.33 | 1.35 |
| 22 | J | 3002 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 22 | A | 837 | CLA | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 22 | A | 810 | CLA | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 29 | 4 | 606 | CHL | C4D-CHA | 2.33 | 1.46 | 1.38 |
| 22 | 9 | 609 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 29 | 7 | 607 | CHL | C1B-NB | -2.33 | 1.33 | 1.35 |
| 22 | B | 827 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 22 | A | 819 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 22 | A | 835 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 22 | B | 820 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 29 | 3 | 608 | CHL | C4D-CHA | 2.33 | 1.46 | 1.38 |
| 22 | A | 802 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 22 | 5 | 606 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |
| 22 | 2 | 609 | CLA | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 22 | 9 | 610 | CLA | C1C-C2C | 2.33 | 1.49 | 1.44 |
| 22 | K | 4003 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 22 | Z | 613 | CLA | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 22 | B | 810 | CLA | C4B-CHC | 2.33 | 1.47 | 1.41 |
| 22 | 5 | 611 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 22 | A | 803 | CLA | C4B-NB | -2.33 | 1.33 | 1.35 |
| 22 | G | 203 | CLA | C3D-C4D | -2.33 | 1.38 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 5 | 617 | CLA | C4C-C3C | 2.33 | 1.49 | 1.45 |
| 22 | A | 807 | CLA | C1B-NB | -2.33 | 1.33 | 1.35 |
| 22 | F | 303 | CLA | C1B-NB | -2.33 | 1.33 | 1.35 |
| 22 | B | 839 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 22 | 5 | 601 | CLA | C3D-C4D | -2.32 | 1.38 | 1.44 |
| 22 | 5 | 617 | CLA | C3D-C4D | -2.32 | 1.38 | 1.44 |
| 22 | 6 | 610 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 22 | A | 815 | CLA | C1C-C2C | 2.32 | 1.49 | 1.44 |
| 22 | B | 837 | CLA | C3D-C4D | -2.32 | 1.38 | 1.44 |
| 22 | 6 | 612 | CLA | C3D-C4D | -2.32 | 1.38 | 1.44 |
| 22 | 6 | 604 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 22 | 5 | 611 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 29 | 8 | 607 | CHL | C1B-NB | -2.32 | 1.33 | 1.35 |
| 22 | 2 | 601 | CLA | C3D-C4D | -2.32 | 1.38 | 1.44 |
| 22 | A | 841 | CLA | C1C-C2C | 2.32 | 1.49 | 1.44 |
| 22 | 7 | 603 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 22 | 5 | 614 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 29 | 1 | 601 | CHL | C2C-C1C | 2.32 | 1.49 | 1.44 |
| 22 | A | 827 | CLA | C1C-C2C | 2.32 | 1.49 | 1.44 |
| 22 | 6 | 614 | CLA | C4C-C3C | 2.32 | 1.49 | 1.45 |
| 22 | B | 806 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 22 | A | 829 | CLA | C4B-CHC | 2.32 | 1.47 | 1.41 |
| 22 | 9 | 610 | CLA | C3D-C4D | -2.32 | 1.38 | 1.44 |
| 22 | B | 824 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 22 | L | 204 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 22 | 3 | 606 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 22 | Z | 604 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 22 | B | 814 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 22 | B | 821 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 22 | Z | 616 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 29 | Z | 607 | CHL | C4D-CHA | 2.31 | 1.46 | 1.38 |
| 22 | B | 811 | CLA | C1B-NB | -2.31 | 1.33 | 1.35 |
| 22 | 6 | 603 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 22 | 8 | 606 | CLA | C1B-NB | -2.31 | 1.33 | 1.35 |
| 29 | 6 | 607 | CHL | C4D-CHA | 2.31 | 1.46 | 1.38 |
| 22 | 2 | 603 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 22 | 8 | 612 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 22 | A | 845 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 22 | A | 827 | CLA | C1B-NB | -2.31 | 1.33 | 1.35 |
| 22 | A | 834 | CLA | C3D-C4D | -2.31 | 1.39 | 1.44 |
| 22 | 9 | 610 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 22 | A | 818 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | B | 840 | CLA | C4C-C3C | 2.31 | 1.49 | 1.45 |
| 22 | B | 841 | CLA | C1C-C2C | 2.31 | 1.49 | 1.44 |
| 22 | 5 | 601 | CLA | C4B-CHC | 2.31 | 1.47 | 1.41 |
| 22 | B | 841 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 22 | B | 830 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 22 | 3 | 609 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | 6 | 602 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | 1 | 614 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | 3 | 611 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 22 | 2 | 607 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 22 | A | 845 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | 2 | 611 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | 1 | 602 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 22 | 3 | 602 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 29 | 6 | 606 | CHL | C4D-CHA | 2.30 | 1.46 | 1.38 |
| 22 | 4 | 604 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 22 | A | 811 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | Z | 609 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 29 | 1 | 601 | CHL | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | A | 845 | CLA | C1B-NB | -2.30 | 1.33 | 1.35 |
| 22 | 4 | 609 | CLA | C1B-NB | -2.30 | 1.33 | 1.35 |
| 22 | 9 | 611 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 22 | 1 | 606 | CLA | C1C-C2C | 2.30 | 1.49 | 1.44 |
| 22 | B | 831 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | 7 | 613 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | A | 823 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | A | 842 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 29 | 1 | 607 | CHL | C1B-NB | -2.30 | 1.33 | 1.35 |
| 22 | Z | 614 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 22 | 1 | 608 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | F | 304 | CLA | C4C-C3C | 2.30 | 1.49 | 1.45 |
| 22 | K | 4003 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | G | 204 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 29 | 4 | 606 | CHL | C1B-NB | -2.30 | 1.33 | 1.35 |
| 22 | A | 836 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | A | 818 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | B | 833 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | F | 304 | CLA | C3D-C4D | -2.30 | 1.39 | 1.44 |
| 22 | 9 | 604 | CLA | C4B-CHC | 2.30 | 1.47 | 1.41 |
| 22 | 8 | 616 | CLA | C1C-C2C | 2.29 | 1.49 | 1.44 |
| 22 | B | 804 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | A | 841 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 3 | 614 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 29 | 7 | 607 | CHL | C4D-CHA | 2.29 | 1.46 | 1.38 |
| 22 | 1 | 613 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 22 | 9 | 614 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | 7 | 614 | CLA | C1B-NB | -2.29 | 1.33 | 1.35 |
| 22 | A | 837 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 22 | 1 | 616 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | Z | 614 | CLA | C1C-C2C | 2.29 | 1.49 | 1.44 |
| 22 | 6 | 612 | CLA | C1C-C2C | 2.29 | 1.49 | 1.44 |
| 22 | B | 839 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 22 | B | 817 | CLA | C1C-NC | -2.29 | 1.34 | 1.37 |
| 22 | J | 3002 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | B | 837 | CLA | C1C-C2C | 2.29 | 1.49 | 1.44 |
| 22 | 7 | 616 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | A | 829 | CLA | C4B-NB | -2.29 | 1.33 | 1.35 |
| 22 | 4 | 611 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 29 | 5 | 608 | CHL | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | A | 829 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 22 | 5 | 612 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 22 | 5 | 612 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 22 | 8 | 604 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 22 | A | 814 | CLA | C1B-NB | -2.29 | 1.33 | 1.35 |
| 22 | B | 806 | CLA | C1B-NB | -2.29 | 1.33 | 1.35 |
| 22 | 6 | 611 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | 6 | 612 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | 6 | 604 | CLA | C4C-C3C | 2.29 | 1.49 | 1.45 |
| 22 | 4 | 602 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | A | 839 | CLA | C1B-NB | -2.29 | 1.33 | 1.35 |
| 22 | A | 831 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 22 | B | 841 | CLA | C1B-CHB | 2.29 | 1.47 | 1.41 |
| 22 | 3 | 614 | CLA | C4B-CHC | 2.29 | 1.47 | 1.41 |
| 22 | 5 | 601 | CLA | C1B-NB | -2.29 | 1.33 | 1.35 |
| 22 | 4 | 616 | CLA | C3D-C4D | -2.29 | 1.39 | 1.44 |
| 22 | 9 | 601 | CLA | C1C-C2C | 2.29 | 1.49 | 1.44 |
| 22 | A | 817 | CLA | C1B-CHB | 2.28 | 1.47 | 1.41 |
| 22 | B | 802 | CLA | C4B-CHC | 2.28 | 1.47 | 1.41 |
| 22 | 9 | 603 | CLA | C4B-CHC | 2.28 | 1.47 | 1.41 |
| 22 | A | 832 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 22 | B | 831 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 22 | 8 | 613 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 22 | A | 809 | CLA | C1B-NB | -2.28 | 1.33 | 1.35 |
| 22 | 3 | 620 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | 1 | 601 | CHL | C4D-CHA | 2.28 | 1.46 | 1.38 |
| 22 | B | 805 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | Z | 606 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | B | 822 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 22 | A | 832 | CLA | C4C-C3C | 2.28 | 1.49 | 1.45 |
| 22 | 6 | 601 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | 8 | 604 | CLA | C1B-NB | -2.28 | 1.33 | 1.35 |
| 22 | 5 | 604 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 29 | 5 | 607 | CHL | C4D-CHA | 2.28 | 1.46 | 1.38 |
| 22 | 5 | 613 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | B | 808 | CLA | C1C-NC | -2.28 | 1.34 | 1.37 |
| 22 | B | 820 | CLA | C4B-CHC | 2.28 | 1.47 | 1.41 |
| 22 | 5 | 614 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | 6 | 622 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 29 | 7 | 607 | CHL | C4C-C3C | 2.28 | 1.49 | 1.45 |
| 22 | 6 | 609 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | 2 | 614 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 22 | G | 203 | CLA | C4C-C3C | 2.28 | 1.49 | 1.45 |
| 22 | 3 | 617 | CLA | C4C-C3C | 2.28 | 1.49 | 1.45 |
| 22 | Z | 611 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | A | 826 | CLA | C1B-NB | -2.28 | 1.33 | 1.35 |
| 22 | A | 802 | CLA | C1B-CHB | 2.28 | 1.47 | 1.41 |
| 22 | A | 828 | CLA | C1C-C2C | 2.28 | 1.49 | 1.44 |
| 22 | A | 823 | CLA | C3D-C4D | -2.28 | 1.39 | 1.44 |
| 22 | 4 | 614 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 22 | B | 835 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | A | 814 | CLA | C4C-C3C | 2.27 | 1.49 | 1.45 |
| 22 | 7 | 614 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | 3 | 612 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 22 | 4 | 601 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 22 | A | 845 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |
| 22 | 6 | 617 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 22 | A | 803 | CLA | C4C-C3C | 2.27 | 1.49 | 1.45 |
| 22 | 7 | 604 | CLA | C1C-C2C | 2.27 | 1.49 | 1.44 |
| 22 | A | 822 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | 1 | 604 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | A | 823 | CLA | C4C-C3C | 2.27 | 1.48 | 1.45 |
| 22 | 6 | 616 | CLA | C4C-C3C | 2.27 | 1.48 | 1.45 |
| 22 | 8 | 602 | CLA | C1C-C2C | 2.27 | 1.49 | 1.44 |
| 22 | 1 | 609 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | 9 | 609 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | A | 814 | CLA | C1C-NC | -2.27 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 5 | 610 | CLA | C3D-C4D | -2.27 | 1.39 | 1.44 |
| 22 | 2 | 601 | CLA | C4B-CHC | 2.27 | 1.47 | 1.41 |
| 22 | B | 834 | CLA | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 22 | 2 | 614 | CLA | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 22 | A | 832 | CLA | C1B-NB | -2.26 | 1.33 | 1.35 |
| 22 | 2 | 602 | CLA | C1C-C2C | 2.26 | 1.48 | 1.44 |
| 22 | 8 | 608 | CLA | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 22 | 1 | 609 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 22 | 3 | 607 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 22 | 4 | 610 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 22 | A | 843 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 22 | 9 | 610 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 22 | 1 | 603 | CLA | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 22 | 5 | 617 | CLA | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 22 | 4 | 612 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 22 | 3 | 617 | CLA | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 22 | A | 826 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 22 | 6 | 617 | CLA | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 22 | 6 | 614 | CLA | C1C-C2C | 2.26 | 1.48 | 1.44 |
| 22 | 9 | 602 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 22 | 2 | 613 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 22 | B | 833 | CLA | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 22 | 1 | 612 | CLA | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 22 | A | 839 | CLA | C3D-C4D | -2.26 | 1.39 | 1.44 |
| 22 | 8 | 609 | CLA | C4C-C3C | 2.26 | 1.48 | 1.45 |
| 22 | A | 835 | CLA | C1B-CHB | 2.26 | 1.47 | 1.41 |
| 22 | A | 816 | CLA | C1C-C2C | 2.26 | 1.48 | 1.44 |
| 22 | 2 | 602 | CLA | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 29 | 9 | 607 | CHL | C4B-CHC | 2.26 | 1.47 | 1.41 |
| 22 | B | 813 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | A | 845 | CLA | C4C-C3C | 2.25 | 1.48 | 1.45 |
| 29 | 5 | 607 | CHL | C1C-NC | -2.25 | 1.34 | 1.37 |
| 22 | Z | 606 | CLA | C4C-C3C | 2.25 | 1.48 | 1.45 |
| 22 | 5 | 606 | CLA | C1B-NB | -2.25 | 1.33 | 1.35 |
| 29 | 4 | 618 | CHL | C4D-CHA | 2.25 | 1.46 | 1.38 |
| 22 | F | 304 | CLA | C4B-CHC | 2.25 | 1.47 | 1.41 |
| 22 | A | 806 | CLA | C4C-C3C | 2.25 | 1.48 | 1.45 |
| 22 | B | 812 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | 9 | 602 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | A | 843 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | 6 | 611 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | A | 828 | CLA | C1C-NC | -2.25 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 2 | 613 | CLA | C4B-CHC | 2.25 | 1.47 | 1.41 |
| 22 | A | 832 | CLA | C4B-CHC | 2.25 | 1.47 | 1.41 |
| 22 | 8 | 603 | CLA | C4C-C3C | 2.25 | 1.48 | 1.45 |
| 22 | 1 | 611 | CLA | C4B-CHC | 2.25 | 1.47 | 1.41 |
| 29 | 3 | 608 | CHL | C2C-C1C | 2.25 | 1.49 | 1.44 |
| 22 | B | 852 | CLA | C1C-C2C | 2.25 | 1.48 | 1.44 |
| 29 | 8 | 607 | CHL | C1C-NC | -2.25 | 1.34 | 1.37 |
| 22 | 7 | 604 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | 4 | 609 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | 5 | 616 | CLA | C4B-CHC | 2.25 | 1.47 | 1.41 |
| 22 | A | 811 | CLA | C1B-NB | -2.25 | 1.33 | 1.35 |
| 22 | Z | 603 | CLA | C1B-NB | -2.25 | 1.33 | 1.35 |
| 22 | B | 815 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 22 | L | 203 | CLA | C1C-C2C | 2.25 | 1.48 | 1.44 |
| 22 | 2 | 612 | CLA | C3D-C4D | -2.25 | 1.39 | 1.44 |
| 29 | 9 | 607 | CHL | C4D-CHA | 2.25 | 1.46 | 1.38 |
| 22 | 3 | 617 | CLA | C1B-NB | -2.24 | 1.33 | 1.35 |
| 22 | 1 | 616 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 22 | B | 823 | CLA | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 29 | 4 | 606 | CHL | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 22 | 2 | 613 | CLA | C1C-C2C | 2.24 | 1.48 | 1.44 |
| 22 | B | 815 | CLA | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 22 | 3 | 611 | CLA | C1B-CHB | 2.24 | 1.47 | 1.41 |
| 29 | 4 | 618 | CHL | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 22 | 4 | 604 | CLA | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 29 | 9 | 606 | CHL | C4D-CHA | 2.24 | 1.46 | 1.38 |
| 22 | B | 821 | CLA | C4C-C3C | 2.24 | 1.48 | 1.45 |
| 22 | A | 811 | CLA | C1C-C2C | 2.24 | 1.48 | 1.44 |
| 22 | Z | 616 | CLA | C1B-CHB | 2.24 | 1.47 | 1.41 |
| 22 | 8 | 616 | CLA | C1B-CHB | 2.24 | 1.47 | 1.41 |
| 22 | Z | 610 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 22 | 8 | 608 | CLA | C1C-C2C | 2.24 | 1.48 | 1.44 |
| 22 | G | 203 | CLA | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 22 | 6 | 614 | CLA | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 22 | Z | 612 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 22 | A | 824 | CLA | C1B-NB | -2.24 | 1.33 | 1.35 |
| 29 | 6 | 608 | CHL | C1B-NB | -2.24 | 1.33 | 1.35 |
| 22 | 5 | 610 | CLA | C1C-C2C | 2.24 | 1.48 | 1.44 |
| 22 | Z | 609 | CLA | C1B-NB | -2.24 | 1.33 | 1.35 |
| 22 | 2 | 607 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 22 | 3 | 609 | CLA | C4B-CHC | 2.24 | 1.47 | 1.41 |
| 22 | B | 835 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | A | 809 | CLA | C3D-C4D | -2.24 | 1.39 | 1.44 |
| 22 | B | 822 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | L | 204 | CLA | C1B-CHB | 2.23 | 1.47 | 1.41 |
| 22 | A | 828 | CLA | C1B-NB | -2.23 | 1.33 | 1.35 |
| 22 | A | 812 | CLA | C4B-CHC | 2.23 | 1.47 | 1.41 |
| 22 | 1 | 616 | CLA | C1B-CHB | 2.23 | 1.47 | 1.41 |
| 22 | A | 824 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | B | 813 | CLA | C1C-NC | -2.23 | 1.34 | 1.37 |
| 22 | 3 | 614 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 22 | 4 | 610 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | 1 | 610 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 22 | A | 813 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | 3 | 620 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | 5 | 606 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | 2 | 614 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 22 | 8 | 612 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 29 | 1 | 607 | CHL | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 22 | 5 | 610 | CLA | C1B-NB | -2.23 | 1.33 | 1.35 |
| 22 | 4 | 614 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | 6 | 617 | CLA | C4C-C3C | 2.23 | 1.48 | 1.45 |
| 22 | A | 812 | CLA | C1C-NC | -2.23 | 1.34 | 1.37 |
| 22 | 4 | 611 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 22 | 9 | 612 | CLA | C1B-CHB | 2.23 | 1.47 | 1.41 |
| 22 | 6 | 610 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 22 | Z | 612 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 22 | 6 | 612 | CLA | C1B-NB | -2.23 | 1.33 | 1.35 |
| 29 | 4 | 618 | CHL | C2C-C1C | 2.23 | 1.49 | 1.44 |
| 22 | K | 4002 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 22 | 9 | 609 | CLA | C3D-C4D | -2.23 | 1.39 | 1.44 |
| 22 | B | 838 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 22 | 5 | 617 | CLA | C1C-C2C | 2.23 | 1.48 | 1.44 |
| 22 | Z | 608 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 22 | B | 832 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |
| 22 | 9 | 611 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 22 | 9 | 611 | CLA | C1B-CHB | 2.22 | 1.47 | 1.41 |
| 22 | B | 833 | CLA | C4C-C3C | 2.22 | 1.48 | 1.45 |
| 22 | 1 | 609 | CLA | C1B-NB | -2.22 | 1.33 | 1.35 |
| 22 | 8 | 616 | CLA | C1B-NB | -2.22 | 1.33 | 1.35 |
| 22 | A | 804 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 5 | 609 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | B | 827 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |
| 22 | K | 4002 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 7 | 604 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | Z | 612 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 3 | 604 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 22 | Z | 614 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 22 | 9 | 613 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 5 | 601 | CLA | C4C-C3C | 2.22 | 1.48 | 1.45 |
| 22 | Z | 602 | CLA | C1B-NB | -2.22 | 1.33 | 1.35 |
| 22 | 9 | 613 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |
| 22 | B | 821 | CLA | C1B-CHB | 2.22 | 1.47 | 1.41 |
| 22 | A | 831 | CLA | C4C-C3C | 2.22 | 1.48 | 1.45 |
| 22 | 1 | 609 | CLA | C3D-C4D | -2.22 | 1.39 | 1.44 |
| 22 | B | 820 | CLA | C1C-C2C | 2.22 | 1.48 | 1.44 |
| 29 | Z | 607 | CHL | C4C-C3C | 2.22 | 1.48 | 1.45 |
| 22 | 3 | 612 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 4 | 616 | CLA | C1B-CHB | 2.22 | 1.47 | 1.41 |
| 22 | B | 819 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 29 | 9 | 606 | CHL | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 1 | 613 | CLA | C1B-NB | -2.22 | 1.33 | 1.35 |
| 22 | 9 | 604 | CLA | C1B-NB | -2.22 | 1.33 | 1.35 |
| 22 | A | 817 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 8 | 603 | CLA | C4B-CHC | 2.22 | 1.47 | 1.41 |
| 22 | 3 | 607 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | 5 | 606 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 4 | 602 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 1 | 613 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 22 | 5 | 609 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 22 | A | 804 | CLA | C4D-CHA | 2.21 | 1.46 | 1.38 |
| 22 | 4 | 616 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | F | 301 | CLA | C1B-NB | -2.21 | 1.33 | 1.35 |
| 22 | 8 | 609 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | A | 835 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | B | 821 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 8 | 614 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 7 | 620 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 9 | 614 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | A | 815 | CLA | C1B-CHB | 2.21 | 1.47 | 1.41 |
| 22 | 7 | 609 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | A | 834 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | K | 4003 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | 7 | 604 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 22 | Z | 616 | CLA | C1B-NB | -2.21 | 1.33 | 1.35 |
| 22 | 5 | 621 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A | 841 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 22 | 8 | 611 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | 3 | 617 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | B | 814 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | B | 827 | CLA | C4B-CHC | 2.21 | 1.47 | 1.41 |
| 22 | 8 | 603 | CLA | C1B-CHB | 2.21 | 1.47 | 1.41 |
| 22 | 8 | 614 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 22 | Z | 606 | CLA | C1B-NB | -2.21 | 1.33 | 1.35 |
| 22 | 5 | 617 | CLA | C1B-NB | -2.21 | 1.33 | 1.35 |
| 22 | L | 203 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 22 | A | 833 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 2 | 609 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 2 | 602 | CLA | C3D-C4D | -2.21 | 1.39 | 1.44 |
| 22 | 3 | 612 | CLA | C1C-NC | -2.21 | 1.34 | 1.37 |
| 22 | 9 | 602 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | 3 | 602 | CLA | C1C-C2C | 2.21 | 1.48 | 1.44 |
| 22 | B | 836 | CLA | C4C-C3C | 2.21 | 1.48 | 1.45 |
| 22 | 8 | 612 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 7 | 602 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 29 | 6 | 618 | CHL | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 29 | 5 | 618 | CHL | C1B-NB | -2.20 | 1.33 | 1.35 |
| 22 | Z | 616 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 22 | 3 | 613 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 22 | 6 | 622 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 22 | L | 204 | CLA | C3D-C4D | -2.20 | 1.39 | 1.44 |
| 22 | 3 | 607 | CLA | C4C-C3C | 2.20 | 1.48 | 1.45 |
| 22 | 7 | 611 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | Z | 604 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 4 | 601 | CLA | C1B-CHB | 2.20 | 1.47 | 1.41 |
| 22 | 5 | 612 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | A | 824 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 2 | 607 | CLA | C1B-CHB | 2.20 | 1.47 | 1.41 |
| 22 | 4 | 603 | CLA | C1B-NB | -2.20 | 1.33 | 1.35 |
| 22 | 3 | 604 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | A | 840 | CLA | C4C-C3C | 2.20 | 1.48 | 1.45 |
| 22 | 5 | 613 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 4 | 609 | CLA | C1C-NC | -2.20 | 1.34 | 1.37 |
| 22 | B | 807 | CLA | C1B-NB | -2.20 | 1.33 | 1.35 |
| 22 | A | 807 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 5 | 603 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 9 | 612 | CLA | C3D-C4D | -2.20 | 1.39 | 1.44 |
| 22 | 6 | 601 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 5 | 614 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 22 | 2 | 612 | CLA | C4B-CHC | 2.20 | 1.47 | 1.41 |
| 22 | 6 | 612 | CLA | C4C-C3C | 2.20 | 1.48 | 1.45 |
| 22 | 7 | 609 | CLA | C1C-C2C | 2.20 | 1.48 | 1.44 |
| 22 | 9 | 604 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 22 | B | 834 | CLA | C1C-C2C | 2.19 | 1.48 | 1.44 |
| 22 | 5 | 601 | CLA | C1C-C2C | 2.19 | 1.48 | 1.44 |
| 22 | A | 840 | CLA | C4B-CHC | 2.19 | 1.47 | 1.41 |
| 22 | A | 807 | CLA | C1C-NC | -2.19 | 1.34 | 1.37 |
| 22 | 7 | 612 | CLA | C4C-C3C | 2.19 | 1.48 | 1.45 |
| 29 | 5 | 618 | CHL | C4D-CHA | 2.19 | 1.46 | 1.38 |
| 22 | 4 | 610 | CLA | C4B-CHC | 2.19 | 1.47 | 1.41 |
| 22 | 2 | 612 | CLA | C1B-CHB | 2.19 | 1.47 | 1.41 |
| 22 | 9 | 604 | CLA | C1C-C2C | 2.19 | 1.48 | 1.44 |
| 22 | 9 | 612 | CLA | C1C-C2C | 2.19 | 1.48 | 1.44 |
| 22 | B | 812 | CLA | C1B-NB | -2.19 | 1.33 | 1.35 |
| 22 | L | 203 | CLA | C1B-CHB | 2.19 | 1.47 | 1.41 |
| 29 | 1 | 607 | CHL | C4B-CHC | 2.19 | 1.47 | 1.41 |
| 22 | 5 | 616 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 22 | L | 203 | CLA | C4C-C3C | 2.19 | 1.48 | 1.45 |
| 22 | 6 | 609 | CLA | C4B-CHC | 2.19 | 1.47 | 1.41 |
| 22 | A | 839 | CLA | C1C-C2C | 2.19 | 1.48 | 1.44 |
| 22 | 8 | 613 | CLA | C4B-CHC | 2.19 | 1.47 | 1.41 |
| 22 | 1 | 608 | CLA | C1B-CHB | 2.19 | 1.47 | 1.41 |
| 22 | 3 | 607 | CLA | C1B-NB | -2.19 | 1.33 | 1.35 |
| 22 | A | 839 | CLA | C4B-CHC | 2.19 | 1.47 | 1.41 |
| 22 | A | 837 | CLA | C1C-C2C | 2.19 | 1.48 | 1.44 |
| 22 | B | 812 | CLA | C4C-C3C | 2.19 | 1.48 | 1.45 |
| 22 | 6 | 616 | CLA | C3D-C4D | -2.19 | 1.39 | 1.44 |
| 22 | 8 | 610 | CLA | C4B-NB | -2.18 | 1.33 | 1.35 |
| 22 | 9 | 603 | CLA | C1B-NB | -2.18 | 1.33 | 1.35 |
| 22 | A | 830 | CLA | C1C-NC | -2.18 | 1.34 | 1.37 |
| 29 | 6 | 607 | CHL | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 22 | 8 | 611 | CLA | C1B-NB | -2.18 | 1.33 | 1.35 |
| 22 | K | 4003 | CLA | C1B-CHB | 2.18 | 1.47 | 1.41 |
| 22 | 3 | 620 | CLA | C1B-CHB | 2.18 | 1.47 | 1.41 |
| 22 | 8 | 606 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 22 | 2 | 611 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 22 | A | 805 | CLA | C1B-CHB | 2.18 | 1.47 | 1.41 |
| 29 | 5 | 608 | CHL | C1B-NB | -2.18 | 1.33 | 1.35 |
| 22 | 6 | 604 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 22 | 1 | 604 | CLA | C1B-NB | -2.18 | 1.33 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | Z | 607 | CHL | C4B-CHC | 2.18 | 1.47 | 1.41 |
| 22 | 3 | 604 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 29 | 8 | 607 | CHL | C4B-CHC | 2.18 | 1.47 | 1.41 |
| 22 | A | 830 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 22 | 8 | 612 | CLA | C1C-NC | -2.18 | 1.34 | 1.37 |
| 22 | Z | 611 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 22 | 2 | 601 | CLA | C1B-CHB | 2.18 | 1.47 | 1.41 |
| 22 | Z | 602 | CLA | C1C-C2C | 2.18 | 1.48 | 1.44 |
| 22 | G | 204 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 22 | 3 | 603 | CLA | C4C-C3C | 2.18 | 1.48 | 1.45 |
| 22 | A | 834 | CLA | C1B-NB | -2.18 | 1.33 | 1.35 |
| 22 | A | 823 | CLA | C1B-CHB | 2.18 | 1.47 | 1.41 |
| 22 | B | 804 | CLA | C3D-C4D | -2.18 | 1.39 | 1.44 |
| 22 | 3 | 611 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 8 | 611 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 8 | 614 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | A | 838 | CLA | C4B-CHC | 2.17 | 1.47 | 1.41 |
| 22 | 3 | 603 | CLA | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | 4 | 613 | CLA | C4B-CHC | 2.17 | 1.47 | 1.41 |
| 22 | 1 | 614 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 1 | 612 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 22 | A | 843 | CLA | C4B-CHC | 2.17 | 1.47 | 1.41 |
| 29 | 6 | 618 | CHL | C4D-CHA | 2.17 | 1.46 | 1.38 |
| 21 | A | 801 | CL0 | C1C-NC | -2.17 | 1.34 | 1.37 |
| 22 | 8 | 604 | CLA | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | A | 805 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 22 | B | 830 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 22 | 7 | 612 | CLA | C4B-CHC | 2.17 | 1.47 | 1.41 |
| 22 | 7 | 611 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 3 | 607 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 22 | 7 | 616 | CLA | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | 9 | 613 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 1 | 608 | CLA | C1C-C2C | 2.17 | 1.48 | 1.44 |
| 22 | 6 | 613 | CLA | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | A | 854 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 6 | 616 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 22 | Z | 608 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 22 | Z | 611 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 22 | Z | 612 | CLA | C4C-C3C | 2.17 | 1.48 | 1.45 |
| 29 | Z | 607 | CHL | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | B | 823 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | A | 815 | CLA | C1D-C2D | 2.17 | 1.49 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 9 | 601 | CLA | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | F | 303 | CLA | C3D-C4D | -2.17 | 1.39 | 1.44 |
| 22 | 8 | 606 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 22 | 4 | 601 | CLA | C1C-NC | -2.17 | 1.34 | 1.37 |
| 22 | A | 818 | CLA | C1B-NB | -2.17 | 1.33 | 1.35 |
| 22 | 2 | 611 | CLA | C1B-CHB | 2.17 | 1.47 | 1.41 |
| 22 | A | 821 | CLA | C4B-CHC | 2.17 | 1.47 | 1.41 |
| 29 | 8 | 607 | CHL | C4D-CHA | 2.17 | 1.46 | 1.38 |
| 22 | 5 | 612 | CLA | C1C-NC | -2.16 | 1.34 | 1.37 |
| 22 | 2 | 606 | CLA | C3D-C4D | -2.16 | 1.39 | 1.44 |
| 22 | 8 | 613 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 22 | B | 841 | CLA | C1D-C2D | 2.16 | 1.49 | 1.45 |
| 22 | Z | 608 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 29 | 4 | 607 | CHL | C4B-CHC | 2.16 | 1.47 | 1.41 |
| 22 | 3 | 602 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 22 | 3 | 609 | CLA | C1B-NB | -2.16 | 1.33 | 1.35 |
| 22 | B | 811 | CLA | C4B-CHC | 2.16 | 1.47 | 1.41 |
| 22 | B | 825 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 22 | 1 | 613 | CLA | C1B-CHB | 2.16 | 1.47 | 1.41 |
| 22 | Z | 608 | CLA | C1B-CHB | 2.16 | 1.47 | 1.41 |
| 29 | 9 | 607 | CHL | C1B-CHB | 2.16 | 1.47 | 1.41 |
| 22 | 2 | 611 | CLA | C3D-C4D | -2.16 | 1.39 | 1.44 |
| 22 | 6 | 601 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 22 | A | 825 | CLA | C1B-NB | -2.16 | 1.33 | 1.35 |
| 22 | A | 812 | CLA | C1A-CHA | 2.16 | 1.52 | 1.43 |
| 22 | A | 840 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 22 | B | 813 | CLA | C4B-CHC | 2.16 | 1.47 | 1.41 |
| 22 | 2 | 612 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 25 | A | 851 | BCR | C21-C22 | -2.16 | 1.32 | 1.35 |
| 22 | 7 | 616 | CLA | C3D-C4D | -2.16 | 1.39 | 1.44 |
| 22 | 7 | 603 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 22 | 2 | 603 | CLA | C4B-CHC | 2.16 | 1.47 | 1.41 |
| 22 | 7 | 606 | CLA | C1C-NC | -2.16 | 1.34 | 1.37 |
| 22 | 1 | 613 | CLA | C4B-CHC | 2.16 | 1.47 | 1.41 |
| 22 | 6 | 611 | CLA | C1B-NB | -2.16 | 1.33 | 1.35 |
| 22 | 1 | 616 | CLA | C1C-C2C | 2.16 | 1.48 | 1.44 |
| 22 | 6 | 610 | CLA | C4C-C3C | 2.16 | 1.48 | 1.45 |
| 29 | 4 | 607 | CHL | C4D-CHA | 2.16 | 1.46 | 1.38 |
| 22 | 3 | 606 | CLA | C1B-NB | -2.16 | 1.33 | 1.35 |
| 22 | 4 | 613 | CLA | C3D-C4D | -2.16 | 1.39 | 1.44 |
| 22 | A | 812 | CLA | C1B-NB | -2.15 | 1.33 | 1.35 |
| 22 | A | 843 | CLA | C1B-NB | -2.15 | 1.33 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 29 | 4 | 607 | CHL | C2C-C1C | 2.15 | 1.49 | 1.44 |
| 29 | 1 | 607 | CHL | C2C-C1C | 2.15 | 1.49 | 1.44 |
| 22 | A | 838 | CLA | C1B-NB | -2.15 | 1.33 | 1.35 |
| 22 | 6 | 604 | CLA | C1B-CHB | 2.15 | 1.47 | 1.41 |
| 22 | B | 810 | CLA | C1B-CHB | 2.15 | 1.47 | 1.41 |
| 22 | B | 852 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 22 | A | 833 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 22 | B | 803 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 29 | 8 | 607 | CHL | C1B-CHB | 2.15 | 1.47 | 1.41 |
| 22 | 8 | 614 | CLA | C1B-NB | -2.15 | 1.33 | 1.35 |
| 22 | 9 | 614 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 22 | 3 | 620 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 22 | B | 837 | CLA | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 22 | A | 823 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 22 | B | 802 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 22 | 9 | 609 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 22 | B | 822 | CLA | C1B-NB | -2.15 | 1.33 | 1.35 |
| 22 | 3 | 613 | CLA | C1B-NB | -2.15 | 1.33 | 1.35 |
| 22 | A | 843 | CLA | C1B-CHB | 2.15 | 1.47 | 1.41 |
| 22 | B | 803 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 22 | 7 | 620 | CLA | C3D-C4D | -2.15 | 1.39 | 1.44 |
| 22 | A | 824 | CLA | C1B-CHB | 2.15 | 1.47 | 1.41 |
| 22 | B | 808 | CLA | C4B-CHC | 2.15 | 1.47 | 1.41 |
| 29 | 6 | 618 | CHL | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 22 | Z | 604 | CLA | C1C-C2C | 2.15 | 1.48 | 1.44 |
| 29 | 1 | 601 | CHL | C4C-C3C | 2.15 | 1.48 | 1.45 |
| 22 | 5 | 604 | CLA | C4B-CHC | 2.14 | 1.47 | 1.41 |
| 22 | 8 | 602 | CLA | C1B-CHB | 2.14 | 1.47 | 1.41 |
| 22 | 8 | 601 | CLA | C1B-CHB | 2.14 | 1.47 | 1.41 |
| 22 | K | 4002 | CLA | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | 9 | 613 | CLA | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | B | 836 | CLA | C4B-CHC | 2.14 | 1.46 | 1.41 |
| 22 | A | 802 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 22 | 8 | 606 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 22 | 6 | 617 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 22 | A | 810 | CLA | C4C-C3C | 2.14 | 1.48 | 1.45 |
| 22 | 3 | 603 | CLA | C4B-CHC | 2.14 | 1.46 | 1.41 |
| 29 | 6 | 608 | CHL | C4D-CHA | 2.14 | 1.46 | 1.38 |
| 22 | 8 | 616 | CLA | C4C-C3C | 2.14 | 1.48 | 1.45 |
| 22 | 6 | 609 | CLA | C1B-NB | -2.14 | 1.33 | 1.35 |
| 22 | G | 204 | CLA | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | B | 833 | CLA | C4B-CHC | 2.14 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 7 | 601 | CLA | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | Z | 612 | CLA | C1B-NB | -2.14 | 1.33 | 1.35 |
| 22 | Z | 613 | CLA | C3D-C4D | -2.14 | 1.39 | 1.44 |
| 22 | 2 | 603 | CLA | C1C-C2C | 2.14 | 1.48 | 1.44 |
| 29 | 4 | 607 | CHL | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | 2 | 606 | CLA | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | 7 | 620 | CLA | C1B-CHB | 2.14 | 1.46 | 1.41 |
| 22 | B | 827 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 22 | 6 | 613 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 28 | 9 | 620 | LMG | O4-C4 | -2.13 | 1.37 | 1.43 |
| 22 | A | 807 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 22 | A | 803 | CLA | C4B-CHC | 2.13 | 1.46 | 1.41 |
| 22 | 6 | 603 | CLA | C4B-CHC | 2.13 | 1.46 | 1.41 |
| 29 | 6 | 607 | CHL | C4B-CHC | 2.13 | 1.46 | 1.41 |
| 22 | B | 805 | CLA | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 22 | 8 | 604 | CLA | C4B-CHC | 2.13 | 1.46 | 1.41 |
| 29 | 9 | 606 | CHL | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 22 | 5 | 611 | CLA | C3D-C4D | -2.13 | 1.39 | 1.44 |
| 22 | B | 811 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 29 | 4 | 618 | CHL | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 22 | 1 | 608 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 22 | 4 | 610 | CLA | C1C-NC | -2.13 | 1.34 | 1.37 |
| 22 | B | 837 | CLA | C1B-NB | -2.13 | 1.33 | 1.35 |
| 22 | B | 839 | CLA | C1C-NC | -2.13 | 1.34 | 1.37 |
| 22 | 6 | 603 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | G | 203 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | Z | 602 | CLA | C1C-NC | -2.13 | 1.34 | 1.37 |
| 22 | 2 | 609 | CLA | C3D-C4D | -2.13 | 1.39 | 1.44 |
| 22 | B | 812 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | B | 815 | CLA | C4C-C3C | 2.13 | 1.48 | 1.45 |
| 22 | 3 | 610 | CLA | C1B-NB | -2.13 | 1.33 | 1.35 |
| 22 | 6 | 622 | CLA | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 22 | 5 | 611 | CLA | C1B-CHB | 2.13 | 1.46 | 1.41 |
| 22 | A | 836 | CLA | C1C-NC | -2.13 | 1.34 | 1.37 |
| 22 | 5 | 602 | CLA | C1B-NB | -2.13 | 1.33 | 1.35 |
| 22 | B | 835 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | G | 204 | CLA | C1C-C2C | 2.13 | 1.48 | 1.44 |
| 22 | 3 | 613 | CLA | C4B-CHC | 2.13 | 1.46 | 1.41 |
| 22 | A | 842 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | L | 204 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | J | 3002 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | 1 | 611 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | Z | 609 | CLA | C4B-CHC | 2.12 | 1.46 | 1.41 |
| 22 | A | 808 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 22 | B | 833 | CLA | C1C-NC | -2.12 | 1.34 | 1.37 |
| 22 | 5 | 616 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | 5 | 609 | CLA | C1A-CHA | 2.12 | 1.51 | 1.43 |
| 22 | A | 824 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 29 | 4 | 606 | CHL | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | B | 835 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 22 | G | 203 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | 2 | 609 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 29 | Z | 601 | CHL | C4D-CHA | 2.12 | 1.45 | 1.38 |
| 22 | 5 | 601 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | 1 | 610 | CLA | C1B-NB | -2.12 | 1.33 | 1.35 |
| 22 | 3 | 607 | CLA | C1C-NC | -2.12 | 1.34 | 1.37 |
| 22 | B | 802 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | B | 805 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | 7 | 603 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | Z | 611 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | 7 | 611 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | A | 822 | CLA | C4C-C3C | 2.12 | 1.48 | 1.45 |
| 22 | Z | 606 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | 4 | 604 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | B | 839 | CLA | C1C-C2C | 2.12 | 1.48 | 1.44 |
| 22 | 5 | 614 | CLA | C1B-CHB | 2.12 | 1.46 | 1.41 |
| 22 | A | 822 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 29 | 5 | 618 | CHL | C2C-C1C | 2.11 | 1.49 | 1.44 |
| 22 | 6 | 616 | CLA | C4B-CHC | 2.11 | 1.46 | 1.41 |
| 22 | A | 824 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 22 | 7 | 612 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 22 | 8 | 609 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |
| 22 | 4 | 612 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 22 | A | 826 | CLA | C4B-CHC | 2.11 | 1.46 | 1.41 |
| 22 | 5 | 617 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 29 | 5 | 607 | CHL | C4B-CHC | 2.11 | 1.46 | 1.41 |
| 22 | 6 | 614 | CLA | C1B-NB | -2.11 | 1.33 | 1.35 |
| 22 | A | 826 | CLA | C1B-CHB | 2.11 | 1.46 | 1.41 |
| 22 | Z | 603 | CLA | C4B-CHC | 2.11 | 1.46 | 1.41 |
| 22 | A | 818 | CLA | C1C-NC | -2.11 | 1.34 | 1.37 |
| 29 | Z | 607 | CHL | C2C-C1C | 2.11 | 1.49 | 1.44 |
| 22 | 6 | 616 | CLA | C1B-CHB | 2.11 | 1.46 | 1.41 |
| 22 | 7 | 608 | CLA | C1B-CHB | 2.11 | 1.46 | 1.41 |
| 22 | A | 810 | CLA | C1C-C2C | 2.11 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | B | 815 | CLA | C1B-NB | -2.11 | 1.33 | 1.35 |
| 22 | B | 830 | CLA | C1B-NB | -2.11 | 1.33 | 1.35 |
| 22 | 6 | 611 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | B | 807 | CLA | C4B-CHC | 2.10 | 1.46 | 1.41 |
| 22 | A | 825 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | 6 | 612 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | 7 | 614 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | 1 | 603 | CLA | C4B-CHC | 2.10 | 1.46 | 1.41 |
| 22 | A | 834 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 29 | 1 | 607 | CHL | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | F | 303 | CLA | C4C-C3C | 2.10 | 1.48 | 1.45 |
| 22 | 5 | 609 | CLA | C1B-NB | -2.10 | 1.33 | 1.35 |
| 22 | 4 | 601 | CLA | C4B-CHC | 2.10 | 1.46 | 1.41 |
| 22 | A | 814 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | A | 820 | CLA | C4B-CHC | 2.10 | 1.46 | 1.41 |
| 22 | B | 838 | CLA | C4C-C3C | 2.10 | 1.48 | 1.45 |
| 22 | 5 | 611 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | A | 803 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | 3 | 609 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | 7 | 606 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 29 | 3 | 608 | CHL | C4B-CHC | 2.10 | 1.46 | 1.41 |
| 22 | A | 823 | CLA | C1B-NB | -2.10 | 1.33 | 1.35 |
| 22 | 5 | 603 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | 4 | 612 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | A | 820 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 22 | G | 204 | CLA | C1B-NB | -2.10 | 1.33 | 1.35 |
| 22 | A | 843 | CLA | C1C-NC | -2.10 | 1.34 | 1.37 |
| 22 | B | 836 | CLA | C1C-NC | -2.10 | 1.34 | 1.37 |
| 22 | B | 810 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 22 | A | 836 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | 2 | 601 | CLA | C1C-C2C | 2.10 | 1.48 | 1.44 |
| 25 | A | 851 | BCR | C10-C9 | -2.10 | 1.33 | 1.35 |
| 22 | 6 | 601 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | A | 835 | CLA | C1D-C2D | 2.10 | 1.49 | 1.45 |
| 22 | 7 | 603 | CLA | C1C-NC | -2.10 | 1.34 | 1.37 |
| 22 | 7 | 614 | CLA | C1A-CHA | 2.10 | 1.51 | 1.43 |
| 22 | A | 810 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | B | 822 | CLA | C1B-CHB | 2.10 | 1.46 | 1.41 |
| 22 | 1 | 616 | CLA | C1B-NB | -2.10 | 1.33 | 1.35 |
| 22 | B | 852 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | Z | 604 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | 5 | 612 | CLA | C1B-NB | -2.09 | 1.33 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21 | A | 801 | CL0 | C4B-CHC | 2.09 | 1.46 | 1.41 |
| 29 | 5 | 618 | CHL | C4B-CHC | 2.09 | 1.46 | 1.41 |
| 22 | 2 | 610 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | A | 817 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 22 | 9 | 604 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | 4 | 604 | CLA | C1B-NB | -2.09 | 1.33 | 1.35 |
| 22 | A | 841 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 22 | B | 818 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 22 | 2 | 603 | CLA | C1D-C2D | 2.09 | 1.49 | 1.45 |
| 22 | A | 828 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | 3 | 602 | CLA | C1B-NB | -2.09 | 1.33 | 1.35 |
| 22 | A | 834 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 22 | B | 812 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 22 | 8 | 610 | CLA | C1C-NC | -2.09 | 1.34 | 1.37 |
| 22 | J | 3002 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | A | 820 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 22 | 4 | 612 | CLA | C1C-C2C | 2.09 | 1.48 | 1.44 |
| 22 | Z | 603 | CLA | C1B-CHB | 2.09 | 1.46 | 1.41 |
| 22 | B | 816 | CLA | C1B-NB | -2.09 | 1.33 | 1.35 |
| 22 | 4 | 609 | CLA | C4C-C3C | 2.09 | 1.48 | 1.45 |
| 22 | F | 304 | CLA | C1B-NB | -2.09 | 1.33 | 1.35 |
| 22 | B | 818 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 22 | A | 819 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 22 | 5 | 603 | CLA | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 22 | Z | 609 | CLA | C1A-CHA | 2.08 | 1.51 | 1.43 |
| 22 | 7 | 611 | CLA | C1C-NC | -2.08 | 1.34 | 1.37 |
| 22 | A | 802 | CLA | C1D-C2D | 2.08 | 1.49 | 1.45 |
| 22 | 5 | 613 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 22 | 5 | 610 | CLA | C4C-C3C | 2.08 | 1.48 | 1.45 |
| 22 | 1 | 613 | CLA | C1C-C2C | 2.08 | 1.48 | 1.44 |
| 22 | 6 | 617 | CLA | C1B-NB | -2.08 | 1.33 | 1.35 |
| 29 | Z | 607 | CHL | C1B-NB | -2.08 | 1.33 | 1.35 |
| 22 | Z | 613 | CLA | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 22 | B | 802 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 22 | 4 | 614 | CLA | C1B-NB | -2.08 | 1.33 | 1.35 |
| 22 | 4 | 614 | CLA | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 22 | 3 | 613 | CLA | C1B-CHB | 2.08 | 1.46 | 1.41 |
| 22 | A | 819 | CLA | C4B-NB | -2.08 | 1.33 | 1.35 |
| 22 | 6 | 613 | CLA | C1B-NB | -2.08 | 1.33 | 1.35 |
| 22 | 1 | 611 | CLA | C1C-NC | -2.08 | 1.34 | 1.37 |
| 22 | 5 | 609 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 22 | B | 814 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | 2 | 602 | CLA | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 22 | A | 831 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |
| 22 | B | 803 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 22 | 7 | 601 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 22 | 9 | 601 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 22 | 1 | 614 | CLA | C1B-NB | -2.07 | 1.33 | 1.35 |
| 22 | Z | 611 | CLA | C1B-NB | -2.07 | 1.33 | 1.35 |
| 22 | 3 | 614 | CLA | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 22 | 1 | 609 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 22 | A | 842 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 29 | 6 | 608 | CHL | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 22 | 8 | 603 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 22 | A | 814 | CLA | C4B-CHC | 2.07 | 1.46 | 1.41 |
| 22 | A | 842 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 22 | B | 828 | CLA | C4B-CHC | 2.07 | 1.46 | 1.41 |
| 22 | 7 | 601 | CLA | C1C-NC | -2.07 | 1.34 | 1.37 |
| 22 | 6 | 609 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 22 | A | 812 | CLA | C4C-C3C | 2.07 | 1.48 | 1.45 |
| 22 | B | 818 | CLA | C4B-CHC | 2.07 | 1.46 | 1.41 |
| 22 | 9 | 609 | CLA | C1A-CHA | 2.07 | 1.51 | 1.43 |
| 22 | B | 838 | CLA | C1B-NB | -2.07 | 1.33 | 1.35 |
| 22 | Z | 606 | CLA | C1C-C2C | 2.07 | 1.48 | 1.44 |
| 29 | 6 | 606 | CHL | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 22 | 6 | 603 | CLA | C1B-CHB | 2.07 | 1.46 | 1.41 |
| 22 | 6 | 622 | CLA | C1B-NB | -2.06 | 1.33 | 1.35 |
| 22 | A | 821 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 22 | 4 | 603 | CLA | C4B-CHC | 2.06 | 1.46 | 1.41 |
| 22 | 1 | 614 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 22 | A | 840 | CLA | C1C-NC | -2.06 | 1.34 | 1.37 |
| 22 | 8 | 603 | CLA | C1B-NB | -2.06 | 1.33 | 1.35 |
| 22 | 5 | 621 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 22 | 8 | 606 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 22 | F | 304 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 29 | 5 | 607 | CHL | C4C-C3C | 2.06 | 1.48 | 1.45 |
| 22 | F | 303 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 29 | 4 | 608 | CHL | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 22 | F | 304 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 22 | B | 827 | CLA | C1A-CHA | 2.06 | 1.51 | 1.43 |
| 22 | 3 | 602 | CLA | C1C-NC | -2.06 | 1.34 | 1.37 |
| 29 | 6 | 608 | CHL | C4B-CHC | 2.06 | 1.46 | 1.41 |
| 22 | A | 816 | CLA | C1B-NB | -2.06 | 1.33 | 1.35 |
| 22 | 3 | 620 | CLA | C1B-NB | -2.06 | 1.33 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 9 | 614 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 22 | 6 | 610 | CLA | C1B-NB | -2.06 | 1.33 | 1.35 |
| 22 | B | 839 | CLA | C1B-CHB | 2.06 | 1.46 | 1.41 |
| 22 | B | 823 | CLA | C1C-C2C | 2.06 | 1.48 | 1.44 |
| 22 | 3 | 606 | CLA | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 22 | 1 | 604 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 22 | 6 | 617 | CLA | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 22 | B | 840 | CLA | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 22 | 3 | 602 | CLA | C4B-NB | -2.05 | 1.33 | 1.35 |
| 22 | A | 806 | CLA | C4B-CHC | 2.05 | 1.46 | 1.41 |
| 22 | 3 | 609 | CLA | C1C-NC | -2.05 | 1.34 | 1.37 |
| 22 | 1 | 602 | CLA | C1B-NB | -2.05 | 1.33 | 1.35 |
| 25 | 7 | 623 | BCR | C38-C26 | 2.05 | 1.54 | 1.50 |
| 29 | 6 | 606 | CHL | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 29 | 1 | 601 | CHL | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 22 | B | 824 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 22 | 7 | 616 | CLA | C1C-C2C | 2.05 | 1.48 | 1.44 |
| 22 | A | 808 | CLA | C1C-NC | -2.05 | 1.34 | 1.37 |
| 22 | 8 | 613 | CLA | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 22 | B | 817 | CLA | C1B-NB | -2.05 | 1.33 | 1.35 |
| 22 | 1 | 611 | CLA | C1B-NB | -2.05 | 1.33 | 1.35 |
| 22 | 5 | 616 | CLA | C1C-NC | -2.05 | 1.34 | 1.37 |
| 22 | B | 803 | CLA | C4B-CHC | 2.05 | 1.46 | 1.41 |
| 22 | 7 | 603 | CLA | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 29 | Z | 601 | CHL | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 22 | 1 | 606 | CLA | C4C-C3C | 2.05 | 1.48 | 1.45 |
| 22 | 4 | 611 | CLA | C1B-CHB | 2.05 | 1.46 | 1.41 |
| 28 | J | 3001 | LMG | O7-C8 | -2.05 | 1.41 | 1.46 |
| 22 | A | 808 | CLA | C4B-CHC | 2.04 | 1.46 | 1.41 |
| 22 | 8 | 614 | CLA | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 29 | 7 | 607 | CHL | C4B-CHC | 2.04 | 1.46 | 1.41 |
| 22 | 5 | 611 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 22 | 8 | 604 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 22 | B | 811 | CLA | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 22 | Z | 614 | CLA | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 22 | 4 | 613 | CLA | C1C-C2C | 2.04 | 1.48 | 1.44 |
| 22 | A | 826 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 22 | 9 | 613 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 22 | 5 | 616 | CLA | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 22 | 3 | 603 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 22 | B | 807 | CLA | C1B-CHB | 2.04 | 1.46 | 1.41 |
| 22 | 8 | 601 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A | 805 | CLA | C1D-C2D | 2.04 | 1.49 | 1.45 |
| 22 | 4 | 602 | CLA | C1B-NB | -2.04 | 1.33 | 1.35 |
| 22 | 7 | 611 | CLA | C1A-CHA | 2.04 | 1.51 | 1.43 |
| 22 | A | 829 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 22 | B | 821 | CLA | C1C-NC | -2.04 | 1.34 | 1.37 |
| 22 | A | 809 | CLA | C4C-C3C | 2.04 | 1.48 | 1.45 |
| 22 | Z | 612 | CLA | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 22 | 9 | 603 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | Z | 606 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 22 | A | 807 | CLA | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 22 | L | 203 | CLA | C1B-NB | -2.03 | 1.33 | 1.35 |
| 22 | 7 | 613 | CLA | C4B-CHC | 2.03 | 1.46 | 1.41 |
| 22 | 6 | 609 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | 1 | 606 | CLA | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 22 | 4 | 611 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 22 | 6 | 611 | CLA | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 22 | 9 | 603 | CLA | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 29 | 1 | 607 | CHL | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 22 | B | 802 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 22 | 4 | 612 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 22 | 4 | 611 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | 5 | 606 | CLA | C1B-CHB | 2.03 | 1.46 | 1.41 |
| 22 | 2 | 609 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 29 | 6 | 607 | CHL | C2C-C1C | 2.03 | 1.48 | 1.44 |
| 22 | F | 304 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 22 | 8 | 608 | CLA | C1B-NB | -2.03 | 1.33 | 1.35 |
| 29 | 4 | 618 | CHL | C1B-NB | -2.03 | 1.33 | 1.35 |
| 22 | B | 829 | CLA | C4C-C3C | 2.03 | 1.48 | 1.45 |
| 29 | 6 | 607 | CHL | C1C-NC | -2.03 | 1.34 | 1.37 |
| 22 | A | 836 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | A | 843 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | A | 809 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 22 | B | 823 | CLA | C1C-NC | -2.03 | 1.34 | 1.37 |
| 22 | 8 | 611 | CLA | C1A-CHA | 2.03 | 1.51 | 1.43 |
| 22 | A | 804 | CLA | C1C-C2C | 2.03 | 1.48 | 1.44 |
| 22 | 4 | 611 | CLA | C1B-NB | -2.03 | 1.33 | 1.35 |
| 22 | B | 836 | CLA | C4B-NB | -2.02 | 1.33 | 1.35 |
| 22 | 7 | 602 | CLA | C1B-NB | -2.02 | 1.33 | 1.35 |
| 28 | 9 | 620 | LMG | C4-C5 | 2.02 | 1.57 | 1.53 |
| 29 | 5 | 607 | CHL | C4B-NB | -2.02 | 1.33 | 1.35 |
| 29 | 5 | 618 | CHL | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 22 | B | 819 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | 7 | 604 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 22 | B | 824 | CLA | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 22 | A | 837 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 22 | 8 | 603 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 22 | 5 | 603 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 22 | G | 203 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 22 | 3 | 612 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 22 | 1 | 603 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 22 | 1 | 612 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 22 | 4 | 602 | CLA | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 29 | 4 | 618 | CHL | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 22 | 6 | 611 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 22 | 1 | 609 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 22 | 8 | 611 | CLA | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 22 | 5 | 612 | CLA | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 22 | A | 830 | CLA | C1A-CHA | 2.02 | 1.51 | 1.43 |
| 22 | B | 810 | CLA | C1C-NC | -2.02 | 1.34 | 1.37 |
| 22 | B | 829 | CLA | C4B-NB | -2.02 | 1.33 | 1.35 |
| 22 | B | 809 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 22 | 7 | 611 | CLA | C1C-C2C | 2.02 | 1.48 | 1.44 |
| 22 | A | 831 | CLA | C1B-CHB | 2.02 | 1.46 | 1.41 |
| 22 | B | 825 | CLA | C4C-C3C | 2.02 | 1.48 | 1.45 |
| 22 | Z | 602 | CLA | C4C-C3C | 2.01 | 1.48 | 1.45 |
| 22 | 7 | 602 | CLA | C4C-C3C | 2.01 | 1.48 | 1.45 |
| 22 | B | 852 | CLA | C1B-NB | -2.01 | 1.33 | 1.35 |
| 22 | 1 | 604 | CLA | C1B-CHB | 2.01 | 1.46 | 1.41 |
| 22 | A | 817 | CLA | C1D-C2D | 2.01 | 1.49 | 1.45 |
| 22 | A | 820 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 22 | 7 | 609 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 22 | A | 812 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 22 | 5 | 621 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 22 | 5 | 604 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 22 | 2 | 613 | CLA | C1B-NB | -2.01 | 1.33 | 1.35 |
| 22 | K | 4002 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 22 | 6 | 601 | CLA | C1C-C2C | 2.01 | 1.48 | 1.44 |
| 22 | 7 | 614 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 22 | B | 835 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 22 | Z | 602 | CLA | C1B-CHB | 2.01 | 1.46 | 1.41 |
| 29 | 7 | 607 | CHL | C1B-CHB | 2.01 | 1.46 | 1.41 |
| 22 | 7 | 613 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 22 | Z | 610 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 22 | 4 | 603 | CLA | C1B-CHB | 2.01 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 22 | L | 203 | CLA | C1C-NC | -2.01 | 1.34 | 1.37 |
| 22 | Z | 608 | CLA | C1B-NB | -2.01 | 1.33 | 1.35 |
| 29 | 6 | 607 | CHL | C1B-NB | -2.01 | 1.33 | 1.35 |
| 22 | F | 301 | CLA | C4C-C3C | 2.01 | 1.48 | 1.45 |
| 22 | A | 840 | CLA | C1A-CHA | 2.01 | 1.51 | 1.43 |
| 22 | B | 814 | CLA | C1B-NB | -2.00 | 1.33 | 1.35 |
| 22 | 7 | 616 | CLA | C1B-NB | -2.00 | 1.33 | 1.35 |
| 22 | B | 804 | CLA | C1C-NC | -2.00 | 1.34 | 1.37 |
| 22 | B | 808 | CLA | C1C-C2C | 2.00 | 1.48 | 1.44 |
| 22 | 3 | 607 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 22 | 6 | 604 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 22 | B | 812 | CLA | C1B-CHB | 2.00 | 1.46 | 1.41 |
| 22 | A | 834 | CLA | C4B-NB | -2.00 | 1.33 | 1.35 |
| 22 | 5 | 616 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 28 | J | 3001 | LMG | C4-C5 | 2.00 | 1.57 | 1.53 |
| 22 | 9 | 610 | CLA | C1B-CHB | 2.00 | 1.46 | 1.41 |
| 22 | 1 | 614 | CLA | C1B-CHB | 2.00 | 1.46 | 1.41 |
| 22 | A | 816 | CLA | C1A-CHA | 2.00 | 1.51 | 1.43 |
| 22 | A | 821 | CLA | C4C-C3C | 2.00 | 1.48 | 1.45 |

All (7074) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 22 | 5 | 617 | CLA | O2A-CGA-O1A | -13.94 | 79.44 | 123.14 |
| 22 | 5 | 617 | CLA | O2A-CGA-CBA | 12.13 | 160.18 | 112.23 |
| 29 | 6 | 608 | CHL | C4A-NA-C1A | -11.78 | 101.41 | 106.71 |
| 22 | 5 | 617 | CLA | O1A-CGA-CBA | -11.02 | 80.75 | 123.73 |
| 29 | Z | 601 | CHL | C4A-NA-C1A | -10.94 | 101.79 | 106.71 |
| 29 | 1 | 601 | CHL | C4A-NA-C1A | -10.61 | 101.94 | 106.71 |
| 22 | L | 203 | CLA | C1D-ND-C4D | -10.34 | 98.99 | 106.33 |
| 29 | 9 | 606 | CHL | C4A-NA-C1A | -10.31 | 102.07 | 106.71 |
| 29 | 4 | 608 | CHL | C2D-C1D-ND | 10.26 | 117.67 | 110.10 |
| 29 | 1 | 607 | CHL | C2D-C1D-ND | 10.25 | 117.66 | 110.10 |
| 22 | B | 829 | CLA | C1D-ND-C4D | -10.16 | 99.11 | 106.33 |
| 29 | 6 | 618 | CHL | C2D-C1D-ND | 10.15 | 117.59 | 110.10 |
| 22 | A | 818 | CLA | C1D-ND-C4D | -10.12 | 99.15 | 106.33 |
| 29 | 4 | 618 | CHL | C4A-NA-C1A | -10.01 | 102.21 | 106.71 |
| 29 | 5 | 618 | CHL | C4A-NA-C1A | -10.00 | 102.21 | 106.71 |
| 22 | 7 | 602 | CLA | C1D-ND-C4D | -10.00 | 99.23 | 106.33 |
| 29 | 3 | 608 | CHL | C2D-C1D-ND | 9.97 | 117.45 | 110.10 |
| 22 | 7 | 604 | CLA | C1D-ND-C4D | -9.96 | 99.26 | 106.33 |
| 22 | B | 838 | CLA | C1D-ND-C4D | -9.95 | 99.27 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22 | B | 802 | CLA | C1D-ND-C4D | -9.93 | 99.28 | 106.33 |
| 22 | A | 823 | CLA | C1D-ND-C4D | -9.88 | 99.31 | 106.33 |
| 22 | 5 | 617 | CLA | C1D-ND-C4D | -9.88 | 99.32 | 106.33 |
| 22 | A | 812 | CLA | C1D-ND-C4D | -9.88 | 99.32 | 106.33 |
| 29 | 6 | 607 | CHL | C2D-C1D-ND | 9.87 | 117.38 | 110.10 |
| 22 | 8 | 602 | CLA | C1D-ND-C4D | -9.87 | 99.32 | 106.33 |
| 22 | 7 | 608 | CLA | C1D-ND-C4D | -9.85 | 99.33 | 106.33 |
| 29 | Z | 607 | CHL | C2D-C1D-ND | 9.82 | 117.34 | 110.10 |
| 22 | A | 854 | CLA | C1D-ND-C4D | -9.80 | 99.37 | 106.33 |
| 29 | 8 | 607 | CHL | C2D-C1D-ND | 9.80 | 117.33 | 110.10 |
| 22 | 7 | 606 | CLA | C1D-ND-C4D | -9.79 | 99.38 | 106.33 |
| 22 | 5 | 602 | CLA | C1D-ND-C4D | -9.78 | 99.39 | 106.33 |
| 29 | Z | 601 | CHL | C2D-C1D-ND | 9.77 | 117.30 | 110.10 |
| 29 | 5 | 607 | CHL | C2D-C1D-ND | 9.77 | 117.30 | 110.10 |
| 29 | 6 | 606 | CHL | C4A-NA-C1A | -9.74 | 102.33 | 106.71 |
| 29 | 6 | 606 | CHL | C2D-C1D-ND | 9.72 | 117.27 | 110.10 |
| 22 | A | 803 | CLA | C1D-ND-C4D | -9.71 | 99.43 | 106.33 |
| 29 | 4 | 607 | CHL | C4A-NA-C1A | -9.71 | 102.34 | 106.71 |
| 29 | 4 | 607 | CHL | C2D-C1D-ND | 9.68 | 117.24 | 110.10 |
| 22 | 6 | 602 | CLA | C1D-ND-C4D | -9.67 | 99.47 | 106.33 |
| 22 | L | 204 | CLA | C1D-ND-C4D | -9.63 | 99.49 | 106.33 |
| 29 | 9 | 606 | CHL | C2D-C1D-ND | 9.63 | 117.20 | 110.10 |
| 29 | 5 | 618 | CHL | C2D-C1D-ND | 9.59 | 117.17 | 110.10 |
| 29 | 4 | 606 | CHL | C2D-C1D-ND | 9.58 | 117.16 | 110.10 |
| 22 | B | 821 | CLA | C1D-ND-C4D | -9.58 | 99.53 | 106.33 |
| 29 | 9 | 607 | CHL | C2D-C1D-ND | 9.55 | 117.14 | 110.10 |
| 22 | B | 837 | CLA | C1D-ND-C4D | -9.55 | 99.55 | 106.33 |
| 22 | 1 | 614 | CLA | C1D-ND-C4D | -9.55 | 99.55 | 106.33 |
| 22 | 5 | 617 | CLA | C2D-C1D-ND | 9.51 | 117.11 | 110.10 |
| 29 | 4 | 618 | CHL | C2D-C1D-ND | 9.50 | 117.10 | 110.10 |
| 29 | 5 | 608 | CHL | C2D-C1D-ND | 9.49 | 117.10 | 110.10 |
| 22 | A | 816 | CLA | C1D-ND-C4D | -9.48 | 99.60 | 106.33 |
| 22 | A | 841 | CLA | C1D-ND-C4D | -9.47 | 99.61 | 106.33 |
| 22 | 2 | 614 | CLA | C1D-ND-C4D | -9.47 | 99.61 | 106.33 |
| 22 | 5 | 614 | CLA | C1D-ND-C4D | -9.46 | 99.62 | 106.33 |
| 22 | A | 845 | CLA | C1D-ND-C4D | -9.45 | 99.62 | 106.33 |
| 22 | 2 | 610 | CLA | C1D-ND-C4D | -9.45 | 99.62 | 106.33 |
| 22 | 9 | 604 | CLA | C1D-ND-C4D | -9.44 | 99.63 | 106.33 |
| 22 | A | 808 | CLA | C1D-ND-C4D | -9.43 | 99.63 | 106.33 |
| 29 | 6 | 608 | CHL | C2D-C1D-ND | 9.43 | 117.05 | 110.10 |
| 22 | A | 828 | CLA | C1D-ND-C4D | -9.43 | 99.64 | 106.33 |
| 22 | B | 816 | CLA | C1D-ND-C4D | -9.42 | 99.64 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22 | B | 822 | CLA | C1D-ND-C4D | -9.42 | 99.64 | 106.33 |
| 22 | B | 812 | CLA | C1D-ND-C4D | -9.42 | 99.64 | 106.33 |
| 22 | A | 842 | CLA | C1D-ND-C4D | -9.41 | 99.65 | 106.33 |
| 22 | L | 203 | CLA | C2D-C1D-ND | 9.41 | 117.04 | 110.10 |
| 22 | A | 827 | CLA | C1D-ND-C4D | -9.40 | 99.66 | 106.33 |
| 22 | B | 831 | CLA | C1D-ND-C4D | -9.39 | 99.67 | 106.33 |
| 22 | B | 841 | CLA | C1D-ND-C4D | -9.39 | 99.67 | 106.33 |
| 22 | Z | 602 | CLA | C1D-ND-C4D | -9.39 | 99.67 | 106.33 |
| 22 | A | 804 | CLA | C1D-ND-C4D | -9.38 | 99.67 | 106.33 |
| 22 | 4 | 616 | CLA | C1D-ND-C4D | -9.38 | 99.67 | 106.33 |
| 22 | 7 | 601 | CLA | C1D-ND-C4D | -9.36 | 99.69 | 106.33 |
| 22 | 6 | 614 | CLA | C1D-ND-C4D | -9.36 | 99.69 | 106.33 |
| 22 | 2 | 607 | CLA | C1D-ND-C4D | -9.35 | 99.69 | 106.33 |
| 22 | Z | 610 | CLA | C1D-ND-C4D | -9.35 | 99.69 | 106.33 |
| 22 | A | 809 | CLA | C1D-ND-C4D | -9.34 | 99.70 | 106.33 |
| 22 | A | 806 | CLA | C1D-ND-C4D | -9.33 | 99.70 | 106.33 |
| 29 | 1 | 601 | CHL | C2D-C1D-ND | 9.33 | 116.98 | 110.10 |
| 22 | B | 805 | CLA | C1D-ND-C4D | -9.32 | 99.72 | 106.33 |
| 22 | A | 811 | CLA | C1D-ND-C4D | -9.32 | 99.72 | 106.33 |
| 22 | A | 836 | CLA | C1D-ND-C4D | -9.29 | 99.73 | 106.33 |
| 22 | 1 | 610 | CLA | C1D-ND-C4D | -9.28 | 99.74 | 106.33 |
| 22 | 3 | 614 | CLA | C1D-ND-C4D | -9.28 | 99.74 | 106.33 |
| 22 | A | 814 | CLA | C1D-ND-C4D | -9.28 | 99.74 | 106.33 |
| 22 | B | 833 | CLA | C1D-ND-C4D | -9.28 | 99.74 | 106.33 |
| 22 | 4 | 614 | CLA | C1D-ND-C4D | -9.28 | 99.74 | 106.33 |
| 29 | 6 | 618 | CHL | C4A-NA-C1A | -9.27 | 102.54 | 106.71 |
| 22 | 3 | 610 | CLA | C1D-ND-C4D | -9.26 | 99.75 | 106.33 |
| 22 | 6 | 613 | CLA | C1D-ND-C4D | -9.24 | 99.77 | 106.33 |
| 22 | 2 | 602 | CLA | C1D-ND-C4D | -9.24 | 99.77 | 106.33 |
| 22 | 8 | 608 | CLA | C1D-ND-C4D | -9.23 | 99.78 | 106.33 |
| 22 | B | 804 | CLA | C1D-ND-C4D | -9.23 | 99.78 | 106.33 |
| 22 | B | 825 | CLA | C1D-ND-C4D | -9.23 | 99.78 | 106.33 |
| 22 | 2 | 611 | CLA | C1D-ND-C4D | -9.21 | 99.79 | 106.33 |
| 22 | A | 805 | CLA | C1D-ND-C4D | -9.21 | 99.79 | 106.33 |
| 22 | 7 | 609 | CLA | C1D-ND-C4D | -9.21 | 99.80 | 106.33 |
| 22 | 4 | 602 | CLA | C1D-ND-C4D | -9.21 | 99.80 | 106.33 |
| 22 | 4 | 601 | CLA | C1D-ND-C4D | -9.20 | 99.80 | 106.33 |
| 22 | A | 802 | CLA | C1D-ND-C4D | -9.19 | 99.81 | 106.33 |
| 22 | 6 | 622 | CLA | C1D-ND-C4D | -9.19 | 99.81 | 106.33 |
| 22 | A | 815 | CLA | C1D-ND-C4D | -9.16 | 99.83 | 106.33 |
| 22 | A | 810 | CLA | C1D-ND-C4D | -9.16 | 99.83 | 106.33 |
| 22 | 7 | 612 | CLA | C1D-ND-C4D | -9.15 | 99.83 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | 6 | 601 | CLA | C1D-ND-C4D | -9.14 | 99.84 | 106.33 |
| 22 | 3 | 602 | CLA | C1D-ND-C4D | -9.14 | 99.84 | 106.33 |
| 22 | G | 203 | CLA | C1D-ND-C4D | -9.14 | 99.84 | 106.33 |
| 22 | A | 834 | CLA | C1D-ND-C4D | -9.13 | 99.85 | 106.33 |
| 22 | 4 | 612 | CLA | C1D-ND-C4D | -9.11 | 99.86 | 106.33 |
| 22 | B | 820 | CLA | C1D-ND-C4D | -9.11 | 99.86 | 106.33 |
| 22 | Z | 614 | CLA | C1D-ND-C4D | -9.11 | 99.86 | 106.33 |
| 22 | 1 | 602 | CLA | C1D-ND-C4D | -9.11 | 99.86 | 106.33 |
| 22 | 7 | 613 | CLA | C1D-ND-C4D | -9.11 | 99.86 | 106.33 |
| 22 | A | 824 | CLA | C1D-ND-C4D | -9.10 | 99.87 | 106.33 |
| 29 | 7 | 607 | CHL | C2D-C1D-ND | 9.09 | 116.80 | 110.10 |
| 22 | 9 | 610 | CLA | C1D-ND-C4D | -9.09 | 99.88 | 106.33 |
| 22 | Z | 611 | CLA | C1D-ND-C4D | -9.07 | 99.89 | 106.33 |
| 22 | 2 | 613 | CLA | C1D-ND-C4D | -9.07 | 99.89 | 106.33 |
| 22 | 9 | 614 | CLA | C1D-ND-C4D | -9.07 | 99.89 | 106.33 |
| 22 | 7 | 620 | CLA | C1D-ND-C4D | -9.07 | 99.89 | 106.33 |
| 22 | 3 | 612 | CLA | C1D-ND-C4D | -9.07 | 99.89 | 106.33 |
| 22 | 3 | 620 | CLA | C1D-ND-C4D | -9.07 | 99.89 | 106.33 |
| 22 | 8 | 614 | CLA | C1D-ND-C4D | -9.06 | 99.90 | 106.33 |
| 22 | 1 | 608 | CLA | C1D-ND-C4D | -9.06 | 99.90 | 106.33 |
| 22 | A | 817 | CLA | C1D-ND-C4D | -9.06 | 99.90 | 106.33 |
| 22 | B | 811 | CLA | C1D-ND-C4D | -9.05 | 99.90 | 106.33 |
| 22 | B | 832 | CLA | C1D-ND-C4D | -9.03 | 99.92 | 106.33 |
| 22 | K | 4002 | CLA | C1D-ND-C4D | -9.03 | 99.92 | 106.33 |
| 29 | 8 | 607 | CHL | C4A-NA-C1A | -9.03 | 102.65 | 106.71 |
| 22 | 4 | 613 | CLA | C1D-ND-C4D | -9.03 | 99.92 | 106.33 |
| 22 | A | 830 | CLA | C1D-ND-C4D | -9.03 | 99.92 | 106.33 |
| 22 | 4 | 604 | CLA | C1D-ND-C4D | -9.02 | 99.92 | 106.33 |
| 22 | 8 | 606 | CLA | C1D-ND-C4D | -9.02 | 99.93 | 106.33 |
| 22 | A | 835 | CLA | C1D-ND-C4D | -9.02 | 99.93 | 106.33 |
| 22 | A | 840 | CLA | C1D-ND-C4D | -9.02 | 99.93 | 106.33 |
| 22 | F | 304 | CLA | C1D-ND-C4D | -9.02 | 99.93 | 106.33 |
| 22 | A | 818 | CLA | C2D-C1D-ND | 9.01 | 116.75 | 110.10 |
| 22 | A | 854 | CLA | C2D-C1D-ND | 9.01 | 116.74 | 110.10 |
| 22 | 9 | 602 | CLA | C1D-ND-C4D | -9.01 | 99.94 | 106.33 |
| 22 | 5 | 610 | CLA | C1D-ND-C4D | -9.01 | 99.94 | 106.33 |
| 22 | A | 813 | CLA | C1D-ND-C4D | -9.00 | 99.94 | 106.33 |
| 22 | A | 825 | CLA | C1D-ND-C4D | -9.00 | 99.94 | 106.33 |
| 22 | 8 | 604 | CLA | C1D-ND-C4D | -9.00 | 99.94 | 106.33 |
| 22 | B | 802 | CLA | C2D-C1D-ND | 8.99 | 116.73 | 110.10 |
| 22 | Z | 613 | CLA | C1D-ND-C4D | -8.99 | 99.95 | 106.33 |
| 22 | F | 303 | CLA | C1D-ND-C4D | -8.99 | 99.95 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | B | 805 | CLA | C2D-C1D-ND | 8.99 | 116.73 | 110.10 |
| 22 | B | 840 | CLA | C1D-ND-C4D | -8.98 | 99.95 | 106.33 |
| 22 | B | 826 | CLA | C1D-ND-C4D | -8.98 | 99.95 | 106.33 |
| 22 | Z | 612 | CLA | C1D-ND-C4D | -8.98 | 99.96 | 106.33 |
| 22 | Z | 608 | CLA | C1D-ND-C4D | -8.98 | 99.96 | 106.33 |
| 22 | B | 830 | CLA | C1D-ND-C4D | -8.98 | 99.96 | 106.33 |
| 22 | B | 815 | CLA | C1D-ND-C4D | -8.97 | 99.96 | 106.33 |
| 22 | 3 | 607 | CLA | C1D-ND-C4D | -8.97 | 99.96 | 106.33 |
| 22 | G | 204 | CLA | C1D-ND-C4D | -8.97 | 99.96 | 106.33 |
| 22 | 7 | 610 | CLA | C1D-ND-C4D | -8.97 | 99.96 | 106.33 |
| 22 | 3 | 604 | CLA | C1D-ND-C4D | -8.97 | 99.96 | 106.33 |
| 22 | 2 | 606 | CLA | C1D-ND-C4D | -8.97 | 99.97 | 106.33 |
| 22 | 7 | 616 | CLA | C1D-ND-C4D | -8.96 | 99.97 | 106.33 |
| 22 | 1 | 613 | CLA | C1D-ND-C4D | -8.96 | 99.97 | 106.33 |
| 22 | 1 | 606 | CLA | C1D-ND-C4D | -8.94 | 99.98 | 106.33 |
| 22 | J | 3002 | CLA | C1D-ND-C4D | -8.93 | 99.99 | 106.33 |
| 22 | B | 810 | CLA | C1D-ND-C4D | -8.92 | 100.00 | 106.33 |
| 22 | 9 | 603 | CLA | C1D-ND-C4D | -8.92 | 100.00 | 106.33 |
| 22 | A | 828 | CLA | C2D-C1D-ND | 8.91 | 116.67 | 110.10 |
| 22 | Z | 606 | CLA | C1D-ND-C4D | -8.90 | 100.01 | 106.33 |
| 22 | 1 | 603 | CLA | C1D-ND-C4D | -8.89 | 100.02 | 106.33 |
| 22 | 4 | 609 | CLA | C1D-ND-C4D | -8.88 | 100.03 | 106.33 |
| 22 | 1 | 609 | CLA | C1D-ND-C4D | -8.87 | 100.03 | 106.33 |
| 22 | 9 | 613 | CLA | C1D-ND-C4D | -8.87 | 100.04 | 106.33 |
| 22 | A | 807 | CLA | C1D-ND-C4D | -8.85 | 100.05 | 106.33 |
| 22 | 5 | 606 | CLA | C1D-ND-C4D | -8.85 | 100.05 | 106.33 |
| 22 | A | 829 | CLA | C1D-ND-C4D | -8.84 | 100.05 | 106.33 |
| 22 | 8 | 612 | CLA | C1D-ND-C4D | -8.84 | 100.05 | 106.33 |
| 22 | 2 | 603 | CLA | C1D-ND-C4D | -8.84 | 100.06 | 106.33 |
| 22 | B | 808 | CLA | C1D-ND-C4D | -8.83 | 100.06 | 106.33 |
| 22 | B | 827 | CLA | C1D-ND-C4D | -8.83 | 100.06 | 106.33 |
| 22 | 6 | 612 | CLA | C1D-ND-C4D | -8.83 | 100.06 | 106.33 |
| 22 | 2 | 601 | CLA | C1D-ND-C4D | -8.82 | 100.07 | 106.33 |
| 22 | 3 | 617 | CLA | C1D-ND-C4D | -8.81 | 100.08 | 106.33 |
| 22 | A | 820 | CLA | C1D-ND-C4D | -8.81 | 100.08 | 106.33 |
| 22 | A | 841 | CLA | C2D-C1D-ND | 8.81 | 116.59 | 110.10 |
| 22 | 3 | 603 | CLA | C1D-ND-C4D | -8.81 | 100.08 | 106.33 |
| 22 | 9 | 612 | CLA | C1D-ND-C4D | -8.81 | 100.08 | 106.33 |
| 22 | 1 | 612 | CLA | C1D-ND-C4D | -8.80 | 100.08 | 106.33 |
| 22 | B | 839 | CLA | C1D-ND-C4D | -8.79 | 100.09 | 106.33 |
| 22 | 7 | 614 | CLA | C1D-ND-C4D | -8.79 | 100.09 | 106.33 |
| 22 | 6 | 603 | CLA | C1D-ND-C4D | -8.77 | 100.10 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21 | A | 801 | CL0 | C1D-ND-C4D | -8.77 | 100.11 | 106.33 |
| 22 | A | 819 | CLA | C1D-ND-C4D | -8.77 | 100.11 | 106.33 |
| 22 | K | 4003 | CLA | C1D-ND-C4D | -8.76 | 100.11 | 106.33 |
| 22 | 6 | 616 | CLA | C1D-ND-C4D | -8.76 | 100.11 | 106.33 |
| 22 | 3 | 609 | CLA | C1D-ND-C4D | -8.76 | 100.11 | 106.33 |
| 22 | 7 | 603 | CLA | C1D-ND-C4D | -8.76 | 100.11 | 106.33 |
| 22 | 6 | 604 | CLA | C1D-ND-C4D | -8.76 | 100.11 | 106.33 |
| 22 | 1 | 611 | CLA | C1D-ND-C4D | -8.76 | 100.11 | 106.33 |
| 22 | B | 852 | CLA | C1D-ND-C4D | -8.75 | 100.12 | 106.33 |
| 22 | 5 | 612 | CLA | C1D-ND-C4D | -8.75 | 100.12 | 106.33 |
| 22 | B | 814 | CLA | C1D-ND-C4D | -8.74 | 100.13 | 106.33 |
| 22 | 9 | 601 | CLA | C1D-ND-C4D | -8.74 | 100.13 | 106.33 |
| 22 | Z | 616 | CLA | C1D-ND-C4D | -8.73 | 100.13 | 106.33 |
| 22 | A | 839 | CLA | C1D-ND-C4D | -8.72 | 100.14 | 106.33 |
| 29 | 5 | 607 | CHL | C4A-NA-C1A | -8.71 | 102.79 | 106.71 |
| 22 | B | 834 | CLA | C1D-ND-C4D | -8.71 | 100.15 | 106.33 |
| 22 | 3 | 606 | CLA | C1D-ND-C4D | -8.70 | 100.15 | 106.33 |
| 22 | B | 806 | CLA | C1D-ND-C4D | -8.66 | 100.18 | 106.33 |
| 22 | B | 824 | CLA | C1D-ND-C4D | -8.66 | 100.18 | 106.33 |
| 22 | A | 823 | CLA | C2D-C1D-ND | 8.65 | 116.48 | 110.10 |
| 22 | Z | 604 | CLA | C1D-ND-C4D | -8.65 | 100.19 | 106.33 |
| 22 | A | 833 | CLA | C1D-ND-C4D | -8.65 | 100.19 | 106.33 |
| 22 | 5 | 601 | CLA | C1D-ND-C4D | -8.65 | 100.19 | 106.33 |
| 22 | A | 821 | CLA | C1D-ND-C4D | -8.65 | 100.19 | 106.33 |
| 22 | B | 813 | CLA | C1D-ND-C4D | -8.65 | 100.19 | 106.33 |
| 22 | B | 816 | CLA | C2D-C1D-ND | 8.65 | 116.47 | 110.10 |
| 22 | 7 | 602 | CLA | C2D-C1D-ND | 8.64 | 116.47 | 110.10 |
| 22 | A | 838 | CLA | C1D-ND-C4D | -8.64 | 100.20 | 106.33 |
| 22 | 1 | 604 | CLA | C1D-ND-C4D | -8.64 | 100.20 | 106.33 |
| 22 | 9 | 611 | CLA | C1D-ND-C4D | -8.63 | 100.20 | 106.33 |
| 22 | 5 | 609 | CLA | C1D-ND-C4D | -8.63 | 100.20 | 106.33 |
| 22 | 6 | 609 | CLA | C1D-ND-C4D | -8.63 | 100.20 | 106.33 |
| 22 | B | 804 | CLA | C2D-C1D-ND | 8.63 | 116.46 | 110.10 |
| 22 | A | 829 | CLA | C2D-C1D-ND | 8.62 | 116.46 | 110.10 |
| 22 | B | 831 | CLA | C2D-C1D-ND | 8.61 | 116.45 | 110.10 |
| 22 | A | 812 | CLA | C2D-C1D-ND | 8.60 | 116.44 | 110.10 |
| 22 | B | 807 | CLA | C1D-ND-C4D | -8.60 | 100.23 | 106.33 |
| 22 | 2 | 612 | CLA | C1D-ND-C4D | -8.59 | 100.23 | 106.33 |
| 22 | 6 | 617 | CLA | C1D-ND-C4D | -8.59 | 100.23 | 106.33 |
| 22 | 5 | 611 | CLA | C1D-ND-C4D | -8.59 | 100.23 | 106.33 |
| 22 | 8 | 613 | CLA | C1D-ND-C4D | -8.59 | 100.24 | 106.33 |
| 22 | 4 | 610 | CLA | C1D-ND-C4D | -8.58 | 100.24 | 106.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22 | 8 | 602 | CLA | C2D-C1D-ND | 8.58 | 116.42 | 110.10 |
| 22 | B | 835 | CLA | C1D-ND-C4D | -8.57 | 100.25 | 106.33 |
| 22 | 5 | 613 | CLA | C1D-ND-C4D | -8.57 | 100.25 | 106.33 |
| 22 | 8 | 603 | CLA | C1D-ND-C4D | -8.56 | 100.25 | 106.33 |
| 22 | B | 828 | CLA | C1D-ND-C4D | -8.56 | 100.25 | 106.33 |
| 22 | A | 831 | CLA | C1D-ND-C4D | -8.55 | 100.26 | 106.33 |
| 22 | 1 | 616 | CLA | C1D-ND-C4D | -8.54 | 100.27 | 106.33 |
| 22 | Z | 603 | CLA | C1D-ND-C4D | -8.54 | 100.27 | 106.33 |
| 22 | F | 301 | CLA | C1D-ND-C4D | -8.53 | 100.27 | 106.33 |
| 29 | 5 | 608 | CHL | C4A-NA-C1A | -8.53 | 102.87 | 106.71 |
| 22 | 6 | 611 | CLA | C1D-ND-C4D | -8.53 | 100.28 | 106.33 |
| 22 | 7 | 608 | CLA | C2D-C1D-ND | 8.51 | 116.38 | 110.10 |
| 22 | 6 | 610 | CLA | C1D-ND-C4D | -8.51 | 100.29 | 106.33 |
| 22 | 8 | 611 | CLA | C1D-ND-C4D | -8.51 | 100.29 | 106.33 |
| 22 | B | 803 | CLA | C2D-C1D-ND | 8.50 | 116.37 | 110.10 |
| 29 | 4 | 608 | CHL | C4A-NA-C1A | -8.50 | 102.89 | 106.71 |
| 22 | 3 | 613 | CLA | C1D-ND-C4D | -8.50 | 100.30 | 106.33 |
| 22 | B | 803 | CLA | C1D-ND-C4D | -8.50 | 100.30 | 106.33 |
| 22 | 7 | 611 | CLA | C1D-ND-C4D | -8.50 | 100.30 | 106.33 |
| 22 | A | 803 | CLA | C2D-C1D-ND | 8.49 | 116.36 | 110.10 |
| 22 | A | 830 | CLA | C2D-C1D-ND | 8.48 | 116.36 | 110.10 |
| 22 | 2 | 609 | CLA | C1D-ND-C4D | -8.48 | 100.31 | 106.33 |
| 22 | 8 | 610 | CLA | C1D-ND-C4D | -8.47 | 100.32 | 106.33 |
| 22 | 8 | 616 | CLA | C1D-ND-C4D | -8.47 | 100.32 | 106.33 |
| 22 | 5 | 616 | CLA | C1D-ND-C4D | -8.45 | 100.33 | 106.33 |
| 22 | B | 819 | CLA | C1D-ND-C4D | -8.44 | 100.34 | 106.33 |
| 22 | 7 | 604 | CLA | C2D-C1D-ND | 8.43 | 116.31 | 110.10 |
| 22 | 3 | 611 | CLA | C1D-ND-C4D | -8.42 | 100.35 | 106.33 |
| 22 | 9 | 609 | CLA | C1D-ND-C4D | -8.40 | 100.36 | 106.33 |
| 22 | A | 809 | CLA | C2D-C1D-ND | 8.40 | 116.29 | 110.10 |
| 22 | 8 | 608 | CLA | C2D-C1D-ND | 8.38 | 116.28 | 110.10 |
| 22 | B | 809 | CLA | C1D-ND-C4D | -8.37 | 100.39 | 106.33 |
| 22 | 4 | 611 | CLA | C1D-ND-C4D | -8.37 | 100.39 | 106.33 |
| 22 | 8 | 601 | CLA | C1D-ND-C4D | -8.36 | 100.39 | 106.33 |
| 22 | 4 | 603 | CLA | C1D-ND-C4D | -8.36 | 100.40 | 106.33 |
| 22 | Z | 609 | CLA | C1D-ND-C4D | -8.35 | 100.40 | 106.33 |
| 22 | A | 832 | CLA | C1D-ND-C4D | -8.34 | 100.41 | 106.33 |
| 22 | 7 | 616 | CLA | C2D-C1D-ND | 8.33 | 116.25 | 110.10 |
| 29 | 4 | 606 | CHL | C4A-NA-C1A | -8.33 | 102.96 | 106.71 |
| 22 | 6 | 602 | CLA | C2D-C1D-ND | 8.33 | 116.24 | 110.10 |
| 22 | 5 | 604 | CLA | C1D-ND-C4D | -8.32 | 100.42 | 106.33 |
| 22 | 1 | 610 | CLA | C2D-C1D-ND | 8.32 | 116.24 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 826 | CLA | C1D-ND-C4D | -8.32 | 100.42 | 106.33 |
| 22 | 7 | 609 | CLA | C2D-C1D-ND | 8.32 | 116.23 | 110.10 |
| 22 | 7 | 606 | CLA | C2D-C1D-ND | 8.31 | 116.23 | 110.10 |
| 22 | A | 840 | CLA | C2D-C1D-ND | 8.31 | 116.23 | 110.10 |
| 22 | F | 303 | CLA | C2D-C1D-ND | 8.31 | 116.23 | 110.10 |
| 22 | Z | 610 | CLA | C2D-C1D-ND | 8.28 | 116.21 | 110.10 |
| 22 | 6 | 614 | CLA | CMD-C2D-C1D | 8.28 | 139.30 | 124.71 |
| 22 | L | 204 | CLA | C2D-C1D-ND | 8.26 | 116.19 | 110.10 |
| 22 | B | 838 | CLA | C2D-C1D-ND | 8.26 | 116.19 | 110.10 |
| 22 | B | 821 | CLA | C2D-C1D-ND | 8.25 | 116.18 | 110.10 |
| 22 | B | 817 | CLA | C1D-ND-C4D | -8.24 | 100.48 | 106.33 |
| 22 | 6 | 622 | CLA | C2D-C1D-ND | 8.24 | 116.18 | 110.10 |
| 22 | B | 823 | CLA | C1D-ND-C4D | -8.22 | 100.50 | 106.33 |
| 22 | A | 822 | CLA | C1D-ND-C4D | -8.21 | 100.50 | 106.33 |
| 22 | A | 811 | CLA | C2D-C1D-ND | 8.20 | 116.15 | 110.10 |
| 22 | 8 | 609 | CLA | C1D-ND-C4D | -8.20 | 100.51 | 106.33 |
| 22 | G | 203 | CLA | C2D-C1D-ND | 8.19 | 116.14 | 110.10 |
| 22 | A | 845 | CLA | C2D-C1D-ND | 8.19 | 116.14 | 110.10 |
| 22 | Z | 602 | CLA | C2D-C1D-ND | 8.18 | 116.13 | 110.10 |
| 22 | B | 827 | CLA | C2D-C1D-ND | 8.17 | 116.12 | 110.10 |
| 29 | 3 | 608 | CHL | C4A-NA-C1A | -8.17 | 103.03 | 106.71 |
| 22 | B | 812 | CLA | C2D-C1D-ND | 8.16 | 116.12 | 110.10 |
| 22 | A | 843 | CLA | C1D-ND-C4D | -8.14 | 100.55 | 106.33 |
| 22 | B | 836 | CLA | C1D-ND-C4D | -8.12 | 100.57 | 106.33 |
| 22 | 7 | 601 | CLA | C2D-C1D-ND | 8.11 | 116.08 | 110.10 |
| 22 | 7 | 613 | CLA | C2D-C1D-ND | 8.10 | 116.08 | 110.10 |
| 22 | 5 | 603 | CLA | C1D-ND-C4D | -8.08 | 100.59 | 106.33 |
| 22 | 1 | 602 | CLA | C2D-C1D-ND | 8.06 | 116.05 | 110.10 |
| 22 | 1 | 614 | CLA | C2D-C1D-ND | 8.06 | 116.05 | 110.10 |
| 22 | A | 842 | CLA | C2D-C1D-ND | 8.06 | 116.05 | 110.10 |
| 22 | B | 837 | CLA | C2D-C1D-ND | 8.06 | 116.04 | 110.10 |
| 22 | A | 837 | CLA | C1D-ND-C4D | -8.04 | 100.62 | 106.33 |
| 22 | 8 | 614 | CLA | C2D-C1D-ND | 8.02 | 116.01 | 110.10 |
| 21 | A | 801 | CL0 | C2D-C1D-ND | 8.02 | 116.01 | 110.10 |
| 22 | B | 815 | CLA | C2D-C1D-ND | 8.01 | 116.01 | 110.10 |
| 22 | A | 836 | CLA | C2D-C1D-ND | 8.01 | 116.00 | 110.10 |
| 22 | 5 | 602 | CLA | C2D-C1D-ND | 8.00 | 116.00 | 110.10 |
| 22 | A | 808 | CLA | C2D-C1D-ND | 7.99 | 115.99 | 110.10 |
| 22 | 2 | 614 | CLA | C2D-C1D-ND | 7.98 | 115.99 | 110.10 |
| 22 | 5 | 614 | CLA | C2D-C1D-ND | 7.98 | 115.98 | 110.10 |
| 22 | A | 817 | CLA | CMD-C2D-C1D | 7.98 | 138.77 | 124.71 |
| 22 | 4 | 612 | CLA | C2D-C1D-ND | 7.97 | 115.98 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 814 | CLA | C2D-C1D-ND | 7.97 | 115.98 | 110.10 |
| 22 | B | 829 | CLA | C2D-C1D-ND | 7.97 | 115.98 | 110.10 |
| 22 | A | 831 | CLA | C2D-C1D-ND | 7.94 | 115.96 | 110.10 |
| 22 | 5 | 610 | CLA | C2D-C1D-ND | 7.94 | 115.95 | 110.10 |
| 22 | A | 816 | CLA | C2D-C1D-ND | 7.93 | 115.95 | 110.10 |
| 22 | 4 | 613 | CLA | C2D-C1D-ND | 7.91 | 115.94 | 110.10 |
| 22 | 2 | 607 | CLA | C2D-C1D-ND | 7.90 | 115.92 | 110.10 |
| 22 | A | 819 | CLA | C2D-C1D-ND | 7.89 | 115.92 | 110.10 |
| 22 | 4 | 614 | CLA | C2D-C1D-ND | 7.89 | 115.92 | 110.10 |
| 22 | 7 | 614 | CLA | C2D-C1D-ND | 7.89 | 115.92 | 110.10 |
| 22 | B | 826 | CLA | C2D-C1D-ND | 7.87 | 115.91 | 110.10 |
| 22 | 3 | 607 | CLA | C2D-C1D-ND | 7.87 | 115.91 | 110.10 |
| 22 | B | 818 | CLA | C1D-ND-C4D | -7.86 | 100.75 | 106.33 |
| 22 | 3 | 604 | CLA | C2D-C1D-ND | 7.86 | 115.90 | 110.10 |
| 22 | A | 820 | CLA | C2D-C1D-ND | 7.86 | 115.90 | 110.10 |
| 22 | 7 | 612 | CLA | C2D-C1D-ND | 7.86 | 115.90 | 110.10 |
| 22 | 2 | 610 | CLA | C2D-C1D-ND | 7.86 | 115.89 | 110.10 |
| 22 | B | 829 | CLA | CMD-C2D-C1D | 7.86 | 138.56 | 124.71 |
| 22 | 5 | 609 | CLA | C2D-C1D-ND | 7.85 | 115.89 | 110.10 |
| 22 | Z | 613 | CLA | C2D-C1D-ND | 7.85 | 115.89 | 110.10 |
| 22 | F | 301 | CLA | CMD-C2D-C1D | 7.84 | 138.53 | 124.71 |
| 22 | 4 | 609 | CLA | C2D-C1D-ND | 7.82 | 115.87 | 110.10 |
| 22 | 9 | 604 | CLA | C2D-C1D-ND | 7.82 | 115.87 | 110.10 |
| 22 | B | 835 | CLA | C2D-C1D-ND | 7.81 | 115.86 | 110.10 |
| 22 | Z | 608 | CLA | C2D-C1D-ND | 7.80 | 115.85 | 110.10 |
| 25 | I | 172 | BCR | C24-C23-C22 | -7.80 | 114.45 | 126.23 |
| 22 | Z | 614 | CLA | C2D-C1D-ND | 7.80 | 115.85 | 110.10 |
| 22 | 1 | 613 | CLA | C2D-C1D-ND | 7.79 | 115.85 | 110.10 |
| 22 | 6 | 603 | CLA | C2D-C1D-ND | 7.79 | 115.84 | 110.10 |
| 22 | A | 834 | CLA | C2D-C1D-ND | 7.79 | 115.84 | 110.10 |
| 22 | 9 | 610 | CLA | C2D-C1D-ND | 7.78 | 115.84 | 110.10 |
| 22 | B | 813 | CLA | C2D-C1D-ND | 7.78 | 115.84 | 110.10 |
| 22 | B | 852 | CLA | C2D-C1D-ND | 7.78 | 115.83 | 110.10 |
| 22 | 3 | 603 | CLA | C2D-C1D-ND | 7.77 | 115.83 | 110.10 |
| 22 | B | 811 | CLA | C2D-C1D-ND | 7.76 | 115.82 | 110.10 |
| 22 | 7 | 620 | CLA | C2D-C1D-ND | 7.76 | 115.82 | 110.10 |
| 22 | 4 | 601 | CLA | C2D-C1D-ND | 7.76 | 115.82 | 110.10 |
| 22 | A | 807 | CLA | C2D-C1D-ND | 7.75 | 115.82 | 110.10 |
| 22 | A | 824 | CLA | C2D-C1D-ND | 7.75 | 115.81 | 110.10 |
| 22 | 5 | 606 | CLA | C2D-C1D-ND | 7.75 | 115.81 | 110.10 |
| 22 | 2 | 611 | CLA | C2D-C1D-ND | 7.75 | 115.81 | 110.10 |
| 22 | 7 | 611 | CLA | C2D-C1D-ND | 7.74 | 115.81 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 6 | 601 | CLA | C2D-C1D-ND | 7.74 | 115.81 | 110.10 |
| 22 | 9 | 614 | CLA | C2D-C1D-ND | 7.74 | 115.81 | 110.10 |
| 22 | 2 | 613 | CLA | C2D-C1D-ND | 7.74 | 115.81 | 110.10 |
| 22 | 3 | 610 | CLA | C2D-C1D-ND | 7.74 | 115.81 | 110.10 |
| 22 | 1 | 608 | CLA | C2D-C1D-ND | 7.74 | 115.81 | 110.10 |
| 22 | 3 | 620 | CLA | C2D-C1D-ND | 7.73 | 115.80 | 110.10 |
| 22 | A | 825 | CLA | C2D-C1D-ND | 7.72 | 115.80 | 110.10 |
| 22 | A | 810 | CLA | C2D-C1D-ND | 7.72 | 115.79 | 110.10 |
| 22 | 5 | 611 | CLA | C2D-C1D-ND | 7.71 | 115.79 | 110.10 |
| 29 | 9 | 607 | CHL | C4A-NA-C1A | -7.71 | 103.24 | 106.71 |
| 22 | B | 833 | CLA | C2D-C1D-ND | 7.71 | 115.79 | 110.10 |
| 22 | B | 832 | CLA | C2D-C1D-ND | 7.71 | 115.79 | 110.10 |
| 22 | 9 | 602 | CLA | C2D-C1D-ND | 7.71 | 115.79 | 110.10 |
| 22 | Z | 612 | CLA | C2D-C1D-ND | 7.71 | 115.78 | 110.10 |
| 22 | 4 | 610 | CLA | C2D-C1D-ND | 7.70 | 115.78 | 110.10 |
| 22 | 5 | 621 | CLA | C1D-ND-C4D | -7.70 | 100.86 | 106.33 |
| 22 | 5 | 616 | CLA | C2D-C1D-ND | 7.70 | 115.78 | 110.10 |
| 22 | B | 806 | CLA | C2D-C1D-ND | 7.69 | 115.77 | 110.10 |
| 22 | B | 822 | CLA | C2D-C1D-ND | 7.69 | 115.77 | 110.10 |
| 22 | 2 | 602 | CLA | C2D-C1D-ND | 7.69 | 115.77 | 110.10 |
| 22 | A | 806 | CLA | C2D-C1D-ND | 7.69 | 115.77 | 110.10 |
| 22 | 1 | 603 | CLA | C2D-C1D-ND | 7.68 | 115.76 | 110.10 |
| 22 | 1 | 606 | CLA | C2D-C1D-ND | 7.67 | 115.76 | 110.10 |
| 22 | 8 | 606 | CLA | C2D-C1D-ND | 7.67 | 115.76 | 110.10 |
| 22 | B | 809 | CLA | C2D-C1D-ND | 7.67 | 115.75 | 110.10 |
| 22 | A | 813 | CLA | C2D-C1D-ND | 7.66 | 115.75 | 110.10 |
| 22 | 5 | 612 | CLA | C2D-C1D-ND | 7.66 | 115.75 | 110.10 |
| 22 | 6 | 609 | CLA | C2D-C1D-ND | 7.66 | 115.75 | 110.10 |
| 22 | 3 | 612 | CLA | C2D-C1D-ND | 7.66 | 115.75 | 110.10 |
| 22 | Z | 611 | CLA | C2D-C1D-ND | 7.66 | 115.75 | 110.10 |
| 22 | 3 | 614 | CLA | C2D-C1D-ND | 7.65 | 115.74 | 110.10 |
| 22 | 4 | 616 | CLA | C2D-C1D-ND | 7.65 | 115.74 | 110.10 |
| 22 | Z | 606 | CLA | C2D-C1D-ND | 7.64 | 115.73 | 110.10 |
| 22 | 8 | 610 | CLA | C2D-C1D-ND | 7.63 | 115.73 | 110.10 |
| 22 | F | 304 | CLA | C2D-C1D-ND | 7.63 | 115.73 | 110.10 |
| 22 | K | 4002 | CLA | C2D-C1D-ND | 7.62 | 115.72 | 110.10 |
| 29 | 3 | 608 | CHL | CMD-C2D-C1D | 7.62 | 138.15 | 124.71 |
| 22 | 4 | 602 | CLA | C2D-C1D-ND | 7.62 | 115.72 | 110.10 |
| 22 | 8 | 611 | CLA | C2D-C1D-ND | 7.61 | 115.71 | 110.10 |
| 29 | 4 | 608 | CHL | CMD-C2D-C1D | 7.61 | 138.13 | 124.71 |
| 22 | B | 807 | CLA | C2D-C1D-ND | 7.61 | 115.71 | 110.10 |
| 22 | G | 204 | CLA | C2D-C1D-ND | 7.61 | 115.71 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 1 | 609 | CLA | C2D-C1D-ND | 7.61 | 115.71 | 110.10 |
| 22 | A | 804 | CLA | CMD-C2D-C1D | 7.61 | 138.12 | 124.71 |
| 22 | 3 | 602 | CLA | C2D-C1D-ND | 7.60 | 115.70 | 110.10 |
| 22 | B | 830 | CLA | C2D-C1D-ND | 7.60 | 115.70 | 110.10 |
| 22 | 3 | 617 | CLA | C2D-C1D-ND | 7.58 | 115.69 | 110.10 |
| 22 | K | 4003 | CLA | C2D-C1D-ND | 7.58 | 115.69 | 110.10 |
| 22 | 5 | 603 | CLA | C2D-C1D-ND | 7.57 | 115.69 | 110.10 |
| 22 | Z | 616 | CLA | C2D-C1D-ND | 7.57 | 115.68 | 110.10 |
| 22 | A | 839 | CLA | C2D-C1D-ND | 7.56 | 115.68 | 110.10 |
| 22 | B | 810 | CLA | C2D-C1D-ND | 7.56 | 115.68 | 110.10 |
| 22 | 9 | 601 | CLA | C2D-C1D-ND | 7.56 | 115.67 | 110.10 |
| 22 | 6 | 616 | CLA | C2D-C1D-ND | 7.55 | 115.67 | 110.10 |
| 29 | 6 | 607 | CHL | C4A-NA-C1A | -7.55 | 103.31 | 106.71 |
| 22 | 2 | 606 | CLA | C2D-C1D-ND | 7.55 | 115.67 | 110.10 |
| 22 | 8 | 601 | CLA | C2D-C1D-ND | 7.55 | 115.67 | 110.10 |
| 22 | 9 | 609 | CLA | C2D-C1D-ND | 7.54 | 115.66 | 110.10 |
| 22 | 5 | 601 | CLA | C2D-C1D-ND | 7.54 | 115.66 | 110.10 |
| 22 | 7 | 616 | CLA | CHD-C1D-ND | -7.53 | 117.54 | 124.45 |
| 22 | B | 840 | CLA | C2D-C1D-ND | 7.52 | 115.65 | 110.10 |
| 22 | A | 827 | CLA | C2D-C1D-ND | 7.52 | 115.65 | 110.10 |
| 22 | B | 808 | CLA | C2D-C1D-ND | 7.50 | 115.63 | 110.10 |
| 22 | 4 | 604 | CLA | C2D-C1D-ND | 7.50 | 115.63 | 110.10 |
| 22 | 9 | 612 | CLA | C2D-C1D-ND | 7.49 | 115.63 | 110.10 |
| 22 | A | 822 | CLA | C2D-C1D-ND | 7.48 | 115.62 | 110.10 |
| 22 | 3 | 609 | CLA | C2D-C1D-ND | 7.48 | 115.62 | 110.10 |
| 22 | 2 | 601 | CLA | C2D-C1D-ND | 7.48 | 115.62 | 110.10 |
| 22 | 6 | 617 | CLA | C2D-C1D-ND | 7.47 | 115.61 | 110.10 |
| 22 | B | 823 | CLA | C2D-C1D-ND | 7.47 | 115.61 | 110.10 |
| 22 | J | 3002 | CLA | C2D-C1D-ND | 7.46 | 115.60 | 110.10 |
| 22 | 9 | 611 | CLA | C2D-C1D-ND | 7.46 | 115.60 | 110.10 |
| 22 | 5 | 613 | CLA | C2D-C1D-ND | 7.45 | 115.60 | 110.10 |
| 22 | 8 | 604 | CLA | C2D-C1D-ND | 7.45 | 115.59 | 110.10 |
| 22 | 9 | 613 | CLA | C2D-C1D-ND | 7.44 | 115.59 | 110.10 |
| 22 | 6 | 612 | CLA | C2D-C1D-ND | 7.44 | 115.59 | 110.10 |
| 22 | A | 821 | CLA | C2D-C1D-ND | 7.43 | 115.58 | 110.10 |
| 22 | 8 | 609 | CLA | C2D-C1D-ND | 7.43 | 115.58 | 110.10 |
| 22 | A | 843 | CLA | C2D-C1D-ND | 7.43 | 115.58 | 110.10 |
| 22 | 6 | 604 | CLA | C2D-C1D-ND | 7.42 | 115.58 | 110.10 |
| 22 | 7 | 610 | CLA | C2D-C1D-ND | 7.42 | 115.57 | 110.10 |
| 29 | 7 | 607 | CHL | CMD-C2D-C1D | 7.42 | 137.79 | 124.71 |
| 22 | 1 | 612 | CLA | C2D-C1D-ND | 7.42 | 115.57 | 110.10 |
| 22 | 8 | 612 | CLA | C2D-C1D-ND | 7.41 | 115.57 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 841 | CLA | C2D-C1D-ND | 7.41 | 115.56 | 110.10 |
| 22 | Z | 604 | CLA | C2D-C1D-ND | 7.41 | 115.56 | 110.10 |
| 22 | 1 | 611 | CLA | C2D-C1D-ND | 7.41 | 115.56 | 110.10 |
| 22 | A | 833 | CLA | C2D-C1D-ND | 7.40 | 115.56 | 110.10 |
| 22 | 6 | 611 | CLA | C2D-C1D-ND | 7.40 | 115.56 | 110.10 |
| 22 | 3 | 611 | CLA | C2D-C1D-ND | 7.38 | 115.55 | 110.10 |
| 22 | 8 | 613 | CLA | C2D-C1D-ND | 7.38 | 115.54 | 110.10 |
| 22 | A | 802 | CLA | C2D-C1D-ND | 7.37 | 115.53 | 110.10 |
| 22 | 4 | 611 | CLA | C2D-C1D-ND | 7.36 | 115.53 | 110.10 |
| 22 | B | 824 | CLA | C2D-C1D-ND | 7.36 | 115.53 | 110.10 |
| 22 | 6 | 613 | CLA | C2D-C1D-ND | 7.36 | 115.53 | 110.10 |
| 22 | 2 | 609 | CLA | C2D-C1D-ND | 7.36 | 115.53 | 110.10 |
| 22 | 7 | 603 | CLA | C2D-C1D-ND | 7.34 | 115.51 | 110.10 |
| 22 | 9 | 603 | CLA | C2D-C1D-ND | 7.33 | 115.51 | 110.10 |
| 22 | A | 805 | CLA | C2D-C1D-ND | 7.32 | 115.50 | 110.10 |
| 22 | 3 | 606 | CLA | C2D-C1D-ND | 7.32 | 115.50 | 110.10 |
| 22 | B | 825 | CLA | C2D-C1D-ND | 7.30 | 115.48 | 110.10 |
| 22 | 1 | 616 | CLA | C2D-C1D-ND | 7.28 | 115.47 | 110.10 |
| 29 | 7 | 607 | CHL | C4A-NA-C1A | -7.27 | 103.44 | 106.71 |
| 22 | 2 | 612 | CLA | C2D-C1D-ND | 7.27 | 115.46 | 110.10 |
| 22 | A | 832 | CLA | C2D-C1D-ND | 7.27 | 115.46 | 110.10 |
| 29 | 6 | 606 | CHL | CMD-C2D-C1D | 7.26 | 137.51 | 124.71 |
| 22 | A | 828 | CLA | CHD-C4C-C3C | -7.26 | 114.16 | 124.84 |
| 22 | 8 | 603 | CLA | C2D-C1D-ND | 7.26 | 115.46 | 110.10 |
| 22 | 6 | 610 | CLA | C2D-C1D-ND | 7.26 | 115.46 | 110.10 |
| 22 | 2 | 603 | CLA | C2D-C1D-ND | 7.26 | 115.45 | 110.10 |
| 22 | B | 839 | CLA | C2D-C1D-ND | 7.23 | 115.43 | 110.10 |
| 22 | 6 | 614 | CLA | C2D-C1D-ND | 7.23 | 115.43 | 110.10 |
| 22 | 8 | 601 | CLA | CMD-C2D-C1D | 7.21 | 137.41 | 124.71 |
| 22 | B | 836 | CLA | C2D-C1D-ND | 7.19 | 115.40 | 110.10 |
| 22 | 8 | 608 | CLA | CMD-C2D-C1D | 7.18 | 137.37 | 124.71 |
| 29 | 5 | 608 | CHL | CMD-C2D-C1D | 7.18 | 137.37 | 124.71 |
| 22 | B | 820 | CLA | C2D-C1D-ND | 7.17 | 115.39 | 110.10 |
| 22 | B | 834 | CLA | CMD-C2D-C1D | 7.17 | 137.34 | 124.71 |
| 22 | B | 828 | CLA | C2D-C1D-ND | 7.17 | 115.39 | 110.10 |
| 22 | F | 301 | CLA | C2D-C1D-ND | 7.15 | 115.38 | 110.10 |
| 29 | 9 | 607 | CHL | CMD-C2D-C1D | 7.15 | 137.32 | 124.71 |
| 22 | 7 | 603 | CLA | CMD-C2D-C1D | 7.15 | 137.32 | 124.71 |
| 22 | 3 | 613 | CLA | C2D-C1D-ND | 7.15 | 115.37 | 110.10 |
| 22 | A | 815 | CLA | C2D-C1D-ND | 7.14 | 115.37 | 110.10 |
| 22 | A | 835 | CLA | C2D-C1D-ND | 7.14 | 115.37 | 110.10 |
| 22 | B | 819 | CLA | C2D-C1D-ND | 7.13 | 115.36 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 3 | 614 | CLA | CMD-C2D-C1D | 7.13 | 137.29 | 124.71 |
| 22 | B | 834 | CLA | C2D-C1D-ND | 7.13 | 115.36 | 110.10 |
| 25 | B | 801 | BCR | C16-C15-C14 | -7.12 | 108.88 | 123.47 |
| 22 | 7 | 601 | CLA | CMD-C2D-C1D | 7.11 | 137.25 | 124.71 |
| 22 | 5 | 604 | CLA | C2D-C1D-ND | 7.10 | 115.34 | 110.10 |
| 22 | A | 838 | CLA | CMD-C2D-C1D | 7.10 | 137.22 | 124.71 |
| 22 | 5 | 602 | CLA | CMD-C2D-C1D | 7.10 | 137.22 | 124.71 |
| 22 | B | 817 | CLA | C2D-C1D-ND | 7.09 | 115.33 | 110.10 |
| 22 | A | 840 | CLA | CMD-C2D-C1D | 7.09 | 137.20 | 124.71 |
| 22 | B | 840 | CLA | C2C-C1C-NC | 7.08 | 116.60 | 109.97 |
| 22 | A | 826 | CLA | CMD-C2D-C1D | 7.07 | 137.18 | 124.71 |
| 22 | Z | 603 | CLA | C2D-C1D-ND | 7.07 | 115.32 | 110.10 |
| 22 | A | 838 | CLA | C2D-C1D-ND | 7.06 | 115.31 | 110.10 |
| 22 | 8 | 616 | CLA | C2D-C1D-ND | 7.06 | 115.31 | 110.10 |
| 22 | 1 | 608 | CLA | CMD-C2D-C1D | 7.06 | 137.16 | 124.71 |
| 22 | B | 826 | CLA | CMD-C2D-C1D | 7.06 | 137.15 | 124.71 |
| 22 | 6 | 613 | CLA | CMD-C2D-C1D | 7.06 | 137.15 | 124.71 |
| 22 | Z | 608 | CLA | CMD-C2D-C1D | 7.06 | 137.15 | 124.71 |
| 22 | J | 3002 | CLA | CMD-C2D-C1D | 7.05 | 137.15 | 124.71 |
| 22 | 9 | 603 | CLA | C4A-NA-C1A | -7.05 | 103.54 | 106.71 |
| 22 | A | 834 | CLA | CMD-C2D-C1D | 7.05 | 137.13 | 124.71 |
| 22 | A | 837 | CLA | C2D-C1D-ND | 7.04 | 115.29 | 110.10 |
| 22 | B | 814 | CLA | CMD-C2D-C1D | 7.04 | 137.12 | 124.71 |
| 22 | A | 826 | CLA | C2D-C1D-ND | 7.03 | 115.28 | 110.10 |
| 22 | Z | 609 | CLA | C2D-C1D-ND | 7.03 | 115.28 | 110.10 |
| 22 | Z | 606 | CLA | CMD-C2D-C1D | 7.03 | 137.10 | 124.71 |
| 29 | 4 | 606 | CHL | CMD-C2D-C1D | 7.03 | 137.09 | 124.71 |
| 22 | 7 | 614 | CLA | O2D-CGD-CBD | 7.02 | 123.75 | 111.27 |
| 29 | 4 | 607 | CHL | CMD-C2D-C1D | 7.02 | 137.08 | 124.71 |
| 22 | 1 | 604 | CLA | CMD-C2D-C1D | 7.02 | 137.08 | 124.71 |
| 22 | B | 816 | CLA | CMD-C2D-C1D | 7.01 | 137.08 | 124.71 |
| 22 | A | 827 | CLA | CMD-C2D-C1D | 7.01 | 137.07 | 124.71 |
| 29 | 1 | 601 | CHL | CMD-C2D-C1D | 7.01 | 137.07 | 124.71 |
| 22 | A | 814 | CLA | CMD-C2D-C1D | 6.99 | 137.03 | 124.71 |
| 29 | 5 | 607 | CHL | CMD-C2D-C1D | 6.99 | 137.03 | 124.71 |
| 22 | B | 802 | CLA | CHD-C4C-C3C | -6.99 | 114.57 | 124.84 |
| 22 | B | 812 | CLA | CMD-C2D-C1D | 6.98 | 137.02 | 124.71 |
| 22 | A | 817 | CLA | C2D-C1D-ND | 6.98 | 115.25 | 110.10 |
| 22 | 9 | 603 | CLA | CMD-C2D-C1D | 6.95 | 136.97 | 124.71 |
| 22 | B | 818 | CLA | C2D-C1D-ND | 6.95 | 115.23 | 110.10 |
| 22 | B | 836 | CLA | CMD-C2D-C1D | 6.95 | 136.96 | 124.71 |
| 22 | A | 802 | CLA | CHD-C1D-ND | -6.95 | 118.07 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 840 | CLA | CMD-C2D-C1D | 6.94 | 136.95 | 124.71 |
| 22 | B | 810 | CLA | CMD-C2D-C1D | 6.94 | 136.94 | 124.71 |
| 22 | B | 817 | CLA | CMD-C2D-C1D | 6.93 | 136.92 | 124.71 |
| 22 | 7 | 606 | CLA | CMD-C2D-C1D | 6.93 | 136.92 | 124.71 |
| 29 | 6 | 608 | CHL | CMD-C2D-C1D | 6.92 | 136.90 | 124.71 |
| 22 | 1 | 609 | CLA | CMD-C2D-C1D | 6.91 | 136.89 | 124.71 |
| 22 | 4 | 603 | CLA | CMD-C2D-C1D | 6.90 | 136.88 | 124.71 |
| 22 | 5 | 603 | CLA | CMD-C2D-C1D | 6.90 | 136.88 | 124.71 |
| 29 | 3 | 608 | CHL | C1C-C2C-C3C | -6.90 | 101.64 | 107.11 |
| 22 | 4 | 603 | CLA | C2D-C1D-ND | 6.89 | 115.18 | 110.10 |
| 22 | 7 | 604 | CLA | CMD-C2D-C1D | 6.89 | 136.86 | 124.71 |
| 22 | 7 | 616 | CLA | CMD-C2D-C1D | 6.89 | 136.86 | 124.71 |
| 29 | 5 | 618 | CHL | CMD-C2D-C1D | 6.89 | 136.86 | 124.71 |
| 22 | 2 | 609 | CLA | CMD-C2D-C1D | 6.89 | 136.86 | 124.71 |
| 22 | 2 | 603 | CLA | CMD-C2D-C1D | 6.89 | 136.86 | 124.71 |
| 22 | B | 816 | CLA | CHD-C4C-C3C | -6.89 | 114.72 | 124.84 |
| 22 | 1 | 604 | CLA | C2D-C1D-ND | 6.88 | 115.17 | 110.10 |
| 22 | 3 | 606 | CLA | CMD-C2D-C1D | 6.88 | 136.84 | 124.71 |
| 22 | 2 | 614 | CLA | CMD-C2D-C1D | 6.88 | 136.83 | 124.71 |
| 22 | 8 | 602 | CLA | CHD-C4C-C3C | -6.88 | 114.73 | 124.84 |
| 22 | Z | 603 | CLA | CMD-C2D-C1D | 6.88 | 136.83 | 124.71 |
| 22 | 3 | 620 | CLA | CMD-C2D-C1D | 6.87 | 136.83 | 124.71 |
| 29 | 9 | 606 | CHL | CMD-C2D-C1D | 6.87 | 136.81 | 124.71 |
| 22 | 2 | 601 | CLA | CMD-C2D-C1D | 6.86 | 136.81 | 124.71 |
| 22 | 5 | 606 | CLA | CMD-C2D-C1D | 6.86 | 136.80 | 124.71 |
| 22 | 6 | 602 | CLA | CMD-C2D-C1D | 6.85 | 136.79 | 124.71 |
| 22 | A | 819 | CLA | CMD-C2D-C1D | 6.85 | 136.79 | 124.71 |
| 22 | B | 832 | CLA | CMD-C2D-C1D | 6.85 | 136.78 | 124.71 |
| 22 | K | 4002 | CLA | CMD-C2D-C1D | 6.85 | 136.78 | 124.71 |
| 22 | B | 806 | CLA | CMD-C2D-C1D | 6.84 | 136.77 | 124.71 |
| 22 | L | 204 | CLA | CMD-C2D-C1D | 6.84 | 136.77 | 124.71 |
| 22 | A | 824 | CLA | CMD-C2D-C1D | 6.84 | 136.76 | 124.71 |
| 22 | A | 815 | CLA | CHD-C1D-ND | -6.84 | 118.17 | 124.45 |
| 29 | Z | 607 | CHL | C4A-NA-C1A | -6.84 | 103.63 | 106.71 |
| 22 | 6 | 603 | CLA | CMD-C2D-C1D | 6.82 | 136.74 | 124.71 |
| 22 | A | 828 | CLA | CMD-C2D-C1D | 6.82 | 136.73 | 124.71 |
| 22 | B | 833 | CLA | CMD-C2D-C1D | 6.81 | 136.72 | 124.71 |
| 22 | Z | 604 | CLA | CMD-C2D-C1D | 6.81 | 136.72 | 124.71 |
| 22 | 4 | 604 | CLA | CMD-C2D-C1D | 6.81 | 136.71 | 124.71 |
| 22 | A | 808 | CLA | CMD-C2D-C1D | 6.80 | 136.71 | 124.71 |
| 22 | 3 | 602 | CLA | CMD-C2D-C1D | 6.80 | 136.69 | 124.71 |
| 22 | B | 831 | CLA | CMD-C2D-C1D | 6.79 | 136.69 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 614 | CLA | CMD-C2D-C1D | 6.79 | 136.68 | 124.71 |
| 22 | 2 | 610 | CLA | CMD-C2D-C1D | 6.79 | 136.68 | 124.71 |
| 22 | 6 | 614 | CLA | CHD-C1D-ND | -6.79 | 118.22 | 124.45 |
| 22 | 3 | 610 | CLA | CMD-C2D-C1D | 6.79 | 136.67 | 124.71 |
| 22 | B | 839 | CLA | CMD-C2D-C1D | 6.78 | 136.67 | 124.71 |
| 29 | 4 | 618 | CHL | CMD-C2D-C1D | 6.76 | 136.63 | 124.71 |
| 22 | K | 4003 | CLA | CMD-C2D-C1D | 6.76 | 136.63 | 124.71 |
| 29 | 6 | 607 | CHL | CMD-C2D-C1D | 6.76 | 136.63 | 124.71 |
| 22 | A | 833 | CLA | CMD-C2D-C1D | 6.76 | 136.62 | 124.71 |
| 22 | 9 | 610 | CLA | CMD-C2D-C1D | 6.75 | 136.61 | 124.71 |
| 22 | G | 204 | CLA | CMD-C2D-C1D | 6.75 | 136.61 | 124.71 |
| 22 | 6 | 601 | CLA | CMD-C2D-C1D | 6.74 | 136.60 | 124.71 |
| 22 | 3 | 612 | CLA | C4A-NA-C1A | -6.73 | 103.68 | 106.71 |
| 22 | 8 | 611 | CLA | CMD-C2D-C1D | 6.73 | 136.57 | 124.71 |
| 22 | B | 837 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.71 |
| 22 | 9 | 601 | CLA | CMD-C2D-C1D | 6.72 | 136.56 | 124.71 |
| 22 | 2 | 602 | CLA | CMD-C2D-C1D | 6.72 | 136.55 | 124.71 |
| 22 | 6 | 616 | CLA | CMD-C2D-C1D | 6.71 | 136.55 | 124.71 |
| 22 | A | 835 | CLA | CMD-C2D-C1D | 6.71 | 136.54 | 124.71 |
| 22 | 1 | 603 | CLA | CMD-C2D-C1D | 6.71 | 136.54 | 124.71 |
| 22 | 7 | 610 | CLA | CMD-C2D-C1D | 6.70 | 136.53 | 124.71 |
| 22 | 4 | 616 | CLA | CMD-C2D-C1D | 6.70 | 136.53 | 124.71 |
| 22 | 2 | 607 | CLA | CMD-C2D-C1D | 6.70 | 136.53 | 124.71 |
| 22 | B | 807 | CLA | CMD-C2D-C1D | 6.70 | 136.52 | 124.71 |
| 29 | 8 | 607 | CHL | C1D-ND-C4D | -6.70 | 101.58 | 106.33 |
| 22 | A | 837 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.71 |
| 22 | A | 820 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.71 |
| 22 | 9 | 614 | CLA | CMD-C2D-C1D | 6.69 | 136.51 | 124.71 |
| 22 | A | 842 | CLA | CMD-C2D-C1D | 6.69 | 136.50 | 124.71 |
| 22 | 9 | 604 | CLA | CMD-C2D-C1D | 6.69 | 136.50 | 124.71 |
| 22 | Z | 609 | CLA | CMD-C2D-C1D | 6.69 | 136.50 | 124.71 |
| 22 | A | 815 | CLA | CMD-C2D-C1D | 6.68 | 136.49 | 124.71 |
| 22 | B | 814 | CLA | C2D-C1D-ND | 6.68 | 115.03 | 110.10 |
| 22 | 6 | 622 | CLA | CMD-C2D-C1D | 6.68 | 136.49 | 124.71 |
| 22 | Z | 614 | CLA | CMD-C2D-C1D | 6.68 | 136.48 | 124.71 |
| 22 | 4 | 602 | CLA | CMD-C2D-C1D | 6.68 | 136.48 | 124.71 |
| 22 | B | 819 | CLA | CMD-C2D-C1D | 6.68 | 136.48 | 124.71 |
| 29 | 4 | 607 | CHL | C1D-ND-C4D | -6.67 | 101.60 | 106.33 |
| 22 | 8 | 602 | CLA | CMD-C2D-C1D | 6.67 | 136.47 | 124.71 |
| 22 | 3 | 609 | CLA | CMD-C2D-C1D | 6.67 | 136.46 | 124.71 |
| 22 | 1 | 614 | CLA | CMD-C2D-C1D | 6.66 | 136.46 | 124.71 |
| 22 | 6 | 610 | CLA | CMD-C2D-C1D | 6.66 | 136.46 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 7 | 608 | CLA | CMD-C2D-C1D | 6.66 | 136.45 | 124.71 |
| 22 | 4 | 601 | CLA | CMD-C2D-C1D | 6.66 | 136.45 | 124.71 |
| 22 | 6 | 604 | CLA | CMD-C2D-C1D | 6.66 | 136.45 | 124.71 |
| 22 | F | 304 | CLA | CMD-C2D-C1D | 6.66 | 136.44 | 124.71 |
| 22 | A | 835 | CLA | CHD-C1D-ND | -6.66 | 118.34 | 124.45 |
| 22 | 2 | 606 | CLA | CMD-C2D-C1D | 6.65 | 136.44 | 124.71 |
| 22 | G | 203 | CLA | CMD-C2D-C1D | 6.65 | 136.44 | 124.71 |
| 22 | F | 303 | CLA | CMD-C2D-C1D | 6.65 | 136.43 | 124.71 |
| 22 | 5 | 604 | CLA | CMD-C2D-C1D | 6.64 | 136.41 | 124.71 |
| 22 | B | 815 | CLA | CMD-C2D-C1D | 6.64 | 136.41 | 124.71 |
| 22 | 7 | 620 | CLA | CMD-C2D-C1D | 6.63 | 136.41 | 124.71 |
| 22 | B | 811 | CLA | CMD-C2D-C1D | 6.63 | 136.39 | 124.71 |
| 22 | 8 | 604 | CLA | CMD-C2D-C1D | 6.62 | 136.38 | 124.71 |
| 22 | 3 | 604 | CLA | CMD-C2D-C1D | 6.61 | 136.37 | 124.71 |
| 22 | A | 809 | CLA | CMD-C2D-C1D | 6.61 | 136.37 | 124.71 |
| 22 | 5 | 616 | CLA | CMD-C2D-C1D | 6.61 | 136.37 | 124.71 |
| 22 | A | 813 | CLA | CMD-C2D-C1D | 6.61 | 136.36 | 124.71 |
| 22 | 9 | 602 | CLA | CMD-C2D-C1D | 6.61 | 136.36 | 124.71 |
| 22 | 5 | 617 | CLA | CMD-C2D-C1D | 6.60 | 136.35 | 124.71 |
| 22 | 8 | 603 | CLA | CMD-C2D-C1D | 6.60 | 136.35 | 124.71 |
| 22 | 1 | 606 | CLA | CMD-C2D-C1D | 6.60 | 136.35 | 124.71 |
| 22 | Z | 602 | CLA | CMD-C2D-C1D | 6.59 | 136.34 | 124.71 |
| 29 | 8 | 607 | CHL | C2C-C3C-C4C | -6.59 | 101.79 | 106.49 |
| 22 | A | 845 | CLA | CMD-C2D-C1D | 6.59 | 136.32 | 124.71 |
| 22 | 9 | 612 | CLA | CMD-C2D-C1D | 6.58 | 136.31 | 124.71 |
| 22 | 5 | 610 | CLA | CMD-C2D-C1D | 6.58 | 136.31 | 124.71 |
| 22 | B | 841 | CLA | CHD-C1D-ND | -6.57 | 118.41 | 124.45 |
| 22 | 9 | 613 | CLA | CMD-C2D-C1D | 6.57 | 136.30 | 124.71 |
| 22 | A | 805 | CLA | CHD-C1D-ND | -6.57 | 118.42 | 124.45 |
| 22 | A | 839 | CLA | CMD-C2D-C1D | 6.56 | 136.27 | 124.71 |
| 22 | B | 825 | CLA | CMD-C2D-C1D | 6.56 | 136.27 | 124.71 |
| 22 | Z | 611 | CLA | CMD-C2D-C1D | 6.56 | 136.27 | 124.71 |
| 22 | 7 | 602 | CLA | CMD-C2D-C1D | 6.55 | 136.26 | 124.71 |
| 22 | B | 830 | CLA | CMD-C2D-C1D | 6.55 | 136.26 | 124.71 |
| 22 | B | 820 | CLA | CMD-C2D-C1D | 6.55 | 136.25 | 124.71 |
| 22 | 5 | 617 | CLA | CHD-C1D-ND | -6.55 | 118.44 | 124.45 |
| 22 | 1 | 614 | CLA | CHD-C1D-ND | -6.54 | 118.44 | 124.45 |
| 22 | 8 | 612 | CLA | CMD-C2D-C1D | 6.53 | 136.23 | 124.71 |
| 22 | B | 818 | CLA | CMD-C2D-C1D | 6.53 | 136.23 | 124.71 |
| 22 | B | 837 | CLA | O2D-CGD-CBD | 6.53 | 122.88 | 111.27 |
| 22 | 7 | 604 | CLA | C2C-C1C-NC | 6.53 | 116.09 | 109.97 |
| 22 | B | 841 | CLA | CMD-C2D-C1D | 6.53 | 136.22 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 806 | CLA | CMD-C2D-C1D | 6.53 | 136.22 | 124.71 |
| 25 | 5 | 625 | BCR | C11-C10-C9 | -6.53 | 117.99 | 127.31 |
| 22 | 2 | 613 | CLA | CMD-C2D-C1D | 6.53 | 136.22 | 124.71 |
| 22 | 2 | 603 | CLA | C4A-NA-C1A | -6.52 | 103.77 | 106.71 |
| 29 | 6 | 618 | CHL | C1D-ND-C4D | -6.52 | 101.70 | 106.33 |
| 22 | B | 836 | CLA | C4A-NA-C1A | -6.51 | 103.78 | 106.71 |
| 22 | B | 822 | CLA | CMD-C2D-C1D | 6.50 | 136.16 | 124.71 |
| 22 | A | 803 | CLA | CMD-C2D-C1D | 6.50 | 136.16 | 124.71 |
| 22 | A | 802 | CLA | CMD-C2D-C1D | 6.49 | 136.16 | 124.71 |
| 22 | B | 805 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.71 |
| 22 | 7 | 612 | CLA | CMD-C2D-C1D | 6.49 | 136.15 | 124.71 |
| 22 | B | 805 | CLA | O2D-CGD-CBD | 6.49 | 122.79 | 111.27 |
| 22 | 2 | 610 | CLA | CHD-C1D-ND | -6.48 | 118.50 | 124.45 |
| 22 | 8 | 606 | CLA | CMD-C2D-C1D | 6.48 | 136.13 | 124.71 |
| 22 | 9 | 611 | CLA | CMD-C2D-C1D | 6.48 | 136.13 | 124.71 |
| 22 | F | 301 | CLA | C4A-NA-C1A | -6.47 | 103.80 | 106.71 |
| 22 | B | 830 | CLA | O2D-CGD-CBD | 6.47 | 122.77 | 111.27 |
| 29 | Z | 607 | CHL | CMD-C2D-C1D | 6.47 | 136.11 | 124.71 |
| 29 | Z | 607 | CHL | C1D-ND-C4D | -6.46 | 101.74 | 106.33 |
| 22 | A | 805 | CLA | CMD-C2D-C1D | 6.46 | 136.10 | 124.71 |
| 22 | 5 | 611 | CLA | CMD-C2D-C1D | 6.46 | 136.10 | 124.71 |
| 22 | 3 | 617 | CLA | CMD-C2D-C1D | 6.46 | 136.10 | 124.71 |
| 22 | A | 817 | CLA | CHD-C1D-ND | -6.46 | 118.52 | 124.45 |
| 22 | A | 829 | CLA | CHD-C4C-C3C | -6.46 | 115.35 | 124.84 |
| 22 | Z | 616 | CLA | CMD-C2D-C1D | 6.45 | 136.09 | 124.71 |
| 22 | B | 838 | CLA | CMD-C2D-C1D | 6.45 | 136.09 | 124.71 |
| 22 | 9 | 609 | CLA | CMD-C2D-C1D | 6.45 | 136.09 | 124.71 |
| 22 | B | 837 | CLA | CHD-C1D-ND | -6.45 | 118.53 | 124.45 |
| 22 | A | 803 | CLA | CHD-C1D-ND | -6.45 | 118.53 | 124.45 |
| 22 | A | 816 | CLA | CMD-C2D-C1D | 6.44 | 136.06 | 124.71 |
| 22 | 2 | 612 | CLA | CMD-C2D-C1D | 6.43 | 136.05 | 124.71 |
| 22 | B | 813 | CLA | CMD-C2D-C1D | 6.43 | 136.04 | 124.71 |
| 22 | 1 | 611 | CLA | CMD-C2D-C1D | 6.43 | 136.04 | 124.71 |
| 22 | 5 | 609 | CLA | CMD-C2D-C1D | 6.43 | 136.04 | 124.71 |
| 22 | 7 | 610 | CLA | CHD-C4C-C3C | -6.42 | 115.40 | 124.84 |
| 22 | A | 812 | CLA | CMD-C2D-C1D | 6.42 | 136.03 | 124.71 |
| 22 | A | 818 | CLA | CMD-C2D-C1D | 6.42 | 136.03 | 124.71 |
| 22 | B | 824 | CLA | O2D-CGD-CBD | 6.42 | 122.67 | 111.27 |
| 22 | B | 804 | CLA | O2D-CGD-CBD | 6.41 | 122.66 | 111.27 |
| 22 | Z | 612 | CLA | CMD-C2D-C1D | 6.40 | 136.00 | 124.71 |
| 22 | B | 832 | CLA | CHD-C1D-ND | -6.40 | 118.57 | 124.45 |
| 22 | A | 809 | CLA | O2D-CGD-CBD | 6.39 | 122.63 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 807 | CLA | CMD-C2D-C1D | 6.39 | 135.97 | 124.71 |
| 22 | 3 | 612 | CLA | CMD-C2D-C1D | 6.39 | 135.97 | 124.71 |
| 22 | 5 | 614 | CLA | O2D-CGD-CBD | 6.38 | 122.61 | 111.27 |
| 29 | Z | 601 | CHL | C1D-ND-C4D | -6.38 | 101.80 | 106.33 |
| 29 | 8 | 607 | CHL | CMD-C2D-C1D | 6.38 | 135.95 | 124.71 |
| 22 | 8 | 608 | CLA | CHD-C4C-C3C | -6.38 | 115.47 | 124.84 |
| 29 | 9 | 606 | CHL | C1D-ND-C4D | -6.37 | 101.81 | 106.33 |
| 22 | B | 805 | CLA | CHD-C4C-C3C | -6.37 | 115.48 | 124.84 |
| 22 | B | 834 | CLA | CHD-C1D-ND | -6.36 | 118.61 | 124.45 |
| 22 | B | 820 | CLA | CHD-C1D-ND | -6.35 | 118.62 | 124.45 |
| 22 | 2 | 614 | CLA | CHD-C1D-ND | -6.35 | 118.62 | 124.45 |
| 22 | 4 | 612 | CLA | CMD-C2D-C1D | 6.34 | 135.90 | 124.71 |
| 22 | A | 808 | CLA | CHD-C1D-ND | -6.34 | 118.62 | 124.45 |
| 22 | A | 812 | CLA | CHD-C1D-ND | -6.34 | 118.63 | 124.45 |
| 29 | 6 | 606 | CHL | C1D-ND-C4D | -6.33 | 101.84 | 106.33 |
| 22 | 8 | 603 | CLA | C4A-NA-C1A | -6.33 | 103.86 | 106.71 |
| 22 | A | 825 | CLA | CMD-C2D-C1D | 6.33 | 135.87 | 124.71 |
| 22 | 7 | 609 | CLA | CMD-C2D-C1D | 6.33 | 135.86 | 124.71 |
| 22 | A | 822 | CLA | CMD-C2D-C1D | 6.32 | 135.85 | 124.71 |
| 29 | 6 | 607 | CHL | C2C-C3C-C4C | -6.32 | 101.98 | 106.49 |
| 22 | A | 854 | CLA | O2D-CGD-CBD | 6.32 | 122.50 | 111.27 |
| 22 | 3 | 603 | CLA | CMD-C2D-C1D | 6.32 | 135.84 | 124.71 |
| 22 | 5 | 613 | CLA | CMD-C2D-C1D | 6.31 | 135.84 | 124.71 |
| 22 | 7 | 608 | CLA | CHD-C4C-C3C | -6.31 | 115.56 | 124.84 |
| 22 | 4 | 604 | CLA | CHD-C1D-ND | -6.31 | 118.66 | 124.45 |
| 22 | 7 | 609 | CLA | CHD-C1D-ND | -6.31 | 118.66 | 124.45 |
| 22 | 5 | 614 | CLA | CMD-C2D-C1D | 6.31 | 135.83 | 124.71 |
| 22 | A | 804 | CLA | C2D-C1D-ND | 6.30 | 114.75 | 110.10 |
| 22 | A | 838 | CLA | C2C-C1C-NC | 6.30 | 115.88 | 109.97 |
| 22 | A | 831 | CLA | O2D-CGD-CBD | 6.30 | 122.46 | 111.27 |
| 29 | 4 | 608 | CHL | C1D-ND-C4D | -6.30 | 101.86 | 106.33 |
| 22 | B | 804 | CLA | CMD-C2D-C1D | 6.30 | 135.81 | 124.71 |
| 22 | Z | 610 | CLA | CHD-C4C-C3C | -6.30 | 115.58 | 124.84 |
| 22 | A | 814 | CLA | CHD-C1D-ND | -6.29 | 118.67 | 124.45 |
| 29 | 3 | 608 | CHL | CHD-C4C-C3C | -6.29 | 115.59 | 124.84 |
| 22 | B | 806 | CLA | CHD-C4C-C3C | -6.29 | 115.60 | 124.84 |
| 22 | L | 204 | CLA | CHD-C1D-ND | -6.29 | 118.68 | 124.45 |
| 22 | A | 839 | CLA | O2D-CGD-CBD | 6.29 | 122.44 | 111.27 |
| 29 | 1 | 607 | CHL | CMD-C2D-C1D | 6.28 | 135.79 | 124.71 |
| 22 | 2 | 602 | CLA | CHD-C1D-ND | -6.28 | 118.68 | 124.45 |
| 22 | 6 | 601 | CLA | CHD-C1D-ND | -6.28 | 118.68 | 124.45 |
| 22 | 2 | 611 | CLA | CMD-C2D-C1D | 6.28 | 135.78 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 826 | CLA | C2C-C1C-NC | 6.27 | 115.85 | 109.97 |
| 22 | A | 809 | CLA | CHD-C1D-ND | -6.27 | 118.69 | 124.45 |
| 22 | F | 301 | CLA | CHD-C1D-ND | -6.27 | 118.69 | 124.45 |
| 22 | 3 | 613 | CLA | C2C-C1C-NC | 6.27 | 115.84 | 109.97 |
| 22 | 1 | 610 | CLA | CHD-C4C-C3C | -6.26 | 115.64 | 124.84 |
| 22 | 1 | 603 | CLA | C2C-C1C-NC | 6.26 | 115.83 | 109.97 |
| 22 | B | 810 | CLA | CHD-C1D-ND | -6.25 | 118.71 | 124.45 |
| 22 | K | 4003 | CLA | CHD-C1D-ND | -6.25 | 118.71 | 124.45 |
| 22 | 7 | 611 | CLA | CMD-C2D-C1D | 6.25 | 135.73 | 124.71 |
| 29 | 5 | 618 | CHL | C1D-ND-C4D | -6.25 | 101.90 | 106.33 |
| 21 | A | 801 | CL0 | CHD-C4C-C3C | -6.25 | 115.66 | 124.84 |
| 22 | B | 827 | CLA | CMD-C2D-C1D | 6.24 | 135.72 | 124.71 |
| 22 | B | 815 | CLA | CHD-C1D-ND | -6.24 | 118.72 | 124.45 |
| 22 | B | 821 | CLA | CMD-C2D-C1D | 6.24 | 135.71 | 124.71 |
| 22 | A | 840 | CLA | O2D-CGD-CBD | 6.24 | 122.35 | 111.27 |
| 29 | 6 | 607 | CHL | C1D-ND-C4D | -6.23 | 101.91 | 106.33 |
| 22 | 7 | 603 | CLA | CHD-C1D-ND | -6.23 | 118.73 | 124.45 |
| 22 | 8 | 610 | CLA | CMD-C2D-C1D | 6.23 | 135.69 | 124.71 |
| 22 | 7 | 614 | CLA | CHD-C1D-ND | -6.23 | 118.73 | 124.45 |
| 29 | 6 | 608 | CHL | C1C-C2C-C3C | -6.23 | 102.17 | 107.11 |
| 22 | 1 | 609 | CLA | CHD-C1D-ND | -6.23 | 118.73 | 124.45 |
| 22 | 4 | 603 | CLA | C2C-C1C-NC | 6.23 | 115.81 | 109.97 |
| 22 | 3 | 614 | CLA | CHD-C1D-ND | -6.22 | 118.73 | 124.45 |
| 22 | 6 | 617 | CLA | CMD-C2D-C1D | 6.22 | 135.68 | 124.71 |
| 25 | 5 | 625 | BCR | C7-C8-C9 | -6.22 | 116.84 | 126.23 |
| 22 | 4 | 603 | CLA | C4A-NA-C1A | -6.22 | 103.91 | 106.71 |
| 22 | B | 832 | CLA | CHD-C4C-C3C | -6.21 | 115.71 | 124.84 |
| 22 | A | 828 | CLA | O2D-CGD-CBD | 6.21 | 122.30 | 111.27 |
| 22 | A | 818 | CLA | CHD-C4C-C3C | -6.21 | 115.71 | 124.84 |
| 22 | 4 | 611 | CLA | CMD-C2D-C1D | 6.21 | 135.66 | 124.71 |
| 22 | 7 | 602 | CLA | CHD-C1D-ND | -6.21 | 118.75 | 124.45 |
| 22 | 1 | 613 | CLA | CMD-C2D-C1D | 6.21 | 135.66 | 124.71 |
| 22 | B | 807 | CLA | C2C-C1C-NC | 6.21 | 115.79 | 109.97 |
| 22 | B | 818 | CLA | C2C-C1C-NC | 6.21 | 115.79 | 109.97 |
| 22 | 5 | 612 | CLA | CMD-C2D-C1D | 6.21 | 135.65 | 124.71 |
| 22 | B | 831 | CLA | CHD-C4C-C3C | -6.21 | 115.72 | 124.84 |
| 22 | 3 | 612 | CLA | C2C-C1C-NC | 6.20 | 115.78 | 109.97 |
| 22 | 3 | 611 | CLA | CMD-C2D-C1D | 6.20 | 135.64 | 124.71 |
| 22 | 5 | 601 | CLA | CMD-C2D-C1D | 6.20 | 135.64 | 124.71 |
| 29 | 1 | 607 | CHL | C1D-ND-C4D | -6.20 | 101.93 | 106.33 |
| 22 | 5 | 604 | CLA | C2C-C1C-NC | 6.20 | 115.78 | 109.97 |
| 22 | 9 | 603 | CLA | C2C-C1C-NC | 6.20 | 115.78 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 1 | 604 | CLA | CHD-C1D-ND | -6.19 | 118.76 | 124.45 |
| 29 | 3 | 608 | CHL | C1D-ND-C4D | -6.19 | 101.94 | 106.33 |
| 22 | 4 | 610 | CLA | CMD-C2D-C1D | 6.19 | 135.62 | 124.71 |
| 22 | 4 | 613 | CLA | CMD-C2D-C1D | 6.19 | 135.61 | 124.71 |
| 22 | 6 | 609 | CLA | CMD-C2D-C1D | 6.19 | 135.61 | 124.71 |
| 22 | 6 | 612 | CLA | CMD-C2D-C1D | 6.18 | 135.61 | 124.71 |
| 22 | 6 | 611 | CLA | CMD-C2D-C1D | 6.18 | 135.61 | 124.71 |
| 22 | 7 | 604 | CLA | CHD-C4C-C3C | -6.18 | 115.76 | 124.84 |
| 22 | A | 817 | CLA | C2C-C1C-NC | 6.17 | 115.76 | 109.97 |
| 22 | 1 | 612 | CLA | CMD-C2D-C1D | 6.17 | 135.59 | 124.71 |
| 22 | 1 | 616 | CLA | CMD-C2D-C1D | 6.17 | 135.59 | 124.71 |
| 22 | 8 | 609 | CLA | CMD-C2D-C1D | 6.17 | 135.59 | 124.71 |
| 22 | A | 827 | CLA | CHD-C1D-ND | -6.17 | 118.78 | 124.45 |
| 22 | Z | 614 | CLA | CHD-C1D-ND | -6.17 | 118.78 | 124.45 |
| 21 | A | 801 | CL0 | C2C-C1C-NC | 6.17 | 115.75 | 109.97 |
| 29 | 1 | 607 | CHL | C4A-NA-C1A | -6.16 | 103.94 | 106.71 |
| 22 | 5 | 602 | CLA | CHD-C1D-ND | -6.16 | 118.79 | 124.45 |
| 30 | 2 | 617 | LUT | C35-C34-C33 | -6.16 | 118.52 | 127.31 |
| 22 | 6 | 602 | CLA | CHD-C4C-C3C | -6.16 | 115.79 | 124.84 |
| 22 | 5 | 621 | CLA | C2D-C1D-ND | 6.16 | 114.64 | 110.10 |
| 22 | A | 818 | CLA | O2D-CGD-CBD | 6.16 | 122.21 | 111.27 |
| 22 | 4 | 616 | CLA | C2C-C1C-NC | 6.16 | 115.74 | 109.97 |
| 22 | A | 823 | CLA | CMD-C2D-C1D | 6.15 | 135.56 | 124.71 |
| 22 | 6 | 601 | CLA | O2D-CGD-CBD | 6.15 | 122.20 | 111.27 |
| 22 | 7 | 606 | CLA | CHD-C4C-C3C | -6.15 | 115.80 | 124.84 |
| 22 | 5 | 602 | CLA | CHD-C4C-C3C | -6.15 | 115.80 | 124.84 |
| 22 | 9 | 614 | CLA | CHD-C1D-ND | -6.14 | 118.81 | 124.45 |
| 22 | 3 | 604 | CLA | CHD-C1D-ND | -6.13 | 118.82 | 124.45 |
| 22 | 6 | 609 | CLA | C2C-C1C-NC | 6.12 | 115.71 | 109.97 |
| 22 | B | 841 | CLA | C4A-NA-C1A | -6.12 | 103.95 | 106.71 |
| 22 | 7 | 603 | CLA | C4A-NA-C1A | -6.12 | 103.95 | 106.71 |
| 22 | 9 | 604 | CLA | CHD-C1D-ND | -6.12 | 118.83 | 124.45 |
| 22 | 7 | 608 | CLA | CHD-C1D-ND | -6.12 | 118.83 | 124.45 |
| 22 | B | 833 | CLA | CHD-C1D-ND | -6.12 | 118.83 | 124.45 |
| 22 | 2 | 607 | CLA | CHD-C1D-ND | -6.11 | 118.84 | 124.45 |
| 22 | Z | 613 | CLA | CMD-C2D-C1D | 6.11 | 135.48 | 124.71 |
| 22 | 5 | 621 | CLA | CMD-C2D-C1D | 6.10 | 135.47 | 124.71 |
| 22 | A | 822 | CLA | CHD-C1D-ND | -6.10 | 118.85 | 124.45 |
| 22 | B | 829 | CLA | CHD-C1D-ND | -6.10 | 118.85 | 124.45 |
| 22 | 5 | 609 | CLA | CHD-C1D-ND | -6.09 | 118.86 | 124.45 |
| 29 | 5 | 607 | CHL | C1D-ND-C4D | -6.09 | 102.01 | 106.33 |
| 22 | B | 826 | CLA | CHD-C4C-C3C | -6.09 | 115.89 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 811 | CLA | CMD-C2D-C1D | 6.09 | 135.44 | 124.71 |
| 22 | A | 821 | CLA | C2C-C1C-NC | 6.09 | 115.67 | 109.97 |
| 22 | A | 823 | CLA | CHD-C1D-ND | -6.09 | 118.86 | 124.45 |
| 22 | 4 | 601 | CLA | CHD-C1D-ND | -6.08 | 118.86 | 124.45 |
| 22 | B | 829 | CLA | CHD-C4C-C3C | -6.08 | 115.90 | 124.84 |
| 22 | 1 | 602 | CLA | CMD-C2D-C1D | 6.08 | 135.43 | 124.71 |
| 22 | 5 | 614 | CLA | CHD-C1D-ND | -6.08 | 118.87 | 124.45 |
| 22 | 6 | 613 | CLA | CHD-C1D-ND | -6.08 | 118.87 | 124.45 |
| 22 | A | 826 | CLA | CHD-C1D-ND | -6.08 | 118.87 | 124.45 |
| 22 | A | 810 | CLA | CMD-C2D-C1D | 6.07 | 135.42 | 124.71 |
| 22 | B | 831 | CLA | CHD-C1D-ND | -6.07 | 118.87 | 124.45 |
| 22 | A | 839 | CLA | CHD-C1D-ND | -6.07 | 118.87 | 124.45 |
| 22 | 2 | 609 | CLA | CHD-C1D-ND | -6.07 | 118.88 | 124.45 |
| 22 | 8 | 601 | CLA | O2D-CGD-CBD | 6.07 | 122.05 | 111.27 |
| 22 | 9 | 603 | CLA | CHD-C1D-ND | -6.07 | 118.88 | 124.45 |
| 22 | B | 806 | CLA | CHD-C1D-ND | -6.07 | 118.88 | 124.45 |
| 22 | A | 811 | CLA | CHD-C4C-C3C | -6.07 | 115.92 | 124.84 |
| 22 | 8 | 612 | CLA | CHD-C4C-C3C | -6.07 | 115.92 | 124.84 |
| 22 | A | 812 | CLA | C2C-C1C-NC | 6.07 | 115.66 | 109.97 |
| 22 | 7 | 610 | CLA | C4A-NA-C1A | -6.07 | 103.98 | 106.71 |
| 29 | 4 | 606 | CHL | C1D-ND-C4D | -6.06 | 102.03 | 106.33 |
| 22 | B | 808 | CLA | C2C-C1C-NC | 6.06 | 115.65 | 109.97 |
| 22 | B | 811 | CLA | C1B-C2B-C3B | -6.06 | 101.28 | 106.92 |
| 22 | 1 | 602 | CLA | CHD-C4C-C3C | -6.06 | 115.93 | 124.84 |
| 22 | B | 809 | CLA | C2C-C1C-NC | 6.06 | 115.65 | 109.97 |
| 22 | 3 | 609 | CLA | CHD-C1D-ND | -6.06 | 118.89 | 124.45 |
| 22 | B | 835 | CLA | CMD-C2D-C1D | 6.06 | 135.39 | 124.71 |
| 22 | A | 825 | CLA | CHD-C1D-ND | -6.05 | 118.89 | 124.45 |
| 22 | B | 803 | CLA | CHD-C1D-ND | -6.05 | 118.89 | 124.45 |
| 22 | 8 | 613 | CLA | CHD-C4C-C3C | -6.05 | 115.95 | 124.84 |
| 22 | A | 836 | CLA | C2C-C1C-NC | 6.05 | 115.64 | 109.97 |
| 22 | 2 | 603 | CLA | C2C-C1C-NC | 6.05 | 115.64 | 109.97 |
| 22 | B | 809 | CLA | CMD-C2D-C1D | 6.04 | 135.36 | 124.71 |
| 25 | 5 | 625 | BCR | C15-C14-C13 | -6.04 | 118.69 | 127.31 |
| 22 | 2 | 606 | CLA | CHD-C1D-ND | -6.04 | 118.90 | 124.45 |
| 22 | A | 838 | CLA | C4A-NA-C1A | -6.04 | 103.99 | 106.71 |
| 22 | 8 | 608 | CLA | CHD-C1D-ND | -6.04 | 118.90 | 124.45 |
| 22 | Z | 609 | CLA | C2C-C1C-NC | 6.04 | 115.63 | 109.97 |
| 22 | 7 | 611 | CLA | CAA-C2A-C3A | -6.04 | 102.01 | 116.10 |
| 22 | 7 | 610 | CLA | CHD-C1D-ND | -6.04 | 118.91 | 124.45 |
| 22 | 2 | 613 | CLA | CHD-C1D-ND | -6.04 | 118.91 | 124.45 |
| 22 | 8 | 613 | CLA | CMD-C2D-C1D | 6.04 | 135.35 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 808 | CLA | CMD-C2D-C1D | 6.04 | 135.35 | 124.71 |
| 22 | 6 | 616 | CLA | CHD-C1D-ND | -6.03 | 118.91 | 124.45 |
| 22 | A | 804 | CLA | C4A-NA-C1A | -6.03 | 103.99 | 106.71 |
| 22 | B | 828 | CLA | C2C-C1C-NC | 6.03 | 115.62 | 109.97 |
| 22 | Z | 606 | CLA | CHD-C1D-ND | -6.03 | 118.91 | 124.45 |
| 22 | B | 840 | CLA | CHD-C1D-ND | -6.03 | 118.91 | 124.45 |
| 22 | 9 | 610 | CLA | CHD-C1D-ND | -6.03 | 118.91 | 124.45 |
| 22 | 7 | 602 | CLA | CHD-C4C-C3C | -6.03 | 115.98 | 124.84 |
| 22 | 1 | 606 | CLA | CHD-C4C-C3C | -6.03 | 115.98 | 124.84 |
| 22 | 4 | 614 | CLA | CMD-C2D-C1D | 6.02 | 135.33 | 124.71 |
| 22 | 5 | 612 | CLA | C2C-C1C-NC | 6.02 | 115.61 | 109.97 |
| 22 | 8 | 610 | CLA | C4A-NA-C1A | -6.02 | 104.00 | 106.71 |
| 22 | 3 | 603 | CLA | C2C-C1C-NC | 6.02 | 115.61 | 109.97 |
| 22 | 3 | 610 | CLA | CHD-C4C-C3C | -6.02 | 115.99 | 124.84 |
| 22 | 5 | 610 | CLA | CHD-C1D-ND | -6.02 | 118.93 | 124.45 |
| 22 | A | 815 | CLA | O2D-CGD-CBD | 6.01 | 121.95 | 111.27 |
| 22 | B | 833 | CLA | O2D-CGD-CBD | 6.01 | 121.95 | 111.27 |
| 29 | Z | 601 | CHL | C2C-C3C-C4C | -6.01 | 102.20 | 106.49 |
| 29 | 1 | 601 | CHL | C1D-ND-C4D | -6.01 | 102.06 | 106.33 |
| 22 | 8 | 611 | CLA | CHD-C1D-ND | -6.01 | 118.93 | 124.45 |
| 29 | 5 | 607 | CHL | C2C-C3C-C4C | -6.01 | 102.21 | 106.49 |
| 22 | B | 826 | CLA | O2D-CGD-CBD | 6.00 | 121.94 | 111.27 |
| 22 | 9 | 602 | CLA | CHD-C1D-ND | -6.00 | 118.94 | 124.45 |
| 22 | 9 | 609 | CLA | CHD-C1D-ND | -6.00 | 118.94 | 124.45 |
| 22 | A | 840 | CLA | CHD-C4C-C3C | -6.00 | 116.02 | 124.84 |
| 22 | B | 838 | CLA | CHD-C1D-ND | -6.00 | 118.94 | 124.45 |
| 22 | B | 817 | CLA | C2C-C1C-NC | 6.00 | 115.59 | 109.97 |
| 22 | 4 | 612 | CLA | CHD-C1D-ND | -6.00 | 118.94 | 124.45 |
| 22 | 8 | 604 | CLA | CHD-C1D-ND | -6.00 | 118.94 | 124.45 |
| 22 | A | 806 | CLA | O2D-CGD-CBD | 6.00 | 121.93 | 111.27 |
| 22 | 2 | 612 | CLA | C4A-NA-C1A | -6.00 | 104.01 | 106.71 |
| 22 | 3 | 620 | CLA | CHD-C1D-ND | -6.00 | 118.94 | 124.45 |
| 22 | 4 | 612 | CLA | C4A-NA-C1A | -6.00 | 104.01 | 106.71 |
| 22 | A | 806 | CLA | CHD-C1D-ND | -5.99 | 118.94 | 124.45 |
| 22 | A | 815 | CLA | C4A-NA-C1A | -5.99 | 104.01 | 106.71 |
| 22 | Z | 603 | CLA | C2C-C1C-NC | 5.99 | 115.59 | 109.97 |
| 29 | 6 | 608 | CHL | C1D-ND-C4D | -5.99 | 102.08 | 106.33 |
| 22 | 8 | 602 | CLA | CHD-C1D-ND | -5.99 | 118.95 | 124.45 |
| 22 | Z | 609 | CLA | CHD-C1D-ND | -5.99 | 118.95 | 124.45 |
| 22 | 9 | 612 | CLA | C2C-C1C-NC | 5.98 | 115.58 | 109.97 |
| 29 | 4 | 618 | CHL | C1D-ND-C4D | -5.98 | 102.09 | 106.33 |
| 22 | A | 831 | CLA | CMD-C2D-C1D | 5.97 | 135.24 | 124.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 6 | 614 | CLA | C4A-NA-C1A | -5.97 | 104.02 | 106.71 |
| 22 | Z | 611 | CLA | CHD-C1D-ND | -5.97 | 118.97 | 124.45 |
| 22 | K | 4002 | CLA | CHD-C1D-ND | -5.97 | 118.97 | 124.45 |
| 22 | 7 | 601 | CLA | CHD-C1D-ND | -5.97 | 118.97 | 124.45 |
| 22 | 7 | 601 | CLA | CHD-C4C-C3C | -5.97 | 116.07 | 124.84 |
| 22 | B | 825 | CLA | CHD-C4C-C3C | -5.96 | 116.07 | 124.84 |
| 22 | 5 | 603 | CLA | CHD-C4C-C3C | -5.96 | 116.07 | 124.84 |
| 22 | 7 | 620 | CLA | CHD-C1D-ND | -5.96 | 118.98 | 124.45 |
| 25 | 6 | 625 | BCR | C15-C14-C13 | -5.96 | 118.81 | 127.31 |
| 22 | Z | 610 | CLA | CMD-C2D-C1D | 5.96 | 135.21 | 124.71 |
| 22 | B | 819 | CLA | CHD-C1D-ND | -5.96 | 118.98 | 124.45 |
| 22 | B | 824 | CLA | CHD-C4C-C3C | -5.96 | 116.08 | 124.84 |
| 22 | B | 822 | CLA | CHD-C1D-ND | -5.95 | 118.98 | 124.45 |
| 22 | 6 | 602 | CLA | CHD-C1D-ND | -5.95 | 118.98 | 124.45 |
| 22 | Z | 613 | CLA | CHD-C4C-C3C | -5.95 | 116.09 | 124.84 |
| 22 | 5 | 616 | CLA | C2C-C1C-NC | 5.95 | 115.55 | 109.97 |
| 22 | 6 | 603 | CLA | C2C-C1C-NC | 5.95 | 115.55 | 109.97 |
| 22 | Z | 612 | CLA | CHD-C4C-C3C | -5.95 | 116.10 | 124.84 |
| 22 | 1 | 608 | CLA | CHD-C1D-ND | -5.95 | 118.99 | 124.45 |
| 22 | B | 812 | CLA | CHD-C1D-ND | -5.94 | 118.99 | 124.45 |
| 22 | 3 | 612 | CLA | CHD-C1D-ND | -5.94 | 118.99 | 124.45 |
| 22 | B | 836 | CLA | O2D-CGD-CBD | 5.94 | 121.83 | 111.27 |
| 22 | F | 301 | CLA | CHD-C4C-C3C | -5.94 | 116.11 | 124.84 |
| 22 | B | 839 | CLA | CHD-C1D-ND | -5.94 | 119.00 | 124.45 |
| 22 | Z | 602 | CLA | CHD-C4C-C3C | -5.94 | 116.11 | 124.84 |
| 22 | 9 | 612 | CLA | CHD-C1D-ND | -5.94 | 119.00 | 124.45 |
| 22 | A | 834 | CLA | CHD-C4C-C3C | -5.93 | 116.12 | 124.84 |
| 22 | 1 | 611 | CLA | CHD-C1D-ND | -5.93 | 119.00 | 124.45 |
| 22 | 5 | 621 | CLA | C2C-C1C-NC | 5.93 | 115.52 | 109.97 |
| 22 | 8 | 616 | CLA | CHD-C4C-C3C | -5.92 | 116.13 | 124.84 |
| 22 | A | 818 | CLA | CHD-C1D-ND | -5.92 | 119.01 | 124.45 |
| 29 | 6 | 608 | CHL | CHD-C4C-C3C | -5.92 | 116.14 | 124.84 |
| 22 | 4 | 614 | CLA | CHD-C4C-C3C | -5.92 | 116.14 | 124.84 |
| 22 | K | 4003 | CLA | C2C-C1C-NC | 5.91 | 115.51 | 109.97 |
| 22 | A | 833 | CLA | CHD-C1D-ND | -5.91 | 119.02 | 124.45 |
| 22 | J | 3002 | CLA | CHD-C1D-ND | -5.91 | 119.02 | 124.45 |
| 22 | 7 | 613 | CLA | CMD-C2D-C1D | 5.91 | 135.13 | 124.71 |
| 29 | 4 | 608 | CHL | CHD-C4C-C3C | -5.91 | 116.15 | 124.84 |
| 22 | A | 842 | CLA | CHD-C4C-C3C | -5.91 | 116.16 | 124.84 |
| 22 | B | 838 | CLA | CHD-C4C-C3C | -5.91 | 116.16 | 124.84 |
| 22 | Z | 608 | CLA | CHD-C1D-ND | -5.91 | 119.03 | 124.45 |
| 22 | 8 | 601 | CLA | C2C-C1C-NC | 5.91 | 115.50 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 814 | CLA | O2D-CGD-CBD | 5.90 | 121.76 | 111.27 |
| 22 | A | 816 | CLA | CHD-C1D-ND | -5.90 | 119.03 | 124.45 |
| 22 | A | 838 | CLA | CHD-C1D-ND | -5.90 | 119.03 | 124.45 |
| 22 | 4 | 609 | CLA | C2C-C1C-NC | 5.90 | 115.50 | 109.97 |
| 22 | K | 4002 | CLA | O2D-CGD-CBD | 5.89 | 121.74 | 111.27 |
| 29 | 9 | 607 | CHL | C1D-ND-C4D | -5.89 | 102.15 | 106.33 |
| 22 | A | 830 | CLA | CHD-C4C-C3C | -5.89 | 116.18 | 124.84 |
| 22 | 1 | 608 | CLA | CHD-C4C-C3C | -5.89 | 116.18 | 124.84 |
| 22 | A | 804 | CLA | CHD-C4C-C3C | -5.89 | 116.18 | 124.84 |
| 22 | 9 | 611 | CLA | CHD-C4C-C3C | -5.89 | 116.19 | 124.84 |
| 22 | A | 829 | CLA | CMD-C2D-C1D | 5.89 | 135.09 | 124.71 |
| 22 | 4 | 602 | CLA | CHD-C1D-ND | -5.89 | 119.04 | 124.45 |
| 22 | 7 | 611 | CLA | C2C-C1C-NC | 5.88 | 115.48 | 109.97 |
| 22 | 8 | 610 | CLA | CHD-C4C-C3C | -5.88 | 116.19 | 124.84 |
| 22 | 8 | 604 | CLA | C2C-C1C-NC | 5.88 | 115.48 | 109.97 |
| 22 | A | 831 | CLA | C2C-C1C-NC | 5.88 | 115.48 | 109.97 |
| 22 | 9 | 601 | CLA | CHD-C1D-ND | -5.88 | 119.05 | 124.45 |
| 22 | 5 | 614 | CLA | C4A-NA-C1A | -5.88 | 104.06 | 106.71 |
| 22 | G | 204 | CLA | CHD-C1D-ND | -5.88 | 119.05 | 124.45 |
| 22 | A | 821 | CLA | CMD-C2D-C1D | 5.88 | 135.07 | 124.71 |
| 22 | G | 203 | CLA | C4A-NA-C1A | -5.88 | 104.06 | 106.71 |
| 22 | B | 821 | CLA | CHD-C1D-ND | -5.88 | 119.05 | 124.45 |
| 22 | 6 | 610 | CLA | CHD-C1D-ND | -5.87 | 119.06 | 124.45 |
| 22 | 6 | 612 | CLA | CHD-C4C-C3C | -5.87 | 116.21 | 124.84 |
| 25 | A | 852 | BCR | C20-C21-C22 | -5.87 | 118.93 | 127.31 |
| 22 | B | 841 | CLA | O2D-CGD-CBD | 5.87 | 121.70 | 111.27 |
| 22 | 2 | 612 | CLA | CHD-C1D-ND | -5.87 | 119.06 | 124.45 |
| 22 | A | 834 | CLA | CHD-C1D-ND | -5.86 | 119.06 | 124.45 |
| 22 | 6 | 609 | CLA | CHD-C1D-ND | -5.86 | 119.06 | 124.45 |
| 22 | B | 806 | CLA | C4A-NA-C1A | -5.86 | 104.07 | 106.71 |
| 22 | 6 | 622 | CLA | CHD-C1D-ND | -5.86 | 119.07 | 124.45 |
| 22 | G | 203 | CLA | CHD-C1D-ND | -5.86 | 119.07 | 124.45 |
| 22 | 7 | 613 | CLA | C2C-C1C-NC | 5.86 | 115.46 | 109.97 |
| 22 | A | 837 | CLA | CHD-C1D-ND | -5.86 | 119.07 | 124.45 |
| 22 | B | 813 | CLA | O2D-CGD-CBD | 5.86 | 121.67 | 111.27 |
| 22 | 5 | 601 | CLA | O2D-CGD-CBD | 5.85 | 121.67 | 111.27 |
| 22 | 2 | 601 | CLA | CHD-C1D-ND | -5.85 | 119.08 | 124.45 |
| 22 | A | 841 | CLA | CHD-C4C-C3C | -5.85 | 116.24 | 124.84 |
| 22 | B | 824 | CLA | CMD-C2D-C1D | 5.85 | 135.02 | 124.71 |
| 22 | A | 843 | CLA | C2C-C1C-NC | 5.85 | 115.45 | 109.97 |
| 22 | B | 807 | CLA | CHD-C1D-ND | -5.85 | 119.08 | 124.45 |
| 22 | 7 | 603 | CLA | CHD-C4C-C3C | -5.84 | 116.25 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 2 | 611 | CLA | CHD-C1D-ND | -5.84 | 119.08 | 124.45 |
| 22 | B | 804 | CLA | CHD-C4C-C3C | -5.84 | 116.25 | 124.84 |
| 22 | A | 812 | CLA | CHD-C4C-C3C | -5.84 | 116.26 | 124.84 |
| 22 | 3 | 606 | CLA | CHD-C1D-ND | -5.84 | 119.09 | 124.45 |
| 22 | A | 804 | CLA | CHD-C1D-ND | -5.84 | 119.09 | 124.45 |
| 22 | 4 | 616 | CLA | CHD-C1D-ND | -5.83 | 119.09 | 124.45 |
| 22 | A | 836 | CLA | CMD-C2D-C1D | 5.83 | 134.99 | 124.71 |
| 22 | A | 826 | CLA | C4A-NA-C1A | -5.83 | 104.08 | 106.71 |
| 22 | 8 | 603 | CLA | C2C-C1C-NC | 5.83 | 115.43 | 109.97 |
| 22 | 9 | 609 | CLA | C2C-C1C-NC | 5.83 | 115.43 | 109.97 |
| 22 | A | 824 | CLA | C2C-C1C-NC | 5.83 | 115.43 | 109.97 |
| 22 | A | 809 | CLA | CHD-C4C-C3C | -5.82 | 116.28 | 124.84 |
| 22 | L | 203 | CLA | CHD-C1D-ND | -5.82 | 119.10 | 124.45 |
| 22 | 2 | 613 | CLA | C2C-C1C-NC | 5.82 | 115.43 | 109.97 |
| 22 | F | 303 | CLA | CHD-C4C-C3C | -5.82 | 116.29 | 124.84 |
| 22 | 4 | 611 | CLA | C2C-C1C-NC | 5.82 | 115.42 | 109.97 |
| 22 | B | 811 | CLA | C2C-C1C-NC | 5.81 | 115.42 | 109.97 |
| 22 | 6 | 603 | CLA | C4A-NA-C1A | -5.81 | 104.09 | 106.71 |
| 22 | B | 805 | CLA | CHD-C1D-ND | -5.81 | 119.11 | 124.45 |
| 22 | A | 843 | CLA | CMD-C2D-C1D | 5.81 | 134.95 | 124.71 |
| 22 | 3 | 602 | CLA | CHD-C1D-ND | -5.81 | 119.12 | 124.45 |
| 22 | 9 | 613 | CLA | CHD-C1D-ND | -5.81 | 119.12 | 124.45 |
| 29 | 5 | 608 | CHL | C1D-ND-C4D | -5.81 | 102.21 | 106.33 |
| 22 | B | 818 | CLA | O2D-CGD-CBD | 5.81 | 121.58 | 111.27 |
| 22 | F | 304 | CLA | CHD-C4C-C3C | -5.80 | 116.31 | 124.84 |
| 22 | B | 813 | CLA | CHD-C1D-ND | -5.80 | 119.12 | 124.45 |
| 22 | A | 835 | CLA | O2D-CGD-CBD | 5.80 | 121.58 | 111.27 |
| 22 | B | 830 | CLA | CHD-C4C-C3C | -5.80 | 116.32 | 124.84 |
| 22 | 9 | 602 | CLA | O2D-CGD-CBD | 5.80 | 121.57 | 111.27 |
| 22 | A | 808 | CLA | CHD-C4C-C3C | -5.79 | 116.33 | 124.84 |
| 22 | B | 811 | CLA | CHD-C1D-ND | -5.79 | 119.13 | 124.45 |
| 22 | F | 303 | CLA | CHD-C1D-ND | -5.79 | 119.13 | 124.45 |
| 22 | 4 | 603 | CLA | CHD-C1D-ND | -5.79 | 119.13 | 124.45 |
| 22 | B | 837 | CLA | CHD-C4C-C3C | -5.79 | 116.33 | 124.84 |
| 22 | 4 | 601 | CLA | O2D-CGD-CBD | 5.79 | 121.55 | 111.27 |
| 22 | 5 | 613 | CLA | C2C-C1C-NC | 5.79 | 115.39 | 109.97 |
| 22 | 4 | 612 | CLA | CHD-C4C-C3C | -5.79 | 116.33 | 124.84 |
| 22 | A | 842 | CLA | CHD-C1D-ND | -5.79 | 119.14 | 124.45 |
| 22 | B | 811 | CLA | CHD-C4C-C3C | -5.78 | 116.34 | 124.84 |
| 22 | 4 | 609 | CLA | CMD-C2D-C1D | 5.78 | 134.90 | 124.71 |
| 29 | 5 | 618 | CHL | O2D-CGD-CBD | 5.78 | 121.54 | 111.27 |
| 22 | 6 | 603 | CLA | CHD-C1D-ND | -5.78 | 119.14 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | Z | 612 | CLA | CHD-C1D-ND | -5.78 | 119.14 | 124.45 |
| 29 | 6 | 618 | CHL | C1C-C2C-C3C | -5.78 | 102.53 | 107.11 |
| 22 | 5 | 601 | CLA | CHD-C1D-ND | -5.77 | 119.15 | 124.45 |
| 25 | 6 | 625 | BCR | C7-C8-C9 | -5.77 | 117.51 | 126.23 |
| 22 | Z | 603 | CLA | CHD-C1D-ND | -5.77 | 119.15 | 124.45 |
| 22 | B | 827 | CLA | CHD-C4C-C3C | -5.77 | 116.37 | 124.84 |
| 22 | A | 813 | CLA | CHD-C1D-ND | -5.76 | 119.16 | 124.45 |
| 22 | A | 819 | CLA | CHD-C1D-ND | -5.76 | 119.16 | 124.45 |
| 22 | A | 807 | CLA | CHD-C4C-C3C | -5.76 | 116.37 | 124.84 |
| 22 | Z | 608 | CLA | CHD-C4C-C3C | -5.76 | 116.38 | 124.84 |
| 22 | 2 | 603 | CLA | CHD-C1D-ND | -5.76 | 119.16 | 124.45 |
| 22 | Z | 604 | CLA | CHD-C1D-ND | -5.76 | 119.16 | 124.45 |
| 22 | A | 832 | CLA | C2C-C1C-NC | 5.75 | 115.36 | 109.97 |
| 22 | B | 835 | CLA | CHD-C4C-C3C | -5.75 | 116.38 | 124.84 |
| 22 | B | 816 | CLA | CHD-C1D-ND | -5.75 | 119.17 | 124.45 |
| 22 | 5 | 601 | CLA | C2C-C1C-NC | 5.75 | 115.36 | 109.97 |
| 22 | 5 | 611 | CLA | CHD-C1D-ND | -5.75 | 119.17 | 124.45 |
| 22 | 2 | 609 | CLA | C2C-C1C-NC | 5.75 | 115.36 | 109.97 |
| 22 | Z | 611 | CLA | CHD-C4C-C3C | -5.75 | 116.39 | 124.84 |
| 22 | 7 | 612 | CLA | CHD-C1D-ND | -5.74 | 119.17 | 124.45 |
| 22 | 5 | 609 | CLA | C2C-C1C-NC | 5.74 | 115.35 | 109.97 |
| 29 | 1 | 607 | CHL | C2C-C3C-C4C | -5.74 | 102.40 | 106.49 |
| 22 | 7 | 613 | CLA | CHD-C1D-ND | -5.74 | 119.18 | 124.45 |
| 22 | G | 203 | CLA | C2C-C1C-NC | 5.74 | 115.35 | 109.97 |
| 22 | A | 832 | CLA | CHD-C4C-C3C | -5.74 | 116.41 | 124.84 |
| 29 | 6 | 618 | CHL | CMD-C2D-C1D | 5.73 | 134.82 | 124.71 |
| 22 | B | 822 | CLA | CHD-C4C-C3C | -5.73 | 116.42 | 124.84 |
| 29 | 4 | 607 | CHL | C1C-C2C-C3C | -5.73 | 102.56 | 107.11 |
| 29 | 1 | 601 | CHL | O2D-CGD-CBD | 5.73 | 121.45 | 111.27 |
| 22 | 9 | 610 | CLA | CHD-C4C-C3C | -5.73 | 116.42 | 124.84 |
| 22 | A | 825 | CLA | C2C-C1C-NC | 5.73 | 115.34 | 109.97 |
| 22 | 8 | 614 | CLA | CHD-C1D-ND | -5.73 | 119.19 | 124.45 |
| 22 | A | 845 | CLA | CHD-C4C-C3C | -5.72 | 116.42 | 124.84 |
| 22 | 1 | 611 | CLA | C2C-C1C-NC | 5.72 | 115.33 | 109.97 |
| 22 | B | 840 | CLA | CHD-C4C-C3C | -5.72 | 116.43 | 124.84 |
| 22 | 1 | 614 | CLA | C2C-C1C-NC | 5.72 | 115.33 | 109.97 |
| 29 | 7 | 607 | CHL | C1D-ND-C4D | -5.72 | 102.27 | 106.33 |
| 29 | 1 | 601 | CHL | C2C-C3C-C4C | -5.72 | 102.41 | 106.49 |
| 22 | Z | 612 | CLA | C2C-C1C-NC | 5.72 | 115.33 | 109.97 |
| 22 | 8 | 606 | CLA | CHD-C1D-ND | -5.72 | 119.20 | 124.45 |
| 22 | B | 813 | CLA | CHD-C4C-C3C | -5.71 | 116.44 | 124.84 |
| 22 | 6 | 604 | CLA | CHD-C4C-C3C | -5.71 | 116.44 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 3 | 620 | CLA | C2C-C1C-NC | 5.71 | 115.32 | 109.97 |
| 29 | 4 | 608 | CHL | C3D-C2D-C1D | -5.71 | 98.04 | 105.83 |
| 22 | A | 827 | CLA | CHD-C4C-C3C | -5.71 | 116.45 | 124.84 |
| 29 | 9 | 607 | CHL | C2C-C3C-C4C | -5.71 | 102.42 | 106.49 |
| 22 | A | 841 | CLA | CHD-C1D-ND | -5.71 | 119.21 | 124.45 |
| 22 | 3 | 604 | CLA | C2C-C1C-NC | 5.71 | 115.32 | 109.97 |
| 22 | 5 | 606 | CLA | CHD-C1D-ND | -5.71 | 119.21 | 124.45 |
| 22 | 3 | 610 | CLA | CHD-C1D-ND | -5.70 | 119.21 | 124.45 |
| 22 | A | 810 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.84 |
| 22 | L | 203 | CLA | CMD-C2D-C1D | 5.70 | 134.76 | 124.71 |
| 22 | 7 | 612 | CLA | C2C-C1C-NC | 5.70 | 115.31 | 109.97 |
| 22 | 5 | 611 | CLA | C2C-C1C-NC | 5.70 | 115.31 | 109.97 |
| 22 | 9 | 604 | CLA | C2C-C1C-NC | 5.70 | 115.31 | 109.97 |
| 22 | A | 845 | CLA | CHD-C1D-ND | -5.70 | 119.22 | 124.45 |
| 22 | B | 836 | CLA | CHD-C1D-ND | -5.70 | 119.22 | 124.45 |
| 22 | 9 | 601 | CLA | C2C-C1C-NC | 5.70 | 115.31 | 109.97 |
| 22 | 9 | 602 | CLA | CHD-C4C-C3C | -5.70 | 116.46 | 124.84 |
| 22 | B | 830 | CLA | CHD-C1D-ND | -5.70 | 119.22 | 124.45 |
| 22 | 6 | 610 | CLA | C4A-NA-C1A | -5.70 | 104.14 | 106.71 |
| 22 | A | 845 | CLA | C2C-C1C-NC | 5.70 | 115.31 | 109.97 |
| 22 | 1 | 603 | CLA | CHD-C1D-ND | -5.70 | 119.22 | 124.45 |
| 22 | A | 820 | CLA | C4A-NA-C1A | -5.69 | 104.15 | 106.71 |
| 22 | A | 824 | CLA | CHD-C1D-ND | -5.69 | 119.22 | 124.45 |
| 22 | B | 817 | CLA | CHD-C1D-ND | -5.69 | 119.22 | 124.45 |
| 22 | 2 | 612 | CLA | C2C-C1C-NC | 5.69 | 115.30 | 109.97 |
| 22 | 4 | 613 | CLA | CHD-C1D-ND | -5.69 | 119.23 | 124.45 |
| 22 | A | 841 | CLA | CMD-C2D-C1D | 5.69 | 134.74 | 124.71 |
| 22 | B | 814 | CLA | CHD-C1D-ND | -5.68 | 119.23 | 124.45 |
| 22 | A | 803 | CLA | CHD-C4C-C3C | -5.68 | 116.49 | 124.84 |
| 22 | 8 | 616 | CLA | CMD-C2D-C1D | 5.68 | 134.73 | 124.71 |
| 22 | A | 842 | CLA | C2C-C1C-NC | 5.68 | 115.30 | 109.97 |
| 22 | B | 804 | CLA | CHD-C1D-ND | -5.68 | 119.24 | 124.45 |
| 22 | 8 | 614 | CLA | CHD-C4C-C3C | -5.68 | 116.50 | 124.84 |
| 22 | 3 | 607 | CLA | C2C-C1C-NC | 5.68 | 115.29 | 109.97 |
| 22 | 5 | 603 | CLA | C2C-C1C-NC | 5.67 | 115.29 | 109.97 |
| 29 | 4 | 608 | CHL | C1C-C2C-C3C | -5.67 | 102.61 | 107.11 |
| 22 | 6 | 617 | CLA | CHD-C4C-C3C | -5.67 | 116.50 | 124.84 |
| 22 | A | 854 | CLA | CHD-C4C-C3C | -5.67 | 116.50 | 124.84 |
| 22 | A | 838 | CLA | O2D-CGD-CBD | 5.66 | 121.33 | 111.27 |
| 22 | 1 | 612 | CLA | C2C-C1C-NC | 5.66 | 115.28 | 109.97 |
| 22 | 1 | 606 | CLA | CHD-C1D-ND | -5.66 | 119.25 | 124.45 |
| 22 | A | 820 | CLA | CHD-C4C-C3C | -5.66 | 116.53 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 802 | CLA | CMD-C2D-C1D | 5.66 | 134.68 | 124.71 |
| 22 | 9 | 613 | CLA | C2C-C1C-NC | 5.66 | 115.27 | 109.97 |
| 22 | B | 820 | CLA | O2D-CGD-CBD | 5.65 | 121.32 | 111.27 |
| 22 | 8 | 611 | CLA | O2D-CGD-CBD | 5.65 | 121.32 | 111.27 |
| 22 | 9 | 614 | CLA | C2C-C1C-NC | 5.65 | 115.27 | 109.97 |
| 29 | 8 | 607 | CHL | CHD-C4C-C3C | -5.65 | 116.53 | 124.84 |
| 22 | 2 | 601 | CLA | C2C-C1C-NC | 5.65 | 115.26 | 109.97 |
| 22 | B | 809 | CLA | CHD-C1D-ND | -5.65 | 119.26 | 124.45 |
| 22 | B | 810 | CLA | C4A-NA-C1A | -5.65 | 104.17 | 106.71 |
| 22 | B | 814 | CLA | CHD-C4C-C3C | -5.65 | 116.54 | 124.84 |
| 22 | 3 | 610 | CLA | C4A-NA-C1A | -5.65 | 104.17 | 106.71 |
| 22 | A | 816 | CLA | O2D-CGD-CBD | 5.64 | 121.30 | 111.27 |
| 22 | 4 | 610 | CLA | CHD-C1D-ND | -5.64 | 119.27 | 124.45 |
| 22 | 6 | 612 | CLA | C4A-NA-C1A | -5.64 | 104.17 | 106.71 |
| 22 | A | 820 | CLA | C2C-C1C-NC | 5.64 | 115.26 | 109.97 |
| 22 | 3 | 617 | CLA | CHD-C1D-ND | -5.64 | 119.27 | 124.45 |
| 22 | 6 | 604 | CLA | CHD-C1D-ND | -5.64 | 119.27 | 124.45 |
| 22 | 3 | 603 | CLA | CHD-C4C-C3C | -5.64 | 116.55 | 124.84 |
| 22 | 3 | 607 | CLA | CHD-C4C-C3C | -5.64 | 116.55 | 124.84 |
| 22 | 5 | 604 | CLA | CHD-C1D-ND | -5.63 | 119.28 | 124.45 |
| 22 | 7 | 616 | CLA | C2C-C1C-NC | 5.63 | 115.25 | 109.97 |
| 22 | A | 821 | CLA | O2D-CGD-CBD | 5.63 | 121.28 | 111.27 |
| 22 | 3 | 607 | CLA | CMD-C2D-C1D | 5.63 | 134.64 | 124.71 |
| 22 | A | 832 | CLA | O2D-CGD-CBD | 5.63 | 121.28 | 111.27 |
| 22 | A | 805 | CLA | CHD-C4C-C3C | -5.63 | 116.56 | 124.84 |
| 22 | 5 | 610 | CLA | CHD-C4C-C3C | -5.63 | 116.57 | 124.84 |
| 22 | B | 815 | CLA | O2D-CGD-CBD | 5.63 | 121.27 | 111.27 |
| 22 | 3 | 613 | CLA | CHD-C4C-C3C | -5.62 | 116.57 | 124.84 |
| 22 | 5 | 601 | CLA | CHD-C4C-C3C | -5.62 | 116.57 | 124.84 |
| 22 | B | 823 | CLA | CMD-C2D-C1D | 5.62 | 134.62 | 124.71 |
| 22 | 7 | 611 | CLA | O2D-CGD-CBD | 5.62 | 121.26 | 111.27 |
| 22 | A | 816 | CLA | CHD-C4C-C3C | -5.62 | 116.58 | 124.84 |
| 22 | 8 | 603 | CLA | CHD-C1D-ND | -5.62 | 119.29 | 124.45 |
| 29 | 5 | 618 | CHL | C1C-C2C-C3C | -5.62 | 102.65 | 107.11 |
| 22 | 5 | 611 | CLA | O2D-CGD-CBD | 5.62 | 121.25 | 111.27 |
| 22 | B | 852 | CLA | CHD-C4C-C3C | -5.62 | 116.58 | 124.84 |
| 22 | 7 | 603 | CLA | O2D-CGD-CBD | 5.61 | 121.25 | 111.27 |
| 29 | 3 | 608 | CHL | C3D-C2D-C1D | -5.61 | 98.17 | 105.83 |
| 29 | 4 | 606 | CHL | CHD-C4C-C3C | -5.61 | 116.59 | 124.84 |
| 22 | 8 | 611 | CLA | C2C-C1C-NC | 5.61 | 115.23 | 109.97 |
| 22 | 9 | 611 | CLA | C2C-C1C-NC | 5.61 | 115.23 | 109.97 |
| 22 | A | 836 | CLA | CHD-C1D-ND | -5.61 | 119.30 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 818 | CLA | CHD-C1D-ND | -5.61 | 119.30 | 124.45 |
| 22 | 5 | 603 | CLA | CHD-C1D-ND | -5.61 | 119.30 | 124.45 |
| 22 | 5 | 612 | CLA | CHD-C1D-ND | -5.61 | 119.30 | 124.45 |
| 29 | Z | 601 | CHL | CMD-C2D-C1D | 5.61 | 134.60 | 124.71 |
| 22 | 5 | 603 | CLA | C4A-NA-C1A | -5.61 | 104.19 | 106.71 |
| 22 | 7 | 606 | CLA | CHD-C1D-ND | -5.61 | 119.30 | 124.45 |
| 29 | Z | 607 | CHL | C2C-C3C-C4C | -5.61 | 102.49 | 106.49 |
| 22 | A | 832 | CLA | CMD-C2D-C1D | 5.61 | 134.59 | 124.71 |
| 22 | A | 805 | CLA | C4A-NA-C1A | -5.61 | 104.19 | 106.71 |
| 22 | A | 813 | CLA | CHD-C4C-C3C | -5.60 | 116.61 | 124.84 |
| 22 | Z | 606 | CLA | CHD-C4C-C3C | -5.60 | 116.61 | 124.84 |
| 22 | 1 | 616 | CLA | C2C-C1C-NC | 5.60 | 115.22 | 109.97 |
| 22 | 1 | 608 | CLA | C2C-C1C-NC | 5.60 | 115.22 | 109.97 |
| 22 | A | 820 | CLA | CHD-C1D-ND | -5.60 | 119.31 | 124.45 |
| 22 | B | 818 | CLA | C4A-NA-C1A | -5.60 | 104.19 | 106.71 |
| 22 | A | 834 | CLA | C2C-C1C-NC | 5.60 | 115.21 | 109.97 |
| 22 | 4 | 613 | CLA | CHD-C4C-C3C | -5.59 | 116.62 | 124.84 |
| 22 | 3 | 617 | CLA | C2C-C1C-NC | 5.59 | 115.21 | 109.97 |
| 22 | 9 | 601 | CLA | CHD-C4C-C3C | -5.59 | 116.62 | 124.84 |
| 22 | 4 | 601 | CLA | C2C-C1C-NC | 5.59 | 115.21 | 109.97 |
| 22 | A | 841 | CLA | C2C-C1C-NC | 5.59 | 115.21 | 109.97 |
| 22 | 8 | 616 | CLA | C2C-C1C-NC | 5.59 | 115.21 | 109.97 |
| 22 | 5 | 606 | CLA | CHD-C4C-C3C | -5.59 | 116.63 | 124.84 |
| 22 | A | 807 | CLA | CHD-C1D-ND | -5.59 | 119.32 | 124.45 |
| 22 | 4 | 609 | CLA | CHD-C1D-ND | -5.58 | 119.32 | 124.45 |
| 22 | 3 | 611 | CLA | C2C-C1C-NC | 5.58 | 115.20 | 109.97 |
| 22 | A | 824 | CLA | CHD-C4C-C3C | -5.58 | 116.63 | 124.84 |
| 22 | B | 803 | CLA | CMD-C2D-C1D | 5.58 | 134.54 | 124.71 |
| 22 | 4 | 609 | CLA | C4A-NA-C1A | -5.58 | 104.20 | 106.71 |
| 22 | Z | 616 | CLA | CHD-C4C-C3C | -5.57 | 116.65 | 124.84 |
| 21 | A | 801 | CL0 | CMD-C2D-C1D | 5.57 | 134.53 | 124.71 |
| 22 | F | 304 | CLA | CHD-C1D-ND | -5.57 | 119.33 | 124.45 |
| 22 | A | 833 | CLA | CHD-C4C-C3C | -5.57 | 116.65 | 124.84 |
| 22 | A | 810 | CLA | C2C-C1C-NC | 5.57 | 115.19 | 109.97 |
| 22 | A | 840 | CLA | C2C-C1C-NC | 5.56 | 115.19 | 109.97 |
| 22 | 6 | 612 | CLA | C2C-C1C-NC | 5.56 | 115.18 | 109.97 |
| 22 | 8 | 613 | CLA | C2C-C1C-NC | 5.56 | 115.18 | 109.97 |
| 22 | B | 852 | CLA | CMD-C2D-C1D | 5.56 | 134.51 | 124.71 |
| 22 | 8 | 603 | CLA | CHD-C4C-C3C | -5.56 | 116.67 | 124.84 |
| 22 | Z | 616 | CLA | CHD-C1D-ND | -5.56 | 119.34 | 124.45 |
| 22 | B | 808 | CLA | O2D-CGD-CBD | 5.56 | 121.14 | 111.27 |
| 22 | B | 812 | CLA | CHD-C4C-C3C | -5.56 | 116.67 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 1 | 602 | CLA | CHD-C1D-ND | -5.56 | 119.35 | 124.45 |
| 22 | A | 819 | CLA | CHD-C4C-C3C | -5.55 | 116.68 | 124.84 |
| 22 | Z | 604 | CLA | C2C-C1C-NC | 5.55 | 115.17 | 109.97 |
| 22 | 7 | 620 | CLA | CHD-C4C-C3C | -5.55 | 116.68 | 124.84 |
| 22 | 3 | 603 | CLA | CHD-C1D-ND | -5.55 | 119.35 | 124.45 |
| 22 | 7 | 613 | CLA | CHD-C4C-C3C | -5.55 | 116.69 | 124.84 |
| 22 | 6 | 603 | CLA | CHD-C4C-C3C | -5.55 | 116.69 | 124.84 |
| 22 | Z | 603 | CLA | O2D-CGD-CBD | 5.54 | 121.12 | 111.27 |
| 22 | Z | 610 | CLA | CHD-C1D-ND | -5.54 | 119.36 | 124.45 |
| 22 | 5 | 611 | CLA | CHD-C4C-C3C | -5.54 | 116.69 | 124.84 |
| 22 | 1 | 612 | CLA | CHD-C1D-ND | -5.54 | 119.36 | 124.45 |
| 22 | 9 | 611 | CLA | CHD-C1D-ND | -5.54 | 119.36 | 124.45 |
| 29 | 4 | 606 | CHL | C1C-C2C-C3C | -5.54 | 102.71 | 107.11 |
| 22 | 4 | 609 | CLA | CHD-C4C-C3C | -5.54 | 116.70 | 124.84 |
| 22 | A | 854 | CLA | CHD-C1D-ND | -5.54 | 119.36 | 124.45 |
| 22 | 1 | 609 | CLA | C2C-C1C-NC | 5.54 | 115.16 | 109.97 |
| 22 | Z | 616 | CLA | C2C-C1C-NC | 5.53 | 115.16 | 109.97 |
| 22 | 7 | 606 | CLA | O2D-CGD-CBD | 5.53 | 121.10 | 111.27 |
| 22 | J | 3002 | CLA | C2C-C1C-NC | 5.53 | 115.16 | 109.97 |
| 22 | 7 | 603 | CLA | C2C-C1C-NC | 5.53 | 115.16 | 109.97 |
| 22 | 8 | 609 | CLA | CHD-C1D-ND | -5.53 | 119.37 | 124.45 |
| 22 | A | 823 | CLA | CHD-C4C-C3C | -5.53 | 116.71 | 124.84 |
| 22 | 3 | 607 | CLA | CHD-C1D-ND | -5.53 | 119.37 | 124.45 |
| 22 | 2 | 606 | CLA | CHD-C4C-C3C | -5.53 | 116.71 | 124.84 |
| 22 | A | 839 | CLA | CHD-C4C-C3C | -5.53 | 116.71 | 124.84 |
| 22 | 1 | 612 | CLA | CHD-C4C-C3C | -5.53 | 116.71 | 124.84 |
| 22 | 1 | 616 | CLA | CHD-C4C-C3C | -5.53 | 116.72 | 124.84 |
| 22 | 8 | 612 | CLA | CHD-C1D-ND | -5.52 | 119.38 | 124.45 |
| 22 | 6 | 601 | CLA | C2C-C1C-NC | 5.52 | 115.15 | 109.97 |
| 22 | 7 | 614 | CLA | CHD-C4C-C3C | -5.52 | 116.72 | 124.84 |
| 22 | 3 | 611 | CLA | CAA-C2A-C3A | -5.52 | 103.22 | 116.10 |
| 29 | 7 | 607 | CHL | C2C-C3C-C4C | -5.52 | 102.55 | 106.49 |
| 22 | 2 | 601 | CLA | CHD-C4C-C3C | -5.52 | 116.73 | 124.84 |
| 22 | B | 821 | CLA | CHD-C4C-C3C | -5.51 | 116.73 | 124.84 |
| 22 | B | 808 | CLA | CHD-C4C-C3C | -5.51 | 116.74 | 124.84 |
| 22 | 4 | 612 | CLA | C2C-C1C-NC | 5.51 | 115.14 | 109.97 |
| 29 | 9 | 606 | CHL | C1C-C2C-C3C | -5.51 | 102.74 | 107.11 |
| 22 | 7 | 612 | CLA | CHD-C4C-C3C | -5.51 | 116.74 | 124.84 |
| 22 | A | 808 | CLA | O2D-CGD-CBD | 5.51 | 121.06 | 111.27 |
| 22 | 5 | 612 | CLA | CHD-C4C-C3C | -5.51 | 116.74 | 124.84 |
| 22 | 4 | 613 | CLA | C2C-C1C-NC | 5.51 | 115.13 | 109.97 |
| 22 | 8 | 609 | CLA | CHD-C4C-C3C | -5.51 | 116.74 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 4 | 614 | CLA | CHD-C1D-ND | -5.50 | 119.40 | 124.45 |
| 22 | 5 | 616 | CLA | CHD-C4C-C3C | -5.50 | 116.75 | 124.84 |
| 22 | B | 832 | CLA | C2C-C1C-NC | 5.50 | 115.13 | 109.97 |
| 22 | 7 | 604 | CLA | CHD-C1D-ND | -5.50 | 119.40 | 124.45 |
| 22 | 9 | 612 | CLA | CHD-C4C-C3C | -5.50 | 116.75 | 124.84 |
| 22 | 1 | 603 | CLA | O2D-CGD-CBD | 5.50 | 121.04 | 111.27 |
| 22 | B | 839 | CLA | CHD-C4C-C3C | -5.50 | 116.76 | 124.84 |
| 22 | 6 | 611 | CLA | CHD-C1D-ND | -5.50 | 119.40 | 124.45 |
| 22 | 7 | 609 | CLA | C2C-C1C-NC | 5.50 | 115.12 | 109.97 |
| 22 | 3 | 602 | CLA | CHD-C4C-C3C | -5.50 | 116.76 | 124.84 |
| 22 | 1 | 613 | CLA | CHD-C4C-C3C | -5.50 | 116.76 | 124.84 |
| 22 | G | 203 | CLA | O2D-CGD-CBD | 5.50 | 121.03 | 111.27 |
| 22 | 3 | 606 | CLA | C2C-C1C-NC | 5.50 | 115.12 | 109.97 |
| 22 | 6 | 617 | CLA | C2C-C1C-NC | 5.50 | 115.12 | 109.97 |
| 22 | 4 | 611 | CLA | CHD-C1D-ND | -5.49 | 119.41 | 124.45 |
| 22 | Z | 614 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.84 |
| 22 | 6 | 614 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.84 |
| 22 | 2 | 610 | CLA | CHD-C4C-C3C | -5.49 | 116.77 | 124.84 |
| 22 | A | 854 | CLA | C4A-NA-C1A | -5.49 | 104.24 | 106.71 |
| 22 | F | 304 | CLA | C2C-C1C-NC | 5.49 | 115.11 | 109.97 |
| 22 | 3 | 609 | CLA | C2C-C1C-NC | 5.48 | 115.11 | 109.97 |
| 22 | Z | 602 | CLA | CHD-C1D-ND | -5.48 | 119.42 | 124.45 |
| 22 | 6 | 604 | CLA | C2C-C1C-NC | 5.48 | 115.11 | 109.97 |
| 22 | B | 807 | CLA | O2D-CGD-CBD | 5.48 | 121.00 | 111.27 |
| 22 | B | 827 | CLA | O2D-CGD-CBD | 5.48 | 121.00 | 111.27 |
| 22 | 1 | 610 | CLA | CMD-C2D-C1D | 5.47 | 134.36 | 124.71 |
| 22 | 6 | 617 | CLA | CHD-C1D-ND | -5.47 | 119.42 | 124.45 |
| 22 | 7 | 606 | CLA | C2C-C1C-NC | 5.47 | 115.10 | 109.97 |
| 22 | 5 | 606 | CLA | C2C-C1C-NC | 5.47 | 115.10 | 109.97 |
| 22 | 3 | 603 | CLA | C4A-NA-C1A | -5.47 | 104.25 | 106.71 |
| 22 | 3 | 602 | CLA | O2D-CGD-CBD | 5.47 | 120.99 | 111.27 |
| 22 | 3 | 617 | CLA | CHD-C4C-C3C | -5.47 | 116.80 | 124.84 |
| 22 | B | 836 | CLA | CHD-C4C-C3C | -5.47 | 116.81 | 124.84 |
| 29 | 1 | 601 | CHL | CHD-C4C-C3C | -5.47 | 116.81 | 124.84 |
| 22 | A | 840 | CLA | CHD-C1D-ND | -5.46 | 119.43 | 124.45 |
| 22 | 1 | 610 | CLA | CHD-C1D-ND | -5.46 | 119.44 | 124.45 |
| 22 | 6 | 611 | CLA | C2C-C1C-NC | 5.46 | 115.08 | 109.97 |
| 22 | K | 4003 | CLA | CHD-C4C-C3C | -5.46 | 116.82 | 124.84 |
| 29 | 9 | 606 | CHL | CHD-C4C-C3C | -5.46 | 116.82 | 124.84 |
| 22 | B | 815 | CLA | CHD-C4C-C3C | -5.46 | 116.82 | 124.84 |
| 22 | J | 3002 | CLA | CHD-C4C-C3C | -5.46 | 116.82 | 124.84 |
| 22 | A | 807 | CLA | C2C-C1C-NC | 5.46 | 115.08 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | F | 303 | CLA | C2C-C1C-NC | 5.46 | 115.08 | 109.97 |
| 22 | 2 | 611 | CLA | C2C-C1C-NC | 5.45 | 115.08 | 109.97 |
| 22 | G | 203 | CLA | CHD-C4C-C3C | -5.45 | 116.83 | 124.84 |
| 22 | 3 | 611 | CLA | CHD-C1D-ND | -5.45 | 119.44 | 124.45 |
| 22 | A | 839 | CLA | C2C-C1C-NC | 5.45 | 115.08 | 109.97 |
| 29 | 4 | 607 | CHL | CHD-C4C-C3C | -5.45 | 116.83 | 124.84 |
| 22 | 8 | 606 | CLA | C2C-C1C-NC | 5.45 | 115.08 | 109.97 |
| 22 | 6 | 616 | CLA | C2C-C1C-NC | 5.45 | 115.08 | 109.97 |
| 22 | A | 815 | CLA | CHD-C4C-C3C | -5.44 | 116.84 | 124.84 |
| 22 | A | 811 | CLA | CHD-C1D-ND | -5.44 | 119.45 | 124.45 |
| 22 | 9 | 614 | CLA | C4A-NA-C1A | -5.44 | 104.26 | 106.71 |
| 22 | L | 204 | CLA | C2C-C1C-NC | 5.44 | 115.07 | 109.97 |
| 22 | 2 | 614 | CLA | C2C-C1C-NC | 5.44 | 115.07 | 109.97 |
| 22 | A | 822 | CLA | CHD-C4C-C3C | -5.44 | 116.84 | 124.84 |
| 22 | A | 829 | CLA | C4A-NA-C1A | -5.44 | 104.26 | 106.71 |
| 29 | 5 | 607 | CHL | C3D-C2D-C1D | -5.44 | 98.41 | 105.83 |
| 22 | A | 835 | CLA | CHD-C4C-C3C | -5.44 | 116.85 | 124.84 |
| 22 | 7 | 602 | CLA | O2D-CGD-CBD | 5.44 | 120.93 | 111.27 |
| 22 | 8 | 606 | CLA | CHD-C4C-C3C | -5.43 | 116.85 | 124.84 |
| 22 | G | 204 | CLA | C2C-C1C-NC | 5.43 | 115.06 | 109.97 |
| 22 | A | 843 | CLA | CHD-C4C-C3C | -5.42 | 116.87 | 124.84 |
| 22 | 1 | 613 | CLA | C2C-C1C-NC | 5.42 | 115.05 | 109.97 |
| 22 | A | 821 | CLA | CHD-C4C-C3C | -5.42 | 116.87 | 124.84 |
| 22 | 2 | 614 | CLA | CHD-C4C-C3C | -5.42 | 116.87 | 124.84 |
| 22 | 7 | 606 | CLA | C4A-NA-C1A | -5.42 | 104.27 | 106.71 |
| 22 | A | 808 | CLA | C2C-C1C-NC | 5.41 | 115.04 | 109.97 |
| 22 | 2 | 603 | CLA | CHD-C4C-C3C | -5.41 | 116.88 | 124.84 |
| 22 | 7 | 614 | CLA | C2C-C1C-NC | 5.41 | 115.04 | 109.97 |
| 22 | F | 303 | CLA | C4A-NA-C1A | -5.41 | 104.27 | 106.71 |
| 22 | B | 810 | CLA | CHD-C4C-C3C | -5.41 | 116.89 | 124.84 |
| 22 | L | 203 | CLA | C2C-C1C-NC | 5.41 | 115.04 | 109.97 |
| 22 | L | 203 | CLA | CHD-C4C-C3C | -5.41 | 116.89 | 124.84 |
| 22 | A | 804 | CLA | O2D-CGD-CBD | 5.41 | 120.88 | 111.27 |
| 29 | 6 | 606 | CHL | C3D-C2D-C1D | -5.41 | 98.45 | 105.83 |
| 22 | 3 | 614 | CLA | CHD-C4C-C3C | -5.41 | 116.89 | 124.84 |
| 29 | 9 | 607 | CHL | O2D-CGD-CBD | 5.41 | 120.88 | 111.27 |
| 22 | B | 828 | CLA | C4A-NA-C1A | -5.41 | 104.28 | 106.71 |
| 22 | B | 839 | CLA | C2C-C1C-NC | 5.40 | 115.03 | 109.97 |
| 22 | K | 4002 | CLA | CHD-C4C-C3C | -5.40 | 116.90 | 124.84 |
| 29 | 4 | 618 | CHL | C1C-C2C-C3C | -5.40 | 102.83 | 107.11 |
| 29 | 1 | 607 | CHL | CHD-C4C-C3C | -5.40 | 116.90 | 124.84 |
| 22 | A | 831 | CLA | CHD-C1D-ND | -5.40 | 119.49 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 814 | CLA | CHD-C4C-C3C | -5.40 | 116.91 | 124.84 |
| 22 | 6 | 610 | CLA | CHD-C4C-C3C | -5.40 | 116.91 | 124.84 |
| 22 | 1 | 613 | CLA | CHD-C1D-ND | -5.40 | 119.49 | 124.45 |
| 29 | 6 | 607 | CHL | CHD-C4C-C3C | -5.40 | 116.91 | 124.84 |
| 22 | A | 837 | CLA | O2D-CGD-CBD | 5.40 | 120.86 | 111.27 |
| 22 | B | 841 | CLA | CHD-C4C-C3C | -5.39 | 116.91 | 124.84 |
| 22 | 2 | 607 | CLA | CHD-C4C-C3C | -5.39 | 116.92 | 124.84 |
| 22 | Z | 606 | CLA | C2C-C1C-NC | 5.39 | 115.02 | 109.97 |
| 22 | 7 | 620 | CLA | C2C-C1C-NC | 5.39 | 115.02 | 109.97 |
| 22 | 8 | 610 | CLA | CHD-C1D-ND | -5.39 | 119.50 | 124.45 |
| 22 | A | 829 | CLA | CHD-C1D-ND | -5.38 | 119.51 | 124.45 |
| 22 | 5 | 617 | CLA | C3D-C2D-C1D | -5.38 | 98.49 | 105.83 |
| 22 | 5 | 614 | CLA | CHD-C4C-C3C | -5.38 | 116.93 | 124.84 |
| 22 | B | 852 | CLA | C2C-C1C-NC | 5.38 | 115.01 | 109.97 |
| 22 | A | 803 | CLA | O2D-CGD-CBD | 5.38 | 120.83 | 111.27 |
| 22 | 2 | 606 | CLA | C2C-C1C-NC | 5.38 | 115.01 | 109.97 |
| 22 | 6 | 622 | CLA | C2C-C1C-NC | 5.37 | 115.01 | 109.97 |
| 22 | B | 835 | CLA | CHD-C1D-ND | -5.37 | 119.52 | 124.45 |
| 22 | 3 | 617 | CLA | O2D-CGD-CBD | 5.37 | 120.82 | 111.27 |
| 22 | A | 802 | CLA | C4A-NA-C1A | -5.37 | 104.29 | 106.71 |
| 25 | B | 846 | BCR | C39-C30-C25 | -5.37 | 101.59 | 110.30 |
| 22 | 9 | 614 | CLA | O2D-CGD-CBD | 5.37 | 120.81 | 111.27 |
| 22 | 5 | 609 | CLA | CHD-C4C-C3C | -5.37 | 116.95 | 124.84 |
| 22 | 8 | 601 | CLA | CHD-C1D-ND | -5.37 | 119.52 | 124.45 |
| 22 | 2 | 612 | CLA | CHD-C4C-C3C | -5.37 | 116.95 | 124.84 |
| 22 | B | 835 | CLA | C2C-C1C-NC | 5.37 | 115.00 | 109.97 |
| 22 | 3 | 614 | CLA | C2C-C1C-NC | 5.37 | 115.00 | 109.97 |
| 22 | 8 | 601 | CLA | CHD-C4C-C3C | -5.37 | 116.95 | 124.84 |
| 29 | 6 | 607 | CHL | C3D-C2D-C1D | -5.37 | 98.51 | 105.83 |
| 22 | A | 819 | CLA | C4A-NA-C1A | -5.37 | 104.29 | 106.71 |
| 22 | Z | 613 | CLA | CHD-C1D-ND | -5.36 | 119.52 | 124.45 |
| 22 | B | 807 | CLA | CHD-C4C-C3C | -5.36 | 116.95 | 124.84 |
| 22 | 5 | 613 | CLA | CHD-C4C-C3C | -5.36 | 116.96 | 124.84 |
| 22 | 3 | 604 | CLA | CHD-C4C-C3C | -5.36 | 116.96 | 124.84 |
| 22 | 4 | 603 | CLA | CHD-C4C-C3C | -5.36 | 116.96 | 124.84 |
| 22 | 6 | 616 | CLA | CHD-C4C-C3C | -5.36 | 116.96 | 124.84 |
| 22 | A | 828 | CLA | C3D-C2D-C1D | -5.36 | 98.52 | 105.83 |
| 22 | 2 | 611 | CLA | CHD-C4C-C3C | -5.36 | 116.96 | 124.84 |
| 22 | B | 827 | CLA | CHD-C1D-ND | -5.36 | 119.53 | 124.45 |
| 22 | B | 821 | CLA | C2C-C1C-NC | 5.36 | 114.99 | 109.97 |
| 22 | 9 | 603 | CLA | CHD-C4C-C3C | -5.36 | 116.97 | 124.84 |
| 22 | 4 | 602 | CLA | C2C-C1C-NC | 5.36 | 114.99 | 109.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 4 | 604 | CLA | C2C-C1C-NC | 5.35 | 114.99 | 109.97 |
| 22 | A | 820 | CLA | O2D-CGD-CBD | 5.35 | 120.78 | 111.27 |
| 22 | 7 | 601 | CLA | O2D-CGD-CBD | 5.35 | 120.78 | 111.27 |
| 29 | 6 | 606 | CHL | CHD-C4C-C3C | -5.35 | 116.98 | 124.84 |
| 22 | B | 815 | CLA | C2C-C1C-NC | 5.35 | 114.98 | 109.97 |
| 22 | B | 809 | CLA | CHD-C4C-C3C | -5.35 | 116.98 | 124.84 |
| 22 | Z | 603 | CLA | C4A-NA-C1A | -5.35 | 104.30 | 106.71 |
| 22 | 8 | 614 | CLA | CMD-C2D-C1D | 5.35 | 134.13 | 124.71 |
| 22 | A | 826 | CLA | O2D-CGD-CBD | 5.35 | 120.77 | 111.27 |
| 22 | B | 810 | CLA | C2C-C1C-NC | 5.34 | 114.98 | 109.97 |
| 22 | A | 831 | CLA | CHD-C4C-C3C | -5.34 | 116.98 | 124.84 |
| 29 | 6 | 606 | CHL | O2D-CGD-CBD | 5.34 | 120.76 | 111.27 |
| 29 | 5 | 608 | CHL | C1C-C2C-C3C | -5.34 | 102.87 | 107.11 |
| 22 | B | 833 | CLA | CHD-C4C-C3C | -5.34 | 116.99 | 124.84 |
| 22 | A | 835 | CLA | C4A-NA-C1A | -5.34 | 104.31 | 106.71 |
| 22 | 1 | 602 | CLA | C4A-NA-C1A | -5.34 | 104.31 | 106.71 |
| 22 | 1 | 611 | CLA | CHD-C4C-C3C | -5.33 | 117.00 | 124.84 |
| 22 | 6 | 613 | CLA | CHD-C4C-C3C | -5.33 | 117.00 | 124.84 |
| 22 | Z | 608 | CLA | C2C-C1C-NC | 5.33 | 114.97 | 109.97 |
| 22 | 7 | 612 | CLA | C4A-NA-C1A | -5.33 | 104.31 | 106.71 |
| 22 | K | 4002 | CLA | C2C-C1C-NC | 5.33 | 114.97 | 109.97 |
| 22 | 6 | 601 | CLA | CHD-C4C-C3C | -5.33 | 117.00 | 124.84 |
| 22 | 5 | 614 | CLA | C2C-C1C-NC | 5.33 | 114.96 | 109.97 |
| 22 | B | 820 | CLA | CHD-C4C-C3C | -5.33 | 117.01 | 124.84 |
| 22 | A | 837 | CLA | C2C-C1C-NC | 5.33 | 114.96 | 109.97 |
| 22 | 5 | 617 | CLA | CHD-C4C-C3C | -5.33 | 117.01 | 124.84 |
| 22 | A | 824 | CLA | O2D-CGD-CBD | 5.32 | 120.73 | 111.27 |
| 22 | 3 | 606 | CLA | CHD-C4C-C3C | -5.32 | 117.02 | 124.84 |
| 22 | 7 | 609 | CLA | CHD-C4C-C3C | -5.32 | 117.02 | 124.84 |
| 22 | A | 813 | CLA | C4A-NA-C1A | -5.32 | 104.31 | 106.71 |
| 22 | B | 830 | CLA | C4A-NA-C1A | -5.32 | 104.31 | 106.71 |
| 22 | 3 | 614 | CLA | C4A-NA-C1A | -5.32 | 104.31 | 106.71 |
| 22 | B | 812 | CLA | C2C-C1C-NC | 5.32 | 114.95 | 109.97 |
| 22 | 4 | 616 | CLA | CHD-C4C-C3C | -5.31 | 117.03 | 124.84 |
| 22 | 2 | 602 | CLA | CHD-C4C-C3C | -5.31 | 117.03 | 124.84 |
| 22 | B | 836 | CLA | C2C-C1C-NC | 5.31 | 114.95 | 109.97 |
| 22 | 5 | 613 | CLA | CHD-C1D-ND | -5.31 | 119.57 | 124.45 |
| 22 | 3 | 609 | CLA | CHD-C4C-C3C | -5.31 | 117.03 | 124.84 |
| 22 | A | 807 | CLA | O2D-CGD-CBD | 5.31 | 120.70 | 111.27 |
| 22 | 1 | 603 | CLA | CHD-C4C-C3C | -5.30 | 117.04 | 124.84 |
| 29 | 1 | 607 | CHL | C3D-C2D-C1D | -5.30 | 98.60 | 105.83 |
| 22 | 9 | 614 | CLA | CHD-C4C-C3C | -5.30 | 117.05 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 818 | CLA | CHD-C4C-C3C | -5.30 | 117.05 | 124.84 |
| 22 | 5 | 612 | CLA | C4A-NA-C1A | -5.30 | 104.33 | 106.71 |
| 22 | B | 811 | CLA | O2D-CGD-CBD | 5.29 | 120.68 | 111.27 |
| 22 | B | 816 | CLA | C3D-C2D-C1D | -5.29 | 98.61 | 105.83 |
| 22 | 7 | 616 | CLA | C3D-C2D-C1D | -5.29 | 98.61 | 105.83 |
| 22 | 6 | 609 | CLA | CHD-C4C-C3C | -5.29 | 117.06 | 124.84 |
| 22 | A | 827 | CLA | C4A-NA-C1A | -5.29 | 104.33 | 106.71 |
| 22 | 9 | 613 | CLA | CHD-C4C-C3C | -5.29 | 117.07 | 124.84 |
| 22 | Z | 614 | CLA | C2C-C1C-NC | 5.29 | 114.92 | 109.97 |
| 22 | G | 204 | CLA | CHD-C4C-C3C | -5.29 | 117.07 | 124.84 |
| 22 | A | 828 | CLA | CHD-C1D-ND | -5.29 | 119.60 | 124.45 |
| 22 | 4 | 610 | CLA | CHD-C4C-C3C | -5.28 | 117.07 | 124.84 |
| 22 | B | 823 | CLA | CHD-C1D-ND | -5.28 | 119.60 | 124.45 |
| 29 | 9 | 607 | CHL | C3D-C2D-C1D | -5.28 | 98.62 | 105.83 |
| 22 | B | 852 | CLA | CHD-C1D-ND | -5.28 | 119.60 | 124.45 |
| 22 | 5 | 616 | CLA | CHD-C1D-ND | -5.28 | 119.60 | 124.45 |
| 22 | Z | 610 | CLA | O2D-CGD-CBD | 5.28 | 120.65 | 111.27 |
| 22 | B | 822 | CLA | C2C-C1C-NC | 5.28 | 114.92 | 109.97 |
| 22 | 7 | 611 | CLA | CHD-C1D-ND | -5.27 | 119.61 | 124.45 |
| 22 | 8 | 612 | CLA | C4A-NA-C1A | -5.27 | 104.33 | 106.71 |
| 22 | 5 | 621 | CLA | O2D-CGD-CBD | 5.27 | 120.64 | 111.27 |
| 22 | 5 | 621 | CLA | CHD-C4C-C3C | -5.27 | 117.09 | 124.84 |
| 22 | 9 | 609 | CLA | CHD-C4C-C3C | -5.27 | 117.09 | 124.84 |
| 22 | 6 | 612 | CLA | CHD-C1D-ND | -5.27 | 119.61 | 124.45 |
| 22 | B | 832 | CLA | O2D-CGD-CBD | 5.27 | 120.63 | 111.27 |
| 22 | B | 831 | CLA | O2D-CGD-CBD | 5.27 | 120.63 | 111.27 |
| 22 | A | 837 | CLA | CHD-C4C-C3C | -5.26 | 117.10 | 124.84 |
| 22 | A | 802 | CLA | CHD-C4C-C3C | -5.26 | 117.11 | 124.84 |
| 22 | 3 | 620 | CLA | CHD-C4C-C3C | -5.26 | 117.11 | 124.84 |
| 29 | 4 | 606 | CHL | C3D-C2D-C1D | -5.26 | 98.66 | 105.83 |
| 22 | 3 | 612 | CLA | CHD-C4C-C3C | -5.26 | 117.11 | 124.84 |
| 22 | 6 | 617 | CLA | C4A-NA-C1A | -5.26 | 104.34 | 106.71 |
| 25 | L | 201 | BCR | C7-C8-C9 | -5.25 | 118.30 | 126.23 |
| 22 | B | 820 | CLA | C4A-NA-C1A | -5.25 | 104.35 | 106.71 |
| 22 | B | 826 | CLA | C4A-NA-C1A | -5.25 | 104.35 | 106.71 |
| 29 | 6 | 606 | CHL | C1C-C2C-C3C | -5.25 | 102.95 | 107.11 |
| 29 | 6 | 618 | CHL | C3D-C2D-C1D | -5.25 | 98.67 | 105.83 |
| 29 | 9 | 606 | CHL | C3D-C2D-C1D | -5.25 | 98.67 | 105.83 |
| 22 | 4 | 610 | CLA | O2D-CGD-CBD | 5.24 | 120.59 | 111.27 |
| 22 | 7 | 611 | CLA | CHD-C4C-C3C | -5.24 | 117.13 | 124.84 |
| 22 | 4 | 616 | CLA | CAA-C2A-C3A | -5.24 | 103.86 | 116.10 |
| 22 | A | 838 | CLA | CHD-C4C-C3C | -5.24 | 117.14 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 8 | 609 | CLA | C4A-NA-C1A | -5.24 | 104.35 | 106.71 |
| 22 | 6 | 622 | CLA | CHD-C4C-C3C | -5.24 | 117.14 | 124.84 |
| 22 | A | 826 | CLA | CHD-C4C-C3C | -5.24 | 117.14 | 124.84 |
| 22 | 1 | 609 | CLA | C4A-NA-C1A | -5.24 | 104.35 | 106.71 |
| 29 | 5 | 608 | CHL | C3D-C2D-C1D | -5.24 | 98.68 | 105.83 |
| 22 | 2 | 607 | CLA | C2C-C1C-NC | 5.24 | 114.88 | 109.97 |
| 22 | B | 826 | CLA | CHD-C1D-ND | -5.23 | 119.65 | 124.45 |
| 22 | B | 811 | CLA | C4A-NA-C1A | -5.23 | 104.36 | 106.71 |
| 22 | Z | 610 | CLA | C4A-NA-C1A | -5.23 | 104.36 | 106.71 |
| 22 | 2 | 602 | CLA | C2C-C1C-NC | 5.23 | 114.87 | 109.97 |
| 29 | 5 | 618 | CHL | C3D-C2D-C1D | -5.22 | 98.70 | 105.83 |
| 22 | 1 | 614 | CLA | CHD-C4C-C3C | -5.22 | 117.16 | 124.84 |
| 22 | 8 | 602 | CLA | O2D-CGD-CBD | 5.22 | 120.54 | 111.27 |
| 22 | Z | 606 | CLA | O2D-CGD-CBD | 5.22 | 120.54 | 111.27 |
| 29 | 6 | 608 | CHL | CHD-C1D-ND | -5.22 | 119.66 | 124.45 |
| 22 | 2 | 613 | CLA | CHD-C4C-C3C | -5.22 | 117.17 | 124.84 |
| 29 | 1 | 601 | CHL | C1C-C2C-C3C | -5.22 | 102.97 | 107.11 |
| 22 | Z | 603 | CLA | CHD-C4C-C3C | -5.21 | 117.17 | 124.84 |
| 22 | 6 | 611 | CLA | CHD-C4C-C3C | -5.21 | 117.18 | 124.84 |
| 22 | A | 823 | CLA | C2C-C1C-NC | 5.21 | 114.86 | 109.97 |
| 22 | A | 813 | CLA | O2D-CGD-CBD | 5.21 | 120.53 | 111.27 |
| 22 | 3 | 611 | CLA | CHD-C4C-C3C | -5.21 | 117.18 | 124.84 |
| 22 | 2 | 610 | CLA | O2D-CGD-CBD | 5.20 | 120.51 | 111.27 |
| 22 | A | 817 | CLA | CHD-C4C-C3C | -5.20 | 117.19 | 124.84 |
| 22 | 8 | 612 | CLA | C2C-C1C-NC | 5.20 | 114.84 | 109.97 |
| 22 | Z | 611 | CLA | C2C-C1C-NC | 5.20 | 114.84 | 109.97 |
| 22 | B | 813 | CLA | C4A-NA-C1A | -5.20 | 104.37 | 106.71 |
| 22 | B | 834 | CLA | CHD-C4C-C3C | -5.20 | 117.20 | 124.84 |
| 22 | 4 | 602 | CLA | CHD-C4C-C3C | -5.20 | 117.20 | 124.84 |
| 22 | 4 | 604 | CLA | CHD-C4C-C3C | -5.20 | 117.20 | 124.84 |
| 22 | 1 | 616 | CLA | CHD-C1D-ND | -5.20 | 119.67 | 124.45 |
| 22 | B | 820 | CLA | C2C-C1C-NC | 5.20 | 114.84 | 109.97 |
| 22 | B | 822 | CLA | O2D-CGD-CBD | 5.20 | 120.50 | 111.27 |
| 22 | 5 | 606 | CLA | C4A-NA-C1A | -5.20 | 104.37 | 106.71 |
| 22 | 1 | 604 | CLA | C2C-C1C-NC | 5.19 | 114.84 | 109.97 |
| 29 | 4 | 618 | CHL | C3D-C2D-C1D | -5.19 | 98.75 | 105.83 |
| 22 | 1 | 609 | CLA | CHD-C4C-C3C | -5.18 | 117.22 | 124.84 |
| 22 | B | 834 | CLA | C2C-C1C-NC | 5.18 | 114.83 | 109.97 |
| 22 | A | 817 | CLA | O2D-CGD-CBD | 5.18 | 120.48 | 111.27 |
| 29 | 6 | 618 | CHL | CHD-C4C-C3C | -5.18 | 117.22 | 124.84 |
| 22 | 3 | 611 | CLA | O2D-CGD-CBD | 5.18 | 120.47 | 111.27 |
| 29 | 5 | 608 | CHL | CHD-C4C-C3C | -5.18 | 117.22 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | Z | 607 | CHL | C1C-C2C-C3C | -5.18 | 103.00 | 107.11 |
| 22 | B | 825 | CLA | CHD-C1D-ND | -5.18 | 119.69 | 124.45 |
| 22 | 1 | 610 | CLA | C4A-NA-C1A | -5.18 | 104.38 | 106.71 |
| 22 | 5 | 617 | CLA | C4A-NA-C1A | -5.18 | 104.38 | 106.71 |
| 22 | 8 | 609 | CLA | C2C-C1C-NC | 5.17 | 114.82 | 109.97 |
| 22 | 3 | 604 | CLA | C4A-NA-C1A | -5.17 | 104.38 | 106.71 |
| 22 | A | 803 | CLA | C2C-C1C-NC | 5.17 | 114.82 | 109.97 |
| 22 | 4 | 610 | CLA | C4A-NA-C1A | -5.17 | 104.38 | 106.71 |
| 29 | 7 | 607 | CHL | C1C-C2C-C3C | -5.17 | 103.01 | 107.11 |
| 29 | 4 | 607 | CHL | C3D-C2D-C1D | -5.16 | 98.78 | 105.83 |
| 25 | A | 852 | BCR | C7-C8-C9 | -5.16 | 118.43 | 126.23 |
| 22 | 1 | 606 | CLA | C4A-NA-C1A | -5.16 | 104.39 | 106.71 |
| 22 | 4 | 612 | CLA | O2D-CGD-CBD | 5.16 | 120.44 | 111.27 |
| 29 | 6 | 608 | CHL | C3D-C2D-C1D | -5.16 | 98.79 | 105.83 |
| 29 | 5 | 618 | CHL | C2C-C3C-C4C | -5.16 | 102.81 | 106.49 |
| 29 | 1 | 601 | CHL | C3D-C2D-C1D | -5.16 | 98.79 | 105.83 |
| 22 | B | 817 | CLA | CHD-C4C-C3C | -5.16 | 117.26 | 124.84 |
| 22 | 7 | 601 | CLA | C2C-C1C-NC | 5.15 | 114.80 | 109.97 |
| 22 | 8 | 614 | CLA | C2C-C1C-NC | 5.15 | 114.80 | 109.97 |
| 22 | B | 824 | CLA | CHD-C1D-ND | -5.15 | 119.72 | 124.45 |
| 29 | 4 | 618 | CHL | O2D-CGD-CBD | 5.15 | 120.41 | 111.27 |
| 22 | B | 829 | CLA | C2C-C1C-NC | 5.15 | 114.79 | 109.97 |
| 22 | 3 | 617 | CLA | C4A-NA-C1A | -5.14 | 104.39 | 106.71 |
| 22 | 8 | 613 | CLA | CHD-C1D-ND | -5.14 | 119.73 | 124.45 |
| 22 | Z | 604 | CLA | CHD-C4C-C3C | -5.14 | 117.28 | 124.84 |
| 22 | B | 834 | CLA | C4A-NA-C1A | -5.14 | 104.39 | 106.71 |
| 22 | A | 833 | CLA | C2C-C1C-NC | 5.14 | 114.79 | 109.97 |
| 22 | B | 806 | CLA | C2C-C1C-NC | 5.14 | 114.79 | 109.97 |
| 22 | B | 838 | CLA | C2C-C1C-NC | 5.14 | 114.79 | 109.97 |
| 29 | 3 | 608 | CHL | CHD-C1D-ND | -5.14 | 119.73 | 124.45 |
| 29 | 7 | 607 | CHL | C3D-C2D-C1D | -5.14 | 98.82 | 105.83 |
| 22 | A | 830 | CLA | C4A-NA-C1A | -5.13 | 104.40 | 106.71 |
| 22 | 6 | 613 | CLA | C2C-C1C-NC | 5.13 | 114.78 | 109.97 |
| 29 | 6 | 607 | CHL | O2D-CGD-CBD | 5.13 | 120.39 | 111.27 |
| 22 | 5 | 603 | CLA | O2D-CGD-CBD | 5.13 | 120.38 | 111.27 |
| 22 | 6 | 622 | CLA | O2D-CGD-CBD | 5.12 | 120.38 | 111.27 |
| 22 | B | 828 | CLA | CHD-C4C-C3C | -5.12 | 117.31 | 124.84 |
| 22 | 8 | 606 | CLA | C4A-NA-C1A | -5.12 | 104.40 | 106.71 |
| 22 | A | 813 | CLA | C2C-C1C-NC | 5.12 | 114.77 | 109.97 |
| 22 | B | 819 | CLA | CHD-C4C-C3C | -5.12 | 117.31 | 124.84 |
| 22 | B | 817 | CLA | O2D-CGD-CBD | 5.12 | 120.37 | 111.27 |
| 22 | 8 | 604 | CLA | CHD-C4C-C3C | -5.12 | 117.32 | 124.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 814 | CLA | C2C-C1C-NC | 5.11 | 114.76 | 109.97 |
| 22 | 3 | 614 | CLA | O2D-CGD-CBD | 5.11 | 120.35 | 111.27 |
| 22 | A | 825 | CLA | CHD-C4C-C3C | -5.11 | 117.33 | 124.84 |
| 22 | 5 | 603 | CLA | C3D-C2D-C1D | -5.11 | 98.86 | 105.83 |
| 22 | A | 836 | CLA | CHD-C4C-C3C | -5.11 | 117.33 | 124.84 |
| 22 | 5 | 602 | CLA | C4A-NA-C1A | -5.11 | 104.41 | 106.71 |
| 22 | 2 | 609 | CLA | CHD-C4C-C3C | -5.11 | 117.34 | 124.84 |
| 25 | A | 850 | BCR | C16-C17-C18 | -5.10 | 120.03 | 127.31 |
| 22 | Z | 612 | CLA | O2D-CGD-CBD | 5.10 | 120.33 | 111.27 |
| 22 | B | 823 | CLA | CHD-C4C-C3C | -5.10 | 117.34 | 124.84 |
| 29 | Z | 601 | CHL | CHD-C4C-C3C | -5.10 | 117.35 | 124.84 |
| 22 | 6 | 601 | CLA | C4A-NA-C1A | -5.10 | 104.41 | 106.71 |
| 22 | L | 204 | CLA | CHD-C4C-C3C | -5.10 | 117.35 | 124.84 |
| 22 | 5 | 617 | CLA | C2C-C1C-NC | 5.09 | 114.75 | 109.97 |
| 29 | Z | 607 | CHL | CHD-C4C-C3C | -5.09 | 117.36 | 124.84 |
| 22 | 2 | 610 | CLA | C2C-C1C-NC | 5.09 | 114.74 | 109.97 |
| 22 | 6 | 614 | CLA | C2C-C1C-NC | 5.09 | 114.74 | 109.97 |
| 29 | Z | 607 | CHL | C3D-C2D-C1D | -5.09 | 98.89 | 105.83 |
| 22 | 1 | 610 | CLA | O2D-CGD-CBD | 5.09 | 120.31 | 111.27 |
| 25 | 6 | 623 | BCR | C7-C8-C9 | -5.09 | 118.55 | 126.23 |
| 22 | A | 818 | CLA | C2C-C1C-NC | 5.09 | 114.74 | 109.97 |
| 22 | 2 | 603 | CLA | O2D-CGD-CBD | 5.08 | 120.30 | 111.27 |
| 22 | B | 830 | CLA | C2C-C1C-NC | 5.08 | 114.73 | 109.97 |
| 22 | 9 | 603 | CLA | O2D-CGD-CBD | 5.08 | 120.30 | 111.27 |
| 22 | 8 | 603 | CLA | O2D-CGD-CBD | 5.08 | 120.30 | 111.27 |
| 22 | 9 | 610 | CLA | C2C-C1C-NC | 5.08 | 114.73 | 109.97 |
| 29 | Z | 601 | CHL | C1C-C2C-C3C | -5.08 | 103.08 | 107.11 |
| 29 | 8 | 607 | CHL | C3D-C2D-C1D | -5.07 | 98.91 | 105.83 |
| 29 | 4 | 618 | CHL | CHD-C1D-ND | -5.07 | 119.79 | 124.45 |
| 22 | 3 | 606 | CLA | C4A-NA-C1A | -5.07 | 104.42 | 106.71 |
| 22 | 3 | 612 | CLA | O2D-CGD-CBD | 5.07 | 120.28 | 111.27 |
| 22 | 6 | 610 | CLA | O2D-CGD-CBD | 5.07 | 120.28 | 111.27 |
| 22 | 2 | 607 | CLA | O2D-CGD-CBD | 5.07 | 120.28 | 111.27 |
| 22 | 8 | 608 | CLA | C3D-C2D-C1D | -5.07 | 98.91 | 105.83 |
| 22 | A | 833 | CLA | O2D-CGD-CBD | 5.07 | 120.27 | 111.27 |
| 22 | 5 | 604 | CLA | CHD-C4C-C3C | -5.07 | 117.39 | 124.84 |
| 22 | A | 833 | CLA | C4A-NA-C1A | -5.07 | 104.43 | 106.71 |
| 22 | A | 829 | CLA | C3D-C2D-C1D | -5.07 | 98.92 | 105.83 |
| 22 | 1 | 612 | CLA | C4A-NA-C1A | -5.06 | 104.43 | 106.71 |
| 22 | B | 819 | CLA | C2C-C1C-NC | 5.06 | 114.72 | 109.97 |
| 22 | A | 823 | CLA | O2D-CGD-CBD | 5.06 | 120.26 | 111.27 |
| 22 | 8 | 610 | CLA | O2D-CGD-CBD | 5.06 | 120.26 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 616 | CLA | CHD-C4C-C3C | -5.06 | 117.41 | 124.84 |
| 22 | 6 | 617 | CLA | O2D-CGD-CBD | 5.06 | 120.25 | 111.27 |
| 22 | 8 | 611 | CLA | CHD-C4C-C3C | -5.06 | 117.41 | 124.84 |
| 22 | 7 | 610 | CLA | O2D-CGD-CBD | 5.05 | 120.25 | 111.27 |
| 22 | A | 806 | CLA | CHD-C4C-C3C | -5.05 | 117.41 | 124.84 |
| 22 | A | 830 | CLA | C2C-C1C-NC | 5.05 | 114.70 | 109.97 |
| 22 | A | 832 | CLA | C4A-NA-C1A | -5.05 | 104.44 | 106.71 |
| 22 | A | 841 | CLA | C4A-NA-C1A | -5.05 | 104.44 | 106.71 |
| 22 | B | 823 | CLA | C2C-C1C-NC | 5.05 | 114.70 | 109.97 |
| 25 | 4 | 621 | BCR | C15-C14-C13 | -5.04 | 120.11 | 127.31 |
| 22 | A | 843 | CLA | CHD-C1D-ND | -5.04 | 119.82 | 124.45 |
| 22 | 6 | 609 | CLA | C4A-NA-C1A | -5.04 | 104.44 | 106.71 |
| 29 | 6 | 606 | CHL | C2C-C3C-C4C | -5.04 | 102.90 | 106.49 |
| 22 | A | 840 | CLA | C3D-C2D-C1D | -5.03 | 98.96 | 105.83 |
| 22 | G | 204 | CLA | O2D-CGD-CBD | 5.03 | 120.21 | 111.27 |
| 22 | 3 | 613 | CLA | CMD-C2D-C1D | 5.03 | 133.57 | 124.71 |
| 22 | 6 | 603 | CLA | O2D-CGD-CBD | 5.03 | 120.20 | 111.27 |
| 22 | A | 816 | CLA | C2C-C1C-NC | 5.02 | 114.68 | 109.97 |
| 22 | B | 805 | CLA | C3D-C2D-C1D | -5.02 | 98.97 | 105.83 |
| 22 | F | 303 | CLA | C3D-C2D-C1D | -5.02 | 98.98 | 105.83 |
| 29 | 9 | 607 | CHL | CHD-C1D-ND | -5.02 | 119.84 | 124.45 |
| 22 | A | 819 | CLA | O2D-CGD-CBD | 5.01 | 120.17 | 111.27 |
| 22 | B | 805 | CLA | C2C-C1C-NC | 5.01 | 114.67 | 109.97 |
| 22 | B | 824 | CLA | C2C-C1C-NC | 5.00 | 114.66 | 109.97 |
| 22 | A | 812 | CLA | O2D-CGD-CBD | 5.00 | 120.16 | 111.27 |
| 22 | 3 | 606 | CLA | O2D-CGD-CBD | 5.00 | 120.16 | 111.27 |
| 22 | B | 816 | CLA | O2D-CGD-CBD | 5.00 | 120.16 | 111.27 |
| 22 | J | 3002 | CLA | O2D-CGD-CBD | 5.00 | 120.16 | 111.27 |
| 22 | 1 | 614 | CLA | C4A-NA-C1A | -5.00 | 104.46 | 106.71 |
| 22 | B | 823 | CLA | C4A-NA-C1A | -5.00 | 104.46 | 106.71 |
| 22 | 1 | 603 | CLA | C4A-NA-C1A | -5.00 | 104.46 | 106.71 |
| 22 | 4 | 611 | CLA | CHD-C4C-C3C | -5.00 | 117.50 | 124.84 |
| 22 | J | 3002 | CLA | C4A-NA-C1A | -5.00 | 104.46 | 106.71 |
| 22 | B | 814 | CLA | C2C-C1C-NC | 4.99 | 114.65 | 109.97 |
| 22 | B | 821 | CLA | O2D-CGD-CBD | 4.99 | 120.13 | 111.27 |
| 22 | A | 815 | CLA | C2C-C1C-NC | 4.99 | 114.64 | 109.97 |
| 22 | Z | 602 | CLA | C4A-NA-C1A | -4.99 | 104.46 | 106.71 |
| 25 | J | 3003 | BCR | C24-C23-C22 | -4.99 | 118.70 | 126.23 |
| 22 | F | 304 | CLA | O2D-CGD-CBD | 4.98 | 120.12 | 111.27 |
| 22 | 5 | 610 | CLA | O2D-CGD-CBD | 4.98 | 120.11 | 111.27 |
| 22 | 6 | 610 | CLA | C2C-C1C-NC | 4.97 | 114.63 | 109.97 |
| 29 | 6 | 618 | CHL | C2C-C3C-C4C | -4.97 | 102.94 | 106.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 2 | 606 | CLA | CAA-C2A-C3A | -4.97 | 104.50 | 116.10 |
| 29 | 5 | 618 | CHL | CHD-C1D-ND | -4.97 | 119.89 | 124.45 |
| 22 | G | 204 | CLA | C4A-NA-C1A | -4.97 | 104.47 | 106.71 |
| 22 | B | 803 | CLA | CAC-C3C-C4C | 4.97 | 131.26 | 124.81 |
| 22 | A | 845 | CLA | O2D-CGD-CBD | 4.97 | 120.10 | 111.27 |
| 22 | 1 | 604 | CLA | CHD-C4C-C3C | -4.97 | 117.54 | 124.84 |
| 22 | Z | 616 | CLA | O2D-CGD-CBD | 4.96 | 120.09 | 111.27 |
| 22 | 9 | 604 | CLA | CHD-C4C-C3C | -4.96 | 117.55 | 124.84 |
| 22 | 9 | 609 | CLA | O2D-CGD-CBD | 4.96 | 120.08 | 111.27 |
| 22 | F | 301 | CLA | C2C-C1C-NC | 4.96 | 114.62 | 109.97 |
| 22 | L | 203 | CLA | O2D-CGD-CBD | 4.96 | 120.08 | 111.27 |
| 22 | B | 831 | CLA | C3D-C2D-C1D | -4.96 | 99.07 | 105.83 |
| 22 | B | 802 | CLA | CHD-C1D-ND | -4.96 | 119.90 | 124.45 |
| 22 | A | 835 | CLA | C2C-C1C-NC | 4.96 | 114.61 | 109.97 |
| 22 | A | 810 | CLA | CHD-C1D-ND | -4.95 | 119.90 | 124.45 |
| 22 | A | 839 | CLA | C4A-NA-C1A | -4.95 | 104.48 | 106.71 |
| 22 | Z | 614 | CLA | C4A-NA-C1A | -4.95 | 104.48 | 106.71 |
| 29 | 6 | 618 | CHL | O2D-CGD-CBD | 4.95 | 120.07 | 111.27 |
| 21 | A | 801 | CL0 | O2D-CGD-CBD | 4.95 | 120.07 | 111.27 |
| 29 | 5 | 607 | CHL | CHD-C4C-C3C | -4.95 | 117.57 | 124.84 |
| 22 | 5 | 617 | CLA | O2D-CGD-CBD | 4.95 | 120.06 | 111.27 |
| 25 | A | 852 | BCR | C16-C17-C18 | -4.94 | 120.26 | 127.31 |
| 25 | B | 801 | BCR | C20-C21-C22 | -4.94 | 120.26 | 127.31 |
| 22 | B | 833 | CLA | C2C-C1C-NC | 4.94 | 114.60 | 109.97 |
| 22 | 5 | 609 | CLA | O2D-CGD-CBD | 4.94 | 120.04 | 111.27 |
| 21 | A | 801 | CL0 | C4A-NA-C1A | -4.94 | 104.49 | 106.71 |
| 22 | B | 841 | CLA | C2C-C1C-NC | 4.93 | 114.59 | 109.97 |
| 25 | B | 848 | BCR | C16-C17-C18 | -4.93 | 120.27 | 127.31 |
| 22 | B | 839 | CLA | O2D-CGD-CBD | 4.93 | 120.03 | 111.27 |
| 22 | 3 | 602 | CLA | C2C-C1C-NC | 4.93 | 114.59 | 109.97 |
| 22 | A | 821 | CLA | CHD-C1D-ND | -4.93 | 119.92 | 124.45 |
| 22 | B | 802 | CLA | C3C-C4C-NC | 4.92 | 116.09 | 110.57 |
| 22 | A | 841 | CLA | C3D-C2D-C1D | -4.92 | 99.12 | 105.83 |
| 22 | 9 | 602 | CLA | C4A-NA-C1A | -4.92 | 104.49 | 106.71 |
| 29 | 5 | 607 | CHL | CHD-C1D-ND | -4.92 | 119.93 | 124.45 |
| 25 | B | 845 | BCR | C24-C23-C22 | -4.92 | 118.81 | 126.23 |
| 22 | 7 | 620 | CLA | O2D-CGD-CBD | 4.92 | 120.00 | 111.27 |
| 22 | 9 | 609 | CLA | C4A-NA-C1A | -4.91 | 104.50 | 106.71 |
| 22 | A | 807 | CLA | C4A-NA-C1A | -4.91 | 104.50 | 106.71 |
| 29 | 4 | 618 | CHL | CHD-C4C-C3C | -4.91 | 117.63 | 124.84 |
| 22 | B | 832 | CLA | C4A-NA-C1A | -4.90 | 104.50 | 106.71 |
| 22 | G | 203 | CLA | C3D-C2D-C1D | -4.90 | 99.14 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 827 | CLA | C2C-C1C-NC | 4.90 | 114.56 | 109.97 |
| 22 | A | 824 | CLA | C4A-NA-C1A | -4.90 | 104.50 | 106.71 |
| 22 | B | 816 | CLA | C4A-NA-C1A | -4.90 | 104.50 | 106.71 |
| 22 | 1 | 611 | CLA | C4A-NA-C1A | -4.90 | 104.50 | 106.71 |
| 22 | 3 | 607 | CLA | C4A-NA-C1A | -4.90 | 104.50 | 106.71 |
| 22 | B | 828 | CLA | CMD-C2D-C1D | 4.89 | 133.34 | 124.71 |
| 22 | 3 | 607 | CLA | O2D-CGD-CBD | 4.89 | 119.96 | 111.27 |
| 22 | A | 818 | CLA | C3D-C2D-C1D | -4.89 | 99.16 | 105.83 |
| 22 | B | 814 | CLA | O2D-CGD-CBD | 4.89 | 119.95 | 111.27 |
| 22 | B | 805 | CLA | C3C-C4C-NC | 4.89 | 116.05 | 110.57 |
| 22 | 7 | 609 | CLA | C3D-C2D-C1D | -4.88 | 99.17 | 105.83 |
| 29 | 9 | 607 | CHL | C1C-C2C-C3C | -4.88 | 103.24 | 107.11 |
| 22 | 5 | 610 | CLA | C4A-NA-C1A | -4.88 | 104.51 | 106.71 |
| 22 | L | 203 | CLA | C3D-C2D-C1D | -4.88 | 99.18 | 105.83 |
| 29 | Z | 601 | CHL | O2D-CGD-CBD | 4.87 | 119.93 | 111.27 |
| 22 | Z | 613 | CLA | C2C-C1C-NC | 4.87 | 114.54 | 109.97 |
| 22 | 4 | 614 | CLA | C2C-C1C-NC | 4.87 | 114.54 | 109.97 |
| 22 | 7 | 602 | CLA | C3D-C2D-C1D | -4.87 | 99.19 | 105.83 |
| 22 | A | 840 | CLA | C4A-NA-C1A | -4.86 | 104.52 | 106.71 |
| 22 | Z | 612 | CLA | C4A-NA-C1A | -4.86 | 104.52 | 106.71 |
| 22 | 6 | 603 | CLA | C3D-C2D-C1D | -4.86 | 99.20 | 105.83 |
| 22 | A | 806 | CLA | C2C-C1C-NC | 4.86 | 114.53 | 109.97 |
| 22 | A | 822 | CLA | C2C-C1C-NC | 4.86 | 114.53 | 109.97 |
| 22 | 9 | 602 | CLA | C2C-C1C-NC | 4.86 | 114.53 | 109.97 |
| 25 | 3 | 718 | BCR | C16-C17-C18 | -4.86 | 120.38 | 127.31 |
| 22 | B | 827 | CLA | C4A-NA-C1A | -4.86 | 104.52 | 106.71 |
| 22 | Z | 609 | CLA | CHD-C4C-C3C | -4.86 | 117.70 | 124.84 |
| 22 | 4 | 614 | CLA | C4A-NA-C1A | -4.86 | 104.52 | 106.71 |
| 22 | L | 204 | CLA | O2D-CGD-CBD | 4.86 | 119.90 | 111.27 |
| 22 | A | 832 | CLA | CHD-C1D-ND | -4.85 | 119.99 | 124.45 |
| 22 | 2 | 610 | CLA | C4A-NA-C1A | -4.85 | 104.53 | 106.71 |
| 22 | B | 804 | CLA | C2C-C1C-NC | 4.85 | 114.51 | 109.97 |
| 25 | 5 | 622 | BCR | C15-C14-C13 | -4.84 | 120.40 | 127.31 |
| 22 | B | 814 | CLA | C4A-NA-C1A | -4.84 | 104.53 | 106.71 |
| 29 | 7 | 607 | CHL | CHD-C4C-C3C | -4.84 | 117.72 | 124.84 |
| 22 | 8 | 602 | CLA | C3D-C2D-C1D | -4.84 | 99.23 | 105.83 |
| 22 | B | 841 | CLA | C3D-C4D-ND | 4.84 | 118.06 | 110.24 |
| 29 | Z | 601 | CHL | C3D-C2D-C1D | -4.84 | 99.23 | 105.83 |
| 22 | B | 806 | CLA | C3D-C2D-C1D | -4.84 | 99.23 | 105.83 |
| 21 | A | 801 | CL0 | CAA-C2A-C3A | -4.83 | 99.54 | 112.78 |
| 22 | 8 | 616 | CLA | O2D-CGD-CBD | 4.83 | 119.86 | 111.27 |
| 22 | A | 831 | CLA | C4A-NA-C1A | -4.83 | 104.53 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 21 | A | 801 | CL0 | CHD-C1D-ND | -4.83 | 120.01 | 124.45 |
| 22 | 8 | 608 | CLA | O2D-CGD-CBD | 4.83 | 119.85 | 111.27 |
| 22 | Z | 604 | CLA | O2D-CGD-CBD | 4.82 | 119.83 | 111.27 |
| 22 | B | 808 | CLA | CHD-C1D-ND | -4.82 | 120.03 | 124.45 |
| 22 | 4 | 603 | CLA | O2D-CGD-CBD | 4.81 | 119.82 | 111.27 |
| 22 | A | 802 | CLA | C2C-C1C-NC | 4.81 | 114.48 | 109.97 |
| 22 | 5 | 610 | CLA | C2C-C1C-NC | 4.81 | 114.48 | 109.97 |
| 22 | A | 809 | CLA | C2C-C1C-NC | 4.81 | 114.48 | 109.97 |
| 29 | 4 | 618 | CHL | C2C-C3C-C4C | -4.80 | 103.06 | 106.49 |
| 22 | 2 | 602 | CLA | O2D-CGD-CBD | 4.80 | 119.81 | 111.27 |
| 22 | 2 | 614 | CLA | O2D-CGD-CBD | 4.80 | 119.80 | 111.27 |
| 22 | 6 | 602 | CLA | C2C-C1C-NC | 4.80 | 114.47 | 109.97 |
| 22 | A | 854 | CLA | CMD-C2D-C1D | 4.80 | 133.16 | 124.71 |
| 22 | B | 804 | CLA | C3D-C2D-C1D | -4.79 | 99.29 | 105.83 |
| 22 | 9 | 612 | CLA | C4A-NA-C1A | -4.79 | 104.55 | 106.71 |
| 22 | 4 | 610 | CLA | C2C-C1C-NC | 4.79 | 114.46 | 109.97 |
| 22 | 7 | 608 | CLA | C3D-C2D-C1D | -4.79 | 99.30 | 105.83 |
| 22 | 2 | 606 | CLA | O2D-CGD-CBD | 4.79 | 119.77 | 111.27 |
| 29 | Z | 607 | CHL | O2D-CGD-CBD | 4.78 | 119.77 | 111.27 |
| 22 | 4 | 602 | CLA | C4A-NA-C1A | -4.78 | 104.56 | 106.71 |
| 29 | 4 | 607 | CHL | CHD-C1D-ND | -4.78 | 120.06 | 124.45 |
| 22 | A | 830 | CLA | CMD-C2D-C1D | 4.78 | 133.13 | 124.71 |
| 22 | A | 803 | CLA | C3D-C2D-C1D | -4.78 | 99.31 | 105.83 |
| 22 | 8 | 608 | CLA | C2C-C1C-NC | 4.77 | 114.44 | 109.97 |
| 22 | A | 842 | CLA | O2D-CGD-CBD | 4.77 | 119.75 | 111.27 |
| 22 | A | 823 | CLA | C3D-C2D-C1D | -4.77 | 99.32 | 105.83 |
| 22 | A | 805 | CLA | O2D-CGD-CBD | 4.77 | 119.74 | 111.27 |
| 22 | 7 | 604 | CLA | C3D-C2D-C1D | -4.77 | 99.33 | 105.83 |
| 22 | 9 | 610 | CLA | O2D-CGD-CBD | 4.77 | 119.74 | 111.27 |
| 22 | B | 803 | CLA | C3D-C2D-C1D | -4.77 | 99.33 | 105.83 |
| 22 | A | 819 | CLA | C3D-C2D-C1D | -4.76 | 99.33 | 105.83 |
| 22 | B | 838 | CLA | O2D-CGD-CBD | 4.76 | 119.73 | 111.27 |
| 22 | Z | 602 | CLA | C2C-C1C-NC | 4.76 | 114.43 | 109.97 |
| 22 | 1 | 606 | CLA | O2D-CGD-CBD | 4.76 | 119.73 | 111.27 |
| 22 | A | 802 | CLA | C3D-C4D-ND | 4.76 | 117.93 | 110.24 |
| 29 | 9 | 606 | CHL | O2D-CGD-CBD | 4.76 | 119.72 | 111.27 |
| 22 | 2 | 609 | CLA | C4A-NA-C1A | -4.76 | 104.57 | 106.71 |
| 22 | A | 805 | CLA | C2C-C1C-NC | 4.75 | 114.43 | 109.97 |
| 22 | B | 813 | CLA | C2C-C1C-NC | 4.75 | 114.42 | 109.97 |
| 25 | A | 848 | BCR | C16-C17-C18 | -4.75 | 120.53 | 127.31 |
| 25 | F | 305 | BCR | C11-C10-C9 | -4.75 | 120.53 | 127.31 |
| 22 | A | 845 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 814 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |
| 22 | 2 | 613 | CLA | O2D-CGD-CBD | 4.75 | 119.71 | 111.27 |
| 22 | A | 811 | CLA | C2C-C1C-NC | 4.75 | 114.42 | 109.97 |
| 22 | B | 807 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |
| 22 | A | 815 | CLA | C3D-C4D-ND | 4.75 | 117.92 | 110.24 |
| 22 | 5 | 606 | CLA | C3D-C2D-C1D | -4.75 | 99.35 | 105.83 |
| 30 | 4 | 619 | LUT | C35-C34-C33 | -4.75 | 120.54 | 127.31 |
| 22 | A | 805 | CLA | C3D-C4D-ND | 4.75 | 117.92 | 110.24 |
| 22 | A | 812 | CLA | C4A-NA-C1A | -4.74 | 104.57 | 106.71 |
| 22 | 9 | 601 | CLA | O2D-CGD-CBD | 4.74 | 119.69 | 111.27 |
| 29 | 4 | 606 | CHL | C2C-C3C-C4C | -4.74 | 103.11 | 106.49 |
| 22 | 5 | 616 | CLA | C3D-C2D-C1D | -4.74 | 99.37 | 105.83 |
| 22 | B | 815 | CLA | C3D-C2D-C1D | -4.74 | 99.37 | 105.83 |
| 22 | 9 | 604 | CLA | O2D-CGD-CBD | 4.73 | 119.68 | 111.27 |
| 22 | 7 | 603 | CLA | C3D-C2D-C1D | -4.73 | 99.37 | 105.83 |
| 22 | 6 | 602 | CLA | C3D-C2D-C1D | -4.73 | 99.37 | 105.83 |
| 22 | 8 | 610 | CLA | C2C-C1C-NC | 4.73 | 114.40 | 109.97 |
| 22 | A | 809 | CLA | C3D-C2D-C1D | -4.73 | 99.38 | 105.83 |
| 22 | B | 837 | CLA | C2C-C1C-NC | 4.73 | 114.40 | 109.97 |
| 25 | 3 | 717 | BCR | C11-C10-C9 | -4.73 | 120.56 | 127.31 |
| 22 | 9 | 610 | CLA | C4A-NA-C1A | -4.73 | 104.58 | 106.71 |
| 22 | B | 812 | CLA | C3D-C2D-C1D | -4.72 | 99.38 | 105.83 |
| 22 | 4 | 611 | CLA | O2D-CGD-CBD | 4.72 | 119.66 | 111.27 |
| 22 | B | 840 | CLA | C1C-C2C-C3C | -4.72 | 101.99 | 106.96 |
| 22 | 9 | 609 | CLA | C1D-CHD-C4C | -4.72 | 115.87 | 126.06 |
| 22 | 4 | 601 | CLA | CHD-C4C-C3C | -4.72 | 117.90 | 124.84 |
| 22 | 6 | 622 | CLA | C3D-C2D-C1D | -4.72 | 99.39 | 105.83 |
| 22 | 1 | 608 | CLA | C4A-NA-C1A | -4.72 | 104.58 | 106.71 |
| 22 | 1 | 614 | CLA | O2D-CGD-CBD | 4.72 | 119.65 | 111.27 |
| 29 | 4 | 606 | CHL | O2D-CGD-CBD | 4.72 | 119.65 | 111.27 |
| 22 | 7 | 608 | CLA | C2C-C1C-NC | 4.72 | 114.39 | 109.97 |
| 22 | B | 836 | CLA | C3D-C2D-C1D | -4.72 | 99.39 | 105.83 |
| 22 | A | 820 | CLA | C3D-C2D-C1D | -4.72 | 99.40 | 105.83 |
| 22 | K | 4003 | CLA | O2D-CGD-CBD | 4.71 | 119.65 | 111.27 |
| 22 | 1 | 608 | CLA | C3D-C2D-C1D | -4.71 | 99.40 | 105.83 |
| 30 | 2 | 616 | LUT | C35-C34-C33 | -4.71 | 120.58 | 127.31 |
| 22 | Z | 602 | CLA | C3D-C2D-C1D | -4.71 | 99.40 | 105.83 |
| 22 | 3 | 613 | CLA | O2D-CGD-CBD | 4.71 | 119.64 | 111.27 |
| 22 | B | 820 | CLA | C3D-C4D-ND | 4.71 | 117.86 | 110.24 |
| 22 | 6 | 611 | CLA | O2D-CGD-CBD | 4.71 | 119.63 | 111.27 |
| 22 | 8 | 603 | CLA | C3D-C2D-C1D | -4.71 | 99.41 | 105.83 |
| 29 | 9 | 606 | CHL | CHD-C1D-ND | -4.71 | 120.13 | 124.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | 1 | 607 | CHL | C1C-C2C-C3C | -4.70 | 103.38 | 107.11 |
| 22 | Z | 608 | CLA | C3D-C2D-C1D | -4.70 | 99.41 | 105.83 |
| 22 | B | 821 | CLA | C3D-C2D-C1D | -4.70 | 99.41 | 105.83 |
| 30 | 6 | 621 | LUT | C35-C34-C33 | -4.70 | 120.60 | 127.31 |
| 22 | 6 | 612 | CLA | O2D-CGD-CBD | 4.70 | 119.62 | 111.27 |
| 29 | 5 | 618 | CHL | CHD-C4C-C3C | -4.70 | 117.93 | 124.84 |
| 22 | 2 | 606 | CLA | C4A-NA-C1A | -4.70 | 104.59 | 106.71 |
| 22 | A | 834 | CLA | C4A-NA-C1A | -4.70 | 104.59 | 106.71 |
| 22 | A | 812 | CLA | C3D-C2D-C1D | -4.70 | 99.42 | 105.83 |
| 30 | Z | 619 | LUT | C31-C30-C29 | -4.69 | 120.61 | 127.31 |
| 22 | B | 813 | CLA | C3D-C2D-C1D | -4.69 | 99.43 | 105.83 |
| 22 | 5 | 602 | CLA | O2D-CGD-CBD | 4.69 | 119.61 | 111.27 |
| 22 | 9 | 613 | CLA | O2D-CGD-CBD | 4.69 | 119.60 | 111.27 |
| 22 | 1 | 602 | CLA | C2C-C1C-NC | 4.69 | 114.37 | 109.97 |
| 22 | Z | 609 | CLA | C4A-NA-C1A | -4.69 | 104.60 | 106.71 |
| 22 | 7 | 606 | CLA | C3D-C2D-C1D | -4.69 | 99.44 | 105.83 |
| 22 | 8 | 614 | CLA | O2D-CGD-CBD | 4.68 | 119.58 | 111.27 |
| 22 | 7 | 601 | CLA | C3D-C2D-C1D | -4.68 | 99.45 | 105.83 |
| 22 | 2 | 614 | CLA | C3D-C2D-C1D | -4.68 | 99.45 | 105.83 |
| 22 | A | 842 | CLA | C3D-C2D-C1D | -4.68 | 99.45 | 105.83 |
| 22 | Z | 606 | CLA | C3D-C2D-C1D | -4.67 | 99.45 | 105.83 |
| 22 | L | 204 | CLA | C3D-C2D-C1D | -4.67 | 99.45 | 105.83 |
| 22 | B | 827 | CLA | C3D-C2D-C1D | -4.67 | 99.46 | 105.83 |
| 22 | B | 802 | CLA | C2C-C1C-NC | 4.67 | 114.35 | 109.97 |
| 22 | 9 | 611 | CLA | O2D-CGD-CBD | 4.67 | 119.56 | 111.27 |
| 22 | A | 806 | CLA | C4A-NA-C1A | -4.66 | 104.61 | 106.71 |
| 22 | 5 | 609 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 22 | A | 828 | CLA | C3C-C4C-NC | 4.66 | 115.80 | 110.57 |
| 22 | 2 | 601 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 29 | 6 | 607 | CHL | C1C-C2C-C3C | -4.66 | 103.42 | 107.11 |
| 22 | 7 | 611 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 22 | 1 | 603 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 22 | 9 | 610 | CLA | C3D-C2D-C1D | -4.66 | 99.47 | 105.83 |
| 22 | B | 826 | CLA | C2C-C1C-NC | 4.66 | 114.34 | 109.97 |
| 22 | B | 828 | CLA | O2D-CGD-CBD | 4.66 | 119.54 | 111.27 |
| 29 | 4 | 607 | CHL | O2D-CGD-CBD | 4.66 | 119.54 | 111.27 |
| 29 | 9 | 607 | CHL | CHD-C4C-C3C | -4.66 | 118.00 | 124.84 |
| 22 | 9 | 609 | CLA | C3D-C2D-C1D | -4.66 | 99.48 | 105.83 |
| 22 | 2 | 602 | CLA | C4A-NA-C1A | -4.65 | 104.61 | 106.71 |
| 22 | A | 804 | CLA | C2C-C1C-NC | 4.65 | 114.33 | 109.97 |
| 22 | A | 819 | CLA | C2C-C1C-NC | 4.65 | 114.33 | 109.97 |
| 22 | 7 | 614 | CLA | C3D-C2D-C1D | -4.65 | 99.48 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 609 | CLA | C3D-C2D-C1D | -4.65 | 99.49 | 105.83 |
| 22 | A | 804 | CLA | C3D-C4D-ND | 4.65 | 117.75 | 110.24 |
| 29 | 4 | 608 | CHL | CHD-C1D-ND | -4.64 | 120.19 | 124.45 |
| 22 | A | 828 | CLA | C4A-NA-C1A | -4.64 | 104.62 | 106.71 |
| 22 | 1 | 602 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 22 | 1 | 612 | CLA | O2D-CGD-CBD | 4.64 | 119.51 | 111.27 |
| 22 | Z | 610 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 22 | B | 825 | CLA | C4A-NA-C1A | -4.64 | 104.62 | 106.71 |
| 22 | B | 852 | CLA | C4A-NA-C1A | -4.64 | 104.62 | 106.71 |
| 22 | B | 826 | CLA | C3D-C2D-C1D | -4.64 | 99.50 | 105.83 |
| 22 | 2 | 613 | CLA | C4A-NA-C1A | -4.64 | 104.62 | 106.71 |
| 22 | 8 | 601 | CLA | C3D-C2D-C1D | -4.63 | 99.51 | 105.83 |
| 22 | 8 | 616 | CLA | CHD-C1D-ND | -4.63 | 120.19 | 124.45 |
| 25 | B | 843 | BCR | C15-C14-C13 | -4.63 | 120.70 | 127.31 |
| 22 | 2 | 607 | CLA | C3D-C2D-C1D | -4.63 | 99.51 | 105.83 |
| 22 | B | 852 | CLA | O2D-CGD-CBD | 4.63 | 119.50 | 111.27 |
| 29 | 6 | 606 | CHL | CHD-C1D-ND | -4.63 | 120.20 | 124.45 |
| 29 | 7 | 607 | CHL | O2D-CGD-CBD | 4.63 | 119.50 | 111.27 |
| 22 | 7 | 611 | CLA | C4A-NA-C1A | -4.63 | 104.62 | 106.71 |
| 22 | 2 | 610 | CLA | C3D-C2D-C1D | -4.63 | 99.52 | 105.83 |
| 22 | 7 | 612 | CLA | O2D-CGD-CBD | 4.63 | 119.49 | 111.27 |
| 22 | Z | 614 | CLA | C3D-C2D-C1D | -4.63 | 99.52 | 105.83 |
| 22 | A | 845 | CLA | C4A-NA-C1A | -4.62 | 104.63 | 106.71 |
| 22 | A | 854 | CLA | C3D-C2D-C1D | -4.62 | 99.52 | 105.83 |
| 22 | 2 | 612 | CLA | O2D-CGD-CBD | 4.62 | 119.48 | 111.27 |
| 22 | B | 832 | CLA | C3D-C2D-C1D | -4.62 | 99.52 | 105.83 |
| 22 | A | 811 | CLA | C4A-NA-C1A | -4.62 | 104.63 | 106.71 |
| 22 | 3 | 620 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 22 | A | 822 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 22 | 7 | 612 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 22 | A | 834 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 22 | B | 817 | CLA | C4A-NA-C1A | -4.62 | 104.63 | 106.71 |
| 22 | A | 831 | CLA | C3D-C2D-C1D | -4.62 | 99.53 | 105.83 |
| 22 | 5 | 610 | CLA | C3D-C2D-C1D | -4.61 | 99.53 | 105.83 |
| 22 | K | 4003 | CLA | C3D-C2D-C1D | -4.61 | 99.54 | 105.83 |
| 22 | Z | 608 | CLA | C4A-NA-C1A | -4.61 | 104.63 | 106.71 |
| 22 | 3 | 620 | CLA | C4A-NA-C1A | -4.61 | 104.63 | 106.71 |
| 22 | 8 | 602 | CLA | C2C-C1C-NC | 4.61 | 114.29 | 109.97 |
| 22 | F | 301 | CLA | C3D-C2D-C1D | -4.61 | 99.54 | 105.83 |
| 22 | A | 816 | CLA | C3D-C2D-C1D | -4.61 | 99.54 | 105.83 |
| 22 | 8 | 611 | CLA | C3D-C2D-C1D | -4.61 | 99.54 | 105.83 |
| 22 | 2 | 613 | CLA | C3D-C2D-C1D | -4.61 | 99.55 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29 | Z | 601 | CHL | C3C-C4C-NC | 4.61 | 115.74 | 110.57 |
| 25 | 6 | 623 | BCR | C28-C27-C26 | -4.60 | 105.86 | 114.08 |
| 22 | 5 | 611 | CLA | C3D-C2D-C1D | -4.60 | 99.55 | 105.83 |
| 22 | A | 835 | CLA | C3D-C4D-ND | 4.60 | 117.69 | 110.24 |
| 22 | 9 | 602 | CLA | C3D-C2D-C1D | -4.60 | 99.55 | 105.83 |
| 22 | 3 | 603 | CLA | C3D-C2D-C1D | -4.60 | 99.56 | 105.83 |
| 22 | 1 | 616 | CLA | O2D-CGD-CBD | 4.60 | 119.43 | 111.27 |
| 22 | 8 | 606 | CLA | C3D-C2D-C1D | -4.59 | 99.56 | 105.83 |
| 22 | 7 | 602 | CLA | C4A-NA-C1A | -4.59 | 104.64 | 106.71 |
| 22 | 8 | 610 | CLA | C3D-C2D-C1D | -4.59 | 99.56 | 105.83 |
| 22 | 5 | 601 | CLA | C4A-NA-C1A | -4.59 | 104.64 | 106.71 |
| 22 | B | 810 | CLA | C3D-C2D-C1D | -4.59 | 99.57 | 105.83 |
| 22 | 7 | 620 | CLA | C3D-C2D-C1D | -4.59 | 99.57 | 105.83 |
| 22 | 4 | 612 | CLA | C3D-C2D-C1D | -4.59 | 99.57 | 105.83 |
| 22 | Z | 606 | CLA | C4A-NA-C1A | -4.58 | 104.64 | 106.71 |
| 22 | A | 808 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 22 | F | 304 | CLA | C4A-NA-C1A | -4.58 | 104.65 | 106.71 |
| 22 | A | 803 | CLA | CAA-C2A-C3A | -4.58 | 100.23 | 112.78 |
| 22 | A | 826 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 22 | B | 837 | CLA | C3D-C2D-C1D | -4.58 | 99.58 | 105.83 |
| 22 | 1 | 606 | CLA | C2C-C1C-NC | 4.58 | 114.26 | 109.97 |
| 22 | 5 | 612 | CLA | C3D-C2D-C1D | -4.57 | 99.59 | 105.83 |
| 22 | 1 | 609 | CLA | C3D-C2D-C1D | -4.57 | 99.59 | 105.83 |
| 22 | A | 807 | CLA | C3D-C2D-C1D | -4.57 | 99.59 | 105.83 |
| 22 | 5 | 606 | CLA | O2D-CGD-CBD | 4.57 | 119.39 | 111.27 |
| 22 | Z | 611 | CLA | C3D-C2D-C1D | -4.57 | 99.59 | 105.83 |
| 22 | 3 | 604 | CLA | C3D-C2D-C1D | -4.57 | 99.59 | 105.83 |
| 22 | B | 811 | CLA | C3D-C2D-C1D | -4.57 | 99.60 | 105.83 |
| 22 | B | 837 | CLA | C4A-NA-C1A | -4.57 | 104.65 | 106.71 |
| 22 | 6 | 616 | CLA | C3D-C2D-C1D | -4.57 | 99.60 | 105.83 |
| 25 | 5 | 625 | BCR | C16-C17-C18 | -4.56 | 120.80 | 127.31 |
| 22 | 1 | 614 | CLA | C3D-C2D-C1D | -4.56 | 99.60 | 105.83 |
| 22 | 5 | 612 | CLA | O2D-CGD-CBD | 4.56 | 119.38 | 111.27 |
| 22 | A | 808 | CLA | C4A-NA-C1A | -4.56 | 104.66 | 106.71 |
| 22 | 9 | 614 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 22 | A | 825 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 22 | 4 | 616 | CLA | O2D-CGD-CBD | 4.56 | 119.36 | 111.27 |
| 22 | 4 | 614 | CLA | O2D-CGD-CBD | 4.56 | 119.36 | 111.27 |
| 25 | K | 4004 | BCR | C16-C17-C18 | -4.56 | 120.81 | 127.31 |
| 22 | B | 831 | CLA | C4A-NA-C1A | -4.56 | 104.66 | 106.71 |
| 22 | 3 | 602 | CLA | C3D-C2D-C1D | -4.56 | 99.61 | 105.83 |
| 22 | A | 833 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | L | 203 | CLA | C3D-C4D-ND | 4.55 | 117.60 | 110.24 |
| 22 | B | 825 | CLA | CAA-C2A-C3A | -4.55 | 100.31 | 112.78 |
| 22 | 3 | 613 | CLA | C3C-C4C-NC | 4.55 | 115.67 | 110.57 |
| 22 | B | 835 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 22 | 3 | 614 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 22 | B | 840 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 22 | 7 | 613 | CLA | C3D-C2D-C1D | -4.55 | 99.62 | 105.83 |
| 22 | F | 301 | CLA | O2D-CGD-CBD | 4.55 | 119.35 | 111.27 |
| 22 | A | 829 | CLA | C3C-C4C-NC | 4.55 | 115.67 | 110.57 |
| 22 | Z | 613 | CLA | O2D-CGD-CBD | 4.55 | 119.35 | 111.27 |
| 22 | 1 | 606 | CLA | C3D-C2D-C1D | -4.55 | 99.63 | 105.83 |
| 22 | 5 | 604 | CLA | O2D-CGD-CBD | 4.55 | 119.35 | 111.27 |
| 25 | F | 305 | BCR | C15-C14-C13 | -4.55 | 120.82 | 127.31 |
| 22 | 4 | 613 | CLA | C3D-C2D-C1D | -4.55 | 99.63 | 105.83 |
| 22 | B | 822 | CLA | C4A-NA-C1A | -4.54 | 104.66 | 106.71 |
| 22 | 6 | 601 | CLA | C3D-C2D-C1D | -4.54 | 99.63 | 105.83 |
| 30 | 1 | 619 | LUT | C15-C14-C13 | -4.54 | 120.83 | 127.31 |
| 22 | 9 | 604 | CLA | C3D-C2D-C1D | -4.54 | 99.63 | 105.83 |
| 22 | B | 802 | CLA | C1D-CHD-C4C | -4.54 | 116.26 | 126.06 |
| 22 | B | 817 | CLA | C3D-C2D-C1D | -4.54 | 99.63 | 105.83 |
| 22 | 9 | 601 | CLA | C3D-C2D-C1D | -4.54 | 99.64 | 105.83 |
| 22 | 2 | 609 | CLA | C3D-C2D-C1D | -4.54 | 99.64 | 105.83 |
| 22 | 1 | 604 | CLA | O2D-CGD-CBD | 4.54 | 119.33 | 111.27 |
| 22 | F | 304 | CLA | C3D-C2D-C1D | -4.54 | 99.64 | 105.83 |
| 22 | B | 818 | CLA | C1C-C2C-C3C | -4.54 | 102.19 | 106.96 |
| 22 | 5 | 613 | CLA | O2D-CGD-CBD | 4.54 | 119.33 | 111.27 |
| 29 | 8 | 607 | CHL | C3C-C4C-NC | 4.54 | 115.66 | 110.57 |
| 22 | A | 830 | CLA | CHD-C1D-ND | -4.53 | 120.29 | 124.45 |
| 22 | 6 | 602 | CLA | O2D-CGD-CBD | 4.53 | 119.32 | 111.27 |
| 22 | 8 | 604 | CLA | O2D-CGD-CBD | 4.53 | 119.32 | 111.27 |
| 29 | 4 | 607 | CHL | C2C-C3C-C4C | -4.53 | 103.26 | 106.49 |
| 22 | 4 | 604 | CLA | O2D-CGD-CBD | 4.53 | 119.31 | 111.27 |
| 22 | 2 | 603 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 22 | 5 | 601 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 22 | 9 | 603 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 22 | 4 | 602 | CLA | O2D-CGD-CBD | 4.52 | 119.30 | 111.27 |
| 22 | 6 | 609 | CLA | C3D-C2D-C1D | -4.52 | 99.66 | 105.83 |
| 22 | 6 | 610 | CLA | C3D-C2D-C1D | -4.52 | 99.67 | 105.83 |
| 22 | 4 | 604 | CLA | C3D-C2D-C1D | -4.52 | 99.67 | 105.83 |
| 25 | K | 4001 | BCR | C11-C10-C9 | -4.52 | 120.86 | 127.31 |
| 22 | 1 | 614 | CLA | C3D-C4D-ND | 4.52 | 117.54 | 110.24 |
| 22 | B | 809 | CLA | C3D-C2D-C1D | -4.52 | 99.67 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | K | 4001 | BCR | C28-C27-C26 | -4.51 | 106.02 | 114.08 |
| 24 | 4 | 622 | LHG | O7-C7-C8 | 4.51 | 121.23 | 111.50 |
| 22 | 7 | 614 | CLA | C4A-NA-C1A | -4.51 | 104.68 | 106.71 |
| 22 | 3 | 609 | CLA | C3D-C2D-C1D | -4.51 | 99.67 | 105.83 |
| 25 | A | 850 | BCR | C3-C4-C5 | -4.51 | 106.02 | 114.08 |
| 22 | 3 | 617 | CLA | C3D-C2D-C1D | -4.51 | 99.68 | 105.83 |
| 25 | B | 843 | BCR | C16-C15-C14 | -4.51 | 114.24 | 123.47 |
| 22 | B | 803 | CLA | C2C-C1C-NC | 4.51 | 114.20 | 109.97 |
| 22 | 9 | 612 | CLA | O2D-CGD-CBD | 4.51 | 119.28 | 111.27 |
| 25 | B | 844 | BCR | C15-C14-C13 | -4.50 | 120.88 | 127.31 |
| 22 | 3 | 610 | CLA | O2D-CGD-CBD | 4.50 | 119.27 | 111.27 |
| 22 | K | 4002 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 22 | 3 | 612 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 22 | 4 | 602 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 22 | B | 838 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 22 | A | 811 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 29 | 5 | 608 | CHL | CHD-C1D-ND | -4.50 | 120.32 | 124.45 |
| 22 | 6 | 609 | CLA | O2D-CGD-CBD | 4.50 | 119.26 | 111.27 |
| 22 | A | 827 | CLA | C3D-C4D-ND | 4.50 | 117.52 | 110.24 |
| 22 | A | 813 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 22 | J | 3002 | CLA | C3D-C2D-C1D | -4.50 | 99.69 | 105.83 |
| 22 | B | 812 | CLA | O2D-CGD-CBD | 4.50 | 119.26 | 111.27 |
| 22 | 2 | 611 | CLA | O2D-CGD-CBD | 4.50 | 119.26 | 111.27 |
| 22 | A | 811 | CLA | O2D-CGD-CBD | 4.50 | 119.26 | 111.27 |
| 22 | B | 818 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 25 | 4 | 621 | BCR | C11-C10-C9 | -4.49 | 120.90 | 127.31 |
| 22 | A | 829 | CLA | C2C-C1C-NC | 4.49 | 114.18 | 109.97 |
| 22 | B | 802 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 22 | Z | 616 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 22 | 6 | 604 | CLA | C4A-NA-C1A | -4.49 | 104.69 | 106.71 |
| 22 | 5 | 602 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 22 | 5 | 602 | CLA | C3D-C4D-ND | 4.49 | 117.50 | 110.24 |
| 22 | 9 | 612 | CLA | C3D-C2D-C1D | -4.49 | 99.70 | 105.83 |
| 22 | 5 | 614 | CLA | C3D-C2D-C1D | -4.49 | 99.71 | 105.83 |
| 22 | Z | 602 | CLA | O2D-CGD-CBD | 4.49 | 119.24 | 111.27 |
| 22 | 4 | 616 | CLA | C3D-C2D-C1D | -4.49 | 99.71 | 105.83 |
| 22 | 5 | 604 | CLA | C3D-C2D-C1D | -4.49 | 99.71 | 105.83 |
| 22 | 4 | 609 | CLA | C3D-C2D-C1D | -4.49 | 99.71 | 105.83 |
| 22 | 3 | 607 | CLA | C3D-C2D-C1D | -4.49 | 99.71 | 105.83 |
| 25 | I | 172 | BCR | C20-C21-C22 | -4.49 | 120.91 | 127.31 |
| 22 | B | 829 | CLA | C3D-C2D-C1D | -4.48 | 99.71 | 105.83 |
| 22 | B | 809 | CLA | C4A-NA-C1A | -4.48 | 104.69 | 106.71 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 6 | 602 | CLA | C4A-NA-C1A | -4.48 | 104.69 | 106.71 |
| 22 | Z | 612 | CLA | C3D-C2D-C1D | -4.48 | 99.71 | 105.83 |
| 22 | A | 832 | CLA | C3C-C4C-NC | 4.48 | 115.60 | 110.57 |
| 22 | 7 | 608 | CLA | O2D-CGD-CBD | 4.48 | 119.23 | 111.27 |
| 22 | Z | 604 | CLA | C3D-C2D-C1D | -4.48 | 99.72 | 105.83 |
| 21 | A | 801 | CL0 | C3D-C2D-C1D | -4.48 | 99.72 | 105.83 |
| 22 | B | 838 | CLA | C3D-C4D-ND | 4.48 | 117.48 | 110.24 |
| 22 | 9 | 601 | CLA | C4A-NA-C1A | -4.48 | 104.69 | 106.71 |
| 30 | 5 | 620 | LUT | C35-C34-C33 | -4.47 | 120.93 | 127.31 |
| 22 | 5 | 602 | CLA | C2C-C1C-NC | 4.47 | 114.16 | 109.97 |
| 22 | G | 204 | CLA | C3D-C2D-C1D | -4.47 | 99.73 | 105.83 |
| 22 | B | 829 | CLA | C3C-C4C-NC | 4.47 | 115.58 | 110.57 |
| 22 | 9 | 604 | CLA | C3D-C4D-ND | 4.47 | 117.47 | 110.24 |
| 22 | 6 | 617 | CLA | C3D-C2D-C1D | -4.47 | 99.73 | 105.83 |
| 22 | B | 810 | CLA | CAA-C2A-C3A | -4.47 | 100.54 | 112.78 |
| 22 | 2 | 602 | CLA | C3D-C2D-C1D | -4.47 | 99.73 | 105.83 |
| 22 | B | 835 | CLA | C4A-NA-C1A | -4.47 | 104.70 | 106.71 |
| 22 | 4 | 610 | CLA | C3D-C2D-C1D | -4.47 | 99.74 | 105.83 |
| 22 | 2 | 606 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 29 | 1 | 601 | CHL | C3C-C4C-NC | 4.46 | 115.58 | 110.57 |
| 22 | 4 | 601 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 22 | 4 | 611 | CLA | C3D-C2D-C1D | -4.46 | 99.74 | 105.83 |
| 25 | A | 849 | BCR | C16-C17-C18 | -4.46 | 120.94 | 127.31 |
| 30 | Z | 619 | LUT | C15-C14-C13 | -4.46 | 120.94 | 127.31 |
| 22 | Z | 609 | CLA | O2D-CGD-CBD | 4.46 | 119.19 | 111.27 |
| 22 | 9 | 611 | CLA | C3D-C2D-C1D | -4.46 | 99.75 | 105.83 |
| 22 | 3 | 606 | CLA | C3D-C2D-C1D | -4.46 | 99.75 | 105.83 |
| 22 | 2 | 610 | CLA | C3D-C4D-ND | 4.46 | 117.45 | 110.24 |
| 22 | 6 | 604 | CLA | O2D-CGD-CBD | 4.46 | 119.19 | 111.27 |
| 29 | 5 | 608 | CHL | O2D-CGD-CBD | 4.46 | 119.19 | 111.27 |
| 22 | B | 839 | CLA | C4A-NA-C1A | -4.46 | 104.70 | 106.71 |
| 22 | 6 | 611 | CLA | C3D-C2D-C1D | -4.45 | 99.75 | 105.83 |
| 22 | 7 | 613 | CLA | O2D-CGD-CBD | 4.45 | 119.18 | 111.27 |
| 22 | 6 | 614 | CLA | O2D-CGD-CBD | 4.45 | 119.18 | 111.27 |
| 22 | Z | 609 | CLA | C3D-C2D-C1D | -4.45 | 99.75 | 105.83 |
| 22 | B | 833 | CLA | C3D-C2D-C1D | -4.45 | 99.76 | 105.83 |
| 27 | B | 850 | DGD | O2G-C1B-C2B | 4.45 | 121.09 | 111.50 |
| 29 | 9 | 606 | CHL | C2C-C3C-C4C | -4.45 | 103.32 | 106.49 |
| 22 | 5 | 609 | CLA | C4A-NA-C1A | -4.44 | 104.71 | 106.71 |
| 22 | A | 841 | CLA | C3C-C4C-NC | 4.44 | 115.56 | 110.57 |
| 22 | 1 | 610 | CLA | C3D-C2D-C1D | -4.44 | 99.77 | 105.83 |
| 22 | A | 837 | CLA | C3D-C2D-C1D | -4.44 | 99.77 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | 6 | 607 | CHL | C3C-C4C-NC | 4.44 | 115.55 | 110.57 |
| 22 | 1 | 613 | CLA | O2D-CGD-CBD | 4.44 | 119.16 | 111.27 |
| 29 | 8 | 607 | CHL | O2D-CGD-CBD | 4.44 | 119.16 | 111.27 |
| 22 | 5 | 614 | CLA | C3D-C4D-ND | 4.44 | 117.42 | 110.24 |
| 22 | B | 834 | CLA | C3D-C2D-C1D | -4.44 | 99.77 | 105.83 |
| 22 | 7 | 610 | CLA | C3D-C2D-C1D | -4.44 | 99.77 | 105.83 |
| 22 | B | 803 | CLA | CHD-C4C-C3C | -4.44 | 118.32 | 124.84 |
| 22 | Z | 610 | CLA | CMC-C2C-C1C | 4.44 | 131.80 | 125.04 |
| 22 | A | 828 | CLA | C1D-CHD-C4C | -4.44 | 116.49 | 126.06 |
| 22 | 2 | 611 | CLA | C3D-C2D-C1D | -4.44 | 99.78 | 105.83 |
| 22 | 7 | 616 | CLA | O2D-CGD-CBD | 4.44 | 119.15 | 111.27 |
| 22 | A | 836 | CLA | C3D-C2D-C1D | -4.43 | 99.78 | 105.83 |
| 22 | A | 843 | CLA | C3D-C2D-C1D | -4.43 | 99.78 | 105.83 |
| 22 | 1 | 611 | CLA | C3D-C2D-C1D | -4.43 | 99.78 | 105.83 |
| 22 | B | 816 | CLA | C3C-C4C-NC | 4.43 | 115.54 | 110.57 |
| 22 | 2 | 614 | CLA | C3D-C4D-ND | 4.43 | 117.41 | 110.24 |
| 22 | 3 | 611 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 22 | A | 802 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 22 | 5 | 621 | CLA | C4A-NA-C1A | -4.43 | 104.72 | 106.71 |
| 22 | 6 | 604 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 22 | 1 | 613 | CLA | C3D-C2D-C1D | -4.43 | 99.79 | 105.83 |
| 22 | A | 810 | CLA | C4A-NA-C1A | -4.42 | 104.72 | 106.71 |
| 22 | B | 822 | CLA | C3D-C4D-ND | 4.42 | 117.39 | 110.24 |
| 25 | 7 | 623 | BCR | C16-C17-C18 | -4.42 | 121.00 | 127.31 |
| 22 | A | 839 | CLA | C3D-C2D-C1D | -4.42 | 99.80 | 105.83 |
| 22 | A | 854 | CLA | C3C-C4C-NC | 4.42 | 115.53 | 110.57 |
| 22 | Z | 603 | CLA | C3D-C2D-C1D | -4.42 | 99.80 | 105.83 |
| 22 | B | 833 | CLA | C4A-NA-C1A | -4.42 | 104.72 | 106.71 |
| 22 | A | 836 | CLA | O2D-CGD-CBD | 4.42 | 119.11 | 111.27 |
| 22 | B | 829 | CLA | C3D-C4D-ND | 4.42 | 117.38 | 110.24 |
| 22 | A | 812 | CLA | C3C-C4C-NC | 4.42 | 115.52 | 110.57 |
| 22 | A | 823 | CLA | C3D-C4D-ND | 4.41 | 117.38 | 110.24 |
| 22 | 8 | 613 | CLA | C3C-C4C-NC | 4.41 | 115.52 | 110.57 |
| 22 | A | 811 | CLA | C1D-CHD-C4C | -4.41 | 116.54 | 126.06 |
| 22 | B | 816 | CLA | C1D-CHD-C4C | -4.41 | 116.55 | 126.06 |
| 29 | 6 | 608 | CHL | O2D-CGD-CBD | 4.41 | 119.10 | 111.27 |
| 22 | 6 | 611 | CLA | C4A-NA-C1A | -4.41 | 104.72 | 106.71 |
| 22 | A | 806 | CLA | CAC-C3C-C4C | 4.41 | 130.53 | 124.81 |
| 22 | 8 | 613 | CLA | C3D-C2D-C1D | -4.41 | 99.82 | 105.83 |
| 25 | G | 205 | BCR | C16-C17-C18 | -4.41 | 121.02 | 127.31 |
| 22 | 5 | 613 | CLA | C3D-C2D-C1D | -4.40 | 99.82 | 105.83 |
| 22 | 6 | 614 | CLA | C3D-C4D-ND | 4.40 | 117.36 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 809 | CLA | C1C-C2C-C3C | -4.40 | 102.33 | 106.96 |
| 22 | 6 | 613 | CLA | C3D-C4D-ND | 4.40 | 117.36 | 110.24 |
| 22 | 7 | 602 | CLA | C3D-C4D-ND | 4.40 | 117.36 | 110.24 |
| 22 | A | 824 | CLA | C3D-C2D-C1D | -4.40 | 99.83 | 105.83 |
| 22 | L | 204 | CLA | C3D-C4D-ND | 4.40 | 117.35 | 110.24 |
| 22 | 2 | 612 | CLA | C3D-C2D-C1D | -4.40 | 99.83 | 105.83 |
| 22 | 4 | 601 | CLA | C4A-NA-C1A | -4.40 | 104.73 | 106.71 |
| 29 | 7 | 607 | CHL | CHD-C1D-ND | -4.40 | 120.42 | 124.45 |
| 25 | B | 844 | BCR | C7-C8-C9 | -4.39 | 119.59 | 126.23 |
| 22 | A | 803 | CLA | C3D-C4D-ND | 4.39 | 117.34 | 110.24 |
| 22 | B | 809 | CLA | O2D-CGD-CBD | 4.39 | 119.07 | 111.27 |
| 25 | 6 | 623 | BCR | C15-C14-C13 | -4.39 | 121.05 | 127.31 |
| 22 | B | 802 | CLA | O2D-CGD-CBD | 4.39 | 119.07 | 111.27 |
| 22 | A | 812 | CLA | C3D-C4D-ND | 4.38 | 117.33 | 110.24 |
| 22 | 4 | 603 | CLA | C3D-C2D-C1D | -4.38 | 99.85 | 105.83 |
| 22 | 4 | 614 | CLA | C3D-C2D-C1D | -4.38 | 99.85 | 105.83 |
| 22 | B | 852 | CLA | C3D-C2D-C1D | -4.38 | 99.85 | 105.83 |
| 22 | A | 835 | CLA | C3D-C2D-C1D | -4.38 | 99.85 | 105.83 |
| 22 | A | 854 | CLA | CAA-C2A-C3A | -4.38 | 100.78 | 112.78 |
| 22 | A | 854 | CLA | C3D-C4D-ND | 4.38 | 117.32 | 110.24 |
| 22 | B | 821 | CLA | C3D-C4D-ND | 4.38 | 117.32 | 110.24 |
| 29 | 4 | 606 | CHL | CHD-C1D-ND | -4.38 | 120.43 | 124.45 |
| 22 | 8 | 610 | CLA | C1D-CHD-C4C | -4.38 | 116.61 | 126.06 |
| 22 | B | 841 | CLA | C3D-C2D-C1D | -4.38 | 99.86 | 105.83 |
| 22 | Z | 611 | CLA | O2D-CGD-CBD | 4.38 | 119.05 | 111.27 |
| 22 | A | 805 | CLA | C3D-C2D-C1D | -4.38 | 99.86 | 105.83 |
| 22 | 2 | 609 | CLA | O2D-CGD-CBD | 4.37 | 119.04 | 111.27 |
| 22 | B | 825 | CLA | C3D-C4D-ND | 4.37 | 117.31 | 110.24 |
| 22 | A | 827 | CLA | C2C-C1C-NC | 4.37 | 114.07 | 109.97 |
| 22 | 2 | 607 | CLA | C3D-C4D-ND | 4.37 | 117.31 | 110.24 |
| 22 | 7 | 616 | CLA | C4A-NA-C1A | -4.37 | 104.74 | 106.71 |
| 22 | 4 | 616 | CLA | C3D-C4D-ND | 4.37 | 117.30 | 110.24 |
| 22 | 6 | 602 | CLA | C3D-C4D-ND | 4.37 | 117.30 | 110.24 |
| 22 | B | 830 | CLA | C3D-C2D-C1D | -4.37 | 99.87 | 105.83 |
| 22 | 6 | 614 | CLA | C3D-C2D-C1D | -4.36 | 99.88 | 105.83 |
| 22 | A | 815 | CLA | C3D-C2D-C1D | -4.36 | 99.88 | 105.83 |
| 22 | B | 833 | CLA | C3D-C4D-ND | 4.36 | 117.29 | 110.24 |
| 22 | 8 | 602 | CLA | C3D-C4D-ND | 4.36 | 117.29 | 110.24 |
| 22 | Z | 613 | CLA | C3D-C2D-C1D | -4.36 | 99.88 | 105.83 |
| 22 | 3 | 612 | CLA | C1D-CHD-C4C | -4.36 | 116.66 | 126.06 |
| 22 | A | 817 | CLA | C3D-C2D-C1D | -4.36 | 99.89 | 105.83 |
| 22 | A | 830 | CLA | C3D-C2D-C1D | -4.35 | 99.89 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 839 | CLA | C3D-C2D-C1D | -4.35 | 99.89 | 105.83 |
| 22 | B | 840 | CLA | O2D-CGD-CBD | 4.35 | 119.00 | 111.27 |
| 22 | 5 | 612 | CLA | C1D-CHD-C4C | -4.35 | 116.67 | 126.06 |
| 22 | B | 828 | CLA | CHD-C1D-ND | -4.35 | 120.45 | 124.45 |
| 22 | K | 4002 | CLA | C4A-NA-C1A | -4.35 | 104.75 | 106.71 |
| 22 | A | 821 | CLA | C1C-C2C-C3C | -4.35 | 102.38 | 106.96 |
| 22 | 1 | 610 | CLA | C1D-CHD-C4C | -4.35 | 116.67 | 126.06 |
| 22 | A | 838 | CLA | C3D-C2D-C1D | -4.35 | 99.90 | 105.83 |
| 22 | 3 | 602 | CLA | C3D-C4D-ND | 4.35 | 117.27 | 110.24 |
| 22 | 7 | 608 | CLA | C3D-C4D-ND | 4.35 | 117.27 | 110.24 |
| 22 | A | 810 | CLA | O2D-CGD-CBD | 4.35 | 118.99 | 111.27 |
| 22 | B | 837 | CLA | C3D-C4D-ND | 4.35 | 117.27 | 110.24 |
| 22 | A | 830 | CLA | C3C-C4C-NC | 4.35 | 115.44 | 110.57 |
| 22 | 3 | 620 | CLA | O2D-CGD-CBD | 4.34 | 118.99 | 111.27 |
| 21 | A | 801 | CL0 | C3C-C4C-NC | 4.34 | 115.44 | 110.57 |
| 22 | B | 823 | CLA | C3D-C2D-C1D | -4.34 | 99.90 | 105.83 |
| 22 | 5 | 609 | CLA | C1D-CHD-C4C | -4.34 | 116.69 | 126.06 |
| 22 | B | 827 | CLA | C3C-C4C-NC | 4.34 | 115.44 | 110.57 |
| 22 | A | 843 | CLA | O2D-CGD-CBD | 4.34 | 118.98 | 111.27 |
| 22 | B | 819 | CLA | C3D-C2D-C1D | -4.34 | 99.91 | 105.83 |
| 22 | 7 | 604 | CLA | C3D-C4D-ND | 4.34 | 117.26 | 110.24 |
| 29 | 5 | 607 | CHL | O2D-CGD-CBD | 4.34 | 118.98 | 111.27 |
| 22 | 9 | 613 | CLA | C3D-C2D-C1D | -4.34 | 99.91 | 105.83 |
| 22 | 8 | 614 | CLA | C3D-C2D-C1D | -4.34 | 99.91 | 105.83 |
| 22 | 5 | 616 | CLA | C4A-NA-C1A | -4.34 | 104.76 | 106.71 |
| 22 | 4 | 604 | CLA | C3D-C4D-ND | 4.34 | 117.25 | 110.24 |
| 22 | 5 | 621 | CLA | C3C-C4C-NC | 4.34 | 115.43 | 110.57 |
| 22 | B | 822 | CLA | C3D-C2D-C1D | -4.33 | 99.92 | 105.83 |
| 22 | 7 | 602 | CLA | C2C-C1C-NC | 4.33 | 114.03 | 109.97 |
| 25 | A | 856 | BCR | C20-C21-C22 | -4.33 | 121.13 | 127.31 |
| 30 | 2 | 617 | LUT | C35-C15-C14 | -4.33 | 114.60 | 123.47 |
| 22 | 6 | 612 | CLA | C3D-C2D-C1D | -4.33 | 99.92 | 105.83 |
| 22 | 2 | 602 | CLA | C3D-C4D-ND | 4.33 | 117.24 | 110.24 |
| 22 | 5 | 621 | CLA | CHD-C1D-ND | -4.33 | 120.48 | 124.45 |
| 22 | A | 808 | CLA | C3D-C4D-ND | 4.33 | 117.24 | 110.24 |
| 22 | B | 820 | CLA | C3D-C2D-C1D | -4.32 | 99.93 | 105.83 |
| 22 | A | 822 | CLA | C4A-NA-C1A | -4.32 | 104.76 | 106.71 |
| 22 | 1 | 612 | CLA | C3D-C2D-C1D | -4.32 | 99.93 | 105.83 |
| 22 | A | 809 | CLA | C4A-NA-C1A | -4.32 | 104.76 | 106.71 |
| 25 | A | 851 | BCR | C16-C17-C18 | -4.32 | 121.15 | 127.31 |
| 22 | A | 817 | CLA | C1C-C2C-C3C | -4.32 | 102.42 | 106.96 |
| 22 | A | 818 | CLA | C3D-C4D-ND | 4.32 | 117.22 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 604 | CLA | C3D-C4D-ND | 4.32 | 117.22 | 110.24 |
| 22 | 3 | 612 | CLA | C3D-C4D-ND | 4.32 | 117.22 | 110.24 |
| 22 | 2 | 611 | CLA | C3D-C4D-ND | 4.32 | 117.22 | 110.24 |
| 22 | B | 840 | CLA | C3C-C4C-NC | 4.32 | 115.41 | 110.57 |
| 22 | 7 | 604 | CLA | C3C-C4C-NC | 4.32 | 115.41 | 110.57 |
| 22 | 4 | 609 | CLA | C1D-CHD-C4C | -4.31 | 116.75 | 126.06 |
| 22 | 4 | 613 | CLA | O2D-CGD-CBD | 4.31 | 118.94 | 111.27 |
| 29 | 5 | 607 | CHL | C1D-CHD-C4C | -4.31 | 116.75 | 126.06 |
| 22 | A | 806 | CLA | C3D-C4D-ND | 4.31 | 117.22 | 110.24 |
| 24 | A | 847 | LHG | O7-C7-C8 | 4.31 | 120.80 | 111.50 |
| 29 | 8 | 607 | CHL | C1C-C2C-C3C | -4.31 | 103.69 | 107.11 |
| 25 | 6 | 625 | BCR | C3-C4-C5 | -4.31 | 106.38 | 114.08 |
| 25 | K | 4001 | BCR | C15-C16-C17 | -4.31 | 114.65 | 123.47 |
| 22 | 6 | 613 | CLA | O2D-CGD-CBD | 4.31 | 118.92 | 111.27 |
| 22 | 8 | 606 | CLA | CAA-C2A-C3A | -4.31 | 103.50 | 114.26 |
| 30 | 2 | 616 | LUT | C7-C8-C9 | -4.30 | 119.73 | 126.23 |
| 22 | A | 843 | CLA | C4A-NA-C1A | -4.30 | 104.77 | 106.71 |
| 22 | A | 816 | CLA | C3D-C4D-ND | 4.30 | 117.19 | 110.24 |
| 22 | B | 829 | CLA | O2D-CGD-CBD | 4.30 | 118.91 | 111.27 |
| 22 | 3 | 614 | CLA | C3D-C4D-ND | 4.30 | 117.19 | 110.24 |
| 22 | 8 | 604 | CLA | C3D-C2D-C1D | -4.29 | 99.97 | 105.83 |
| 22 | 6 | 613 | CLA | C3D-C2D-C1D | -4.29 | 99.97 | 105.83 |
| 29 | 4 | 608 | CHL | O2D-CGD-CBD | 4.29 | 118.89 | 111.27 |
| 25 | A | 850 | BCR | C15-C14-C13 | -4.29 | 121.19 | 127.31 |
| 22 | 1 | 602 | CLA | O2D-CGD-CBD | 4.28 | 118.88 | 111.27 |
| 22 | 6 | 601 | CLA | C3D-C4D-ND | 4.28 | 117.17 | 110.24 |
| 22 | A | 830 | CLA | O2D-CGD-CBD | 4.28 | 118.87 | 111.27 |
| 22 | A | 827 | CLA | C3D-C2D-C1D | -4.28 | 99.99 | 105.83 |
| 22 | A | 836 | CLA | C3D-C4D-ND | 4.28 | 117.16 | 110.24 |
| 22 | 3 | 607 | CLA | C3D-C4D-ND | 4.28 | 117.16 | 110.24 |
| 22 | 9 | 603 | CLA | C1D-CHD-C4C | -4.28 | 116.83 | 126.06 |
| 22 | 9 | 614 | CLA | C3D-C4D-ND | 4.28 | 117.16 | 110.24 |
| 22 | A | 806 | CLA | C3D-C2D-C1D | -4.27 | 100.00 | 105.83 |
| 25 | I | 172 | BCR | C3-C4-C5 | -4.27 | 106.45 | 114.08 |
| 29 | 1 | 607 | CHL | CHD-C1D-ND | -4.27 | 120.53 | 124.45 |
| 22 | B | 816 | CLA | C2C-C1C-NC | 4.27 | 113.97 | 109.97 |
| 22 | 4 | 602 | CLA | C3D-C4D-ND | 4.27 | 117.14 | 110.24 |
| 22 | 7 | 604 | CLA | C1C-C2C-C3C | -4.27 | 102.47 | 106.96 |
| 22 | A | 817 | CLA | C3D-C4D-ND | 4.27 | 117.14 | 110.24 |
| 22 | 7 | 608 | CLA | C4A-NA-C1A | -4.27 | 104.79 | 106.71 |
| 25 | K | 4001 | BCR | C16-C17-C18 | -4.27 | 121.22 | 127.31 |
| 22 | 8 | 612 | CLA | C3D-C2D-C1D | -4.26 | 100.01 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 829 | CLA | C1D-CHD-C4C | -4.26 | 116.86 | 126.06 |
| 22 | 8 | 613 | CLA | O2D-CGD-CBD | 4.26 | 118.84 | 111.27 |
| 22 | 8 | 616 | CLA | C3C-C4C-NC | 4.26 | 115.35 | 110.57 |
| 22 | 4 | 604 | CLA | C4A-NA-C1A | -4.26 | 104.79 | 106.71 |
| 22 | 2 | 614 | CLA | C4A-NA-C1A | -4.26 | 104.79 | 106.71 |
| 29 | 5 | 607 | CHL | C1C-C2C-C3C | -4.25 | 103.74 | 107.11 |
| 25 | 6 | 625 | BCR | C11-C10-C9 | -4.25 | 121.24 | 127.31 |
| 22 | B | 825 | CLA | C2C-C1C-NC | 4.25 | 113.95 | 109.97 |
| 22 | 4 | 614 | CLA | C3D-C4D-ND | 4.25 | 117.11 | 110.24 |
| 22 | 1 | 604 | CLA | C3D-C4D-ND | 4.25 | 117.11 | 110.24 |
| 21 | A | 801 | CL0 | C1D-CHD-C4C | -4.24 | 116.90 | 126.06 |
| 22 | B | 835 | CLA | O2D-CGD-CBD | 4.24 | 118.81 | 111.27 |
| 22 | B | 814 | CLA | C3D-C4D-ND | 4.24 | 117.10 | 110.24 |
| 22 | B | 819 | CLA | C4A-NA-C1A | -4.24 | 104.80 | 106.71 |
| 22 | 3 | 610 | CLA | CMC-C2C-C1C | 4.24 | 131.50 | 125.04 |
| 22 | B | 810 | CLA | O2D-CGD-CBD | 4.24 | 118.80 | 111.27 |
| 22 | 1 | 616 | CLA | C3D-C2D-C1D | -4.24 | 100.05 | 105.83 |
| 22 | Z | 614 | CLA | C3D-C4D-ND | 4.24 | 117.09 | 110.24 |
| 22 | 9 | 610 | CLA | C3D-C4D-ND | 4.24 | 117.09 | 110.24 |
| 22 | 3 | 613 | CLA | CHD-C1D-ND | -4.24 | 120.56 | 124.45 |
| 22 | Z | 611 | CLA | C3D-C4D-ND | 4.24 | 117.09 | 110.24 |
| 22 | 2 | 613 | CLA | C3D-C4D-ND | 4.23 | 117.09 | 110.24 |
| 22 | 1 | 610 | CLA | CMC-C2C-C1C | 4.23 | 131.49 | 125.04 |
| 22 | B | 812 | CLA | C3D-C4D-ND | 4.23 | 117.08 | 110.24 |
| 22 | 9 | 603 | CLA | C3D-C4D-ND | 4.23 | 117.08 | 110.24 |
| 22 | A | 814 | CLA | C3C-C4C-NC | 4.23 | 115.31 | 110.57 |
| 22 | 8 | 614 | CLA | C3D-C4D-ND | 4.23 | 117.08 | 110.24 |
| 22 | Z | 602 | CLA | C3D-C4D-ND | 4.23 | 117.08 | 110.24 |
| 22 | 3 | 610 | CLA | C3D-C2D-C1D | -4.23 | 100.06 | 105.83 |
| 22 | B | 826 | CLA | C3C-C4C-NC | 4.23 | 115.31 | 110.57 |
| 22 | K | 4003 | CLA | C4A-NA-C1A | -4.23 | 104.81 | 106.71 |
| 29 | 8 | 607 | CHL | C1D-CHD-C4C | -4.22 | 116.94 | 126.06 |
| 22 | A | 825 | CLA | C3D-C4D-ND | 4.22 | 117.07 | 110.24 |
| 22 | 2 | 603 | CLA | C3D-C4D-ND | 4.22 | 117.07 | 110.24 |
| 22 | A | 841 | CLA | O2D-CGD-CBD | 4.22 | 118.77 | 111.27 |
| 22 | A | 821 | CLA | C4A-NA-C1A | -4.22 | 104.81 | 106.71 |
| 22 | 3 | 611 | CLA | C4A-NA-C1A | -4.22 | 104.81 | 106.71 |
| 22 | 6 | 612 | CLA | C3D-C4D-ND | 4.22 | 117.07 | 110.24 |
| 22 | 4 | 616 | CLA | C4A-NA-C1A | -4.22 | 104.81 | 106.71 |
| 22 | 3 | 604 | CLA | O2D-CGD-CBD | 4.22 | 118.76 | 111.27 |
| 22 | F | 303 | CLA | C1D-CHD-C4C | -4.22 | 116.96 | 126.06 |
| 22 | 7 | 606 | CLA | C3D-C4D-ND | 4.22 | 117.06 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 612 | CLA | C3D-C4D-ND | 4.22 | 117.06 | 110.24 |
| 22 | 4 | 612 | CLA | C1D-CHD-C4C | -4.22 | 116.96 | 126.06 |
| 22 | 4 | 612 | CLA | C3D-C4D-ND | 4.22 | 117.06 | 110.24 |
| 22 | B | 815 | CLA | C4A-NA-C1A | -4.21 | 104.81 | 106.71 |
| 22 | 9 | 613 | CLA | C3D-C4D-ND | 4.21 | 117.05 | 110.24 |
| 22 | 8 | 606 | CLA | C3D-C4D-ND | 4.21 | 117.05 | 110.24 |
| 22 | 7 | 612 | CLA | C1D-CHD-C4C | -4.21 | 116.97 | 126.06 |
| 25 | 6 | 623 | BCR | C11-C10-C9 | -4.21 | 121.30 | 127.31 |
| 25 | 5 | 625 | BCR | C11-C12-C13 | -4.21 | 114.59 | 126.42 |
| 22 | 1 | 604 | CLA | C4A-NA-C1A | -4.21 | 104.81 | 106.71 |
| 22 | 4 | 601 | CLA | C3D-C4D-ND | 4.21 | 117.04 | 110.24 |
| 22 | B | 836 | CLA | CMB-C2B-C3B | 4.21 | 132.55 | 124.68 |
| 22 | Z | 610 | CLA | C1D-CHD-C4C | -4.21 | 116.98 | 126.06 |
| 22 | A | 802 | CLA | O2D-CGD-CBD | 4.21 | 118.74 | 111.27 |
| 22 | Z | 612 | CLA | C1D-CHD-C4C | -4.21 | 116.98 | 126.06 |
| 22 | A | 842 | CLA | O2A-C1-C2 | 4.21 | 119.69 | 108.64 |
| 24 | 1 | 620 | LHG | O7-C7-C8 | 4.20 | 120.56 | 111.50 |
| 22 | 8 | 612 | CLA | C3D-C4D-ND | 4.20 | 117.04 | 110.24 |
| 22 | A | 810 | CLA | C3D-C2D-C1D | -4.20 | 100.09 | 105.83 |
| 22 | 2 | 606 | CLA | C3D-C4D-ND | 4.20 | 117.04 | 110.24 |
| 22 | A | 829 | CLA | C1D-CHD-C4C | -4.20 | 116.99 | 126.06 |
| 22 | 1 | 603 | CLA | C1C-C2C-C3C | -4.20 | 102.54 | 106.96 |
| 29 | 6 | 618 | CHL | C3C-C4C-NC | 4.20 | 115.28 | 110.57 |
| 22 | A | 842 | CLA | C1-C2-C3 | -4.20 | 118.79 | 126.04 |
| 25 | 7 | 623 | BCR | C21-C20-C19 | -4.20 | 110.12 | 123.22 |
| 22 | G | 204 | CLA | C3D-C4D-ND | 4.20 | 117.03 | 110.24 |
| 22 | A | 845 | CLA | C3C-C4C-NC | 4.20 | 115.28 | 110.57 |
| 22 | 1 | 612 | CLA | C3D-C4D-ND | 4.19 | 117.02 | 110.24 |
| 22 | B | 813 | CLA | C3C-C4C-NC | 4.19 | 115.27 | 110.57 |
| 22 | 6 | 609 | CLA | C1D-CHD-C4C | -4.19 | 117.02 | 126.06 |
| 25 | A | 849 | BCR | C11-C10-C9 | -4.19 | 121.33 | 127.31 |
| 25 | 4 | 621 | BCR | C33-C5-C6 | -4.19 | 119.82 | 124.53 |
| 22 | B | 840 | CLA | CAC-C3C-C2C | 4.19 | 134.70 | 127.53 |
| 22 | A | 842 | CLA | C3D-C4D-ND | 4.19 | 117.02 | 110.24 |
| 25 | 3 | 718 | BCR | C15-C14-C13 | -4.19 | 121.33 | 127.31 |
| 22 | 8 | 602 | CLA | C3C-C4C-NC | 4.19 | 115.27 | 110.57 |
| 22 | 2 | 612 | CLA | C3D-C4D-ND | 4.19 | 117.01 | 110.24 |
| 22 | A | 812 | CLA | C1D-CHD-C4C | -4.19 | 117.03 | 126.06 |
| 22 | B | 830 | CLA | C3D-C4D-ND | 4.19 | 117.01 | 110.24 |
| 22 | A | 821 | CLA | C3D-C2D-C1D | -4.18 | 100.12 | 105.83 |
| 22 | B | 808 | CLA | C3C-C4C-NC | 4.18 | 115.26 | 110.57 |
| 22 | K | 4002 | CLA | C3D-C4D-ND | 4.18 | 117.00 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | Z | 612 | CLA | C3D-C4D-ND | 4.18 | 117.00 | 110.24 |
| 22 | Z | 610 | CLA | C3D-C4D-ND | 4.18 | 117.00 | 110.24 |
| 22 | A | 818 | CLA | C1D-CHD-C4C | -4.18 | 117.04 | 126.06 |
| 22 | 5 | 616 | CLA | C1D-CHD-C4C | -4.18 | 117.04 | 126.06 |
| 29 | 4 | 606 | CHL | C3C-C4C-NC | 4.18 | 115.26 | 110.57 |
| 22 | B | 828 | CLA | C3D-C4D-ND | 4.18 | 117.00 | 110.24 |
| 25 | A | 856 | BCR | C16-C17-C18 | -4.18 | 121.35 | 127.31 |
| 22 | 6 | 616 | CLA | O2D-CGD-CBD | 4.18 | 118.69 | 111.27 |
| 22 | 6 | 613 | CLA | C4A-NA-C1A | -4.18 | 104.83 | 106.71 |
| 22 | B | 812 | CLA | C4A-NA-C1A | -4.17 | 104.83 | 106.71 |
| 22 | A | 813 | CLA | C3D-C4D-ND | 4.17 | 116.99 | 110.24 |
| 22 | Z | 608 | CLA | O2D-CGD-CBD | 4.17 | 118.68 | 111.27 |
| 29 | 1 | 607 | CHL | C1D-CHD-C4C | -4.17 | 117.06 | 126.06 |
| 22 | 2 | 601 | CLA | C4A-NA-C1A | -4.17 | 104.83 | 106.71 |
| 22 | 1 | 611 | CLA | C3D-C4D-ND | 4.17 | 116.98 | 110.24 |
| 22 | B | 824 | CLA | C3D-C2D-C1D | -4.17 | 100.14 | 105.83 |
| 22 | B | 802 | CLA | C4A-NA-C1A | -4.17 | 104.83 | 106.71 |
| 22 | B | 810 | CLA | C3D-C4D-ND | 4.17 | 116.98 | 110.24 |
| 22 | 7 | 601 | CLA | C3D-C4D-ND | 4.17 | 116.98 | 110.24 |
| 22 | Z | 609 | CLA | C1C-C2C-C3C | -4.17 | 102.58 | 106.96 |
| 22 | 8 | 616 | CLA | C4A-NA-C1A | -4.16 | 104.83 | 106.71 |
| 22 | Z | 614 | CLA | O2D-CGD-CBD | 4.16 | 118.67 | 111.27 |
| 22 | A | 811 | CLA | C3D-C4D-ND | 4.16 | 116.97 | 110.24 |
| 22 | B | 804 | CLA | C3C-C4C-NC | 4.16 | 115.24 | 110.57 |
| 22 | 4 | 603 | CLA | C1C-C2C-C3C | -4.16 | 102.58 | 106.96 |
| 29 | Z | 607 | CHL | C1D-CHD-C4C | -4.16 | 117.08 | 126.06 |
| 22 | A | 810 | CLA | C3D-C4D-ND | 4.16 | 116.97 | 110.24 |
| 22 | B | 834 | CLA | C3D-C4D-ND | 4.16 | 116.97 | 110.24 |
| 22 | B | 832 | CLA | C3D-C4D-ND | 4.16 | 116.97 | 110.24 |
| 25 | A | 856 | BCR | C15-C16-C17 | -4.16 | 114.95 | 123.47 |
| 22 | 7 | 620 | CLA | C3D-C4D-ND | 4.16 | 116.96 | 110.24 |
| 30 | 8 | 617 | LUT | C35-C34-C33 | -4.16 | 121.38 | 127.31 |
| 22 | B | 806 | CLA | C3C-C4C-NC | 4.16 | 115.23 | 110.57 |
| 22 | 1 | 602 | CLA | C3D-C4D-ND | 4.16 | 116.96 | 110.24 |
| 22 | B | 815 | CLA | C1D-CHD-C4C | -4.16 | 117.09 | 126.06 |
| 22 | A | 811 | CLA | C3C-C4C-NC | 4.16 | 115.23 | 110.57 |
| 25 | 3 | 719 | BCR | C16-C17-C18 | -4.16 | 121.38 | 127.31 |
| 22 | 1 | 608 | CLA | O2D-CGD-CBD | 4.16 | 118.65 | 111.27 |
| 22 | A | 810 | CLA | C3C-C4C-NC | 4.15 | 115.23 | 110.57 |
| 22 | A | 809 | CLA | C3D-C4D-ND | 4.15 | 116.96 | 110.24 |
| 29 | 6 | 607 | CHL | CHD-C1D-ND | -4.15 | 120.64 | 124.45 |
| 22 | 1 | 604 | CLA | C3D-C2D-C1D | -4.15 | 100.17 | 105.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 9 | 602 | CLA | C3D-C4D-ND | 4.15 | 116.95 | 110.24 |
| 25 | K | 4004 | BCR | C15-C14-C13 | -4.15 | 121.39 | 127.31 |
| 22 | B | 808 | CLA | C3D-C4D-ND | 4.15 | 116.95 | 110.24 |
| 22 | 9 | 612 | CLA | C3D-C4D-ND | 4.15 | 116.95 | 110.24 |
| 25 | B | 846 | BCR | C40-C30-C25 | 4.15 | 117.03 | 110.30 |
| 22 | A | 838 | CLA | C1D-CHD-C4C | -4.15 | 117.11 | 126.06 |
| 22 | A | 834 | CLA | C3D-C4D-ND | 4.15 | 116.95 | 110.24 |
| 22 | A | 840 | CLA | C3C-C4C-NC | 4.15 | 115.22 | 110.57 |
| 22 | B | 852 | CLA | C3D-C4D-ND | 4.15 | 116.94 | 110.24 |
| 22 | A | 814 | CLA | C3D-C4D-ND | 4.14 | 116.94 | 110.24 |
| 22 | F | 301 | CLA | C1D-CHD-C4C | -4.14 | 117.12 | 126.06 |
| 22 | 7 | 610 | CLA | C1D-CHD-C4C | -4.14 | 117.12 | 126.06 |
| 29 | Z | 607 | CHL | C3C-C4C-NC | 4.14 | 115.22 | 110.57 |
| 22 | 2 | 607 | CLA | C4A-NA-C1A | -4.14 | 104.84 | 106.71 |
| 22 | B | 834 | CLA | O2D-CGD-CBD | 4.14 | 118.63 | 111.27 |
| 22 | Z | 610 | CLA | C3C-C4C-NC | 4.14 | 115.22 | 110.57 |
| 29 | 1 | 607 | CHL | C3C-C4C-NC | 4.14 | 115.22 | 110.57 |
| 29 | 3 | 608 | CHL | C1D-CHD-C4C | -4.14 | 117.13 | 126.06 |
| 22 | J | 3002 | CLA | CAA-C2A-C3A | -4.14 | 103.92 | 114.26 |
| 22 | 7 | 616 | CLA | C3D-C4D-ND | 4.14 | 116.93 | 110.24 |
| 22 | A | 810 | CLA | O2A-CGA-CBA | 4.14 | 124.89 | 111.91 |
| 22 | A | 821 | CLA | C1D-CHD-C4C | -4.14 | 117.14 | 126.06 |
| 22 | B | 811 | CLA | C3D-C4D-ND | 4.13 | 116.92 | 110.24 |
| 22 | 4 | 613 | CLA | C3D-C4D-ND | 4.13 | 116.92 | 110.24 |
| 22 | A | 845 | CLA | C3D-C4D-ND | 4.13 | 116.92 | 110.24 |
| 22 | B | 840 | CLA | C3D-C4D-ND | 4.13 | 116.92 | 110.24 |
| 22 | 2 | 601 | CLA | C3D-C4D-ND | 4.13 | 116.92 | 110.24 |
| 22 | 6 | 616 | CLA | C3D-C4D-ND | 4.13 | 116.92 | 110.24 |
| 22 | B | 832 | CLA | C1C-C2C-C3C | -4.13 | 102.62 | 106.96 |
| 22 | 9 | 609 | CLA | C3C-C4C-NC | 4.13 | 115.20 | 110.57 |
| 22 | B | 839 | CLA | C3D-C4D-ND | 4.13 | 116.91 | 110.24 |
| 22 | 8 | 612 | CLA | C3C-C4C-NC | 4.13 | 115.20 | 110.57 |
| 22 | B | 838 | CLA | C3C-C4C-NC | 4.13 | 115.20 | 110.57 |
| 22 | 7 | 613 | CLA | C3D-C4D-ND | 4.13 | 116.91 | 110.24 |
| 22 | 6 | 612 | CLA | C1D-CHD-C4C | -4.13 | 117.16 | 126.06 |
| 22 | 3 | 602 | CLA | CMB-C2B-C3B | 4.13 | 132.40 | 124.68 |
| 22 | 3 | 604 | CLA | C3D-C4D-ND | 4.12 | 116.91 | 110.24 |
| 25 | L | 205 | BCR | C24-C23-C22 | 4.12 | 132.47 | 126.23 |
| 22 | 1 | 610 | CLA | C3D-C4D-ND | 4.12 | 116.91 | 110.24 |
| 22 | 2 | 611 | CLA | C4A-NA-C1A | -4.12 | 104.85 | 106.71 |
| 22 | Z | 603 | CLA | C3D-C4D-ND | 4.12 | 116.91 | 110.24 |
| 25 | L | 201 | BCR | C15-C14-C13 | -4.12 | 121.43 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 616 | CLA | C1D-CHD-C4C | -4.12 | 117.16 | 126.06 |
| 22 | Z | 603 | CLA | C1C-C2C-C3C | -4.12 | 102.62 | 106.96 |
| 22 | 7 | 610 | CLA | C3D-C4D-ND | 4.12 | 116.91 | 110.24 |
| 22 | A | 824 | CLA | C3D-C4D-ND | 4.12 | 116.91 | 110.24 |
| 22 | 7 | 609 | CLA | CMA-C3A-C4A | -4.12 | 100.70 | 111.77 |
| 22 | 7 | 609 | CLA | C3D-C4D-ND | 4.12 | 116.90 | 110.24 |
| 29 | 7 | 607 | CHL | C1D-CHD-C4C | -4.12 | 117.17 | 126.06 |
| 22 | B | 830 | CLA | C3C-C4C-NC | 4.12 | 115.19 | 110.57 |
| 22 | 8 | 612 | CLA | C1D-CHD-C4C | -4.11 | 117.18 | 126.06 |
| 22 | B | 813 | CLA | CAC-C3C-C4C | 4.11 | 130.15 | 124.81 |
| 25 | A | 851 | BCR | C15-C14-C13 | -4.11 | 121.44 | 127.31 |
| 22 | 3 | 620 | CLA | C3D-C4D-ND | 4.11 | 116.89 | 110.24 |
| 25 | B | 844 | BCR | C16-C17-C18 | -4.11 | 121.44 | 127.31 |
| 22 | A | 836 | CLA | C1C-C2C-C3C | -4.11 | 102.64 | 106.96 |
| 22 | A | 831 | CLA | C3C-C4C-NC | 4.11 | 115.18 | 110.57 |
| 22 | 3 | 610 | CLA | C3D-C4D-ND | 4.11 | 116.88 | 110.24 |
| 22 | Z | 602 | CLA | C1D-CHD-C4C | -4.11 | 117.20 | 126.06 |
| 22 | 3 | 617 | CLA | C3D-C4D-ND | 4.11 | 116.88 | 110.24 |
| 22 | 1 | 612 | CLA | C1D-CHD-C4C | -4.10 | 117.20 | 126.06 |
| 22 | 1 | 611 | CLA | O2D-CGD-CBD | 4.10 | 118.56 | 111.27 |
| 22 | 7 | 603 | CLA | C3D-C4D-ND | 4.10 | 116.88 | 110.24 |
| 22 | A | 842 | CLA | C1D-CHD-C4C | -4.10 | 117.21 | 126.06 |
| 22 | B | 808 | CLA | C3D-C2D-C1D | -4.10 | 100.23 | 105.83 |
| 22 | 3 | 606 | CLA | C3D-C4D-ND | 4.10 | 116.87 | 110.24 |
| 22 | B | 840 | CLA | C4A-NA-C1A | -4.10 | 104.86 | 106.71 |
| 22 | Z | 609 | CLA | C1D-CHD-C4C | -4.10 | 117.21 | 126.06 |
| 29 | 5 | 608 | CHL | C2C-C3C-C4C | -4.10 | 103.57 | 106.49 |
| 22 | 8 | 603 | CLA | C1D-CHD-C4C | -4.10 | 117.22 | 126.06 |
| 29 | 6 | 606 | CHL | C3C-C4C-NC | 4.10 | 115.17 | 110.57 |
| 22 | 2 | 609 | CLA | C1D-CHD-C4C | -4.10 | 117.22 | 126.06 |
| 22 | J | 3002 | CLA | C3D-C4D-ND | 4.10 | 116.86 | 110.24 |
| 22 | B | 802 | CLA | C3D-C4D-ND | 4.09 | 116.86 | 110.24 |
| 22 | K | 4003 | CLA | C3D-C4D-ND | 4.09 | 116.86 | 110.24 |
| 22 | B | 825 | CLA | C1D-CHD-C4C | -4.09 | 117.23 | 126.06 |
| 22 | 3 | 613 | CLA | C3D-C4D-ND | 4.09 | 116.86 | 110.24 |
| 22 | B | 807 | CLA | C3C-C4C-NC | 4.09 | 115.16 | 110.57 |
| 22 | 6 | 609 | CLA | C3C-C4C-NC | 4.09 | 115.16 | 110.57 |
| 22 | Z | 606 | CLA | C3D-C4D-ND | 4.09 | 116.86 | 110.24 |
| 25 | 5 | 622 | BCR | C3-C4-C5 | -4.09 | 106.77 | 114.08 |
| 22 | 1 | 613 | CLA | C1D-CHD-C4C | -4.09 | 117.23 | 126.06 |
| 22 | 5 | 601 | CLA | C3D-C4D-ND | 4.09 | 116.86 | 110.24 |
| 22 | 6 | 604 | CLA | C3D-C4D-ND | 4.09 | 116.86 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 826 | CLA | C1C-C2C-C3C | -4.09 | 102.66 | 106.96 |
| 22 | A | 829 | CLA | O2D-CGD-CBD | 4.09 | 118.53 | 111.27 |
| 22 | 3 | 612 | CLA | C1C-C2C-C3C | -4.09 | 102.66 | 106.96 |
| 22 | B | 804 | CLA | C1D-CHD-C4C | -4.09 | 117.24 | 126.06 |
| 22 | F | 304 | CLA | C3D-C4D-ND | 4.09 | 116.85 | 110.24 |
| 22 | A | 832 | CLA | C3D-C2D-C1D | -4.09 | 100.25 | 105.83 |
| 22 | A | 803 | CLA | C4A-NA-C1A | -4.09 | 104.87 | 106.71 |
| 22 | B | 831 | CLA | C3C-C4C-NC | 4.09 | 115.16 | 110.57 |
| 22 | 8 | 614 | CLA | C3C-C4C-NC | 4.09 | 115.16 | 110.57 |
| 22 | A | 837 | CLA | C4A-NA-C1A | -4.09 | 104.87 | 106.71 |
| 22 | A | 838 | CLA | C3D-C4D-ND | 4.09 | 116.85 | 110.24 |
| 22 | A | 841 | CLA | C3D-C4D-ND | 4.09 | 116.85 | 110.24 |
| 25 | 3 | 718 | BCR | C3-C4-C5 | -4.09 | 106.78 | 114.08 |
| 29 | 4 | 608 | CHL | C2C-C3C-C4C | -4.09 | 103.58 | 106.49 |
| 22 | B | 811 | CLA | C3C-C4C-NC | 4.08 | 115.15 | 110.57 |
| 22 | Z | 612 | CLA | C3C-C4C-NC | 4.08 | 115.15 | 110.57 |
| 22 | 5 | 617 | CLA | C3C-C4C-NC | 4.08 | 115.15 | 110.57 |
| 22 | A | 818 | CLA | C3C-C4C-NC | 4.08 | 115.15 | 110.57 |
| 25 | 7 | 624 | BCR | C3-C4-C5 | -4.08 | 106.79 | 114.08 |
| 22 | 3 | 610 | CLA | O2A-CGA-CBA | 4.08 | 124.71 | 111.91 |
| 22 | 8 | 614 | CLA | C4A-NA-C1A | -4.08 | 104.87 | 106.71 |
| 22 | 4 | 609 | CLA | C1C-C2C-C3C | -4.08 | 102.67 | 106.96 |
| 22 | A | 839 | CLA | C3D-C4D-ND | 4.08 | 116.83 | 110.24 |
| 22 | B | 819 | CLA | C3D-C4D-ND | 4.08 | 116.83 | 110.24 |
| 22 | 5 | 610 | CLA | C3D-C4D-ND | 4.08 | 116.83 | 110.24 |
| 22 | 1 | 610 | CLA | O2A-CGA-CBA | 4.07 | 124.69 | 111.91 |
| 22 | A | 843 | CLA | C3C-C4C-NC | 4.07 | 115.14 | 110.57 |
| 22 | 8 | 608 | CLA | C4A-NA-C1A | -4.07 | 104.88 | 106.71 |
| 22 | 1 | 602 | CLA | C1D-CHD-C4C | -4.07 | 117.27 | 126.06 |
| 25 | 6 | 623 | BCR | C3-C4-C5 | -4.07 | 106.81 | 114.08 |
| 22 | 6 | 610 | CLA | C3D-C4D-ND | 4.07 | 116.82 | 110.24 |
| 22 | 7 | 606 | CLA | C1D-CHD-C4C | -4.07 | 117.28 | 126.06 |
| 22 | A | 817 | CLA | C4A-NA-C1A | -4.07 | 104.88 | 106.71 |
| 25 | 8 | 619 | BCR | C15-C14-C13 | -4.07 | 121.50 | 127.31 |
| 22 | B | 802 | CLA | CAA-C2A-C3A | -4.07 | 101.64 | 112.78 |
| 22 | A | 807 | CLA | C3D-C4D-ND | 4.07 | 116.81 | 110.24 |
| 22 | 7 | 608 | CLA | C3C-C4C-NC | 4.06 | 115.13 | 110.57 |
| 22 | A | 845 | CLA | C1D-CHD-C4C | -4.06 | 117.29 | 126.06 |
| 22 | 8 | 613 | CLA | C3D-C4D-ND | 4.06 | 116.81 | 110.24 |
| 22 | 5 | 612 | CLA | C3D-C4D-ND | 4.06 | 116.81 | 110.24 |
| 22 | A | 825 | CLA | O2D-CGD-CBD | 4.06 | 118.48 | 111.27 |
| 22 | 7 | 613 | CLA | C3C-C4C-NC | 4.06 | 115.12 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 831 | CLA | C3D-C4D-ND | 4.06 | 116.80 | 110.24 |
| 22 | 8 | 616 | CLA | C3D-C4D-ND | 4.06 | 116.80 | 110.24 |
| 22 | 9 | 601 | CLA | C3D-C4D-ND | 4.06 | 116.80 | 110.24 |
| 22 | 2 | 612 | CLA | C1D-CHD-C4C | -4.06 | 117.31 | 126.06 |
| 22 | G | 203 | CLA | C3D-C4D-ND | 4.06 | 116.80 | 110.24 |
| 22 | 3 | 609 | CLA | C3D-C4D-ND | 4.06 | 116.80 | 110.24 |
| 22 | A | 824 | CLA | C3C-C4C-NC | 4.05 | 115.12 | 110.57 |
| 22 | B | 824 | CLA | C3D-C4D-ND | 4.05 | 116.80 | 110.24 |
| 25 | B | 845 | BCR | C7-C8-C9 | -4.05 | 120.11 | 126.23 |
| 22 | L | 204 | CLA | C4A-NA-C1A | -4.05 | 104.88 | 106.71 |
| 22 | A | 825 | CLA | C3B-C4B-NB | 4.05 | 114.45 | 109.21 |
| 22 | 5 | 606 | CLA | C3D-C4D-ND | 4.05 | 116.79 | 110.24 |
| 25 | F | 305 | BCR | C7-C8-C9 | -4.05 | 120.11 | 126.23 |
| 21 | A | 801 | CL0 | C1C-C2C-C3C | -4.05 | 102.70 | 106.96 |
| 22 | 8 | 602 | CLA | C1D-CHD-C4C | -4.05 | 117.32 | 126.06 |
| 22 | 2 | 614 | CLA | C1D-CHD-C4C | -4.05 | 117.32 | 126.06 |
| 22 | 5 | 604 | CLA | C3D-C4D-ND | 4.05 | 116.79 | 110.24 |
| 22 | 1 | 613 | CLA | C3D-C4D-ND | 4.05 | 116.79 | 110.24 |
| 22 | A | 841 | CLA | C1D-CHD-C4C | -4.05 | 117.32 | 126.06 |
| 29 | 3 | 608 | CHL | C3C-C4C-NC | 4.05 | 115.11 | 110.57 |
| 22 | 7 | 604 | CLA | C1D-CHD-C4C | -4.05 | 117.33 | 126.06 |
| 22 | 7 | 616 | CLA | C1C-C2C-C3C | -4.05 | 102.70 | 106.96 |
| 22 | A | 828 | CLA | C2C-C1C-NC | 4.05 | 113.76 | 109.97 |
| 22 | Z | 613 | CLA | C3D-C4D-ND | 4.05 | 116.78 | 110.24 |
| 22 | 6 | 602 | CLA | C3C-C4C-NC | 4.05 | 115.11 | 110.57 |
| 22 | 4 | 609 | CLA | C3D-C4D-ND | 4.05 | 116.78 | 110.24 |
| 22 | 5 | 617 | CLA | C3D-C4D-ND | 4.04 | 116.78 | 110.24 |
| 22 | A | 816 | CLA | C3C-C4C-NC | 4.04 | 115.11 | 110.57 |
| 29 | 6 | 618 | CHL | CHD-C1D-ND | -4.04 | 120.74 | 124.45 |
| 22 | B | 810 | CLA | C1D-CHD-C4C | -4.04 | 117.34 | 126.06 |
| 22 | B | 824 | CLA | C1D-CHD-C4C | -4.04 | 117.34 | 126.06 |
| 22 | A | 838 | CLA | C1C-C2C-C3C | -4.04 | 102.71 | 106.96 |
| 22 | 8 | 601 | CLA | C4A-NA-C1A | -4.04 | 104.89 | 106.71 |
| 22 | 9 | 611 | CLA | C3C-C4C-NC | 4.04 | 115.10 | 110.57 |
| 22 | K | 4003 | CLA | C1D-CHD-C4C | -4.04 | 117.34 | 126.06 |
| 22 | 3 | 606 | CLA | CAA-C2A-C3A | -4.04 | 104.17 | 114.26 |
| 22 | 6 | 616 | CLA | C4A-NA-C1A | -4.04 | 104.89 | 106.71 |
| 22 | B | 840 | CLA | C3B-C4B-NB | 4.04 | 114.43 | 109.21 |
| 22 | B | 815 | CLA | C3D-C4D-ND | 4.04 | 116.77 | 110.24 |
| 22 | 1 | 616 | CLA | C3D-C4D-ND | 4.04 | 116.77 | 110.24 |
| 29 | 6 | 607 | CHL | C1D-CHD-C4C | -4.04 | 117.35 | 126.06 |
| 22 | 8 | 608 | CLA | C1D-CHD-C4C | -4.04 | 117.35 | 126.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 606 | CLA | C3C-C4C-NC | 4.04 | 115.10 | 110.57 |
| 22 | 3 | 613 | CLA | CAC-C3C-C4C | 4.04 | 130.05 | 124.81 |
| 22 | A | 834 | CLA | O2D-CGD-CBD | 4.03 | 118.44 | 111.27 |
| 22 | A | 833 | CLA | C3D-C4D-ND | 4.03 | 116.77 | 110.24 |
| 22 | B | 823 | CLA | CAC-C3C-C4C | 4.03 | 130.04 | 124.81 |
| 22 | A | 826 | CLA | C3C-C4C-NC | 4.03 | 115.09 | 110.57 |
| 25 | K | 4001 | BCR | C7-C8-C9 | -4.03 | 120.14 | 126.23 |
| 22 | 2 | 609 | CLA | C1C-C2C-C3C | -4.03 | 102.72 | 106.96 |
| 22 | B | 819 | CLA | O2D-CGD-CBD | 4.03 | 118.43 | 111.27 |
| 22 | A | 803 | CLA | C3C-C4C-NC | 4.03 | 115.09 | 110.57 |
| 22 | 3 | 613 | CLA | C1D-CHD-C4C | -4.03 | 117.37 | 126.06 |
| 22 | 1 | 606 | CLA | C3D-C4D-ND | 4.03 | 116.75 | 110.24 |
| 22 | 8 | 603 | CLA | C3D-C4D-ND | 4.03 | 116.75 | 110.24 |
| 22 | 5 | 604 | CLA | C1C-C2C-C3C | -4.03 | 102.72 | 106.96 |
| 22 | Z | 613 | CLA | C4A-NA-C1A | -4.03 | 104.90 | 106.71 |
| 22 | 4 | 616 | CLA | C1C-C2C-C3C | -4.03 | 102.72 | 106.96 |
| 22 | 3 | 603 | CLA | C3D-C4D-ND | 4.03 | 116.75 | 110.24 |
| 22 | A | 831 | CLA | C1D-CHD-C4C | -4.02 | 117.38 | 126.06 |
| 22 | 5 | 612 | CLA | C3C-C4C-NC | 4.02 | 115.08 | 110.57 |
| 22 | A | 808 | CLA | C3C-C4C-NC | 4.02 | 115.08 | 110.57 |
| 29 | 1 | 601 | CHL | CHD-C1D-ND | -4.02 | 120.76 | 124.45 |
| 22 | B | 808 | CLA | C1D-CHD-C4C | -4.02 | 117.38 | 126.06 |
| 22 | A | 834 | CLA | C1D-CHD-C4C | -4.02 | 117.39 | 126.06 |
| 22 | B | 817 | CLA | C1D-CHD-C4C | -4.02 | 117.39 | 126.06 |
| 22 | B | 809 | CLA | C3B-C4B-NB | 4.02 | 114.40 | 109.21 |
| 22 | A | 840 | CLA | C1D-CHD-C4C | -4.02 | 117.40 | 126.06 |
| 22 | A | 818 | CLA | C4A-NA-C1A | -4.01 | 104.90 | 106.71 |
| 22 | B | 826 | CLA | C1D-CHD-C4C | -4.01 | 117.40 | 126.06 |
| 22 | A | 820 | CLA | C3D-C4D-ND | 4.01 | 116.73 | 110.24 |
| 22 | B | 814 | CLA | C1D-CHD-C4C | -4.01 | 117.40 | 126.06 |
| 22 | 1 | 608 | CLA | C3D-C4D-ND | 4.01 | 116.72 | 110.24 |
| 25 | 7 | 623 | BCR | C15-C14-C13 | -4.01 | 121.59 | 127.31 |
| 22 | 6 | 616 | CLA | CAA-C2A-C3A | -4.01 | 101.80 | 112.78 |
| 22 | B | 803 | CLA | O2D-CGD-CBD | 4.01 | 118.39 | 111.27 |
| 22 | Z | 604 | CLA | C3D-C4D-ND | 4.01 | 116.72 | 110.24 |
| 22 | A | 831 | CLA | C3B-C4B-NB | 4.01 | 114.39 | 109.21 |
| 22 | 6 | 617 | CLA | C3C-C4C-NC | 4.01 | 115.06 | 110.57 |
| 22 | A | 813 | CLA | C3C-C4C-NC | 4.01 | 115.06 | 110.57 |
| 22 | 3 | 620 | CLA | C1C-C2C-C3C | -4.01 | 102.75 | 106.96 |
| 22 | 9 | 603 | CLA | C1C-C2C-C3C | -4.00 | 102.75 | 106.96 |
| 29 | 4 | 608 | CHL | C3C-C4C-NC | 4.00 | 115.06 | 110.57 |
| 29 | 9 | 607 | CHL | C3C-C4C-NC | 4.00 | 115.06 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | B | 843 | BCR | C20-C21-C22 | -4.00 | 121.60 | 127.31 |
| 22 | 6 | 617 | CLA | C3D-C4D-ND | 4.00 | 116.71 | 110.24 |
| 30 | 8 | 618 | LUT | C15-C14-C13 | -4.00 | 121.60 | 127.31 |
| 22 | 5 | 616 | CLA | C3C-C4C-NC | 4.00 | 115.06 | 110.57 |
| 22 | 5 | 613 | CLA | C3D-C4D-ND | 4.00 | 116.71 | 110.24 |
| 22 | A | 819 | CLA | C3C-C4C-NC | 4.00 | 115.06 | 110.57 |
| 25 | A | 852 | BCR | C20-C19-C18 | -4.00 | 115.18 | 126.42 |
| 22 | 6 | 612 | CLA | C3C-C4C-NC | 4.00 | 115.06 | 110.57 |
| 22 | 2 | 603 | CLA | C1C-C2C-C3C | -4.00 | 102.75 | 106.96 |
| 22 | 6 | 622 | CLA | C3D-C4D-ND | 4.00 | 116.70 | 110.24 |
| 22 | 7 | 620 | CLA | C4A-NA-C1A | -4.00 | 104.91 | 106.71 |
| 22 | A | 842 | CLA | C3C-C4C-NC | 4.00 | 115.05 | 110.57 |
| 22 | Z | 613 | CLA | C3C-C4C-NC | 4.00 | 115.05 | 110.57 |
| 22 | A | 822 | CLA | O2D-CGD-CBD | 4.00 | 118.37 | 111.27 |
| 22 | A | 807 | CLA | CAA-C2A-C3A | -3.99 | 101.84 | 112.78 |
| 25 | 4 | 621 | BCR | C38-C26-C25 | -3.99 | 120.04 | 124.53 |
| 22 | B | 803 | CLA | C1D-CHD-C4C | -3.99 | 117.44 | 126.06 |
| 22 | A | 825 | CLA | C4A-NA-C1A | -3.99 | 104.91 | 106.71 |
| 22 | Z | 616 | CLA | C4A-NA-C1A | -3.99 | 104.91 | 106.71 |
| 22 | 1 | 609 | CLA | C3D-C4D-ND | 3.99 | 116.69 | 110.24 |
| 22 | B | 832 | CLA | C3C-C4C-NC | 3.99 | 115.05 | 110.57 |
| 29 | 3 | 608 | CHL | O2D-CGD-CBD | 3.99 | 118.36 | 111.27 |
| 29 | 6 | 608 | CHL | C3C-C4C-NC | 3.99 | 115.05 | 110.57 |
| 25 | 5 | 622 | BCR | C28-C27-C26 | -3.99 | 106.95 | 114.08 |
| 22 | Z | 608 | CLA | C3D-C4D-ND | 3.99 | 116.69 | 110.24 |
| 29 | 6 | 606 | CHL | C1D-CHD-C4C | -3.99 | 117.46 | 126.06 |
| 22 | 8 | 604 | CLA | C1C-C2C-C3C | -3.98 | 102.77 | 106.96 |
| 22 | 6 | 611 | CLA | C3D-C4D-ND | 3.98 | 116.68 | 110.24 |
| 22 | A | 809 | CLA | C3C-C4C-NC | 3.98 | 115.04 | 110.57 |
| 22 | B | 852 | CLA | C3C-C4C-NC | 3.98 | 115.04 | 110.57 |
| 22 | 3 | 604 | CLA | C1C-C2C-C3C | -3.98 | 102.77 | 106.96 |
| 22 | 1 | 610 | CLA | CAA-C2A-C3A | -3.98 | 101.87 | 112.78 |
| 22 | 5 | 601 | CLA | C1C-C2C-C3C | -3.98 | 102.77 | 106.96 |
| 22 | 1 | 609 | CLA | C1C-C2C-C3C | -3.98 | 102.77 | 106.96 |
| 22 | 3 | 609 | CLA | C4A-NA-C1A | -3.98 | 104.92 | 106.71 |
| 22 | A | 804 | CLA | C1D-CHD-C4C | -3.98 | 117.48 | 126.06 |
| 22 | 8 | 601 | CLA | C1C-C2C-C3C | -3.98 | 102.78 | 106.96 |
| 22 | A | 832 | CLA | C3D-C4D-ND | 3.97 | 116.67 | 110.24 |
| 29 | 1 | 607 | CHL | O2D-CGD-CBD | 3.97 | 118.33 | 111.27 |
| 25 | 3 | 717 | BCR | C28-C27-C26 | -3.97 | 106.98 | 114.08 |
| 22 | 7 | 609 | CLA | C3C-C4C-NC | 3.97 | 115.03 | 110.57 |
| 22 | 1 | 606 | CLA | C3C-C4C-NC | 3.97 | 115.02 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 4 | 611 | CLA | C4A-NA-C1A | -3.97 | 104.92 | 106.71 |
| 22 | B | 825 | CLA | C3D-C2D-C1D | -3.97 | 100.42 | 105.83 |
| 22 | A | 830 | CLA | C3D-C4D-ND | 3.97 | 116.66 | 110.24 |
| 25 | 7 | 624 | BCR | C16-C17-C18 | -3.97 | 121.65 | 127.31 |
| 30 | 9 | 616 | LUT | C35-C34-C33 | -3.97 | 121.65 | 127.31 |
| 22 | 5 | 603 | CLA | C3C-C4C-NC | 3.97 | 115.02 | 110.57 |
| 22 | 7 | 604 | CLA | C4A-NA-C1A | -3.97 | 104.92 | 106.71 |
| 22 | F | 304 | CLA | C1D-CHD-C4C | -3.96 | 117.50 | 126.06 |
| 22 | 6 | 603 | CLA | C1D-CHD-C4C | -3.96 | 117.50 | 126.06 |
| 22 | 7 | 601 | CLA | O2A-CGA-CBA | 3.96 | 124.35 | 111.91 |
| 22 | 1 | 603 | CLA | C3D-C4D-ND | 3.96 | 116.65 | 110.24 |
| 22 | 6 | 609 | CLA | C1C-C2C-C3C | -3.96 | 102.79 | 106.96 |
| 22 | 6 | 601 | CLA | C1C-C2C-C3C | -3.96 | 102.79 | 106.96 |
| 22 | 4 | 603 | CLA | C3D-C4D-ND | 3.96 | 116.65 | 110.24 |
| 22 | 3 | 610 | CLA | C2C-C1C-NC | 3.96 | 113.68 | 109.97 |
| 22 | Z | 613 | CLA | C1D-CHD-C4C | -3.96 | 117.52 | 126.06 |
| 22 | 7 | 611 | CLA | C1D-CHD-C4C | -3.96 | 117.52 | 126.06 |
| 22 | 7 | 601 | CLA | C3C-C4C-NC | 3.96 | 115.01 | 110.57 |
| 22 | 2 | 603 | CLA | C3B-C4B-NB | 3.95 | 114.32 | 109.21 |
| 22 | 2 | 601 | CLA | C1D-CHD-C4C | -3.95 | 117.53 | 126.06 |
| 22 | Z | 612 | CLA | C1C-C2C-C3C | -3.95 | 102.80 | 106.96 |
| 22 | B | 814 | CLA | C3D-C2D-C1D | -3.95 | 100.44 | 105.83 |
| 22 | 5 | 603 | CLA | C1D-CHD-C4C | -3.95 | 117.53 | 126.06 |
| 25 | 4 | 621 | BCR | C7-C8-C9 | -3.95 | 120.26 | 126.23 |
| 22 | A | 820 | CLA | C1C-C2C-C3C | -3.95 | 102.80 | 106.96 |
| 22 | 5 | 611 | CLA | C1C-C2C-C3C | -3.95 | 102.80 | 106.96 |
| 22 | 5 | 613 | CLA | C3C-C4C-NC | 3.95 | 115.00 | 110.57 |
| 22 | 8 | 613 | CLA | C1D-CHD-C4C | -3.95 | 117.53 | 126.06 |
| 22 | A | 834 | CLA | C1C-C2C-C3C | -3.95 | 102.80 | 106.96 |
| 22 | B | 807 | CLA | C3D-C4D-ND | 3.95 | 116.63 | 110.24 |
| 22 | 9 | 612 | CLA | C1C-C2C-C3C | -3.95 | 102.80 | 106.96 |
| 22 | 7 | 610 | CLA | C3C-C4C-NC | 3.95 | 115.00 | 110.57 |
| 22 | 3 | 613 | CLA | C3D-C2D-C1D | -3.95 | 100.44 | 105.83 |
| 22 | 1 | 610 | CLA | C3C-C4C-NC | 3.95 | 115.00 | 110.57 |
| 22 | A | 821 | CLA | C3D-C4D-ND | 3.95 | 116.63 | 110.24 |
| 22 | 4 | 611 | CLA | C1D-CHD-C4C | -3.95 | 117.55 | 126.06 |
| 25 | 8 | 619 | BCR | C16-C17-C18 | -3.94 | 121.68 | 127.31 |
| 22 | 3 | 603 | CLA | C3C-C4C-NC | 3.94 | 114.99 | 110.57 |
| 22 | 6 | 603 | CLA | C3C-C4C-NC | 3.94 | 114.99 | 110.57 |
| 22 | A | 827 | CLA | CAA-C2A-C3A | -3.94 | 101.98 | 112.78 |
| 22 | Z | 609 | CLA | C3D-C4D-ND | 3.94 | 116.61 | 110.24 |
| 22 | Z | 616 | CLA | C3D-C4D-ND | 3.94 | 116.61 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 1 | 609 | CLA | CAA-C2A-C3A | -3.94 | 101.99 | 112.78 |
| 22 | L | 203 | CLA | C3C-C4C-NC | 3.94 | 114.99 | 110.57 |
| 25 | B | 845 | BCR | C3-C4-C5 | -3.94 | 107.04 | 114.08 |
| 22 | 5 | 609 | CLA | C3C-C4C-NC | 3.94 | 114.99 | 110.57 |
| 22 | 9 | 611 | CLA | C3D-C4D-ND | 3.94 | 116.61 | 110.24 |
| 22 | F | 301 | CLA | C3C-C4C-NC | 3.93 | 114.98 | 110.57 |
| 22 | 4 | 613 | CLA | C1D-CHD-C4C | -3.93 | 117.57 | 126.06 |
| 22 | 8 | 610 | CLA | C3C-C4C-NC | 3.93 | 114.98 | 110.57 |
| 22 | A | 834 | CLA | CAA-C2A-C3A | -3.93 | 102.01 | 112.78 |
| 22 | 3 | 602 | CLA | C4A-NA-C1A | -3.93 | 104.94 | 106.71 |
| 22 | 4 | 610 | CLA | C3D-C4D-ND | 3.93 | 116.60 | 110.24 |
| 22 | 7 | 614 | CLA | C3D-C4D-ND | 3.93 | 116.60 | 110.24 |
| 22 | 9 | 614 | CLA | C1C-C2C-C3C | -3.93 | 102.82 | 106.96 |
| 22 | 1 | 603 | CLA | C1D-CHD-C4C | -3.93 | 117.58 | 126.06 |
| 22 | 1 | 614 | CLA | C1C-C2C-C3C | -3.93 | 102.82 | 106.96 |
| 22 | 5 | 606 | CLA | C1C-C2C-C3C | -3.93 | 102.82 | 106.96 |
| 22 | 6 | 603 | CLA | C1C-C2C-C3C | -3.93 | 102.83 | 106.96 |
| 22 | 4 | 612 | CLA | C3C-C4C-NC | 3.93 | 114.98 | 110.57 |
| 29 | 9 | 607 | CHL | C1D-CHD-C4C | -3.93 | 117.58 | 126.06 |
| 22 | 8 | 608 | CLA | CMC-C2C-C1C | 3.93 | 131.02 | 125.04 |
| 22 | 8 | 603 | CLA | C1C-C2C-C3C | -3.93 | 102.83 | 106.96 |
| 22 | F | 304 | CLA | C3C-C4C-NC | 3.93 | 114.97 | 110.57 |
| 22 | G | 203 | CLA | C3C-C4C-NC | 3.93 | 114.97 | 110.57 |
| 22 | K | 4003 | CLA | C3C-C4C-NC | 3.93 | 114.97 | 110.57 |
| 29 | 6 | 618 | CHL | C1D-CHD-C4C | -3.92 | 117.59 | 126.06 |
| 22 | Z | 616 | CLA | C3C-C4C-NC | 3.92 | 114.97 | 110.57 |
| 22 | 1 | 608 | CLA | C3C-C4C-NC | 3.92 | 114.97 | 110.57 |
| 22 | 6 | 610 | CLA | C1D-CHD-C4C | -3.92 | 117.59 | 126.06 |
| 22 | 4 | 603 | CLA | C1D-CHD-C4C | -3.92 | 117.60 | 126.06 |
| 22 | 3 | 603 | CLA | C1C-C2C-C3C | -3.92 | 102.83 | 106.96 |
| 22 | 2 | 603 | CLA | C1D-CHD-C4C | -3.92 | 117.60 | 126.06 |
| 22 | Z | 611 | CLA | C4A-NA-C1A | -3.92 | 104.94 | 106.71 |
| 22 | B | 824 | CLA | C4A-NA-C1A | -3.92 | 104.94 | 106.71 |
| 22 | 5 | 604 | CLA | C4A-NA-C1A | -3.92 | 104.94 | 106.71 |
| 22 | A | 838 | CLA | C3C-C4C-NC | 3.92 | 114.96 | 110.57 |
| 22 | 8 | 601 | CLA | C3C-C4C-NC | 3.92 | 114.96 | 110.57 |
| 22 | A | 826 | CLA | C3D-C4D-ND | 3.92 | 116.57 | 110.24 |
| 29 | 5 | 618 | CHL | C3C-C4C-NC | 3.92 | 114.96 | 110.57 |
| 25 | 7 | 623 | BCR | C27-C26-C25 | -3.91 | 117.05 | 122.73 |
| 22 | A | 803 | CLA | C1D-CHD-C4C | -3.91 | 117.62 | 126.06 |
| 22 | F | 303 | CLA | C3D-C4D-ND | 3.91 | 116.56 | 110.24 |
| 25 | A | 850 | BCR | C28-C27-C26 | -3.91 | 107.09 | 114.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 602 | CLA | C3C-C4C-NC | 3.91 | 114.95 | 110.57 |
| 22 | B | 804 | CLA | C3D-C4D-ND | 3.91 | 116.56 | 110.24 |
| 25 | J | 3003 | BCR | C20-C21-C22 | -3.91 | 121.73 | 127.31 |
| 22 | L | 203 | CLA | C4A-NA-C1A | -3.91 | 104.95 | 106.71 |
| 22 | B | 809 | CLA | C3D-C4D-ND | 3.91 | 116.56 | 110.24 |
| 22 | 6 | 603 | CLA | C3D-C4D-ND | 3.91 | 116.56 | 110.24 |
| 22 | A | 804 | CLA | CAA-C2A-C3A | -3.91 | 102.08 | 112.78 |
| 22 | 7 | 603 | CLA | C1D-CHD-C4C | -3.91 | 117.63 | 126.06 |
| 29 | 4 | 608 | CHL | C1D-CHD-C4C | -3.91 | 117.63 | 126.06 |
| 22 | 5 | 621 | CLA | CAC-C3C-C4C | 3.91 | 129.88 | 124.81 |
| 22 | A | 823 | CLA | C4A-NA-C1A | -3.90 | 104.95 | 106.71 |
| 22 | 5 | 602 | CLA | C1D-CHD-C4C | -3.90 | 117.64 | 126.06 |
| 22 | A | 842 | CLA | C1C-C2C-C3C | -3.90 | 102.85 | 106.96 |
| 22 | A | 810 | CLA | C1D-CHD-C4C | -3.90 | 117.64 | 126.06 |
| 30 | 1 | 619 | LUT | C35-C34-C33 | -3.90 | 121.74 | 127.31 |
| 22 | B | 828 | CLA | C3C-C4C-NC | 3.90 | 114.95 | 110.57 |
| 22 | 7 | 609 | CLA | C4A-NA-C1A | -3.90 | 104.95 | 106.71 |
| 22 | 3 | 609 | CLA | O2D-CGD-CBD | 3.90 | 118.20 | 111.27 |
| 22 | B | 813 | CLA | C3D-C4D-ND | 3.90 | 116.55 | 110.24 |
| 22 | 1 | 611 | CLA | C1D-CHD-C4C | -3.90 | 117.65 | 126.06 |
| 22 | B | 816 | CLA | C3D-C4D-ND | 3.90 | 116.54 | 110.24 |
| 22 | 6 | 604 | CLA | C3C-C4C-NC | 3.90 | 114.94 | 110.57 |
| 22 | 3 | 607 | CLA | C1D-CHD-C4C | -3.90 | 117.65 | 126.06 |
| 22 | 9 | 612 | CLA | C3C-C4C-NC | 3.90 | 114.94 | 110.57 |
| 25 | A | 849 | BCR | C15-C14-C13 | -3.90 | 121.75 | 127.31 |
| 22 | B | 828 | CLA | C1D-CHD-C4C | -3.90 | 117.65 | 126.06 |
| 22 | B | 807 | CLA | C1C-C2C-C3C | -3.90 | 102.86 | 106.96 |
| 22 | 7 | 611 | CLA | C1C-C2C-C3C | -3.90 | 102.86 | 106.96 |
| 22 | 5 | 603 | CLA | C1C-C2C-C3C | -3.89 | 102.86 | 106.96 |
| 22 | B | 826 | CLA | C3D-C4D-ND | 3.89 | 116.54 | 110.24 |
| 29 | 4 | 606 | CHL | C1D-CHD-C4C | -3.89 | 117.66 | 126.06 |
| 22 | B | 811 | CLA | C1D-CHD-C4C | -3.89 | 117.66 | 126.06 |
| 22 | 1 | 616 | CLA | C1D-CHD-C4C | -3.89 | 117.66 | 126.06 |
| 22 | B | 823 | CLA | C3D-C4D-ND | 3.89 | 116.53 | 110.24 |
| 22 | 3 | 611 | CLA | C3D-C4D-ND | 3.89 | 116.53 | 110.24 |
| 22 | 1 | 608 | CLA | C1C-C2C-C3C | -3.89 | 102.87 | 106.96 |
| 22 | 3 | 611 | CLA | C1C-C2C-C3C | -3.89 | 102.87 | 106.96 |
| 22 | A | 817 | CLA | C1D-CHD-C4C | -3.89 | 117.67 | 126.06 |
| 22 | 1 | 609 | CLA | C1D-CHD-C4C | -3.89 | 117.67 | 126.06 |
| 22 | 5 | 613 | CLA | C1D-CHD-C4C | -3.89 | 117.67 | 126.06 |
| 22 | B | 835 | CLA | C3C-C4C-NC | 3.89 | 114.93 | 110.57 |
| 22 | 3 | 607 | CLA | C3C-C4C-NC | 3.89 | 114.93 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 817 | CLA | C3D-C4D-ND | 3.88 | 116.52 | 110.24 |
| 25 | B | 846 | BCR | C3-C4-C5 | -3.88 | 107.14 | 114.08 |
| 22 | 7 | 610 | CLA | O2A-CGA-CBA | 3.88 | 124.09 | 111.91 |
| 22 | 1 | 612 | CLA | C1C-C2C-C3C | -3.88 | 102.87 | 106.96 |
| 25 | 8 | 619 | BCR | C28-C27-C26 | -3.88 | 107.14 | 114.08 |
| 22 | 6 | 612 | CLA | C1C-C2C-C3C | -3.88 | 102.88 | 106.96 |
| 22 | A | 819 | CLA | C3D-C4D-ND | 3.88 | 116.52 | 110.24 |
| 22 | 2 | 609 | CLA | C3D-C4D-ND | 3.88 | 116.51 | 110.24 |
| 22 | B | 852 | CLA | C1D-CHD-C4C | -3.88 | 117.69 | 126.06 |
| 22 | A | 839 | CLA | C3C-C4C-NC | 3.88 | 114.92 | 110.57 |
| 22 | 4 | 616 | CLA | C1D-CHD-C4C | -3.88 | 117.70 | 126.06 |
| 22 | B | 823 | CLA | C3C-C4C-NC | 3.88 | 114.92 | 110.57 |
| 22 | G | 203 | CLA | C1D-CHD-C4C | -3.88 | 117.70 | 126.06 |
| 22 | 4 | 610 | CLA | C1D-CHD-C4C | -3.88 | 117.70 | 126.06 |
| 22 | A | 839 | CLA | C1D-CHD-C4C | -3.88 | 117.70 | 126.06 |
| 22 | Z | 602 | CLA | C3C-C4C-NC | 3.88 | 114.92 | 110.57 |
| 22 | B | 806 | CLA | C3D-C4D-ND | 3.87 | 116.50 | 110.24 |
| 22 | 4 | 611 | CLA | C1C-C2C-C3C | -3.87 | 102.88 | 106.96 |
| 29 | 9 | 606 | CHL | C3C-C4C-NC | 3.87 | 114.92 | 110.57 |
| 22 | 3 | 606 | CLA | C1D-CHD-C4C | -3.87 | 117.70 | 126.06 |
| 22 | A | 830 | CLA | C1D-CHD-C4C | -3.87 | 117.70 | 126.06 |
| 29 | 7 | 607 | CHL | C3C-C4C-NC | 3.87 | 114.91 | 110.57 |
| 22 | 4 | 614 | CLA | C3C-C4C-NC | 3.87 | 114.91 | 110.57 |
| 22 | A | 836 | CLA | C1D-CHD-C4C | -3.87 | 117.71 | 126.06 |
| 22 | 9 | 611 | CLA | C1D-CHD-C4C | -3.87 | 117.71 | 126.06 |
| 22 | 3 | 607 | CLA | C1C-C2C-C3C | -3.87 | 102.89 | 106.96 |
| 22 | 5 | 609 | CLA | C1C-C2C-C3C | -3.87 | 102.89 | 106.96 |
| 25 | K | 4004 | BCR | C20-C21-C22 | -3.87 | 121.79 | 127.31 |
| 22 | 8 | 616 | CLA | C3D-C2D-C1D | -3.87 | 100.55 | 105.83 |
| 25 | 3 | 719 | BCR | C3-C4-C5 | -3.87 | 107.17 | 114.08 |
| 22 | Z | 608 | CLA | C3C-C4C-NC | 3.87 | 114.91 | 110.57 |
| 22 | 9 | 601 | CLA | C1C-C2C-C3C | -3.87 | 102.89 | 106.96 |
| 22 | B | 836 | CLA | C3B-C4B-NB | 3.87 | 114.21 | 109.21 |
| 25 | B | 844 | BCR | C24-C23-C22 | -3.87 | 120.39 | 126.23 |
| 22 | B | 824 | CLA | C3C-C4C-NC | 3.86 | 114.91 | 110.57 |
| 22 | Z | 611 | CLA | C3C-C4C-NC | 3.86 | 114.91 | 110.57 |
| 22 | 5 | 601 | CLA | C3C-C4C-NC | 3.86 | 114.91 | 110.57 |
| 22 | B | 836 | CLA | C1D-CHD-C4C | -3.86 | 117.72 | 126.06 |
| 22 | 1 | 606 | CLA | C1D-CHD-C4C | -3.86 | 117.72 | 126.06 |
| 22 | A | 807 | CLA | C3C-C4C-NC | 3.86 | 114.90 | 110.57 |
| 22 | B | 834 | CLA | CMA-C3A-C4A | -3.86 | 101.39 | 111.77 |
| 22 | B | 822 | CLA | C3C-C4C-NC | 3.86 | 114.90 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24 | Z | 620 | LHG | O7-C7-C8 | 3.86 | 119.82 | 111.50 |
| 25 | 6 | 625 | BCR | C28-C27-C26 | -3.86 | 107.18 | 114.08 |
| 29 | 4 | 618 | CHL | C1D-CHD-C4C | -3.86 | 117.73 | 126.06 |
| 22 | 5 | 609 | CLA | C1-C2-C3 | -3.86 | 120.51 | 126.75 |
| 22 | 7 | 606 | CLA | CAA-C2A-C3A | -3.86 | 104.62 | 114.26 |
| 22 | 5 | 616 | CLA | C1C-C2C-C3C | -3.86 | 102.90 | 106.96 |
| 22 | B | 831 | CLA | C2C-C1C-NC | 3.86 | 113.59 | 109.97 |
| 22 | 1 | 611 | CLA | C1C-C2C-C3C | -3.86 | 102.90 | 106.96 |
| 22 | 8 | 610 | CLA | CAA-C2A-C3A | -3.86 | 102.22 | 112.78 |
| 22 | A | 822 | CLA | C3D-C4D-ND | 3.86 | 116.47 | 110.24 |
| 29 | 4 | 607 | CHL | C1D-CHD-C4C | -3.85 | 117.74 | 126.06 |
| 22 | 8 | 608 | CLA | C3D-C4D-ND | 3.85 | 116.47 | 110.24 |
| 22 | A | 808 | CLA | C1C-C2C-C3C | -3.85 | 102.91 | 106.96 |
| 30 | 4 | 620 | LUT | C35-C34-C33 | -3.85 | 121.81 | 127.31 |
| 22 | 5 | 610 | CLA | C1D-CHD-C4C | -3.85 | 117.75 | 126.06 |
| 29 | 5 | 607 | CHL | C2A-C3A-C4A | -3.85 | 95.65 | 101.87 |
| 22 | Z | 604 | CLA | C1C-C2C-C3C | -3.85 | 102.91 | 106.96 |
| 22 | Z | 614 | CLA | C1C-C2C-C3C | -3.85 | 102.91 | 106.96 |
| 22 | 6 | 617 | CLA | C1D-CHD-C4C | -3.85 | 117.75 | 126.06 |
| 22 | 4 | 611 | CLA | C3D-C4D-ND | 3.85 | 116.47 | 110.24 |
| 22 | 9 | 603 | CLA | C3C-C4C-NC | 3.85 | 114.89 | 110.57 |
| 22 | 4 | 604 | CLA | C1C-C2C-C3C | -3.85 | 102.91 | 106.96 |
| 22 | B | 835 | CLA | C3D-C4D-ND | 3.85 | 116.46 | 110.24 |
| 22 | 2 | 613 | CLA | C1C-C2C-C3C | -3.85 | 102.91 | 106.96 |
| 29 | 9 | 606 | CHL | C1D-CHD-C4C | -3.85 | 117.76 | 126.06 |
| 22 | 9 | 610 | CLA | C1D-CHD-C4C | -3.84 | 117.76 | 126.06 |
| 22 | B | 803 | CLA | C3C-C4C-NC | 3.84 | 114.88 | 110.57 |
| 22 | 6 | 602 | CLA | C1D-CHD-C4C | -3.84 | 117.77 | 126.06 |
| 22 | B | 828 | CLA | C3D-C2D-C1D | -3.84 | 100.59 | 105.83 |
| 22 | B | 821 | CLA | C4A-NA-C1A | -3.84 | 104.98 | 106.71 |
| 22 | 9 | 611 | CLA | C1C-C2C-C3C | -3.84 | 102.92 | 106.96 |
| 22 | J | 3002 | CLA | C1D-CHD-C4C | -3.84 | 117.78 | 126.06 |
| 22 | 6 | 616 | CLA | C1D-CHD-C4C | -3.84 | 117.78 | 126.06 |
| 22 | A | 812 | CLA | C1C-C2C-C3C | -3.84 | 102.92 | 106.96 |
| 22 | 3 | 610 | CLA | C1D-CHD-C4C | -3.84 | 117.78 | 126.06 |
| 22 | A | 825 | CLA | C1C-C2C-C3C | -3.84 | 102.92 | 106.96 |
| 22 | 5 | 614 | CLA | C1D-CHD-C4C | -3.84 | 117.78 | 126.06 |
| 22 | Z | 610 | CLA | O2A-CGA-CBA | 3.84 | 123.94 | 111.91 |
| 22 | B | 827 | CLA | C3D-C4D-ND | 3.84 | 116.44 | 110.24 |
| 22 | 6 | 609 | CLA | C3D-C4D-ND | 3.84 | 116.44 | 110.24 |
| 22 | 1 | 604 | CLA | C1C-C2C-C3C | -3.83 | 102.92 | 106.96 |
| 24 | 6 | 619 | LHG | O7-C7-C8 | 3.83 | 119.76 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 804 | CLA | CMB-C2B-C3B | 3.83 | 131.85 | 124.68 |
| 22 | 6 | 604 | CLA | C1C-C2C-C3C | -3.83 | 102.93 | 106.96 |
| 22 | 7 | 602 | CLA | C1D-CHD-C4C | -3.83 | 117.79 | 126.06 |
| 22 | B | 836 | CLA | C3C-C4C-NC | 3.83 | 114.87 | 110.57 |
| 22 | B | 837 | CLA | C3C-C4C-NC | 3.83 | 114.87 | 110.57 |
| 22 | B | 805 | CLA | C3D-C4D-ND | 3.83 | 116.43 | 110.24 |
| 22 | 2 | 613 | CLA | C1D-CHD-C4C | -3.83 | 117.80 | 126.06 |
| 22 | F | 303 | CLA | O2D-CGD-CBD | 3.83 | 118.07 | 111.27 |
| 22 | 8 | 613 | CLA | C4A-NA-C1A | -3.83 | 104.98 | 106.71 |
| 22 | 7 | 603 | CLA | C1C-C2C-C3C | -3.83 | 102.93 | 106.96 |
| 22 | Z | 611 | CLA | C1D-CHD-C4C | -3.83 | 117.80 | 126.06 |
| 22 | 1 | 603 | CLA | C3B-C4B-NB | 3.83 | 114.16 | 109.21 |
| 22 | B | 808 | CLA | C1C-C2C-C3C | -3.83 | 102.93 | 106.96 |
| 22 | 3 | 602 | CLA | C1D-CHD-C4C | -3.83 | 117.81 | 126.06 |
| 22 | A | 831 | CLA | C3D-C4D-ND | 3.82 | 116.42 | 110.24 |
| 22 | A | 824 | CLA | C1C-C2C-C3C | -3.82 | 102.94 | 106.96 |
| 22 | L | 203 | CLA | C1C-C2C-C3C | -3.82 | 102.94 | 106.96 |
| 29 | 4 | 607 | CHL | CBC-CAC-C3C | -3.82 | 101.89 | 112.43 |
| 22 | 4 | 602 | CLA | C1D-CHD-C4C | -3.82 | 117.81 | 126.06 |
| 22 | A | 820 | CLA | C3C-C4C-NC | 3.82 | 114.86 | 110.57 |
| 22 | B | 818 | CLA | C1D-CHD-C4C | -3.82 | 117.82 | 126.06 |
| 22 | 5 | 604 | CLA | CAC-C3C-C4C | 3.82 | 129.77 | 124.81 |
| 22 | 7 | 601 | CLA | C1D-CHD-C4C | -3.82 | 117.82 | 126.06 |
| 22 | 1 | 613 | CLA | C3C-C4C-NC | 3.82 | 114.86 | 110.57 |
| 22 | 9 | 613 | CLA | C1D-CHD-C4C | -3.82 | 117.82 | 126.06 |
| 22 | A | 803 | CLA | CMB-C2B-C3B | 3.82 | 131.82 | 124.68 |
| 22 | 1 | 609 | CLA | O2D-CGD-CBD | 3.82 | 118.05 | 111.27 |
| 22 | A | 843 | CLA | C3D-C4D-ND | 3.82 | 116.41 | 110.24 |
| 22 | 3 | 612 | CLA | C3C-C4C-NC | 3.81 | 114.85 | 110.57 |
| 22 | Z | 606 | CLA | C1D-CHD-C4C | -3.81 | 117.83 | 126.06 |
| 22 | 9 | 613 | CLA | C1C-C2C-C3C | -3.81 | 102.95 | 106.96 |
| 22 | A | 820 | CLA | C1D-CHD-C4C | -3.81 | 117.83 | 126.06 |
| 22 | 1 | 611 | CLA | C3C-C4C-NC | 3.81 | 114.85 | 110.57 |
| 22 | 3 | 617 | CLA | C1C-C2C-C3C | -3.81 | 102.95 | 106.96 |
| 29 | Z | 607 | CHL | CHD-C1D-ND | -3.81 | 120.95 | 124.45 |
| 22 | 9 | 601 | CLA | C1D-CHD-C4C | -3.81 | 117.84 | 126.06 |
| 29 | 6 | 608 | CHL | C1D-CHD-C4C | -3.81 | 117.84 | 126.06 |
| 22 | 4 | 601 | CLA | C3B-C4B-NB | 3.81 | 114.14 | 109.21 |
| 22 | 2 | 614 | CLA | C3C-C4C-NC | 3.81 | 114.84 | 110.57 |
| 22 | 4 | 613 | CLA | C4A-NA-C1A | -3.81 | 104.99 | 106.71 |
| 29 | 6 | 608 | CHL | C2C-C3C-C4C | -3.81 | 103.78 | 106.49 |
| 22 | Z | 608 | CLA | C1D-CHD-C4C | -3.81 | 117.84 | 126.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 606 | CLA | C1D-CHD-C4C | -3.81 | 117.85 | 126.06 |
| 29 | 8 | 607 | CHL | CHD-C1D-ND | -3.81 | 120.96 | 124.45 |
| 22 | B | 833 | CLA | C1D-CHD-C4C | -3.81 | 117.85 | 126.06 |
| 22 | A | 820 | CLA | C3B-C4B-NB | 3.81 | 114.13 | 109.21 |
| 22 | A | 843 | CLA | C1D-CHD-C4C | -3.81 | 117.85 | 126.06 |
| 22 | B | 811 | CLA | C1C-C2C-C3C | -3.81 | 102.96 | 106.96 |
| 22 | 2 | 606 | CLA | C1C-C2C-C3C | -3.81 | 102.96 | 106.96 |
| 22 | J | 3002 | CLA | C1C-C2C-C3C | -3.80 | 102.96 | 106.96 |
| 22 | A | 839 | CLA | C1-C2-C3 | -3.80 | 119.46 | 126.04 |
| 22 | 7 | 612 | CLA | C3C-C4C-NC | 3.80 | 114.84 | 110.57 |
| 22 | B | 835 | CLA | C1D-CHD-C4C | -3.80 | 117.86 | 126.06 |
| 22 | 7 | 608 | CLA | C1C-C2C-C3C | -3.80 | 102.96 | 106.96 |
| 22 | 9 | 609 | CLA | C1C-C2C-C3C | -3.80 | 102.96 | 106.96 |
| 22 | B | 839 | CLA | C1D-CHD-C4C | -3.80 | 117.87 | 126.06 |
| 22 | 5 | 604 | CLA | C1D-CHD-C4C | -3.80 | 117.87 | 126.06 |
| 22 | Z | 610 | CLA | C2C-C1C-NC | 3.79 | 113.53 | 109.97 |
| 22 | B | 812 | CLA | C1D-CHD-C4C | -3.79 | 117.87 | 126.06 |
| 29 | Z | 601 | CHL | CHD-C1D-ND | -3.79 | 120.97 | 124.45 |
| 22 | 2 | 613 | CLA | C3C-C4C-NC | 3.79 | 114.83 | 110.57 |
| 22 | F | 301 | CLA | C3D-C4D-ND | 3.79 | 116.37 | 110.24 |
| 22 | 4 | 614 | CLA | C1D-CHD-C4C | -3.79 | 117.88 | 126.06 |
| 22 | A | 833 | CLA | C3C-C4C-NC | 3.79 | 114.83 | 110.57 |
| 22 | 7 | 608 | CLA | C1D-CHD-C4C | -3.79 | 117.88 | 126.06 |
| 22 | A | 837 | CLA | C3D-C4D-ND | 3.79 | 116.37 | 110.24 |
| 22 | 6 | 616 | CLA | C3B-C4B-NB | 3.79 | 114.11 | 109.21 |
| 22 | B | 832 | CLA | C1D-CHD-C4C | -3.79 | 117.88 | 126.06 |
| 22 | 2 | 601 | CLA | C1C-C2C-C3C | -3.79 | 102.97 | 106.96 |
| 22 | 7 | 606 | CLA | C1C-C2C-C3C | -3.79 | 102.97 | 106.96 |
| 22 | 3 | 617 | CLA | C1D-CHD-C4C | -3.79 | 117.89 | 126.06 |
| 22 | 8 | 609 | CLA | C3D-C4D-ND | 3.79 | 116.37 | 110.24 |
| 22 | 6 | 611 | CLA | C1D-CHD-C4C | -3.79 | 117.89 | 126.06 |
| 22 | 9 | 601 | CLA | C3C-C4C-NC | 3.79 | 114.82 | 110.57 |
| 22 | B | 821 | CLA | C1D-CHD-C4C | -3.79 | 117.89 | 126.06 |
| 22 | 7 | 610 | CLA | CAA-C2A-C3A | -3.79 | 102.41 | 112.78 |
| 22 | 9 | 609 | CLA | C3D-C4D-ND | 3.79 | 116.36 | 110.24 |
| 22 | A | 834 | CLA | C3C-C4C-NC | 3.79 | 114.82 | 110.57 |
| 22 | A | 843 | CLA | CAC-C3C-C4C | 3.79 | 129.72 | 124.81 |
| 22 | A | 807 | CLA | C1D-CHD-C4C | -3.78 | 117.89 | 126.06 |
| 22 | B | 821 | CLA | C3C-C4C-NC | 3.78 | 114.81 | 110.57 |
| 22 | 3 | 617 | CLA | C3C-C4C-NC | 3.78 | 114.81 | 110.57 |
| 25 | 5 | 622 | BCR | C16-C17-C18 | -3.78 | 121.91 | 127.31 |
| 21 | A | 801 | CL0 | C3D-C4D-ND | 3.78 | 116.36 | 110.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 9 | 612 | CLA | C1D-CHD-C4C | -3.78 | 117.90 | 126.06 |
| 22 | A | 827 | CLA | C1D-CHD-C4C | -3.78 | 117.90 | 126.06 |
| 22 | 5 | 621 | CLA | C1D-CHD-C4C | -3.78 | 117.91 | 126.06 |
| 22 | 4 | 602 | CLA | C1C-C2C-C3C | -3.78 | 102.98 | 106.96 |
| 22 | A | 826 | CLA | C1D-CHD-C4C | -3.78 | 117.91 | 126.06 |
| 22 | 5 | 611 | CLA | C1D-CHD-C4C | -3.78 | 117.91 | 126.06 |
| 22 | 1 | 616 | CLA | C3C-C4C-NC | 3.78 | 114.81 | 110.57 |
| 22 | 5 | 602 | CLA | C3C-C4C-NC | 3.78 | 114.81 | 110.57 |
| 30 | Z | 619 | LUT | C35-C34-C33 | -3.78 | 121.92 | 127.31 |
| 22 | A | 832 | CLA | C1D-CHD-C4C | -3.77 | 117.92 | 126.06 |
| 22 | 2 | 612 | CLA | C3C-C4C-NC | 3.77 | 114.80 | 110.57 |
| 22 | 8 | 611 | CLA | CAC-C3C-C4C | 3.77 | 129.70 | 124.81 |
| 25 | 7 | 624 | BCR | C15-C14-C13 | -3.77 | 121.93 | 127.31 |
| 22 | A | 840 | CLA | C3D-C4D-ND | 3.77 | 116.34 | 110.24 |
| 22 | 8 | 609 | CLA | C1D-CHD-C4C | -3.77 | 117.92 | 126.06 |
| 22 | A | 804 | CLA | C3C-C4C-NC | 3.77 | 114.80 | 110.57 |
| 22 | B | 815 | CLA | C3C-C4C-NC | 3.77 | 114.80 | 110.57 |
| 22 | G | 203 | CLA | C1C-C2C-C3C | -3.77 | 102.99 | 106.96 |
| 22 | 1 | 614 | CLA | C1D-CHD-C4C | -3.77 | 117.93 | 126.06 |
| 22 | 2 | 611 | CLA | C1C-C2C-C3C | -3.77 | 103.00 | 106.96 |
| 22 | 3 | 603 | CLA | C1D-CHD-C4C | -3.77 | 117.93 | 126.06 |
| 24 | 7 | 625 | LHG | O7-C7-C8 | 3.77 | 119.62 | 111.50 |
| 22 | Z | 616 | CLA | C1D-CHD-C4C | -3.77 | 117.93 | 126.06 |
| 22 | 5 | 606 | CLA | C1D-CHD-C4C | -3.77 | 117.93 | 126.06 |
| 22 | 9 | 604 | CLA | C4A-NA-C1A | -3.77 | 105.01 | 106.71 |
| 22 | 8 | 606 | CLA | C3C-C4C-NC | 3.77 | 114.79 | 110.57 |
| 22 | F | 303 | CLA | C3C-C4C-NC | 3.76 | 114.79 | 110.57 |
| 22 | B | 806 | CLA | C1C-C2C-C3C | -3.76 | 103.00 | 106.96 |
| 22 | 7 | 612 | CLA | C1C-C2C-C3C | -3.76 | 103.00 | 106.96 |
| 22 | 5 | 609 | CLA | C3D-C4D-ND | 3.76 | 116.33 | 110.24 |
| 22 | 7 | 613 | CLA | C3B-C4B-NB | 3.76 | 114.07 | 109.21 |
| 22 | 7 | 601 | CLA | C1C-C2C-C3C | -3.76 | 103.00 | 106.96 |
| 22 | A | 823 | CLA | C3C-C4C-NC | 3.76 | 114.79 | 110.57 |
| 22 | 9 | 613 | CLA | C3C-C4C-NC | 3.76 | 114.79 | 110.57 |
| 22 | B | 807 | CLA | C4A-NA-C1A | -3.76 | 105.02 | 106.71 |
| 22 | 7 | 613 | CLA | C1C-C2C-C3C | -3.76 | 103.00 | 106.96 |
| 22 | 5 | 612 | CLA | C1C-C2C-C3C | -3.76 | 103.00 | 106.96 |
| 25 | B | 844 | BCR | C28-C27-C26 | -3.76 | 107.37 | 114.08 |
| 24 | 4 | 623 | LHG | O7-C7-C8 | 3.76 | 119.60 | 111.50 |
| 22 | B | 809 | CLA | C1D-CHD-C4C | -3.76 | 117.95 | 126.06 |
| 22 | 9 | 602 | CLA | C1D-CHD-C4C | -3.76 | 117.95 | 126.06 |
| 22 | 3 | 611 | CLA | C1D-CHD-C4C | -3.76 | 117.95 | 126.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 4 | 616 | CLA | C3B-C4B-NB | 3.76 | 114.07 | 109.21 |
| 22 | 1 | 608 | CLA | C1D-CHD-C4C | -3.76 | 117.96 | 126.06 |
| 22 | A | 836 | CLA | C4A-NA-C1A | -3.75 | 105.02 | 106.71 |
| 22 | A | 814 | CLA | C3B-C4B-NB | 3.75 | 114.06 | 109.21 |
| 22 | 8 | 608 | CLA | C3C-C4C-NC | 3.75 | 114.78 | 110.57 |
| 22 | B | 803 | CLA | C3D-C4D-ND | 3.75 | 116.31 | 110.24 |
| 22 | 5 | 601 | CLA | C1D-CHD-C4C | -3.75 | 117.96 | 126.06 |
| 25 | K | 4004 | BCR | C24-C23-C22 | -3.75 | 120.57 | 126.23 |
| 29 | 4 | 607 | CHL | C3C-C4C-NC | 3.75 | 114.78 | 110.57 |
| 22 | 3 | 614 | CLA | C1D-CHD-C4C | -3.75 | 117.97 | 126.06 |
| 22 | 4 | 610 | CLA | O2A-CGA-CBA | 3.75 | 123.67 | 111.91 |
| 22 | 8 | 609 | CLA | C3C-C4C-NC | 3.75 | 114.77 | 110.57 |
| 22 | B | 833 | CLA | C3B-C4B-NB | 3.75 | 114.05 | 109.21 |
| 22 | 9 | 610 | CLA | C3C-C4C-NC | 3.75 | 114.77 | 110.57 |
| 22 | 3 | 609 | CLA | C1D-CHD-C4C | -3.75 | 117.98 | 126.06 |
| 22 | 8 | 610 | CLA | C3D-C4D-ND | 3.75 | 116.30 | 110.24 |
| 22 | 5 | 611 | CLA | C3D-C4D-ND | 3.75 | 116.30 | 110.24 |
| 22 | B | 821 | CLA | C1C-C2C-C3C | -3.75 | 103.02 | 106.96 |
| 22 | A | 842 | CLA | C4A-NA-C1A | -3.74 | 105.02 | 106.71 |
| 29 | 1 | 601 | CHL | C1D-CHD-C4C | -3.74 | 117.98 | 126.06 |
| 29 | 5 | 607 | CHL | C3C-C4C-NC | 3.74 | 114.77 | 110.57 |
| 22 | 3 | 609 | CLA | CAA-C2A-C3A | -3.74 | 102.53 | 112.78 |
| 22 | B | 807 | CLA | C1D-CHD-C4C | -3.74 | 117.99 | 126.06 |
| 22 | 1 | 616 | CLA | C1C-C2C-C3C | -3.74 | 103.02 | 106.96 |
| 22 | Z | 603 | CLA | C3B-C4B-NB | 3.74 | 114.05 | 109.21 |
| 22 | A | 854 | CLA | C1D-CHD-C4C | -3.74 | 117.99 | 126.06 |
| 22 | 2 | 607 | CLA | C1D-CHD-C4C | -3.74 | 117.99 | 126.06 |
| 22 | 1 | 602 | CLA | C3C-C4C-NC | 3.74 | 114.76 | 110.57 |
| 22 | Z | 603 | CLA | C1D-CHD-C4C | -3.73 | 118.00 | 126.06 |
| 22 | 2 | 610 | CLA | C1D-CHD-C4C | -3.73 | 118.00 | 126.06 |
| 22 | K | 4002 | CLA | C1C-C2C-C3C | -3.73 | 103.03 | 106.96 |
| 22 | B | 803 | CLA | C4C-C3C-C2C | -3.73 | 101.46 | 106.90 |
| 22 | B | 806 | CLA | C1D-CHD-C4C | -3.73 | 118.01 | 126.06 |
| 22 | 7 | 620 | CLA | C1D-CHD-C4C | -3.73 | 118.01 | 126.06 |
| 22 | 4 | 612 | CLA | C1C-C2C-C3C | -3.73 | 103.03 | 106.96 |
| 22 | 9 | 604 | CLA | C1C-C2C-C3C | -3.73 | 103.03 | 106.96 |
| 22 | B | 817 | CLA | C1C-C2C-C3C | -3.73 | 103.04 | 106.96 |
| 22 | 3 | 614 | CLA | C1C-C2C-C3C | -3.73 | 103.04 | 106.96 |
| 22 | 4 | 601 | CLA | C1C-C2C-C3C | -3.73 | 103.04 | 106.96 |
| 30 | 5 | 620 | LUT | C18-C5-C6 | -3.73 | 120.34 | 124.53 |
| 22 | 7 | 603 | CLA | C3C-C4C-NC | 3.73 | 114.75 | 110.57 |
| 22 | B | 802 | CLA | CMA-C3A-C4A | -3.73 | 101.75 | 111.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 836 | CLA | C3D-C4D-ND | 3.73 | 116.27 | 110.24 |
| 22 | A | 836 | CLA | C3C-C4C-NC | 3.73 | 114.75 | 110.57 |
| 22 | A | 814 | CLA | CAC-C3C-C4C | 3.72 | 129.64 | 124.81 |
| 22 | 8 | 611 | CLA | C3D-C4D-ND | 3.72 | 116.26 | 110.24 |
| 22 | B | 835 | CLA | C1C-C2C-C3C | -3.72 | 103.04 | 106.96 |
| 22 | 5 | 613 | CLA | C3B-C4B-NB | 3.72 | 114.02 | 109.21 |
| 22 | B | 829 | CLA | CMB-C2B-C1B | 3.72 | 134.19 | 128.46 |
| 25 | B | 847 | BCR | C15-C16-C17 | -3.72 | 115.85 | 123.47 |
| 22 | 4 | 604 | CLA | C1D-CHD-C4C | -3.72 | 118.03 | 126.06 |
| 22 | Z | 609 | CLA | C3B-C4B-NB | 3.72 | 114.02 | 109.21 |
| 22 | 8 | 606 | CLA | C1C-C2C-C3C | -3.72 | 103.05 | 106.96 |
| 22 | B | 818 | CLA | C3D-C4D-ND | 3.72 | 116.25 | 110.24 |
| 22 | 4 | 613 | CLA | C3C-C4C-NC | 3.72 | 114.74 | 110.57 |
| 22 | 6 | 622 | CLA | C4A-NA-C1A | -3.72 | 105.03 | 106.71 |
| 22 | 9 | 611 | CLA | C4A-NA-C1A | -3.72 | 105.03 | 106.71 |
| 22 | 9 | 613 | CLA | C4A-NA-C1A | -3.72 | 105.03 | 106.71 |
| 29 | 4 | 618 | CHL | C3C-C4C-NC | 3.72 | 114.74 | 110.57 |
| 22 | B | 825 | CLA | C3C-C4C-NC | 3.72 | 114.74 | 110.57 |
| 22 | 7 | 620 | CLA | C3C-C4C-NC | 3.72 | 114.74 | 110.57 |
| 22 | B | 830 | CLA | C1D-CHD-C4C | -3.72 | 118.04 | 126.06 |
| 22 | A | 841 | CLA | C1C-C2C-C3C | -3.72 | 103.05 | 106.96 |
| 22 | 1 | 612 | CLA | C3C-C4C-NC | 3.72 | 114.74 | 110.57 |
| 22 | A | 819 | CLA | CAC-C3C-C4C | 3.72 | 129.63 | 124.81 |
| 22 | B | 828 | CLA | C1C-C2C-C3C | -3.72 | 103.05 | 106.96 |
| 22 | 6 | 622 | CLA | C3C-C4C-NC | 3.72 | 114.74 | 110.57 |
| 24 | A | 855 | LHG | O7-C7-C8 | 3.71 | 119.51 | 111.50 |
| 25 | A | 851 | BCR | C11-C10-C9 | -3.71 | 122.01 | 127.31 |
| 22 | 2 | 606 | CLA | C3C-C4C-NC | 3.71 | 114.74 | 110.57 |
| 22 | 2 | 612 | CLA | C1C-C2C-C3C | -3.71 | 103.05 | 106.96 |
| 22 | B | 839 | CLA | C1C-C2C-C3C | -3.71 | 103.05 | 106.96 |
| 22 | 8 | 616 | CLA | C1C-C2C-C3C | -3.71 | 103.05 | 106.96 |
| 22 | 5 | 611 | CLA | C4A-NA-C1A | -3.71 | 105.04 | 106.71 |
| 22 | 5 | 611 | CLA | C3C-C4C-NC | 3.71 | 114.73 | 110.57 |
| 22 | 6 | 613 | CLA | C3C-C4C-NC | 3.71 | 114.73 | 110.57 |
| 25 | 7 | 623 | BCR | C29-C30-C25 | 3.71 | 116.19 | 110.48 |
| 22 | 4 | 609 | CLA | C3C-C4C-NC | 3.71 | 114.73 | 110.57 |
| 22 | 2 | 611 | CLA | C1D-CHD-C4C | -3.71 | 118.05 | 126.06 |
| 22 | B | 808 | CLA | C4A-NA-C1A | -3.71 | 105.04 | 106.71 |
| 22 | 3 | 609 | CLA | C1C-C2C-C3C | -3.71 | 103.06 | 106.96 |
| 22 | B | 813 | CLA | C1D-CHD-C4C | -3.71 | 118.06 | 126.06 |
| 22 | B | 834 | CLA | C1C-C2C-C3C | -3.71 | 103.06 | 106.96 |
| 22 | 6 | 622 | CLA | C1C-C2C-C3C | -3.71 | 103.06 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 5 | 621 | CLA | C3D-C4D-ND | 3.71 | 116.24 | 110.24 |
| 22 | F | 301 | CLA | CAA-C2A-C3A | -3.71 | 102.63 | 112.78 |
| 22 | B | 806 | CLA | O2D-CGD-CBD | 3.71 | 117.86 | 111.27 |
| 25 | 7 | 623 | BCR | C3-C4-C5 | -3.71 | 107.46 | 114.08 |
| 30 | 8 | 617 | LUT | C7-C8-C9 | -3.71 | 120.64 | 126.23 |
| 22 | B | 812 | CLA | C1C-C2C-C3C | -3.71 | 103.06 | 106.96 |
| 22 | 4 | 616 | CLA | CAC-C3C-C4C | 3.70 | 129.62 | 124.81 |
| 22 | 8 | 606 | CLA | O2D-CGD-CBD | 3.70 | 117.85 | 111.27 |
| 25 | B | 801 | BCR | C3-C4-C5 | -3.70 | 107.47 | 114.08 |
| 22 | A | 837 | CLA | C1C-C2C-C3C | -3.70 | 103.06 | 106.96 |
| 21 | A | 801 | CL0 | C3B-C4B-NB | 3.70 | 114.00 | 109.21 |
| 22 | 4 | 603 | CLA | C3B-C4B-NB | 3.70 | 114.00 | 109.21 |
| 22 | 9 | 613 | CLA | C3B-C4B-NB | 3.70 | 114.00 | 109.21 |
| 22 | A | 828 | CLA | CHD-C4C-NC | 3.70 | 130.03 | 124.20 |
| 22 | A | 828 | CLA | C3D-C4D-ND | 3.70 | 116.22 | 110.24 |
| 25 | B | 843 | BCR | C11-C10-C9 | -3.70 | 122.03 | 127.31 |
| 22 | 3 | 620 | CLA | C1D-CHD-C4C | -3.70 | 118.08 | 126.06 |
| 22 | 5 | 616 | CLA | C3D-C4D-ND | 3.70 | 116.22 | 110.24 |
| 22 | B | 814 | CLA | C1C-C2C-C3C | -3.70 | 103.07 | 106.96 |
| 22 | 5 | 614 | CLA | C1C-C2C-C3C | -3.70 | 103.07 | 106.96 |
| 24 | B | 851 | LHG | O7-C7-C8 | 3.69 | 119.46 | 111.50 |
| 22 | B | 822 | CLA | C1C-C2C-C3C | -3.69 | 103.07 | 106.96 |
| 22 | A | 814 | CLA | C4A-NA-C1A | -3.69 | 105.05 | 106.71 |
| 22 | A | 813 | CLA | C1D-CHD-C4C | -3.69 | 118.09 | 126.06 |
| 22 | 5 | 613 | CLA | C1C-C2C-C3C | -3.69 | 103.07 | 106.96 |
| 22 | A | 806 | CLA | C3B-C4B-NB | 3.69 | 113.98 | 109.21 |
| 22 | 5 | 621 | CLA | C3D-C2D-C1D | -3.69 | 100.79 | 105.83 |
| 22 | A | 806 | CLA | C1D-CHD-C4C | -3.69 | 118.09 | 126.06 |
| 22 | B | 820 | CLA | C1C-C2C-C3C | -3.69 | 103.08 | 106.96 |
| 22 | A | 821 | CLA | C3C-C4C-NC | 3.69 | 114.71 | 110.57 |
| 22 | A | 803 | CLA | C3B-C4B-NB | 3.69 | 113.98 | 109.21 |
| 22 | B | 840 | CLA | C1D-CHD-C4C | -3.69 | 118.10 | 126.06 |
| 22 | A | 839 | CLA | C1C-C2C-C3C | -3.69 | 103.08 | 106.96 |
| 22 | B | 810 | CLA | C3C-C4C-NC | 3.69 | 114.71 | 110.57 |
| 22 | L | 204 | CLA | C3C-C4C-NC | 3.69 | 114.71 | 110.57 |
| 22 | G | 204 | CLA | C1C-C2C-C3C | -3.69 | 103.08 | 106.96 |
| 22 | 6 | 611 | CLA | C1C-C2C-C3C | -3.68 | 103.08 | 106.96 |
| 22 | A | 810 | CLA | C1C-C2C-C3C | -3.68 | 103.08 | 106.96 |
| 25 | 8 | 619 | BCR | C21-C20-C19 | -3.68 | 111.73 | 123.22 |
| 22 | 2 | 606 | CLA | C1D-CHD-C4C | -3.68 | 118.12 | 126.06 |
| 22 | 3 | 610 | CLA | C3C-C4C-NC | 3.68 | 114.70 | 110.57 |
| 22 | A | 805 | CLA | C1D-CHD-C4C | -3.68 | 118.12 | 126.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 602 | CLA | CHD-C4C-NC | 3.68 | 130.00 | 124.20 |
| 22 | A | 809 | CLA | C1C-C2C-C3C | -3.68 | 103.09 | 106.96 |
| 22 | 8 | 603 | CLA | C3C-C4C-NC | 3.68 | 114.70 | 110.57 |
| 22 | A | 837 | CLA | C3C-C4C-NC | 3.68 | 114.69 | 110.57 |
| 22 | 4 | 603 | CLA | C3C-C4C-NC | 3.68 | 114.69 | 110.57 |
| 22 | A | 843 | CLA | C1C-C2C-C3C | -3.68 | 103.09 | 106.96 |
| 22 | A | 807 | CLA | C1C-C2C-C3C | -3.67 | 103.09 | 106.96 |
| 22 | 1 | 616 | CLA | C4A-NA-C1A | -3.67 | 105.05 | 106.71 |
| 22 | 3 | 607 | CLA | CAA-C2A-C3A | -3.67 | 102.72 | 112.78 |
| 30 | 7 | 621 | LUT | C7-C8-C9 | -3.67 | 120.69 | 126.23 |
| 30 | 4 | 619 | LUT | C7-C8-C9 | -3.67 | 120.69 | 126.23 |
| 22 | A | 833 | CLA | C1D-CHD-C4C | -3.67 | 118.14 | 126.06 |
| 22 | 6 | 614 | CLA | C1D-CHD-C4C | -3.67 | 118.14 | 126.06 |
| 22 | B | 839 | CLA | C3C-C4C-NC | 3.67 | 114.69 | 110.57 |
| 22 | 7 | 620 | CLA | C1C-C2C-C3C | -3.67 | 103.10 | 106.96 |
| 30 | 3 | 622 | LUT | C7-C8-C9 | -3.67 | 120.69 | 126.23 |
| 22 | 8 | 608 | CLA | C1C-C2C-C3C | -3.67 | 103.10 | 106.96 |
| 22 | A | 822 | CLA | C3C-C4C-NC | 3.67 | 114.69 | 110.57 |
| 22 | 1 | 614 | CLA | C3C-C4C-NC | 3.67 | 114.69 | 110.57 |
| 22 | B | 811 | CLA | C4B-C3B-C2B | -3.67 | 103.51 | 106.92 |
| 22 | Z | 616 | CLA | C1C-C2C-C3C | -3.67 | 103.10 | 106.96 |
| 22 | 5 | 617 | CLA | C1D-CHD-C4C | -3.67 | 118.14 | 126.06 |
| 22 | B | 808 | CLA | C3B-C4B-NB | 3.67 | 113.95 | 109.21 |
| 22 | B | 813 | CLA | C4C-C3C-C2C | -3.67 | 101.55 | 106.90 |
| 22 | 4 | 610 | CLA | C3C-C4C-NC | 3.67 | 114.68 | 110.57 |
| 22 | A | 811 | CLA | C1-C2-C3 | -3.67 | 119.70 | 126.04 |
| 22 | A | 808 | CLA | C3B-C4B-NB | 3.67 | 113.95 | 109.21 |
| 22 | Z | 604 | CLA | C1D-CHD-C4C | -3.67 | 118.15 | 126.06 |
| 22 | B | 805 | CLA | C1D-CHD-C4C | -3.66 | 118.15 | 126.06 |
| 22 | K | 4003 | CLA | C1C-C2C-C3C | -3.66 | 103.10 | 106.96 |
| 22 | B | 817 | CLA | C3C-C4C-NC | 3.66 | 114.68 | 110.57 |
| 22 | 8 | 611 | CLA | C1C-C2C-C3C | -3.66 | 103.11 | 106.96 |
| 22 | K | 4002 | CLA | C1D-CHD-C4C | -3.66 | 118.16 | 126.06 |
| 22 | Z | 614 | CLA | C1D-CHD-C4C | -3.66 | 118.16 | 126.06 |
| 22 | 7 | 613 | CLA | C1D-CHD-C4C | -3.66 | 118.16 | 126.06 |
| 22 | F | 304 | CLA | C3B-C4B-NB | 3.66 | 113.94 | 109.21 |
| 22 | Z | 610 | CLA | CAA-C2A-C3A | -3.66 | 102.75 | 112.78 |
| 25 | 3 | 718 | BCR | C28-C27-C26 | -3.66 | 107.54 | 114.08 |
| 22 | 7 | 611 | CLA | C3B-C4B-NB | 3.66 | 113.94 | 109.21 |
| 22 | 9 | 602 | CLA | C3C-C4C-NC | 3.66 | 114.67 | 110.57 |
| 22 | A | 823 | CLA | C1D-CHD-C4C | -3.66 | 118.17 | 126.06 |
| 22 | 8 | 601 | CLA | C1D-CHD-C4C | -3.66 | 118.17 | 126.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 611 | CLA | C3D-C4D-ND | 3.65 | 116.15 | 110.24 |
| 22 | A | 802 | CLA | C1D-CHD-C4C | -3.65 | 118.18 | 126.06 |
| 22 | A | 835 | CLA | C1D-CHD-C4C | -3.65 | 118.18 | 126.06 |
| 22 | L | 203 | CLA | C1D-CHD-C4C | -3.65 | 118.18 | 126.06 |
| 29 | 5 | 608 | CHL | CAC-C3C-C4C | 3.65 | 129.55 | 124.81 |
| 22 | 9 | 604 | CLA | C1D-CHD-C4C | -3.65 | 118.18 | 126.06 |
| 22 | 7 | 614 | CLA | C1C-C2C-C3C | -3.65 | 103.12 | 106.96 |
| 22 | 4 | 616 | CLA | C3C-C4C-NC | 3.65 | 114.67 | 110.57 |
| 22 | 3 | 613 | CLA | C1C-C2C-C3C | -3.65 | 103.12 | 106.96 |
| 22 | 7 | 601 | CLA | C3B-C4B-NB | 3.65 | 113.93 | 109.21 |
| 22 | A | 827 | CLA | C3C-C4C-NC | 3.65 | 114.66 | 110.57 |
| 22 | 2 | 601 | CLA | C3C-C4C-NC | 3.65 | 114.66 | 110.57 |
| 29 | 5 | 607 | CHL | C3B-C4B-NB | 3.65 | 113.92 | 109.21 |
| 22 | 2 | 602 | CLA | C1C-C2C-C3C | -3.65 | 103.12 | 106.96 |
| 30 | 5 | 620 | LUT | C15-C14-C13 | -3.64 | 122.11 | 127.31 |
| 22 | A | 825 | CLA | CAC-C3C-C4C | 3.64 | 129.54 | 124.81 |
| 22 | Z | 604 | CLA | C4A-NA-C1A | -3.64 | 105.07 | 106.71 |
| 22 | 3 | 602 | CLA | C3C-C4C-NC | 3.64 | 114.66 | 110.57 |
| 25 | K | 4001 | BCR | C2-C3-C4 | -3.64 | 103.24 | 111.38 |
| 29 | 5 | 608 | CHL | C1D-CHD-C4C | -3.64 | 118.20 | 126.06 |
| 25 | B | 801 | BCR | C21-C20-C19 | -3.64 | 111.86 | 123.22 |
| 22 | 7 | 609 | CLA | C1C-C2C-C3C | -3.64 | 103.13 | 106.96 |
| 22 | 4 | 613 | CLA | C3B-C4B-NB | 3.64 | 113.92 | 109.21 |
| 22 | 5 | 617 | CLA | CAA-C2A-C3A | -3.64 | 102.81 | 112.78 |
| 22 | 2 | 607 | CLA | C1C-C2C-C3C | -3.64 | 103.13 | 106.96 |
| 22 | 7 | 604 | CLA | O2D-CGD-CBD | 3.64 | 117.73 | 111.27 |
| 22 | B | 841 | CLA | C1C-C2C-C3C | -3.64 | 103.13 | 106.96 |
| 22 | B | 822 | CLA | C1D-CHD-C4C | -3.64 | 118.21 | 126.06 |
| 29 | 9 | 607 | CHL | CAC-C3C-C4C | 3.64 | 129.53 | 124.81 |
| 22 | A | 808 | CLA | C1D-CHD-C4C | -3.64 | 118.22 | 126.06 |
| 22 | B | 841 | CLA | C1D-CHD-C4C | -3.64 | 118.22 | 126.06 |
| 22 | 3 | 606 | CLA | C1C-C2C-C3C | -3.63 | 103.14 | 106.96 |
| 22 | Z | 606 | CLA | C1C-C2C-C3C | -3.63 | 103.14 | 106.96 |
| 22 | A | 837 | CLA | C1D-CHD-C4C | -3.63 | 118.22 | 126.06 |
| 22 | A | 823 | CLA | C1C-C2C-C3C | -3.63 | 103.14 | 106.96 |
| 22 | 3 | 611 | CLA | C3C-C4C-NC | 3.63 | 114.64 | 110.57 |
| 22 | F | 301 | CLA | C1C-C2C-C3C | -3.63 | 103.14 | 106.96 |
| 22 | 3 | 604 | CLA | C3C-C4C-NC | 3.63 | 114.64 | 110.57 |
| 22 | 8 | 611 | CLA | C1D-CHD-C4C | -3.63 | 118.23 | 126.06 |
| 22 | A | 821 | CLA | CBC-CAC-C3C | -3.63 | 102.43 | 112.43 |
| 22 | B | 827 | CLA | C1D-CHD-C4C | -3.62 | 118.24 | 126.06 |
| 25 | F | 305 | BCR | C38-C26-C25 | -3.62 | 120.46 | 124.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29 | 5 | 618 | CHL | C1D-CHD-C4C | -3.62 | 118.24 | 126.06 |
| 22 | A | 831 | CLA | C1C-C2C-C3C | -3.62 | 103.15 | 106.96 |
| 22 | B | 833 | CLA | C3C-C4C-NC | 3.62 | 114.63 | 110.57 |
| 22 | A | 834 | CLA | C3B-C4B-NB | 3.62 | 113.89 | 109.21 |
| 22 | A | 820 | CLA | CBA-CAA-C2A | 3.62 | 124.56 | 113.86 |
| 22 | B | 809 | CLA | C3C-C4C-NC | 3.62 | 114.63 | 110.57 |
| 22 | B | 828 | CLA | C3B-C4B-NB | 3.62 | 113.89 | 109.21 |
| 22 | 8 | 612 | CLA | O2D-CGD-CBD | 3.62 | 117.70 | 111.27 |
| 22 | 6 | 611 | CLA | C3C-C4C-NC | 3.62 | 114.63 | 110.57 |
| 24 | 8 | 620 | LHG | O7-C7-C8 | 3.62 | 119.30 | 111.50 |
| 22 | A | 824 | CLA | C1D-CHD-C4C | -3.62 | 118.25 | 126.06 |
| 22 | 3 | 606 | CLA | C3C-C4C-NC | 3.62 | 114.63 | 110.57 |
| 22 | K | 4002 | CLA | C3C-C4C-NC | 3.62 | 114.63 | 110.57 |
| 22 | 8 | 611 | CLA | C3C-C4C-NC | 3.62 | 114.63 | 110.57 |
| 25 | B | 846 | BCR | C21-C20-C19 | -3.62 | 111.93 | 123.22 |
| 22 | 6 | 614 | CLA | C1C-C2C-C3C | -3.62 | 103.15 | 106.96 |
| 22 | A | 819 | CLA | C1D-CHD-C4C | -3.62 | 118.25 | 126.06 |
| 22 | B | 840 | CLA | CHC-C1C-C2C | -3.62 | 116.72 | 126.72 |
| 22 | 9 | 614 | CLA | C1D-CHD-C4C | -3.62 | 118.26 | 126.06 |
| 22 | Z | 614 | CLA | C3C-C4C-NC | 3.61 | 114.62 | 110.57 |
| 22 | B | 819 | CLA | C1C-C2C-C3C | -3.61 | 103.16 | 106.96 |
| 22 | B | 823 | CLA | C1D-CHD-C4C | -3.61 | 118.26 | 126.06 |
| 22 | 6 | 622 | CLA | C1D-CHD-C4C | -3.61 | 118.26 | 126.06 |
| 22 | 3 | 620 | CLA | C3C-C4C-NC | 3.61 | 114.62 | 110.57 |
| 22 | Z | 606 | CLA | C3C-C4C-NC | 3.61 | 114.62 | 110.57 |
| 22 | 2 | 603 | CLA | C3C-C4C-NC | 3.61 | 114.62 | 110.57 |
| 30 | Z | 617 | LUT | C35-C15-C14 | -3.61 | 116.07 | 123.47 |
| 22 | B | 820 | CLA | C1D-CHD-C4C | -3.61 | 118.26 | 126.06 |
| 22 | 7 | 614 | CLA | C1D-CHD-C4C | -3.61 | 118.26 | 126.06 |
| 22 | 2 | 602 | CLA | C1D-CHD-C4C | -3.61 | 118.27 | 126.06 |
| 22 | 6 | 616 | CLA | C3C-C4C-NC | 3.61 | 114.62 | 110.57 |
| 22 | F | 303 | CLA | C1C-C2C-C3C | -3.61 | 103.16 | 106.96 |
| 25 | B | 845 | BCR | C16-C17-C18 | -3.61 | 122.16 | 127.31 |
| 22 | 1 | 609 | CLA | C3B-C4B-NB | 3.61 | 113.88 | 109.21 |
| 22 | 6 | 604 | CLA | C1D-CHD-C4C | -3.61 | 118.27 | 126.06 |
| 22 | 6 | 603 | CLA | C3B-C4B-NB | 3.61 | 113.88 | 109.21 |
| 22 | A | 832 | CLA | C1C-C2C-C3C | -3.61 | 103.16 | 106.96 |
| 22 | Z | 608 | CLA | C1C-C2C-C3C | -3.61 | 103.16 | 106.96 |
| 22 | Z | 610 | CLA | CAC-C3C-C4C | 3.61 | 129.49 | 124.81 |
| 22 | B | 807 | CLA | C3B-C4B-NB | 3.61 | 113.87 | 109.21 |
| 22 | 3 | 602 | CLA | C3B-C4B-NB | 3.61 | 113.87 | 109.21 |
| 22 | 4 | 613 | CLA | O2A-CGA-CBA | 3.60 | 123.22 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 838 | CLA | C1C-C2C-C3C | -3.60 | 103.17 | 106.96 |
| 25 | J | 3003 | BCR | C15-C14-C13 | -3.60 | 122.17 | 127.31 |
| 22 | J | 3002 | CLA | C3C-C4C-NC | 3.60 | 114.61 | 110.57 |
| 22 | 7 | 609 | CLA | CHB-C4A-NA | 3.60 | 129.49 | 124.51 |
| 22 | 3 | 603 | CLA | C3B-C4B-NB | 3.60 | 113.87 | 109.21 |
| 22 | 7 | 612 | CLA | C3B-C4B-NB | 3.60 | 113.86 | 109.21 |
| 22 | 4 | 613 | CLA | C1C-C2C-C3C | -3.60 | 103.17 | 106.96 |
| 22 | 7 | 614 | CLA | C3C-C4C-NC | 3.60 | 114.61 | 110.57 |
| 22 | A | 805 | CLA | C1C-C2C-C3C | -3.60 | 103.17 | 106.96 |
| 22 | 2 | 612 | CLA | C3B-C4B-NB | 3.60 | 113.86 | 109.21 |
| 29 | 6 | 607 | CHL | C3B-C4B-NB | 3.60 | 113.86 | 109.21 |
| 22 | 5 | 606 | CLA | C3C-C4C-NC | 3.60 | 114.61 | 110.57 |
| 22 | B | 834 | CLA | C1D-CHD-C4C | -3.60 | 118.30 | 126.06 |
| 22 | 2 | 607 | CLA | C3C-C4C-NC | 3.60 | 114.61 | 110.57 |
| 22 | 8 | 602 | CLA | C4A-NA-C1A | -3.60 | 105.09 | 106.71 |
| 22 | A | 825 | CLA | C1D-CHD-C4C | -3.60 | 118.30 | 126.06 |
| 22 | 9 | 604 | CLA | C3C-C4C-NC | 3.60 | 114.60 | 110.57 |
| 24 | 5 | 623 | LHG | O7-C7-C8 | 3.60 | 119.25 | 111.50 |
| 22 | B | 817 | CLA | CAA-C2A-C3A | -3.60 | 102.93 | 112.78 |
| 22 | 8 | 610 | CLA | O2A-CGA-CBA | 3.59 | 123.19 | 111.91 |
| 22 | 6 | 614 | CLA | C3C-C4C-NC | 3.59 | 114.60 | 110.57 |
| 22 | 2 | 611 | CLA | C3C-C4C-NC | 3.59 | 114.60 | 110.57 |
| 22 | B | 812 | CLA | C3C-C4C-NC | 3.59 | 114.60 | 110.57 |
| 22 | A | 829 | CLA | C3D-C4D-ND | 3.59 | 116.05 | 110.24 |
| 22 | G | 204 | CLA | C3C-C4C-NC | 3.59 | 114.60 | 110.57 |
| 22 | 3 | 614 | CLA | C3C-C4C-NC | 3.59 | 114.60 | 110.57 |
| 25 | B | 846 | BCR | C15-C14-C13 | -3.59 | 122.19 | 127.31 |
| 22 | B | 816 | CLA | CMC-C2C-C1C | 3.59 | 130.50 | 125.04 |
| 22 | Z | 611 | CLA | C1C-C2C-C3C | -3.59 | 103.19 | 106.96 |
| 22 | 6 | 612 | CLA | C3B-C4B-NB | 3.58 | 113.84 | 109.21 |
| 22 | 6 | 613 | CLA | C1D-CHD-C4C | -3.58 | 118.33 | 126.06 |
| 22 | 2 | 602 | CLA | C3C-C4C-NC | 3.58 | 114.59 | 110.57 |
| 25 | K | 4004 | BCR | C3-C4-C5 | -3.58 | 107.68 | 114.08 |
| 22 | 5 | 610 | CLA | C3C-C4C-NC | 3.58 | 114.59 | 110.57 |
| 22 | B | 819 | CLA | C1D-CHD-C4C | -3.58 | 118.33 | 126.06 |
| 22 | 6 | 616 | CLA | CHC-C1C-C2C | -3.58 | 116.82 | 126.72 |
| 22 | 1 | 603 | CLA | C3C-C4C-NC | 3.58 | 114.59 | 110.57 |
| 22 | 3 | 609 | CLA | C3C-C4C-NC | 3.58 | 114.58 | 110.57 |
| 22 | 3 | 613 | CLA | C3B-C4B-NB | 3.58 | 113.84 | 109.21 |
| 22 | 7 | 611 | CLA | C3C-C4C-NC | 3.58 | 114.58 | 110.57 |
| 22 | B | 831 | CLA | C1D-CHD-C4C | -3.58 | 118.34 | 126.06 |
| 22 | A | 828 | CLA | C4C-C3C-C2C | -3.58 | 101.69 | 106.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 5 | 612 | CLA | C3B-C4B-NB | 3.58 | 113.83 | 109.21 |
| 22 | A | 825 | CLA | C3C-C4C-NC | 3.57 | 114.58 | 110.57 |
| 30 | Z | 617 | LUT | C35-C34-C33 | -3.57 | 122.21 | 127.31 |
| 25 | 3 | 717 | BCR | C21-C20-C19 | -3.57 | 112.06 | 123.22 |
| 22 | 2 | 614 | CLA | C1C-C2C-C3C | -3.57 | 103.20 | 106.96 |
| 22 | A | 815 | CLA | C1D-CHD-C4C | -3.57 | 118.35 | 126.06 |
| 22 | 2 | 609 | CLA | C3B-C4B-NB | 3.57 | 113.83 | 109.21 |
| 22 | G | 204 | CLA | C1D-CHD-C4C | -3.57 | 118.35 | 126.06 |
| 22 | A | 815 | CLA | C1C-C2C-C3C | -3.57 | 103.20 | 106.96 |
| 29 | 9 | 606 | CHL | C2A-C3A-C4A | -3.57 | 97.23 | 101.78 |
| 25 | 5 | 625 | BCR | C3-C4-C5 | -3.57 | 107.70 | 114.08 |
| 25 | 7 | 624 | BCR | C11-C10-C9 | -3.57 | 122.22 | 127.31 |
| 22 | 6 | 614 | CLA | CAA-C2A-C3A | -3.57 | 103.00 | 112.78 |
| 22 | B | 815 | CLA | C1C-C2C-C3C | -3.57 | 103.20 | 106.96 |
| 22 | 4 | 610 | CLA | CAA-C2A-C3A | -3.57 | 103.01 | 112.78 |
| 22 | 5 | 614 | CLA | C3C-C4C-NC | 3.57 | 114.57 | 110.57 |
| 22 | 6 | 617 | CLA | C1C-C2C-C3C | -3.57 | 103.21 | 106.96 |
| 22 | 8 | 613 | CLA | C3B-C4B-NB | 3.57 | 113.82 | 109.21 |
| 22 | 5 | 614 | CLA | C3B-C4B-NB | 3.56 | 113.82 | 109.21 |
| 25 | B | 848 | BCR | C15-C14-C13 | -3.56 | 122.22 | 127.31 |
| 22 | 8 | 601 | CLA | C3D-C4D-ND | 3.56 | 116.00 | 110.24 |
| 22 | A | 833 | CLA | C1C-C2C-C3C | -3.56 | 103.21 | 106.96 |
| 22 | 8 | 612 | CLA | C1C-C2C-C3C | -3.56 | 103.21 | 106.96 |
| 22 | 1 | 613 | CLA | C1C-C2C-C3C | -3.56 | 103.21 | 106.96 |
| 22 | 8 | 604 | CLA | C3C-C4C-NC | 3.56 | 114.56 | 110.57 |
| 29 | 3 | 608 | CHL | C2C-C3C-C4C | -3.56 | 103.95 | 106.49 |
| 30 | 8 | 617 | LUT | C15-C14-C13 | -3.56 | 122.23 | 127.31 |
| 22 | 8 | 614 | CLA | C1D-CHD-C4C | -3.56 | 118.38 | 126.06 |
| 22 | A | 817 | CLA | C3B-C4B-NB | 3.56 | 113.81 | 109.21 |
| 25 | B | 846 | BCR | C16-C17-C18 | -3.56 | 122.24 | 127.31 |
| 22 | A | 854 | CLA | C4C-C3C-C2C | -3.55 | 101.72 | 106.90 |
| 22 | 2 | 610 | CLA | C3C-C4C-NC | 3.55 | 114.56 | 110.57 |
| 22 | B | 810 | CLA | C1C-C2C-C3C | -3.55 | 103.22 | 106.96 |
| 22 | A | 840 | CLA | C3B-C4B-NB | 3.55 | 113.80 | 109.21 |
| 22 | 5 | 609 | CLA | C3B-C4B-NB | 3.55 | 113.80 | 109.21 |
| 29 | 9 | 606 | CHL | CAC-C3C-C4C | 3.55 | 129.42 | 124.81 |
| 22 | 8 | 602 | CLA | C1C-C2C-C3C | -3.55 | 103.22 | 106.96 |
| 25 | A | 850 | BCR | C11-C10-C9 | -3.55 | 122.24 | 127.31 |
| 30 | 1 | 618 | LUT | C35-C34-C33 | -3.55 | 122.24 | 127.31 |
| 22 | 6 | 616 | CLA | CAC-C3C-C4C | 3.55 | 129.42 | 124.81 |
| 22 | A | 824 | CLA | C3B-C4B-NB | 3.55 | 113.80 | 109.21 |
| 22 | B | 805 | CLA | C4C-C3C-C2C | -3.55 | 101.73 | 106.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 3 | 602 | CLA | O2A-CGA-CBA | 3.55 | 123.04 | 111.91 |
| 30 | 4 | 619 | LUT | C35-C15-C14 | -3.55 | 116.21 | 123.47 |
| 22 | B | 837 | CLA | C4-C3-C5 | 3.55 | 121.24 | 115.27 |
| 25 | 7 | 624 | BCR | C7-C8-C9 | -3.55 | 120.88 | 126.23 |
| 22 | 8 | 604 | CLA | C1D-CHD-C4C | -3.55 | 118.41 | 126.06 |
| 22 | A | 854 | CLA | C2C-C1C-NC | 3.54 | 113.29 | 109.97 |
| 22 | Z | 604 | CLA | C3C-C4C-NC | 3.54 | 114.55 | 110.57 |
| 22 | A | 810 | CLA | C11-C10-C8 | -3.54 | 104.47 | 115.92 |
| 29 | 1 | 601 | CHL | O2D-CGD-O1D | -3.54 | 116.91 | 123.84 |
| 22 | 2 | 613 | CLA | CAC-C3C-C4C | 3.54 | 129.40 | 124.81 |
| 22 | A | 835 | CLA | C1C-C2C-C3C | -3.54 | 103.24 | 106.96 |
| 22 | 8 | 614 | CLA | C1C-C2C-C3C | -3.54 | 103.24 | 106.96 |
| 22 | A | 816 | CLA | C1D-CHD-C4C | -3.54 | 118.42 | 126.06 |
| 22 | 5 | 610 | CLA | C1C-C2C-C3C | -3.54 | 103.24 | 106.96 |
| 22 | B | 804 | CLA | C4A-NA-C1A | -3.54 | 105.12 | 106.71 |
| 22 | A | 802 | CLA | C1C-C2C-C3C | -3.54 | 103.24 | 106.96 |
| 22 | 2 | 610 | CLA | C1C-C2C-C3C | -3.53 | 103.24 | 106.96 |
| 22 | 2 | 613 | CLA | C3B-C4B-NB | 3.53 | 113.78 | 109.21 |
| 22 | F | 304 | CLA | C1C-C2C-C3C | -3.53 | 103.24 | 106.96 |
| 22 | 4 | 614 | CLA | C1C-C2C-C3C | -3.53 | 103.24 | 106.96 |
| 22 | B | 837 | CLA | C1D-CHD-C4C | -3.53 | 118.44 | 126.06 |
| 22 | A | 814 | CLA | C1-O2A-CGA | 3.53 | 125.71 | 116.44 |
| 22 | A | 822 | CLA | C1D-CHD-C4C | -3.53 | 118.44 | 126.06 |
| 22 | 8 | 604 | CLA | C4A-NA-C1A | -3.53 | 105.12 | 106.71 |
| 22 | 6 | 610 | CLA | C1C-C2C-C3C | -3.53 | 103.25 | 106.96 |
| 29 | 4 | 607 | CHL | C3D-C4D-ND | 3.53 | 115.94 | 110.24 |
| 22 | B | 838 | CLA | C1D-CHD-C4C | -3.53 | 118.45 | 126.06 |
| 22 | 9 | 603 | CLA | C3B-C4B-NB | 3.53 | 113.77 | 109.21 |
| 22 | 8 | 609 | CLA | C1C-C2C-C3C | -3.53 | 103.25 | 106.96 |
| 25 | B | 846 | BCR | C24-C23-C22 | -3.52 | 120.91 | 126.23 |
| 29 | Z | 607 | CHL | C3B-C4B-NB | 3.52 | 113.77 | 109.21 |
| 22 | 8 | 613 | CLA | C1C-C2C-C3C | -3.52 | 103.25 | 106.96 |
| 22 | A | 807 | CLA | C3B-C4B-NB | 3.52 | 113.77 | 109.21 |
| 29 | 5 | 608 | CHL | C3C-C4C-NC | 3.52 | 114.52 | 110.57 |
| 22 | B | 826 | CLA | C4C-C3C-C2C | -3.52 | 101.76 | 106.90 |
| 22 | 8 | 608 | CLA | CHD-C4C-NC | 3.52 | 129.75 | 124.20 |
| 22 | 4 | 611 | CLA | CAC-C3C-C4C | 3.52 | 129.38 | 124.81 |
| 22 | 6 | 610 | CLA | C3C-C4C-NC | 3.52 | 114.52 | 110.57 |
| 22 | Z | 612 | CLA | C3B-C4B-NB | 3.52 | 113.76 | 109.21 |
| 30 | 6 | 624 | LUT | C15-C14-C13 | -3.52 | 122.29 | 127.31 |
| 22 | B | 803 | CLA | CAA-C2A-C3A | -3.51 | 103.15 | 112.78 |
| 22 | A | 854 | CLA | O2D-CGD-O1D | -3.51 | 116.97 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 816 | CLA | CHD-C4C-NC | 3.51 | 129.74 | 124.20 |
| 22 | A | 829 | CLA | CMC-C2C-C1C | 3.51 | 130.39 | 125.04 |
| 29 | 5 | 608 | CHL | C1B-CHB-C4A | -3.51 | 123.16 | 130.12 |
| 25 | K | 4001 | BCR | C3-C4-C5 | -3.51 | 107.80 | 114.08 |
| 22 | 2 | 601 | CLA | C3B-C4B-NB | 3.51 | 113.75 | 109.21 |
| 22 | 1 | 604 | CLA | C1D-CHD-C4C | -3.51 | 118.48 | 126.06 |
| 22 | B | 805 | CLA | O2A-CGA-CBA | 3.51 | 122.93 | 111.91 |
| 22 | G | 203 | CLA | C3B-C4B-NB | 3.51 | 113.75 | 109.21 |
| 22 | A | 814 | CLA | C4C-C3C-C2C | -3.51 | 101.78 | 106.90 |
| 30 | Z | 617 | LUT | C10-C11-C12 | -3.51 | 112.27 | 123.22 |
| 22 | Z | 603 | CLA | C3C-C4C-NC | 3.51 | 114.50 | 110.57 |
| 22 | K | 4003 | CLA | C3B-C4B-NB | 3.51 | 113.75 | 109.21 |
| 22 | 3 | 604 | CLA | C1D-CHD-C4C | -3.51 | 118.49 | 126.06 |
| 22 | A | 813 | CLA | C1-O2A-CGA | 3.51 | 125.64 | 116.44 |
| 24 | A | 846 | LHG | O7-C7-C8 | 3.51 | 119.06 | 111.50 |
| 22 | 6 | 609 | CLA | C3B-C4B-NB | 3.51 | 113.74 | 109.21 |
| 22 | B | 802 | CLA | C4C-C3C-C2C | -3.50 | 101.79 | 106.90 |
| 22 | A | 822 | CLA | C1C-C2C-C3C | -3.50 | 103.27 | 106.96 |
| 22 | A | 840 | CLA | C1C-C2C-C3C | -3.50 | 103.27 | 106.96 |
| 30 | 1 | 617 | LUT | C35-C34-C33 | -3.50 | 122.31 | 127.31 |
| 22 | A | 813 | CLA | C1C-C2C-C3C | -3.50 | 103.27 | 106.96 |
| 22 | 6 | 601 | CLA | C3C-C4C-NC | 3.50 | 114.50 | 110.57 |
| 22 | Z | 604 | CLA | C3B-C4B-NB | 3.50 | 113.73 | 109.21 |
| 22 | B | 814 | CLA | C3C-C4C-NC | 3.50 | 114.50 | 110.57 |
| 22 | 5 | 621 | CLA | C1C-C2C-C3C | -3.50 | 103.28 | 106.96 |
| 25 | A | 848 | BCR | C28-C27-C26 | -3.50 | 107.83 | 114.08 |
| 22 | 6 | 601 | CLA | C1D-CHD-C4C | -3.50 | 118.51 | 126.06 |
| 25 | A | 849 | BCR | C20-C21-C22 | -3.50 | 122.32 | 127.31 |
| 30 | 1 | 617 | LUT | C10-C11-C12 | -3.50 | 112.30 | 123.22 |
| 22 | B | 823 | CLA | O2D-CGD-CBD | 3.50 | 117.48 | 111.27 |
| 22 | 2 | 609 | CLA | C3C-C4C-NC | 3.50 | 114.49 | 110.57 |
| 22 | 9 | 604 | CLA | C3B-C4B-NB | 3.50 | 113.73 | 109.21 |
| 22 | 4 | 611 | CLA | C3C-C4C-NC | 3.50 | 114.49 | 110.57 |
| 22 | 6 | 602 | CLA | C1C-C2C-C3C | -3.49 | 103.28 | 106.96 |
| 22 | 9 | 614 | CLA | C3C-C4C-NC | 3.49 | 114.49 | 110.57 |
| 22 | 2 | 601 | CLA | O2D-CGD-CBD | 3.49 | 117.47 | 111.27 |
| 22 | 6 | 617 | CLA | CAA-C2A-C3A | -3.49 | 103.22 | 112.78 |
| 30 | 6 | 621 | LUT | C35-C15-C14 | -3.49 | 116.32 | 123.47 |
| 22 | A | 803 | CLA | C1C-C2C-C3C | -3.49 | 103.29 | 106.96 |
| 22 | B | 841 | CLA | C1-C2-C3 | -3.49 | 120.01 | 126.04 |
| 22 | 9 | 610 | CLA | C1C-C2C-C3C | -3.49 | 103.29 | 106.96 |
| 22 | 5 | 614 | CLA | CAC-C3C-C4C | 3.49 | 129.34 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 805 | CLA | C3C-C4C-NC | 3.49 | 114.48 | 110.57 |
| 22 | Z | 613 | CLA | C1C-C2C-C3C | -3.49 | 103.29 | 106.96 |
| 22 | A | 804 | CLA | C3D-C2D-C1D | -3.48 | 101.08 | 105.83 |
| 22 | 6 | 610 | CLA | CAA-C2A-C3A | -3.48 | 103.24 | 112.78 |
| 22 | 9 | 602 | CLA | CAC-C3C-C4C | 3.48 | 129.33 | 124.81 |
| 22 | Z | 609 | CLA | CAA-C2A-C3A | -3.48 | 103.24 | 112.78 |
| 22 | A | 841 | CLA | O2A-CGA-CBA | 3.48 | 122.84 | 111.91 |
| 29 | Z | 601 | CHL | C3D-C4D-ND | 3.48 | 115.87 | 110.24 |
| 22 | A | 815 | CLA | C3C-C4C-NC | 3.48 | 114.47 | 110.57 |
| 22 | 7 | 609 | CLA | C1D-CHD-C4C | -3.48 | 118.56 | 126.06 |
| 22 | 5 | 604 | CLA | C3B-C4B-NB | 3.48 | 113.71 | 109.21 |
| 29 | 8 | 607 | CHL | C3D-C4D-ND | 3.48 | 115.86 | 110.24 |
| 25 | B | 845 | BCR | C34-C9-C10 | -3.48 | 118.05 | 122.92 |
| 29 | Z | 601 | CHL | C1D-CHD-C4C | -3.48 | 118.56 | 126.06 |
| 22 | B | 837 | CLA | O2D-CGD-O1D | -3.47 | 117.05 | 123.84 |
| 22 | B | 816 | CLA | CAC-C3C-C4C | 3.47 | 129.32 | 124.81 |
| 22 | 9 | 614 | CLA | C3B-C4B-NB | 3.47 | 113.70 | 109.21 |
| 22 | B | 824 | CLA | C1C-C2C-C3C | -3.47 | 103.31 | 106.96 |
| 25 | B | 846 | BCR | C11-C10-C9 | -3.47 | 122.36 | 127.31 |
| 29 | 3 | 608 | CHL | CBC-CAC-C3C | -3.47 | 102.86 | 112.43 |
| 22 | A | 845 | CLA | C1C-C2C-C3C | -3.47 | 103.31 | 106.96 |
| 22 | A | 827 | CLA | O2D-CGD-CBD | 3.47 | 117.44 | 111.27 |
| 22 | 2 | 609 | CLA | CAA-C2A-C3A | -3.47 | 103.27 | 112.78 |
| 22 | A | 812 | CLA | C3B-C4B-NB | 3.47 | 113.70 | 109.21 |
| 22 | 5 | 604 | CLA | C3C-C4C-NC | 3.47 | 114.46 | 110.57 |
| 22 | 1 | 610 | CLA | C2C-C1C-NC | 3.47 | 113.22 | 109.97 |
| 22 | L | 204 | CLA | C1D-CHD-C4C | -3.47 | 118.58 | 126.06 |
| 22 | K | 4003 | CLA | CHC-C1C-C2C | -3.47 | 117.13 | 126.72 |
| 25 | 5 | 625 | BCR | C23-C22-C21 | -3.46 | 113.62 | 118.94 |
| 22 | A | 820 | CLA | CMB-C2B-C3B | 3.46 | 131.16 | 124.68 |
| 22 | Z | 609 | CLA | CHC-C1C-C2C | -3.46 | 117.14 | 126.72 |
| 22 | B | 809 | CLA | CAA-C2A-C3A | -3.46 | 103.30 | 112.78 |
| 22 | 8 | 610 | CLA | C1C-C2C-C3C | -3.46 | 103.32 | 106.96 |
| 30 | 1 | 619 | LUT | C31-C30-C29 | -3.46 | 122.37 | 127.31 |
| 22 | L | 204 | CLA | C1C-C2C-C3C | -3.46 | 103.32 | 106.96 |
| 22 | B | 832 | CLA | O2A-CGA-CBA | 3.46 | 122.75 | 111.91 |
| 22 | B | 836 | CLA | CAC-C3C-C4C | 3.46 | 129.29 | 124.81 |
| 22 | B | 820 | CLA | C3C-C4C-NC | 3.46 | 114.45 | 110.57 |
| 22 | B | 852 | CLA | C1C-C2C-C3C | -3.46 | 103.32 | 106.96 |
| 22 | 3 | 602 | CLA | CAC-C3C-C4C | 3.45 | 129.29 | 124.81 |
| 22 | B | 829 | CLA | C1C-C2C-C3C | -3.45 | 103.33 | 106.96 |
| 22 | A | 817 | CLA | CHC-C1C-C2C | -3.45 | 117.18 | 126.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 9 | 604 | CLA | CAC-C3C-C4C | 3.45 | 129.28 | 124.81 |
| 21 | A | 801 | CL0 | O2A-CGA-CBA | 3.45 | 122.73 | 111.91 |
| 22 | A | 832 | CLA | CAC-C3C-C4C | 3.45 | 129.28 | 124.81 |
| 25 | 3 | 717 | BCR | C16-C17-C18 | -3.45 | 122.39 | 127.31 |
| 22 | 6 | 613 | CLA | C1C-C2C-C3C | -3.44 | 103.34 | 106.96 |
| 22 | 3 | 609 | CLA | C3B-C4B-NB | 3.44 | 113.66 | 109.21 |
| 22 | A | 806 | CLA | CMB-C2B-C3B | 3.44 | 131.12 | 124.68 |
| 30 | 9 | 617 | LUT | C35-C15-C14 | -3.44 | 116.42 | 123.47 |
| 22 | 5 | 616 | CLA | O2D-CGD-CBD | 3.44 | 117.38 | 111.27 |
| 25 | A | 856 | BCR | C38-C26-C25 | -3.44 | 120.67 | 124.53 |
| 25 | F | 305 | BCR | C33-C5-C6 | -3.44 | 120.67 | 124.53 |
| 22 | 8 | 612 | CLA | C3B-C4B-NB | 3.44 | 113.65 | 109.21 |
| 29 | Z | 601 | CHL | CAC-C3C-C4C | 3.44 | 129.27 | 124.81 |
| 25 | B | 801 | BCR | C11-C10-C9 | -3.43 | 122.41 | 127.31 |
| 22 | A | 830 | CLA | C1-C2-C3 | -3.43 | 120.10 | 126.04 |
| 29 | 5 | 618 | CHL | C3B-C4B-NB | 3.43 | 113.65 | 109.21 |
| 22 | B | 833 | CLA | CAA-C2A-C3A | -3.43 | 103.37 | 112.78 |
| 22 | 7 | 610 | CLA | CMC-C2C-C1C | 3.43 | 130.26 | 125.04 |
| 25 | B | 847 | BCR | C21-C20-C19 | -3.43 | 112.51 | 123.22 |
| 22 | 9 | 601 | CLA | CAA-C2A-C3A | -3.43 | 103.39 | 112.78 |
| 22 | 7 | 610 | CLA | CHD-C4C-NC | 3.43 | 129.60 | 124.20 |
| 22 | A | 830 | CLA | C4C-C3C-C2C | -3.43 | 101.90 | 106.90 |
| 22 | 5 | 603 | CLA | C3D-C4D-ND | 3.43 | 115.78 | 110.24 |
| 29 | 7 | 607 | CHL | C3B-C4B-NB | 3.43 | 113.64 | 109.21 |
| 22 | A | 802 | CLA | C1-C2-C3 | -3.43 | 120.12 | 126.04 |
| 22 | B | 810 | CLA | C3B-C4B-NB | 3.43 | 113.64 | 109.21 |
| 22 | 1 | 614 | CLA | C3B-C4B-NB | 3.43 | 113.64 | 109.21 |
| 22 | A | 818 | CLA | C1C-C2C-C3C | -3.42 | 103.36 | 106.96 |
| 25 | K | 4001 | BCR | C32-C1-C6 | -3.42 | 104.75 | 110.30 |
| 22 | F | 303 | CLA | CAC-C3C-C4C | 3.42 | 129.25 | 124.81 |
| 22 | 1 | 606 | CLA | CAA-C2A-C3A | -3.42 | 103.41 | 112.78 |
| 22 | A | 809 | CLA | C1D-CHD-C4C | -3.42 | 118.68 | 126.06 |
| 27 | B | 850 | DGD | C2G-O2G-C1B | -3.42 | 109.37 | 117.79 |
| 22 | A | 814 | CLA | C1D-CHD-C4C | -3.42 | 118.68 | 126.06 |
| 22 | A | 840 | CLA | O2D-CGD-O1D | -3.42 | 117.16 | 123.84 |
| 22 | 1 | 613 | CLA | C3B-C4B-NB | 3.42 | 113.63 | 109.21 |
| 22 | 3 | 612 | CLA | C3B-C4B-NB | 3.42 | 113.63 | 109.21 |
| 22 | B | 830 | CLA | C1C-C2C-C3C | -3.42 | 103.36 | 106.96 |
| 22 | 8 | 611 | CLA | C3B-C4B-NB | 3.42 | 113.63 | 109.21 |
| 22 | A | 835 | CLA | C3C-C4C-NC | 3.41 | 114.40 | 110.57 |
| 22 | B | 828 | CLA | CHC-C1C-C2C | -3.41 | 117.28 | 126.72 |
| 30 | Z | 618 | LUT | C10-C11-C12 | -3.41 | 112.57 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 4 | 611 | CLA | C3B-C4B-NB | 3.41 | 113.62 | 109.21 |
| 22 | 4 | 601 | CLA | C1D-CHD-C4C | -3.41 | 118.70 | 126.06 |
| 22 | 4 | 612 | CLA | C3B-C4B-NB | 3.41 | 113.62 | 109.21 |
| 22 | B | 818 | CLA | C3C-C4C-NC | 3.41 | 114.39 | 110.57 |
| 22 | F | 303 | CLA | CAA-C2A-C3A | -3.41 | 103.45 | 112.78 |
| 22 | 5 | 604 | CLA | CHC-C1C-C2C | -3.41 | 117.30 | 126.72 |
| 22 | A | 845 | CLA | C3B-C4B-NB | 3.41 | 113.61 | 109.21 |
| 22 | B | 802 | CLA | CMA-C3A-C2A | -3.40 | 100.10 | 113.83 |
| 22 | A | 825 | CLA | O2A-CGA-CBA | 3.40 | 122.59 | 111.91 |
| 22 | 2 | 611 | CLA | C3B-C4B-NB | 3.40 | 113.61 | 109.21 |
| 22 | B | 827 | CLA | C4C-C3C-C2C | -3.40 | 101.94 | 106.90 |
| 22 | 3 | 610 | CLA | CAC-C3C-C4C | 3.40 | 129.22 | 124.81 |
| 29 | 6 | 618 | CHL | C3B-C4B-NB | 3.40 | 113.60 | 109.21 |
| 30 | 5 | 620 | LUT | C8-C7-C6 | -3.40 | 117.67 | 127.20 |
| 25 | A | 856 | BCR | C15-C14-C13 | -3.39 | 122.47 | 127.31 |
| 25 | J | 3003 | BCR | C16-C17-C18 | -3.39 | 122.47 | 127.31 |
| 25 | B | 848 | BCR | C10-C11-C12 | -3.39 | 112.63 | 123.22 |
| 29 | 8 | 607 | CHL | C3B-C4B-NB | 3.39 | 113.60 | 109.21 |
| 25 | B | 846 | BCR | C7-C8-C9 | -3.39 | 121.11 | 126.23 |
| 22 | 7 | 604 | CLA | C3B-C4B-NB | 3.39 | 113.59 | 109.21 |
| 25 | A | 856 | BCR | C33-C5-C6 | -3.39 | 120.72 | 124.53 |
| 22 | B | 817 | CLA | CAC-C3C-C4C | 3.39 | 129.21 | 124.81 |
| 29 | 5 | 618 | CHL | C3D-C4D-ND | 3.39 | 115.72 | 110.24 |
| 22 | A | 819 | CLA | C1-C2-C3 | -3.39 | 120.18 | 126.04 |
| 22 | A | 831 | CLA | CHC-C1C-C2C | -3.39 | 117.35 | 126.72 |
| 22 | 5 | 603 | CLA | C3B-C4B-NB | 3.39 | 113.59 | 109.21 |
| 22 | A | 817 | CLA | CBC-CAC-C3C | -3.38 | 103.10 | 112.43 |
| 22 | 9 | 612 | CLA | C3B-C4B-NB | 3.38 | 113.58 | 109.21 |
| 22 | 9 | 614 | CLA | CAC-C3C-C4C | 3.38 | 129.20 | 124.81 |
| 22 | 5 | 621 | CLA | CMB-C2B-C3B | 3.38 | 131.01 | 124.68 |
| 30 | 3 | 622 | LUT | C2-C3-C4 | 3.38 | 114.94 | 110.30 |
| 22 | 5 | 611 | CLA | C3B-C4B-NB | 3.38 | 113.58 | 109.21 |
| 22 | 8 | 612 | CLA | C4-C3-C5 | 3.38 | 120.96 | 115.27 |
| 22 | B | 802 | CLA | C3B-C4B-NB | 3.38 | 113.58 | 109.21 |
| 22 | A | 845 | CLA | C4C-C3C-C2C | -3.38 | 101.98 | 106.90 |
| 22 | A | 803 | CLA | CAC-C3C-C4C | 3.37 | 129.19 | 124.81 |
| 22 | 3 | 614 | CLA | C3B-C4B-NB | 3.37 | 113.57 | 109.21 |
| 22 | A | 838 | CLA | C4-C3-C5 | 3.37 | 119.84 | 115.98 |
| 22 | 8 | 603 | CLA | C3B-C4B-NB | 3.37 | 113.57 | 109.21 |
| 22 | 3 | 611 | CLA | C3B-C4B-NB | 3.37 | 113.56 | 109.21 |
| 22 | 1 | 602 | CLA | C1C-C2C-C3C | -3.37 | 103.42 | 106.96 |
| 22 | G | 204 | CLA | C3B-C4B-NB | 3.37 | 113.56 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 6 | 622 | CLA | CAC-C3C-C4C | 3.37 | 129.18 | 124.81 |
| 22 | B | 815 | CLA | C3B-C4B-NB | 3.37 | 113.56 | 109.21 |
| 22 | 7 | 604 | CLA | CAC-C3C-C4C | 3.36 | 129.17 | 124.81 |
| 25 | 3 | 718 | BCR | C7-C8-C9 | -3.36 | 121.15 | 126.23 |
| 22 | A | 825 | CLA | CHC-C1C-C2C | -3.36 | 117.42 | 126.72 |
| 22 | 7 | 609 | CLA | C1-C2-C3 | -3.36 | 121.32 | 126.75 |
| 25 | 3 | 719 | BCR | C15-C14-C13 | -3.36 | 122.52 | 127.31 |
| 22 | A | 828 | CLA | O2D-CGD-O1D | -3.36 | 117.28 | 123.84 |
| 22 | A | 841 | CLA | CMA-C3A-C4A | -3.36 | 102.75 | 111.77 |
| 25 | A | 848 | BCR | C7-C8-C9 | -3.36 | 121.17 | 126.23 |
| 22 | A | 834 | CLA | C4-C3-C5 | 3.36 | 120.92 | 115.27 |
| 22 | 7 | 611 | CLA | O2D-CGD-O1D | -3.35 | 117.28 | 123.84 |
| 29 | 6 | 618 | CHL | C3D-C4D-ND | 3.35 | 115.66 | 110.24 |
| 22 | 5 | 613 | CLA | CAC-C3C-C4C | 3.35 | 129.16 | 124.81 |
| 22 | 2 | 603 | CLA | CAC-C3C-C4C | 3.35 | 129.16 | 124.81 |
| 22 | 7 | 603 | CLA | CAA-C2A-C3A | -3.35 | 103.60 | 112.78 |
| 22 | A | 827 | CLA | C1C-C2C-C3C | -3.35 | 103.43 | 106.96 |
| 22 | Z | 603 | CLA | CHC-C1C-C2C | -3.35 | 117.46 | 126.72 |
| 22 | 5 | 613 | CLA | CHC-C1C-C2C | -3.35 | 117.46 | 126.72 |
| 22 | B | 822 | CLA | C3B-C4B-NB | 3.35 | 113.54 | 109.21 |
| 22 | A | 837 | CLA | CMB-C2B-C3B | 3.35 | 130.94 | 124.68 |
| 22 | 7 | 616 | CLA | C3B-C4B-NB | 3.35 | 113.54 | 109.21 |
| 22 | A | 805 | CLA | C1-C2-C3 | -3.35 | 120.26 | 126.04 |
| 25 | B | 847 | BCR | C24-C23-C22 | -3.35 | 121.18 | 126.23 |
| 22 | B | 817 | CLA | CHC-C1C-C2C | -3.34 | 117.48 | 126.72 |
| 22 | 1 | 609 | CLA | O2A-CGA-CBA | 3.34 | 122.39 | 111.91 |
| 29 | 4 | 618 | CHL | C2A-C3A-C4A | -3.34 | 96.48 | 101.87 |
| 22 | 3 | 612 | CLA | CHC-C1C-C2C | -3.34 | 117.48 | 126.72 |
| 22 | 6 | 609 | CLA | CHC-C1C-C2C | -3.34 | 117.49 | 126.72 |
| 22 | A | 806 | CLA | C3C-C4C-NC | 3.34 | 114.31 | 110.57 |
| 22 | A | 819 | CLA | C4C-C3C-C2C | -3.34 | 102.03 | 106.90 |
| 22 | 5 | 602 | CLA | CMC-C2C-C1C | 3.34 | 130.12 | 125.04 |
| 22 | B | 821 | CLA | C3B-C4B-NB | 3.34 | 113.52 | 109.21 |
| 22 | Z | 602 | CLA | CAC-C3C-C4C | 3.33 | 129.14 | 124.81 |
| 22 | B | 823 | CLA | C4C-C3C-C2C | -3.33 | 102.04 | 106.90 |
| 22 | 7 | 616 | CLA | C3C-C4C-NC | 3.33 | 114.31 | 110.57 |
| 22 | B | 818 | CLA | CHC-C1C-C2C | -3.33 | 117.50 | 126.72 |
| 30 | Z | 617 | LUT | C30-C31-C32 | -3.33 | 112.82 | 123.22 |
| 22 | B | 804 | CLA | C1C-C2C-C3C | -3.33 | 103.45 | 106.96 |
| 22 | 1 | 612 | CLA | C3B-C4B-NB | 3.33 | 113.52 | 109.21 |
| 22 | 8 | 604 | CLA | C3B-C4B-NB | 3.33 | 113.52 | 109.21 |
| 22 | B | 837 | CLA | C1C-C2C-C3C | -3.33 | 103.45 | 106.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 9 | 601 | CLA | C3B-C4B-NB | 3.33 | 113.51 | 109.21 |
| 22 | Z | 609 | CLA | C3C-C4C-NC | 3.33 | 114.30 | 110.57 |
| 22 | B | 839 | CLA | C3B-C4B-NB | 3.33 | 113.51 | 109.21 |
| 29 | 6 | 608 | CHL | C2A-C3A-C4A | -3.33 | 96.49 | 101.87 |
| 22 | 6 | 617 | CLA | C3B-C4B-NB | 3.33 | 113.51 | 109.21 |
| 22 | 8 | 613 | CLA | CAC-C3C-C4C | 3.32 | 129.12 | 124.81 |
| 29 | 9 | 607 | CHL | C3B-C4B-NB | 3.32 | 113.51 | 109.21 |
| 25 | B | 844 | BCR | C11-C10-C9 | -3.32 | 122.57 | 127.31 |
| 22 | Z | 604 | CLA | CAC-C3C-C4C | 3.32 | 129.12 | 124.81 |
| 22 | A | 831 | CLA | O2D-CGD-O1D | -3.32 | 117.35 | 123.84 |
| 22 | A | 831 | CLA | C4-C3-C5 | 3.32 | 120.85 | 115.27 |
| 22 | B | 809 | CLA | CHC-C1C-C2C | -3.32 | 117.54 | 126.72 |
| 22 | 1 | 609 | CLA | C3C-C4C-NC | 3.31 | 114.29 | 110.57 |
| 22 | A | 838 | CLA | CHC-C1C-C2C | -3.31 | 117.56 | 126.72 |
| 22 | L | 204 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 109.21 |
| 22 | 3 | 607 | CLA | O2A-CGA-CBA | 3.31 | 122.31 | 111.91 |
| 22 | 4 | 616 | CLA | CHC-C1C-C2C | -3.31 | 117.56 | 126.72 |
| 22 | 8 | 609 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 109.21 |
| 22 | 5 | 602 | CLA | C1C-C2C-C3C | -3.31 | 103.47 | 106.96 |
| 30 | 8 | 618 | LUT | C35-C34-C33 | -3.31 | 122.58 | 127.31 |
| 22 | 9 | 609 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 109.21 |
| 22 | 7 | 614 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 109.21 |
| 22 | A | 821 | CLA | CHC-C1C-C2C | -3.31 | 117.57 | 126.72 |
| 29 | 5 | 607 | CHL | CAC-C3C-C4C | 3.31 | 129.10 | 124.81 |
| 22 | A | 842 | CLA | C3B-C4B-NB | 3.31 | 113.49 | 109.21 |
| 22 | A | 839 | CLA | C4-C3-C5 | 3.31 | 120.84 | 115.27 |
| 29 | 9 | 606 | CHL | C3D-C4D-ND | 3.31 | 115.59 | 110.24 |
| 22 | 5 | 606 | CLA | CAA-C2A-C3A | -3.31 | 103.72 | 112.78 |
| 22 | A | 804 | CLA | O2D-CGD-O1D | -3.31 | 117.38 | 123.84 |
| 29 | 6 | 608 | CHL | C3D-C4D-ND | 3.30 | 115.58 | 110.24 |
| 22 | 3 | 603 | CLA | CAA-C2A-C3A | -3.30 | 103.73 | 112.78 |
| 22 | A | 802 | CLA | C3C-C4C-NC | 3.30 | 114.28 | 110.57 |
| 22 | 3 | 602 | CLA | C1C-C2C-C3C | -3.30 | 103.48 | 106.96 |
| 22 | F | 304 | CLA | CAA-C2A-C3A | -3.30 | 103.73 | 112.78 |
| 22 | 5 | 612 | CLA | CHC-C1C-C2C | -3.30 | 117.59 | 126.72 |
| 22 | B | 838 | CLA | C4A-NA-C1A | -3.30 | 105.22 | 106.71 |
| 22 | 6 | 616 | CLA | CMB-C2B-C3B | 3.30 | 130.85 | 124.68 |
| 22 | 6 | 613 | CLA | CAC-C3C-C4C | 3.30 | 129.09 | 124.81 |
| 22 | 9 | 613 | CLA | CAC-C3C-C4C | 3.30 | 129.09 | 124.81 |
| 22 | 9 | 602 | CLA | C1C-C2C-C3C | -3.30 | 103.49 | 106.96 |
| 22 | B | 831 | CLA | C4C-C3C-C2C | -3.30 | 102.09 | 106.90 |
| 22 | 4 | 602 | CLA | C3C-C4C-NC | 3.30 | 114.27 | 110.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 6 | 601 | CLA | C3B-C4B-NB | 3.30 | 113.47 | 109.21 |
| 22 | 5 | 616 | CLA | C3B-C4B-NB | 3.30 | 113.47 | 109.21 |
| 22 | 1 | 616 | CLA | C3B-C4B-NB | 3.29 | 113.47 | 109.21 |
| 22 | A | 834 | CLA | C1-C2-C3 | -3.29 | 120.35 | 126.04 |
| 25 | 8 | 619 | BCR | C11-C10-C9 | -3.29 | 122.61 | 127.31 |
| 22 | B | 819 | CLA | CAC-C3C-C4C | 3.29 | 129.08 | 124.81 |
| 22 | 4 | 610 | CLA | CHC-C1C-C2C | -3.29 | 117.62 | 126.72 |
| 22 | B | 829 | CLA | C3B-C4B-NB | 3.29 | 113.47 | 109.21 |
| 22 | 5 | 602 | CLA | CHD-C4C-NC | 3.29 | 129.39 | 124.20 |
| 22 | B | 803 | CLA | CHC-C1C-C2C | -3.29 | 117.62 | 126.72 |
| 22 | B | 819 | CLA | C3C-C4C-NC | 3.29 | 114.26 | 110.57 |
| 22 | 5 | 617 | CLA | C1C-C2C-C3C | -3.29 | 103.50 | 106.96 |
| 22 | 4 | 601 | CLA | CHC-C1C-C2C | -3.29 | 117.63 | 126.72 |
| 30 | 1 | 619 | LUT | C10-C11-C12 | -3.29 | 112.96 | 123.22 |
| 22 | 4 | 603 | CLA | CHC-C1C-C2C | -3.29 | 117.63 | 126.72 |
| 22 | B | 829 | CLA | CMA-C3A-C2A | -3.29 | 100.57 | 113.83 |
| 22 | 1 | 613 | CLA | C4A-NA-C1A | -3.29 | 105.23 | 106.71 |
| 22 | 5 | 617 | CLA | C4C-C3C-C2C | -3.28 | 102.11 | 106.90 |
| 22 | 5 | 611 | CLA | CAA-C2A-C3A | -3.28 | 103.79 | 112.78 |
| 22 | 4 | 610 | CLA | C4C-C3C-C2C | -3.28 | 102.11 | 106.90 |
| 22 | 7 | 610 | CLA | C4C-C3C-C2C | -3.28 | 102.11 | 106.90 |
| 22 | 1 | 604 | CLA | C3B-C4B-NB | 3.28 | 113.45 | 109.21 |
| 22 | Z | 602 | CLA | C4-C3-C5 | 3.28 | 120.79 | 115.27 |
| 22 | B | 841 | CLA | C3C-C4C-NC | 3.28 | 114.25 | 110.57 |
| 22 | 3 | 613 | CLA | C4C-C3C-C2C | -3.28 | 102.12 | 106.90 |
| 22 | 3 | 620 | CLA | C3B-C4B-NB | 3.28 | 113.45 | 109.21 |
| 22 | B | 828 | CLA | CAC-C3C-C4C | 3.28 | 129.06 | 124.81 |
| 22 | 7 | 613 | CLA | CAC-C3C-C4C | 3.28 | 129.06 | 124.81 |
| 22 | Z | 610 | CLA | C1-C2-C3 | -3.28 | 120.38 | 126.04 |
| 22 | A | 840 | CLA | CAC-C3C-C4C | 3.28 | 129.06 | 124.81 |
| 25 | A | 851 | BCR | C20-C21-C22 | -3.28 | 122.64 | 127.31 |
| 22 | B | 826 | CLA | C3B-C4B-NB | 3.27 | 113.44 | 109.21 |
| 25 | B | 845 | BCR | C15-C14-C13 | -3.27 | 122.64 | 127.31 |
| 22 | 1 | 610 | CLA | CAC-C3C-C4C | 3.27 | 129.06 | 124.81 |
| 22 | 1 | 610 | CLA | CHD-C4C-NC | 3.27 | 129.36 | 124.20 |
| 21 | A | 801 | CL0 | C1-C2-C3 | -3.27 | 120.38 | 126.04 |
| 25 | L | 201 | BCR | C16-C17-C18 | -3.27 | 122.64 | 127.31 |
| 22 | 4 | 604 | CLA | C3C-C4C-NC | 3.27 | 114.24 | 110.57 |
| 30 | 3 | 622 | LUT | C18-C5-C6 | -3.27 | 120.85 | 124.53 |
| 25 | F | 305 | BCR | C15-C16-C17 | -3.27 | 116.77 | 123.47 |
| 25 | L | 201 | BCR | C34-C9-C10 | -3.27 | 118.34 | 122.92 |
| 22 | 9 | 603 | CLA | CAC-C3C-C4C | 3.27 | 129.05 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 3 | 610 | CLA | CAA-C2A-C3A | -3.27 | 103.83 | 112.78 |
| 22 | A | 843 | CLA | C3B-C4B-NB | 3.27 | 113.44 | 109.21 |
| 22 | 7 | 611 | CLA | CHC-C1C-C2C | -3.27 | 117.69 | 126.72 |
| 22 | 5 | 601 | CLA | O2A-CGA-CBA | 3.27 | 122.16 | 111.91 |
| 22 | A | 816 | CLA | C4C-C3C-C2C | -3.27 | 102.14 | 106.90 |
| 22 | A | 826 | CLA | CHC-C1C-C2C | -3.27 | 117.69 | 126.72 |
| 22 | G | 203 | CLA | CAC-C3C-C4C | 3.26 | 129.05 | 124.81 |
| 22 | 7 | 616 | CLA | CAC-C3C-C4C | 3.26 | 129.05 | 124.81 |
| 22 | 6 | 616 | CLA | C1C-C2C-C3C | -3.26 | 103.52 | 106.96 |
| 22 | A | 822 | CLA | C1-O2A-CGA | 3.26 | 125.01 | 116.44 |
| 22 | B | 840 | CLA | C4C-C3C-C2C | -3.26 | 102.14 | 106.90 |
| 22 | L | 204 | CLA | CAC-C3C-C4C | 3.26 | 129.04 | 124.81 |
| 22 | J | 3002 | CLA | C3B-C4B-NB | 3.26 | 113.43 | 109.21 |
| 22 | A | 809 | CLA | O2D-CGD-O1D | -3.26 | 117.46 | 123.84 |
| 22 | Z | 608 | CLA | C3B-C4B-NB | 3.26 | 113.42 | 109.21 |
| 22 | A | 830 | CLA | CAC-C3C-C4C | 3.26 | 129.04 | 124.81 |
| 22 | B | 802 | CLA | CHD-C4C-NC | 3.26 | 129.34 | 124.20 |
| 22 | B | 804 | CLA | C3B-C4B-NB | 3.26 | 113.42 | 109.21 |
| 22 | 5 | 621 | CLA | C4C-C3C-C2C | -3.26 | 102.15 | 106.90 |
| 29 | Z | 601 | CHL | C2A-C1A-CHA | -3.26 | 118.16 | 123.86 |
| 22 | 3 | 614 | CLA | CAC-C3C-C4C | 3.26 | 129.04 | 124.81 |
| 22 | 5 | 609 | CLA | CHC-C1C-C2C | -3.26 | 117.71 | 126.72 |
| 22 | 8 | 604 | CLA | CHC-C1C-C2C | -3.26 | 117.71 | 126.72 |
| 22 | 7 | 602 | CLA | C4C-C3C-C2C | -3.25 | 102.16 | 106.90 |
| 22 | 5 | 616 | CLA | CAA-C2A-C3A | -3.25 | 103.87 | 112.78 |
| 30 | 7 | 621 | LUT | C35-C15-C14 | -3.25 | 116.81 | 123.47 |
| 29 | 4 | 606 | CHL | CAC-C3C-C4C | 3.25 | 129.03 | 124.81 |
| 22 | B | 804 | CLA | CHB-C4A-NA | 3.25 | 129.01 | 124.51 |
| 30 | 8 | 618 | LUT | C10-C11-C12 | -3.25 | 113.07 | 123.22 |
| 22 | B | 834 | CLA | C3C-C4C-NC | 3.25 | 114.22 | 110.57 |
| 22 | A | 811 | CLA | CAA-C2A-C3A | -3.25 | 103.88 | 112.78 |
| 22 | 8 | 611 | CLA | CHC-C1C-C2C | -3.25 | 117.74 | 126.72 |
| 22 | A | 811 | CLA | C3B-C4B-NB | 3.25 | 113.41 | 109.21 |
| 22 | A | 808 | CLA | CMC-C2C-C1C | 3.25 | 129.98 | 125.04 |
| 25 | G | 205 | BCR | C11-C10-C9 | -3.25 | 122.68 | 127.31 |
| 22 | A | 837 | CLA | CHC-C1C-C2C | -3.25 | 117.74 | 126.72 |
| 25 | 6 | 625 | BCR | C16-C17-C18 | -3.25 | 122.68 | 127.31 |
| 22 | B | 829 | CLA | C4A-NA-C1A | -3.25 | 105.25 | 106.71 |
| 22 | 7 | 610 | CLA | C2C-C1C-NC | 3.25 | 113.01 | 109.97 |
| 22 | A | 804 | CLA | C3B-C4B-NB | 3.24 | 113.41 | 109.21 |
| 22 | B | 834 | CLA | CAC-C3C-C4C | 3.24 | 129.02 | 124.81 |
| 22 | 3 | 613 | CLA | CHC-C1C-C2C | -3.24 | 117.75 | 126.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 7 | 616 | CLA | CHC-C1C-C2C | -3.24 | 117.75 | 126.72 |
| 29 | 4 | 618 | CHL | C3D-C4D-ND | 3.24 | 115.48 | 110.24 |
| 22 | A | 831 | CLA | CAC-C3C-C4C | 3.24 | 129.02 | 124.81 |
| 22 | 8 | 616 | CLA | CAA-C2A-C3A | -3.24 | 103.91 | 112.78 |
| 22 | 7 | 608 | CLA | CHD-C4C-NC | 3.24 | 129.31 | 124.20 |
| 22 | 6 | 613 | CLA | C3B-C4B-NB | 3.24 | 113.40 | 109.21 |
| 22 | A | 831 | CLA | CMB-C2B-C3B | 3.24 | 130.74 | 124.68 |
| 22 | 5 | 617 | CLA | CAC-C3C-C4C | 3.24 | 129.01 | 124.81 |
| 29 | 1 | 607 | CHL | C3B-C4B-NB | 3.24 | 113.40 | 109.21 |
| 22 | 1 | 602 | CLA | CHD-C4C-NC | 3.24 | 129.30 | 124.20 |
| 22 | 3 | 610 | CLA | CHD-C4C-NC | 3.24 | 129.30 | 124.20 |
| 22 | B | 836 | CLA | C1C-C2C-C3C | -3.24 | 103.55 | 106.96 |
| 22 | 3 | 609 | CLA | CHB-C4A-NA | 3.24 | 128.99 | 124.51 |
| 22 | 7 | 603 | CLA | C3B-C4B-NB | 3.24 | 113.39 | 109.21 |
| 22 | Z | 611 | CLA | C3B-C4B-NB | 3.24 | 113.39 | 109.21 |
| 22 | B | 816 | CLA | C4C-C3C-C2C | -3.23 | 102.18 | 106.90 |
| 22 | 6 | 614 | CLA | C3B-C4B-NB | 3.23 | 113.39 | 109.21 |
| 22 | 2 | 607 | CLA | C3B-C4B-NB | 3.23 | 113.39 | 109.21 |
| 22 | Z | 616 | CLA | C3B-C4B-NB | 3.23 | 113.39 | 109.21 |
| 22 | A | 841 | CLA | C4C-C3C-C2C | -3.23 | 102.19 | 106.90 |
| 22 | A | 833 | CLA | CMB-C2B-C3B | 3.23 | 130.72 | 124.68 |
| 22 | A | 817 | CLA | C3C-C4C-NC | 3.23 | 114.19 | 110.57 |
| 25 | 6 | 623 | BCR | C16-C17-C18 | -3.23 | 122.71 | 127.31 |
| 22 | 1 | 609 | CLA | CHC-C1C-C2C | -3.23 | 117.80 | 126.72 |
| 22 | 2 | 612 | CLA | CHC-C1C-C2C | -3.23 | 117.80 | 126.72 |
| 22 | 4 | 602 | CLA | CAC-C3C-C4C | 3.22 | 128.99 | 124.81 |
| 22 | 6 | 611 | CLA | CAA-C2A-C3A | -3.22 | 103.95 | 112.78 |
| 22 | A | 835 | CLA | O2D-CGD-O1D | -3.22 | 117.54 | 123.84 |
| 29 | 3 | 608 | CHL | CHD-C4C-NC | 3.22 | 129.28 | 124.20 |
| 25 | 4 | 621 | BCR | C15-C16-C17 | -3.22 | 116.88 | 123.47 |
| 22 | 2 | 602 | CLA | CAC-C3C-C4C | 3.22 | 128.99 | 124.81 |
| 22 | 7 | 604 | CLA | CMC-C2C-C1C | 3.22 | 129.94 | 125.04 |
| 22 | 5 | 617 | CLA | C3B-C4B-NB | 3.22 | 113.37 | 109.21 |
| 22 | A | 832 | CLA | C3B-C4B-NB | 3.22 | 113.37 | 109.21 |
| 22 | 4 | 604 | CLA | C1-C2-C3 | -3.22 | 121.55 | 126.75 |
| 22 | 7 | 616 | CLA | C1D-CHD-C4C | -3.22 | 119.12 | 126.06 |
| 22 | 2 | 609 | CLA | CHC-C1C-C2C | -3.22 | 117.83 | 126.72 |
| 22 | 3 | 609 | CLA | CAC-C3C-C4C | 3.22 | 128.98 | 124.81 |
| 22 | 4 | 611 | CLA | CHC-C1C-C2C | -3.22 | 117.83 | 126.72 |
| 22 | 3 | 610 | CLA | CMA-C3A-C2A | -3.21 | 100.86 | 113.83 |
| 22 | 9 | 613 | CLA | CHC-C1C-C2C | -3.21 | 117.83 | 126.72 |
| 22 | B | 820 | CLA | C3B-C4B-NB | 3.21 | 113.37 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30 | 1 | 617 | LUT | C30-C31-C32 | -3.21 | 113.19 | 123.22 |
| 22 | B | 830 | CLA | CAA-C2A-C3A | -3.21 | 103.98 | 112.78 |
| 22 | Z | 606 | CLA | CAA-C2A-C3A | -3.21 | 103.98 | 112.78 |
| 22 | A | 823 | CLA | C3B-C4B-NB | 3.21 | 113.36 | 109.21 |
| 29 | Z | 607 | CHL | C3D-C4D-ND | 3.21 | 115.43 | 110.24 |
| 22 | 9 | 611 | CLA | C3B-C4B-NB | 3.21 | 113.36 | 109.21 |
| 22 | 5 | 610 | CLA | CAA-C2A-C3A | -3.21 | 103.99 | 112.78 |
| 22 | A | 830 | CLA | C3B-C4B-NB | 3.21 | 113.36 | 109.21 |
| 25 | A | 848 | BCR | C16-C15-C14 | -3.21 | 116.90 | 123.47 |
| 22 | A | 836 | CLA | CHC-C1C-C2C | -3.21 | 117.85 | 126.72 |
| 30 | 2 | 617 | LUT | C7-C8-C9 | -3.21 | 121.39 | 126.23 |
| 22 | 8 | 603 | CLA | CHC-C1C-C2C | -3.21 | 117.85 | 126.72 |
| 25 | I | 172 | BCR | C20-C19-C18 | -3.21 | 117.41 | 126.42 |
| 22 | 4 | 609 | CLA | CHC-C1C-C2C | -3.21 | 117.86 | 126.72 |
| 25 | J | 3003 | BCR | C3-C4-C5 | -3.21 | 108.35 | 114.08 |
| 22 | 9 | 604 | CLA | CHC-C1C-C2C | -3.20 | 117.86 | 126.72 |
| 22 | A | 804 | CLA | C1C-C2C-C3C | -3.20 | 103.59 | 106.96 |
| 22 | B | 818 | CLA | C4-C3-C5 | 3.20 | 120.66 | 115.27 |
| 22 | B | 820 | CLA | C1-C2-C3 | -3.20 | 120.50 | 126.04 |
| 22 | A | 816 | CLA | C1C-C2C-C3C | -3.20 | 103.59 | 106.96 |
| 22 | 1 | 609 | CLA | CAC-C3C-C4C | 3.20 | 128.97 | 124.81 |
| 25 | J | 3003 | BCR | C38-C26-C25 | -3.20 | 120.93 | 124.53 |
| 22 | B | 829 | CLA | C4C-C3C-C2C | -3.20 | 102.23 | 106.90 |
| 22 | 3 | 611 | CLA | CAC-C3C-C4C | 3.20 | 128.96 | 124.81 |
| 22 | Z | 616 | CLA | CAC-C3C-C4C | 3.20 | 128.96 | 124.81 |
| 22 | A | 807 | CLA | O2A-CGA-CBA | 3.20 | 121.95 | 111.91 |
| 22 | 9 | 603 | CLA | CHC-C1C-C2C | -3.20 | 117.87 | 126.72 |
| 22 | B | 832 | CLA | CHD-C4C-NC | 3.20 | 129.24 | 124.20 |
| 22 | A | 829 | CLA | C4C-C3C-C2C | -3.20 | 102.23 | 106.90 |
| 29 | 8 | 607 | CHL | CAC-C3C-C4C | 3.20 | 128.96 | 124.81 |
| 22 | 4 | 601 | CLA | C3C-C4C-NC | 3.20 | 114.16 | 110.57 |
| 22 | A | 826 | CLA | CAC-C3C-C4C | 3.20 | 128.96 | 124.81 |
| 22 | 6 | 603 | CLA | CHC-C1C-C2C | -3.19 | 117.88 | 126.72 |
| 22 | 3 | 603 | CLA | O2D-CGD-CBD | 3.19 | 116.94 | 111.27 |
| 22 | 1 | 611 | CLA | CAA-C2A-C3A | -3.19 | 104.03 | 112.78 |
| 22 | F | 304 | CLA | CAC-C3C-C4C | 3.19 | 128.95 | 124.81 |
| 22 | 5 | 614 | CLA | O2D-CGD-O1D | -3.19 | 117.59 | 123.84 |
| 22 | 1 | 616 | CLA | CHC-C1C-C2C | -3.19 | 117.89 | 126.72 |
| 22 | A | 819 | CLA | CMB-C2B-C3B | 3.19 | 130.65 | 124.68 |
| 22 | B | 824 | CLA | CAC-C3C-C4C | 3.19 | 128.95 | 124.81 |
| 22 | 7 | 609 | CLA | O2D-CGD-CBD | 3.19 | 116.94 | 111.27 |
| 21 | A | 801 | CL0 | CBC-CAC-C3C | -3.19 | 103.63 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | 3 | 608 | CHL | C3B-C4B-NB | 3.19 | 113.33 | 109.21 |
| 25 | B | 847 | BCR | C15-C14-C13 | -3.19 | 122.76 | 127.31 |
| 22 | 1 | 604 | CLA | CAC-C3C-C4C | 3.19 | 128.94 | 124.81 |
| 29 | 1 | 601 | CHL | O2A-C1-C2 | 3.19 | 117.01 | 108.64 |
| 22 | 5 | 609 | CLA | CMB-C2B-C3B | 3.19 | 130.64 | 124.68 |
| 25 | B | 847 | BCR | C16-C17-C18 | -3.19 | 122.76 | 127.31 |
| 22 | A | 831 | CLA | C4C-C3C-C2C | -3.19 | 102.25 | 106.90 |
| 22 | 3 | 603 | CLA | CAC-C3C-C4C | 3.18 | 128.94 | 124.81 |
| 22 | B | 807 | CLA | CAC-C3C-C4C | 3.18 | 128.94 | 124.81 |
| 22 | A | 839 | CLA | O2D-CGD-O1D | -3.18 | 117.61 | 123.84 |
| 22 | 5 | 611 | CLA | CHC-C1C-C2C | -3.18 | 117.92 | 126.72 |
| 22 | 1 | 603 | CLA | CAC-C3C-C4C | 3.18 | 128.94 | 124.81 |
| 22 | 1 | 612 | CLA | CHC-C1C-C2C | -3.18 | 117.92 | 126.72 |
| 22 | A | 837 | CLA | CAC-C3C-C4C | 3.18 | 128.94 | 124.81 |
| 22 | A | 821 | CLA | C3B-C4B-NB | 3.18 | 113.32 | 109.21 |
| 22 | 1 | 606 | CLA | C4-C3-C5 | 3.18 | 120.62 | 115.27 |
| 22 | 7 | 613 | CLA | CHC-C1C-C2C | -3.18 | 117.92 | 126.72 |
| 22 | 6 | 610 | CLA | CMB-C2B-C3B | 3.18 | 130.63 | 124.68 |
| 22 | 2 | 610 | CLA | CMB-C2B-C3B | 3.18 | 130.63 | 124.68 |
| 22 | A | 804 | CLA | C4C-C3C-C2C | -3.18 | 102.26 | 106.90 |
| 22 | A | 802 | CLA | C2A-C1A-CHA | -3.18 | 118.30 | 123.86 |
| 22 | 3 | 606 | CLA | CHC-C1C-C2C | -3.18 | 117.93 | 126.72 |
| 22 | 2 | 602 | CLA | C3B-C4B-NB | 3.18 | 113.32 | 109.21 |
| 22 | A | 845 | CLA | CHC-C1C-C2C | -3.18 | 117.93 | 126.72 |
| 22 | G | 204 | CLA | CAC-C3C-C4C | 3.18 | 128.93 | 124.81 |
| 22 | 2 | 611 | CLA | CAA-C2A-C3A | -3.18 | 104.08 | 112.78 |
| 22 | A | 809 | CLA | C1-C2-C3 | -3.18 | 120.55 | 126.04 |
| 22 | B | 810 | CLA | CHC-C1C-C2C | -3.18 | 117.94 | 126.72 |
| 21 | A | 801 | CL0 | CHC-C1C-C2C | -3.18 | 117.94 | 126.72 |
| 30 | Z | 618 | LUT | C15-C14-C13 | -3.17 | 122.78 | 127.31 |
| 22 | 9 | 611 | CLA | C4-C3-C5 | 3.17 | 120.61 | 115.27 |
| 22 | 7 | 612 | CLA | CHC-C1C-C2C | -3.17 | 117.94 | 126.72 |
| 29 | 4 | 607 | CHL | C3B-C4B-NB | 3.17 | 113.31 | 109.21 |
| 22 | B | 833 | CLA | C4C-C3C-C2C | -3.17 | 102.27 | 106.90 |
| 22 | B | 813 | CLA | C3B-C4B-NB | 3.17 | 113.31 | 109.21 |
| 22 | 3 | 604 | CLA | CHC-C1C-C2C | -3.17 | 117.95 | 126.72 |
| 22 | Z | 614 | CLA | C3B-C4B-NB | 3.17 | 113.31 | 109.21 |
| 22 | 9 | 610 | CLA | CAC-C3C-C4C | 3.17 | 128.92 | 124.81 |
| 22 | Z | 610 | CLA | CHD-C4C-NC | 3.17 | 129.20 | 124.20 |
| 22 | 3 | 620 | CLA | CHC-C1C-C2C | -3.17 | 117.95 | 126.72 |
| 30 | 6 | 621 | LUT | C7-C8-C9 | -3.17 | 121.45 | 126.23 |
| 22 | B | 834 | CLA | C3B-C4B-NB | 3.17 | 113.31 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 807 | CLA | CHC-C1C-C2C | -3.17 | 117.96 | 126.72 |
| 22 | A | 839 | CLA | C3B-C4B-NB | 3.17 | 113.30 | 109.21 |
| 22 | B | 818 | CLA | C3B-C4B-NB | 3.17 | 113.30 | 109.21 |
| 22 | 1 | 603 | CLA | CHC-C1C-C2C | -3.17 | 117.96 | 126.72 |
| 22 | G | 203 | CLA | C1-C2-C3 | -3.17 | 121.63 | 126.75 |
| 25 | I | 172 | BCR | C16-C17-C18 | -3.17 | 122.79 | 127.31 |
| 30 | 1 | 617 | LUT | C35-C15-C14 | -3.16 | 116.99 | 123.47 |
| 29 | 6 | 608 | CHL | C2A-C1A-CHA | -3.16 | 118.33 | 123.86 |
| 22 | 5 | 616 | CLA | CHC-C1C-C2C | -3.16 | 117.97 | 126.72 |
| 22 | A | 835 | CLA | C1-C2-C3 | -3.16 | 120.57 | 126.04 |
| 25 | L | 205 | BCR | C28-C27-C26 | -3.16 | 108.43 | 114.08 |
| 25 | 6 | 623 | BCR | C11-C12-C13 | -3.16 | 117.53 | 126.42 |
| 22 | A | 812 | CLA | C4C-C3C-C2C | -3.16 | 102.29 | 106.90 |
| 22 | B | 808 | CLA | C4C-C3C-C2C | -3.16 | 102.29 | 106.90 |
| 22 | 5 | 611 | CLA | O2D-CGD-O1D | -3.16 | 117.66 | 123.84 |
| 22 | B | 826 | CLA | CAA-C2A-C3A | -3.16 | 104.12 | 112.78 |
| 22 | 7 | 606 | CLA | C3B-C4B-NB | 3.16 | 113.30 | 109.21 |
| 22 | A | 811 | CLA | CAC-C3C-C4C | 3.16 | 128.91 | 124.81 |
| 25 | A | 850 | BCR | C24-C23-C22 | -3.16 | 121.46 | 126.23 |
| 22 | B | 825 | CLA | CHD-C4C-NC | 3.16 | 129.18 | 124.20 |
| 22 | A | 816 | CLA | CAC-C3C-C4C | 3.16 | 128.91 | 124.81 |
| 22 | 2 | 601 | CLA | CHC-C1C-C2C | -3.16 | 117.99 | 126.72 |
| 22 | 6 | 622 | CLA | C3B-C4B-NB | 3.16 | 113.29 | 109.21 |
| 29 | 9 | 606 | CHL | C3B-C4B-NB | 3.16 | 113.29 | 109.21 |
| 25 | L | 205 | BCR | C29-C30-C25 | 3.16 | 115.34 | 110.48 |
| 22 | Z | 603 | CLA | CAC-C3C-C4C | 3.16 | 128.91 | 124.81 |
| 22 | B | 808 | CLA | CAA-C2A-C3A | -3.16 | 104.14 | 112.78 |
| 22 | B | 852 | CLA | C3B-C4B-NB | 3.16 | 113.29 | 109.21 |
| 22 | 8 | 601 | CLA | C3B-C4B-NB | 3.16 | 113.29 | 109.21 |
| 22 | 9 | 610 | CLA | CAA-C2A-C3A | -3.16 | 104.14 | 112.78 |
| 22 | Z | 604 | CLA | CHC-C1C-C2C | -3.16 | 117.99 | 126.72 |
| 22 | A | 806 | CLA | O2D-CGD-O1D | -3.15 | 117.67 | 123.84 |
| 22 | B | 810 | CLA | CAC-C3C-C4C | 3.15 | 128.90 | 124.81 |
| 22 | B | 807 | CLA | O2A-CGA-CBA | 3.15 | 121.80 | 111.91 |
| 22 | 4 | 613 | CLA | CAC-C3C-C4C | 3.15 | 128.90 | 124.81 |
| 22 | Z | 616 | CLA | CHC-C1C-C2C | -3.15 | 118.00 | 126.72 |
| 22 | 3 | 609 | CLA | CHC-C1C-C2C | -3.15 | 118.00 | 126.72 |
| 22 | 1 | 604 | CLA | C3C-C4C-NC | 3.15 | 114.10 | 110.57 |
| 22 | B | 830 | CLA | C4C-C3C-C2C | -3.15 | 102.31 | 106.90 |
| 22 | 2 | 613 | CLA | CHC-C1C-C2C | -3.15 | 118.01 | 126.72 |
| 22 | A | 839 | CLA | CHC-C1C-C2C | -3.15 | 118.01 | 126.72 |
| 22 | B | 819 | CLA | CAA-C2A-C3A | -3.15 | 104.15 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 802 | CLA | C3B-C4B-NB | 3.15 | 113.28 | 109.21 |
| 22 | 4 | 613 | CLA | CHC-C1C-C2C | -3.15 | 118.01 | 126.72 |
| 22 | Z | 606 | CLA | C4-C3-C5 | 3.15 | 120.57 | 115.27 |
| 22 | A | 843 | CLA | CHC-C1C-C2C | -3.15 | 118.01 | 126.72 |
| 29 | 4 | 618 | CHL | CAC-C3C-C4C | 3.15 | 128.89 | 124.81 |
| 22 | B | 806 | CLA | CHD-C4C-NC | 3.15 | 129.16 | 124.20 |
| 22 | 1 | 613 | CLA | CAC-C3C-C4C | 3.15 | 128.89 | 124.81 |
| 22 | A | 811 | CLA | C4C-C3C-C2C | -3.15 | 102.31 | 106.90 |
| 22 | A | 832 | CLA | C4C-C3C-C2C | -3.15 | 102.31 | 106.90 |
| 22 | 8 | 609 | CLA | CHC-C1C-C2C | -3.15 | 118.02 | 126.72 |
| 22 | B | 833 | CLA | CAC-C3C-C4C | 3.15 | 128.89 | 124.81 |
| 22 | 2 | 613 | CLA | O2A-CGA-CBA | 3.15 | 121.78 | 111.91 |
| 22 | B | 839 | CLA | CAC-C3C-C4C | 3.15 | 128.89 | 124.81 |
| 22 | G | 203 | CLA | CHC-C1C-C2C | -3.14 | 118.02 | 126.72 |
| 22 | Z | 609 | CLA | CAC-C3C-C4C | 3.14 | 128.89 | 124.81 |
| 22 | 8 | 610 | CLA | CMC-C2C-C1C | 3.14 | 129.83 | 125.04 |
| 22 | L | 204 | CLA | C4C-C3C-C2C | -3.14 | 102.31 | 106.90 |
| 22 | 9 | 601 | CLA | CHC-C1C-C2C | -3.14 | 118.03 | 126.72 |
| 22 | 5 | 601 | CLA | CHC-C1C-C2C | -3.14 | 118.03 | 126.72 |
| 22 | A | 811 | CLA | C1C-C2C-C3C | -3.14 | 103.65 | 106.96 |
| 22 | A | 815 | CLA | C1-C2-C3 | -3.14 | 120.61 | 126.04 |
| 29 | 5 | 618 | CHL | CAC-C3C-C4C | 3.14 | 128.88 | 124.81 |
| 22 | 8 | 611 | CLA | CAA-C2A-C3A | -3.14 | 104.18 | 112.78 |
| 22 | 1 | 616 | CLA | CAC-C3C-C4C | 3.14 | 128.88 | 124.81 |
| 22 | 1 | 606 | CLA | C4C-C3C-C2C | -3.14 | 102.32 | 106.90 |
| 22 | B | 819 | CLA | CHC-C1C-C2C | -3.14 | 118.04 | 126.72 |
| 25 | A | 851 | BCR | C21-C20-C19 | -3.14 | 113.43 | 123.22 |
| 22 | 7 | 609 | CLA | CHC-C1C-C2C | -3.14 | 118.05 | 126.72 |
| 25 | 7 | 624 | BCR | C28-C27-C26 | -3.14 | 108.48 | 114.08 |
| 22 | 2 | 601 | CLA | CAC-C3C-C4C | 3.14 | 128.88 | 124.81 |
| 22 | F | 303 | CLA | CHC-C1C-C2C | -3.14 | 118.05 | 126.72 |
| 22 | 4 | 601 | CLA | CAC-C3C-C4C | 3.13 | 128.88 | 124.81 |
| 22 | Z | 602 | CLA | C1C-C2C-C3C | -3.13 | 103.66 | 106.96 |
| 22 | B | 828 | CLA | C4C-C3C-C2C | -3.13 | 102.33 | 106.90 |
| 22 | B | 825 | CLA | C4C-C3C-C2C | -3.13 | 102.33 | 106.90 |
| 22 | 5 | 621 | CLA | CHC-C1C-C2C | -3.13 | 118.06 | 126.72 |
| 22 | 9 | 612 | CLA | CHC-C1C-C2C | -3.13 | 118.06 | 126.72 |
| 22 | 4 | 609 | CLA | CHB-C4A-NA | 3.13 | 128.84 | 124.51 |
| 22 | 9 | 609 | CLA | CHC-C1C-C2C | -3.13 | 118.06 | 126.72 |
| 22 | 6 | 610 | CLA | O2A-CGA-CBA | 3.13 | 121.73 | 111.91 |
| 22 | A | 818 | CLA | CHD-C4C-NC | 3.13 | 129.14 | 124.20 |
| 29 | 1 | 601 | CHL | C1-C2-C3 | 3.13 | 131.46 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 835 | CLA | C3B-C4B-NB | 3.13 | 113.26 | 109.21 |
| 29 | 6 | 607 | CHL | C4-C3-C5 | 3.13 | 120.53 | 115.27 |
| 22 | 5 | 603 | CLA | CMB-C2B-C3B | 3.13 | 130.53 | 124.68 |
| 22 | B | 823 | CLA | CHC-C1C-C2C | -3.13 | 118.07 | 126.72 |
| 22 | 6 | 611 | CLA | CHC-C1C-C2C | -3.13 | 118.07 | 126.72 |
| 22 | A | 816 | CLA | C4A-NA-C1A | -3.13 | 105.30 | 106.71 |
| 22 | A | 806 | CLA | C1C-C2C-C3C | -3.13 | 103.67 | 106.96 |
| 22 | B | 824 | CLA | O2D-CGD-O1D | -3.13 | 117.72 | 123.84 |
| 22 | A | 826 | CLA | C4-C3-C5 | 3.13 | 120.53 | 115.27 |
| 22 | 6 | 603 | CLA | CAC-C3C-C4C | 3.13 | 128.87 | 124.81 |
| 22 | 5 | 601 | CLA | C3B-C4B-NB | 3.12 | 113.25 | 109.21 |
| 22 | B | 831 | CLA | CHD-C4C-NC | 3.12 | 129.13 | 124.20 |
| 22 | A | 829 | CLA | C1C-C2C-C3C | -3.12 | 103.67 | 106.96 |
| 22 | 7 | 614 | CLA | CAC-C3C-C4C | 3.12 | 128.86 | 124.81 |
| 22 | A | 833 | CLA | C4-C3-C5 | 3.12 | 120.52 | 115.27 |
| 22 | 7 | 620 | CLA | C3B-C4B-NB | 3.12 | 113.25 | 109.21 |
| 22 | B | 836 | CLA | C4C-C3C-C2C | -3.12 | 102.35 | 106.90 |
| 22 | B | 841 | CLA | C3B-C4B-NB | 3.12 | 113.24 | 109.21 |
| 22 | 4 | 610 | CLA | C3B-C4B-NB | 3.12 | 113.24 | 109.21 |
| 25 | 3 | 717 | BCR | C15-C14-C13 | -3.12 | 122.86 | 127.31 |
| 22 | B | 804 | CLA | C4C-C3C-C2C | -3.12 | 102.35 | 106.90 |
| 22 | 3 | 610 | CLA | C1C-C2C-C3C | -3.12 | 103.68 | 106.96 |
| 22 | Z | 604 | CLA | C4-C3-C5 | 3.12 | 120.52 | 115.27 |
| 22 | 1 | 606 | CLA | C1C-C2C-C3C | -3.12 | 103.68 | 106.96 |
| 22 | Z | 602 | CLA | C4C-C3C-C2C | -3.12 | 102.35 | 106.90 |
| 22 | 2 | 607 | CLA | CAC-C3C-C4C | 3.12 | 128.85 | 124.81 |
| 22 | 7 | 614 | CLA | CHC-C1C-C2C | -3.12 | 118.10 | 126.72 |
| 30 | 2 | 616 | LUT | C15-C14-C13 | -3.12 | 122.86 | 127.31 |
| 30 | 5 | 624 | LUT | C10-C11-C12 | -3.11 | 113.50 | 123.22 |
| 22 | B | 808 | CLA | CHC-C1C-C2C | -3.11 | 118.11 | 126.72 |
| 22 | 5 | 621 | CLA | C3B-C4B-NB | 3.11 | 113.23 | 109.21 |
| 22 | 6 | 622 | CLA | CHC-C1C-C2C | -3.11 | 118.11 | 126.72 |
| 22 | 7 | 611 | CLA | CAC-C3C-C4C | 3.11 | 128.85 | 124.81 |
| 22 | 3 | 604 | CLA | C3B-C4B-NB | 3.11 | 113.23 | 109.21 |
| 22 | 7 | 612 | CLA | O2A-CGA-CBA | 3.11 | 121.67 | 111.91 |
| 22 | B | 824 | CLA | C3B-C4B-NB | 3.11 | 113.23 | 109.21 |
| 22 | A | 840 | CLA | C4C-C3C-C2C | -3.11 | 102.36 | 106.90 |
| 29 | 6 | 606 | CHL | C3D-C4D-ND | 3.11 | 115.27 | 110.24 |
| 22 | 6 | 602 | CLA | CHD-C4C-NC | 3.11 | 129.10 | 124.20 |
| 22 | B | 827 | CLA | C1C-C2C-C3C | -3.11 | 103.69 | 106.96 |
| 22 | 1 | 604 | CLA | CHC-C1C-C2C | -3.11 | 118.12 | 126.72 |
| 22 | Z | 612 | CLA | CHC-C1C-C2C | -3.11 | 118.12 | 126.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 2 | 606 | CLA | C3B-C4B-NB | 3.11 | 113.23 | 109.21 |
| 22 | 7 | 606 | CLA | CHD-C4C-NC | 3.11 | 129.10 | 124.20 |
| 25 | 7 | 623 | BCR | C38-C26-C27 | 3.11 | 119.58 | 113.62 |
| 22 | A | 805 | CLA | O2D-CGD-O1D | -3.11 | 117.77 | 123.84 |
| 22 | 8 | 610 | CLA | C1-C2-C3 | -3.11 | 120.67 | 126.04 |
| 22 | 7 | 606 | CLA | CBC-CAC-C3C | -3.11 | 103.87 | 112.43 |
| 29 | 6 | 606 | CHL | CAC-C3C-C4C | 3.11 | 128.84 | 124.81 |
| 22 | 1 | 614 | CLA | CHC-C1C-C2C | -3.10 | 118.13 | 126.72 |
| 22 | B | 852 | CLA | C4C-C3C-C2C | -3.10 | 102.37 | 106.90 |
| 22 | 8 | 611 | CLA | C4A-NA-C1A | -3.10 | 105.31 | 106.71 |
| 22 | B | 808 | CLA | CBA-CAA-C2A | 3.10 | 123.02 | 113.86 |
| 22 | 6 | 602 | CLA | CMC-C2C-C1C | 3.10 | 129.76 | 125.04 |
| 22 | 7 | 609 | CLA | C4C-C3C-C2C | -3.10 | 102.38 | 106.90 |
| 22 | 2 | 610 | CLA | C3B-C4B-NB | 3.10 | 113.22 | 109.21 |
| 22 | A | 804 | CLA | C1-C2-C3 | -3.10 | 120.68 | 126.04 |
| 22 | A | 842 | CLA | C4-C3-C5 | 3.10 | 120.48 | 115.27 |
| 22 | B | 813 | CLA | O2A-CGA-CBA | 3.10 | 121.63 | 111.91 |
| 22 | 8 | 601 | CLA | CAC-C3C-C4C | 3.10 | 128.83 | 124.81 |
| 22 | A | 836 | CLA | CAC-C3C-C4C | 3.10 | 128.83 | 124.81 |
| 22 | 4 | 614 | CLA | C3B-C4B-NB | 3.10 | 113.21 | 109.21 |
| 22 | B | 808 | CLA | CAC-C3C-C4C | 3.10 | 128.83 | 124.81 |
| 29 | 6 | 606 | CHL | C4-C3-C5 | 3.10 | 120.48 | 115.27 |
| 22 | 7 | 614 | CLA | O2D-CGD-O1D | -3.10 | 117.78 | 123.84 |
| 22 | B | 817 | CLA | C3B-C4B-NB | 3.10 | 113.21 | 109.21 |
| 22 | A | 814 | CLA | CHC-C1C-C2C | -3.10 | 118.16 | 126.72 |
| 22 | 8 | 609 | CLA | CHB-C4A-NA | 3.10 | 128.79 | 124.51 |
| 22 | 4 | 604 | CLA | C3B-C4B-NB | 3.09 | 113.21 | 109.21 |
| 22 | B | 811 | CLA | CHC-C1C-C2C | -3.09 | 118.16 | 126.72 |
| 22 | 3 | 603 | CLA | CHC-C1C-C2C | -3.09 | 118.16 | 126.72 |
| 30 | 9 | 616 | LUT | C10-C11-C12 | -3.09 | 113.56 | 123.22 |
| 22 | A | 838 | CLA | C3B-C4B-NB | 3.09 | 113.21 | 109.21 |
| 22 | A | 817 | CLA | CAC-C3C-C4C | 3.09 | 128.82 | 124.81 |
| 30 | 1 | 617 | LUT | C15-C14-C13 | -3.09 | 122.90 | 127.31 |
| 22 | 6 | 616 | CLA | C4C-C3C-C2C | -3.09 | 102.39 | 106.90 |
| 22 | K | 4002 | CLA | C3B-C4B-NB | 3.09 | 113.21 | 109.21 |
| 22 | G | 203 | CLA | O2A-CGA-CBA | 3.09 | 121.61 | 111.91 |
| 22 | A | 803 | CLA | C4C-C3C-C2C | -3.09 | 102.39 | 106.90 |
| 22 | 4 | 604 | CLA | CHC-C1C-C2C | -3.09 | 118.17 | 126.72 |
| 22 | 1 | 608 | CLA | C3B-C4B-NB | 3.09 | 113.21 | 109.21 |
| 22 | A | 839 | CLA | CAC-C3C-C4C | 3.09 | 128.82 | 124.81 |
| 22 | B | 825 | CLA | C3B-C4B-NB | 3.09 | 113.21 | 109.21 |
| 22 | 4 | 612 | CLA | CHC-C1C-C2C | -3.09 | 118.17 | 126.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | B | 801 | BCR | C15-C16-C17 | 3.09 | 129.80 | 123.47 |
| 25 | 6 | 625 | BCR | C15-C16-C17 | -3.09 | 117.15 | 123.47 |
| 22 | A | 834 | CLA | CHC-C1C-C2C | -3.09 | 118.18 | 126.72 |
| 22 | A | 818 | CLA | C4C-C3C-C2C | -3.09 | 102.40 | 106.90 |
| 22 | 3 | 617 | CLA | CAA-C2A-C3A | -3.09 | 104.33 | 112.78 |
| 30 | 9 | 617 | LUT | C10-C11-C12 | -3.09 | 113.59 | 123.22 |
| 22 | A | 834 | CLA | CHD-C4C-NC | 3.09 | 129.06 | 124.20 |
| 22 | B | 804 | CLA | CMA-C3A-C4A | -3.08 | 103.48 | 111.77 |
| 22 | 3 | 610 | CLA | C1-C2-C3 | -3.08 | 120.71 | 126.04 |
| 22 | 7 | 602 | CLA | CHD-C4C-NC | 3.08 | 129.06 | 124.20 |
| 22 | 2 | 603 | CLA | CHC-C1C-C2C | -3.08 | 118.19 | 126.72 |
| 25 | 3 | 719 | BCR | C20-C21-C22 | -3.08 | 122.91 | 127.31 |
| 22 | 1 | 611 | CLA | CHC-C1C-C2C | -3.08 | 118.19 | 126.72 |
| 22 | 6 | 611 | CLA | CAC-C3C-C4C | 3.08 | 128.81 | 124.81 |
| 22 | 9 | 611 | CLA | CHC-C1C-C2C | -3.08 | 118.20 | 126.72 |
| 22 | 8 | 613 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.90 |
| 22 | 2 | 614 | CLA | CAC-C3C-C4C | 3.08 | 128.81 | 124.81 |
| 22 | A | 841 | CLA | CHB-C4A-NA | 3.08 | 128.77 | 124.51 |
| 22 | F | 301 | CLA | O2A-CGA-CBA | 3.08 | 121.57 | 111.91 |
| 22 | 8 | 614 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.90 |
| 29 | 6 | 618 | CHL | CAC-C3C-C4C | 3.08 | 128.81 | 124.81 |
| 22 | B | 824 | CLA | O2A-CGA-CBA | 3.08 | 121.57 | 111.91 |
| 22 | 5 | 612 | CLA | C4C-C3C-C2C | -3.08 | 102.41 | 106.90 |
| 22 | A | 818 | CLA | C3B-C4B-NB | 3.08 | 113.19 | 109.21 |
| 22 | A | 813 | CLA | CAC-C3C-C4C | 3.08 | 128.80 | 124.81 |
| 25 | A | 850 | BCR | C20-C21-C22 | -3.08 | 122.92 | 127.31 |
| 22 | J | 3002 | CLA | CHC-C1C-C2C | -3.07 | 118.22 | 126.72 |
| 29 | 5 | 608 | CHL | C2A-C3A-C4A | -3.07 | 96.90 | 101.87 |
| 22 | A | 842 | CLA | CHC-C1C-C2C | -3.07 | 118.22 | 126.72 |
| 22 | Z | 611 | CLA | CAA-C2A-C3A | -3.07 | 104.36 | 112.78 |
| 22 | Z | 606 | CLA | C3B-C4B-NB | 3.07 | 113.18 | 109.21 |
| 22 | 5 | 603 | CLA | CHC-C1C-C2C | -3.07 | 118.22 | 126.72 |
| 22 | 7 | 609 | CLA | C3B-C4B-NB | 3.07 | 113.18 | 109.21 |
| 22 | 4 | 602 | CLA | CHC-C1C-C2C | -3.07 | 118.22 | 126.72 |
| 22 | A | 814 | CLA | CHB-C4A-NA | 3.07 | 128.76 | 124.51 |
| 22 | 8 | 606 | CLA | CHC-C1C-C2C | -3.07 | 118.23 | 126.72 |
| 22 | K | 4003 | CLA | C4C-C3C-C2C | -3.07 | 102.42 | 106.90 |
| 22 | B | 833 | CLA | CHC-C1C-C2C | -3.07 | 118.23 | 126.72 |
| 22 | A | 810 | CLA | C3B-C4B-NB | 3.07 | 113.18 | 109.21 |
| 22 | A | 835 | CLA | C3B-C4B-NB | 3.07 | 113.18 | 109.21 |
| 22 | 6 | 611 | CLA | C3B-C4B-NB | 3.07 | 113.18 | 109.21 |
| 25 | A | 856 | BCR | C11-C10-C9 | -3.07 | 122.93 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | Z | 610 | CLA | C4C-C3C-C2C | -3.07 | 102.43 | 106.90 |
| 22 | A | 837 | CLA | C3B-C4B-NB | 3.07 | 113.17 | 109.21 |
| 22 | B | 836 | CLA | O2D-CGD-O1D | -3.07 | 117.84 | 123.84 |
| 22 | B | 852 | CLA | CAC-C3C-C4C | 3.07 | 128.79 | 124.81 |
| 22 | B | 836 | CLA | CHC-C1C-C2C | -3.07 | 118.24 | 126.72 |
| 22 | G | 204 | CLA | CHC-C1C-C2C | -3.07 | 118.24 | 126.72 |
| 22 | 8 | 602 | CLA | C3B-C4B-NB | 3.07 | 113.17 | 109.21 |
| 22 | 8 | 616 | CLA | C3B-C4B-NB | 3.07 | 113.17 | 109.21 |
| 22 | 5 | 610 | CLA | C3B-C4B-NB | 3.07 | 113.17 | 109.21 |
| 22 | A | 810 | CLA | CAC-C3C-C4C | 3.07 | 128.79 | 124.81 |
| 22 | 8 | 612 | CLA | C4C-C3C-C2C | -3.06 | 102.43 | 106.90 |
| 22 | 2 | 601 | CLA | CAA-C2A-C3A | -3.06 | 104.39 | 112.78 |
| 22 | 7 | 616 | CLA | CAA-C2A-C3A | -3.06 | 104.39 | 112.78 |
| 22 | B | 814 | CLA | CMA-C3A-C4A | -3.06 | 103.54 | 111.77 |
| 30 | 1 | 619 | LUT | C19-C9-C8 | 3.06 | 122.90 | 118.08 |
| 22 | L | 203 | CLA | C3B-C4B-NB | 3.06 | 113.17 | 109.21 |
| 22 | 2 | 612 | CLA | C4-C3-C5 | 3.06 | 120.42 | 115.27 |
| 29 | 6 | 607 | CHL | C3D-C4D-ND | 3.06 | 115.19 | 110.24 |
| 22 | Z | 613 | CLA | C3B-C4B-NB | 3.06 | 113.17 | 109.21 |
| 22 | B | 825 | CLA | C1C-C2C-C3C | -3.06 | 103.74 | 106.96 |
| 22 | 2 | 612 | CLA | CAC-C3C-C4C | 3.06 | 128.78 | 124.81 |
| 22 | A | 808 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 25 | A | 848 | BCR | C11-C10-C9 | -3.06 | 122.94 | 127.31 |
| 22 | 4 | 602 | CLA | C3B-C4B-NB | 3.06 | 113.17 | 109.21 |
| 29 | 4 | 618 | CHL | C3B-C4B-NB | 3.06 | 113.17 | 109.21 |
| 22 | 6 | 609 | CLA | C4C-C3C-C2C | -3.06 | 102.44 | 106.90 |
| 22 | 8 | 614 | CLA | O2A-CGA-CBA | 3.06 | 121.51 | 111.91 |
| 22 | B | 815 | CLA | CHC-C1C-C2C | -3.06 | 118.26 | 126.72 |
| 22 | B | 815 | CLA | O2D-CGD-O1D | -3.06 | 117.86 | 123.84 |
| 22 | 2 | 614 | CLA | C3B-C4B-NB | 3.06 | 113.16 | 109.21 |
| 22 | F | 304 | CLA | CHC-C1C-C2C | -3.06 | 118.26 | 126.72 |
| 22 | 6 | 617 | CLA | CHC-C1C-C2C | -3.06 | 118.26 | 126.72 |
| 22 | 7 | 601 | CLA | O2A-CGA-O1A | -3.06 | 115.88 | 123.59 |
| 22 | A | 813 | CLA | C4C-C3C-C2C | -3.06 | 102.44 | 106.90 |
| 22 | A | 810 | CLA | C4C-C3C-C2C | -3.06 | 102.44 | 106.90 |
| 25 | 3 | 717 | BCR | C24-C23-C22 | -3.05 | 121.62 | 126.23 |
| 22 | 3 | 611 | CLA | CHC-C1C-C2C | -3.05 | 118.27 | 126.72 |
| 22 | 3 | 606 | CLA | C3B-C4B-NB | 3.05 | 113.16 | 109.21 |
| 22 | 6 | 617 | CLA | C4C-C3C-C2C | -3.05 | 102.45 | 106.90 |
| 22 | B | 835 | CLA | CHC-C1C-C2C | -3.05 | 118.28 | 126.72 |
| 22 | A | 804 | CLA | CHD-C4C-NC | 3.05 | 129.01 | 124.20 |
| 22 | A | 812 | CLA | C1-C2-C3 | -3.05 | 120.76 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30 | 4 | 619 | LUT | C30-C31-C32 | -3.05 | 113.69 | 123.22 |
| 22 | F | 304 | CLA | C4C-C3C-C2C | -3.05 | 102.45 | 106.90 |
| 22 | 1 | 613 | CLA | CHC-C1C-C2C | -3.05 | 118.28 | 126.72 |
| 22 | B | 827 | CLA | CAA-C2A-C3A | -3.05 | 104.42 | 112.78 |
| 22 | B | 824 | CLA | CHD-C4C-NC | 3.05 | 129.01 | 124.20 |
| 22 | B | 840 | CLA | CMC-C2C-C3C | 3.05 | 134.40 | 126.12 |
| 25 | 5 | 625 | BCR | C37-C22-C23 | 3.05 | 122.88 | 118.08 |
| 22 | B | 813 | CLA | CHC-C1C-C2C | -3.05 | 118.28 | 126.72 |
| 29 | 5 | 607 | CHL | C3D-C4D-ND | 3.05 | 115.17 | 110.24 |
| 30 | 8 | 617 | LUT | C39-C29-C28 | 3.05 | 122.88 | 118.08 |
| 29 | 9 | 606 | CHL | CBC-CAC-C3C | -3.05 | 104.03 | 112.43 |
| 22 | 7 | 620 | CLA | CHC-C1C-C2C | -3.05 | 118.29 | 126.72 |
| 22 | 8 | 604 | CLA | CAA-C2A-C3A | -3.05 | 104.43 | 112.78 |
| 29 | 9 | 607 | CHL | C3D-C4D-ND | 3.05 | 115.17 | 110.24 |
| 22 | Z | 608 | CLA | CHC-C1C-C2C | -3.05 | 118.29 | 126.72 |
| 22 | 4 | 610 | CLA | C1C-C2C-C3C | -3.05 | 103.75 | 106.96 |
| 22 | B | 832 | CLA | C3B-C4B-NB | 3.05 | 113.15 | 109.21 |
| 22 | 3 | 607 | CLA | C3B-C4B-NB | 3.05 | 113.15 | 109.21 |
| 22 | 6 | 617 | CLA | CAC-C3C-C4C | 3.05 | 128.76 | 124.81 |
| 22 | A | 803 | CLA | O2A-CGA-CBA | 3.05 | 121.47 | 111.91 |
| 22 | 1 | 610 | CLA | C4C-C3C-C2C | -3.04 | 102.46 | 106.90 |
| 22 | 7 | 603 | CLA | CHD-C4C-NC | 3.04 | 129.00 | 124.20 |
| 22 | A | 812 | CLA | CAC-C3C-C4C | 3.04 | 128.76 | 124.81 |
| 22 | 1 | 606 | CLA | CHD-C4C-NC | 3.04 | 129.00 | 124.20 |
| 22 | 7 | 603 | CLA | CHC-C1C-C2C | -3.04 | 118.31 | 126.72 |
| 22 | B | 841 | CLA | O2A-CGA-CBA | 3.04 | 121.45 | 111.91 |
| 22 | B | 823 | CLA | CMA-C3A-C2A | -3.04 | 101.57 | 113.83 |
| 22 | 4 | 603 | CLA | CAC-C3C-C4C | 3.04 | 128.75 | 124.81 |
| 22 | 3 | 617 | CLA | CHC-C1C-C2C | -3.04 | 118.32 | 126.72 |
| 21 | A | 801 | CL0 | CMA-C3A-C4A | -3.04 | 103.61 | 111.77 |
| 22 | A | 803 | CLA | CMC-C2C-C1C | 3.04 | 129.66 | 125.04 |
| 22 | B | 839 | CLA | CHC-C1C-C2C | -3.04 | 118.32 | 126.72 |
| 29 | 4 | 606 | CHL | C3D-C4D-ND | 3.04 | 115.15 | 110.24 |
| 29 | 1 | 601 | CHL | O2A-CGA-CBA | 3.03 | 121.43 | 111.91 |
| 22 | 9 | 610 | CLA | C1-C2-C3 | -3.03 | 120.80 | 126.04 |
| 22 | 9 | 602 | CLA | C3B-C4B-NB | 3.03 | 113.13 | 109.21 |
| 22 | 9 | 609 | CLA | C4C-C3C-C2C | -3.03 | 102.48 | 106.90 |
| 22 | B | 833 | CLA | C1C-C2C-C3C | -3.03 | 103.77 | 106.96 |
| 22 | A | 843 | CLA | C4-C3-C5 | 3.03 | 120.37 | 115.27 |
| 22 | 7 | 620 | CLA | O2A-CGA-CBA | 3.03 | 121.42 | 111.91 |
| 22 | A | 807 | CLA | C4C-C3C-C2C | -3.03 | 102.48 | 106.90 |
| 22 | 8 | 608 | CLA | C3B-C4B-NB | 3.03 | 113.13 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 5 | 611 | CLA | C4-C3-C5 | 3.03 | 120.37 | 115.27 |
| 22 | Z | 606 | CLA | CHC-C1C-C2C | -3.03 | 118.34 | 126.72 |
| 22 | 6 | 601 | CLA | CAA-C2A-C3A | -3.03 | 104.48 | 112.78 |
| 22 | 5 | 610 | CLA | O2A-CGA-CBA | 3.03 | 121.42 | 111.91 |
| 22 | A | 829 | CLA | CHD-C4C-NC | 3.03 | 128.98 | 124.20 |
| 25 | A | 851 | BCR | C24-C23-C22 | -3.03 | 121.66 | 126.23 |
| 22 | 7 | 610 | CLA | CAC-C3C-C4C | 3.03 | 128.74 | 124.81 |
| 22 | 5 | 609 | CLA | O2A-CGA-CBA | 3.03 | 121.42 | 111.91 |
| 22 | B | 830 | CLA | O2D-CGD-O1D | -3.03 | 117.92 | 123.84 |
| 22 | B | 805 | CLA | CHC-C1C-C2C | -3.03 | 118.34 | 126.72 |
| 25 | 4 | 621 | BCR | C23-C24-C25 | -3.03 | 118.70 | 127.20 |
| 22 | A | 836 | CLA | C3B-C4B-NB | 3.03 | 113.12 | 109.21 |
| 22 | 1 | 611 | CLA | C3B-C4B-NB | 3.03 | 113.12 | 109.21 |
| 22 | 2 | 606 | CLA | CHC-C1C-C2C | -3.03 | 118.34 | 126.72 |
| 22 | 3 | 606 | CLA | CAC-C3C-C4C | 3.03 | 128.74 | 124.81 |
| 22 | Z | 602 | CLA | CHD-C4C-NC | 3.03 | 128.97 | 124.20 |
| 22 | B | 825 | CLA | CMB-C2B-C3B | 3.03 | 130.34 | 124.68 |
| 22 | 3 | 607 | CLA | CHC-C1C-C2C | -3.03 | 118.35 | 126.72 |
| 22 | Z | 603 | CLA | C4-C3-C2 | -3.03 | 115.92 | 123.68 |
| 22 | 8 | 616 | CLA | C4C-C3C-C2C | -3.03 | 102.49 | 106.90 |
| 22 | B | 821 | CLA | CAC-C3C-C4C | 3.03 | 128.74 | 124.81 |
| 22 | B | 830 | CLA | C1-C2-C3 | -3.02 | 121.86 | 126.75 |
| 22 | 2 | 614 | CLA | CHC-C1C-C2C | -3.02 | 118.36 | 126.72 |
| 22 | 8 | 609 | CLA | CMA-C3A-C4A | -3.02 | 103.65 | 111.77 |
| 22 | Z | 616 | CLA | CAA-C2A-C3A | -3.02 | 104.50 | 112.78 |
| 22 | A | 833 | CLA | CHC-C1C-C2C | -3.02 | 118.36 | 126.72 |
| 22 | 6 | 601 | CLA | CHC-C1C-C2C | -3.02 | 118.36 | 126.72 |
| 22 | 1 | 608 | CLA | CHC-C1C-C2C | -3.02 | 118.36 | 126.72 |
| 30 | 4 | 620 | LUT | C15-C14-C13 | -3.02 | 123.00 | 127.31 |
| 22 | B | 814 | CLA | CHD-C4C-NC | 3.02 | 128.96 | 124.20 |
| 22 | A | 811 | CLA | CMC-C2C-C1C | 3.02 | 129.64 | 125.04 |
| 22 | A | 843 | CLA | C4C-C3C-C2C | -3.02 | 102.50 | 106.90 |
| 22 | A | 830 | CLA | C1C-C2C-C3C | -3.02 | 103.78 | 106.96 |
| 22 | 1 | 610 | CLA | O2A-CGA-O1A | -3.02 | 115.97 | 123.59 |
| 22 | A | 824 | CLA | C4C-C3C-C2C | -3.02 | 102.50 | 106.90 |
| 22 | 8 | 614 | CLA | C3B-C4B-NB | 3.02 | 113.11 | 109.21 |
| 22 | A | 808 | CLA | CAC-C3C-C4C | 3.02 | 128.73 | 124.81 |
| 22 | B | 835 | CLA | CMB-C2B-C3B | 3.02 | 130.33 | 124.68 |
| 22 | B | 832 | CLA | CHC-C1C-C2C | -3.02 | 118.37 | 126.72 |
| 22 | B | 811 | CLA | C4C-C3C-C2C | -3.02 | 102.50 | 106.90 |
| 22 | 7 | 613 | CLA | C4C-C3C-C2C | -3.02 | 102.50 | 106.90 |
| 22 | 1 | 610 | CLA | CMB-C2B-C3B | 3.02 | 130.32 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 824 | CLA | CMC-C2C-C1C | 3.02 | 129.63 | 125.04 |
| 30 | Z | 618 | LUT | C7-C8-C9 | -3.02 | 121.68 | 126.23 |
| 29 | 1 | 601 | CHL | C3D-C4D-ND | 3.02 | 115.12 | 110.24 |
| 22 | B | 808 | CLA | C4-C3-C5 | 3.02 | 120.35 | 115.27 |
| 22 | Z | 612 | CLA | O2A-CGA-CBA | 3.02 | 121.37 | 111.91 |
| 22 | A | 812 | CLA | CHC-C1C-C2C | -3.02 | 118.38 | 126.72 |
| 22 | A | 805 | CLA | CHD-C4C-NC | 3.01 | 128.95 | 124.20 |
| 22 | A | 806 | CLA | CHC-C1C-C2C | -3.01 | 118.38 | 126.72 |
| 22 | A | 820 | CLA | C1-C2-C3 | -3.01 | 120.83 | 126.04 |
| 22 | A | 813 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 22 | 8 | 610 | CLA | C3B-C4B-NB | 3.01 | 113.11 | 109.21 |
| 22 | 6 | 601 | CLA | O2D-CGD-O1D | -3.01 | 117.95 | 123.84 |
| 22 | B | 838 | CLA | C4C-C3C-C2C | -3.01 | 102.51 | 106.90 |
| 25 | L | 205 | BCR | C23-C24-C25 | -3.01 | 118.75 | 127.20 |
| 22 | A | 807 | CLA | CHC-C1C-C2C | -3.01 | 118.40 | 126.72 |
| 25 | 6 | 625 | BCR | C11-C12-C13 | -3.01 | 117.96 | 126.42 |
| 22 | B | 807 | CLA | C4C-C3C-C2C | -3.01 | 102.51 | 106.90 |
| 22 | 8 | 609 | CLA | CAC-C3C-C4C | 3.01 | 128.71 | 124.81 |
| 30 | 5 | 624 | LUT | C38-C25-C24 | -3.01 | 117.12 | 123.56 |
| 22 | 4 | 614 | CLA | CHD-C4C-NC | 3.01 | 128.94 | 124.20 |
| 22 | 1 | 603 | CLA | CAA-C2A-C3A | -3.01 | 104.55 | 112.78 |
| 29 | 4 | 618 | CHL | CBC-CAC-C3C | -3.01 | 104.14 | 112.43 |
| 22 | B | 837 | CLA | C4C-C3C-C2C | -3.01 | 102.52 | 106.90 |
| 22 | A | 815 | CLA | C3B-C4B-NB | 3.01 | 113.09 | 109.21 |
| 22 | 6 | 610 | CLA | C3B-C4B-NB | 3.00 | 113.09 | 109.21 |
| 22 | B | 833 | CLA | O2D-CGD-O1D | -3.00 | 117.97 | 123.84 |
| 22 | B | 821 | CLA | CHC-C1C-C2C | -3.00 | 118.41 | 126.72 |
| 25 | B | 847 | BCR | C11-C10-C9 | -3.00 | 123.02 | 127.31 |
| 22 | B | 812 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.72 |
| 22 | A | 854 | CLA | C3B-C4B-NB | 3.00 | 113.09 | 109.21 |
| 22 | 6 | 613 | CLA | C4C-C3C-C2C | -3.00 | 102.52 | 106.90 |
| 22 | 8 | 616 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.72 |
| 22 | A | 833 | CLA | C3B-C4B-NB | 3.00 | 113.09 | 109.21 |
| 22 | 6 | 610 | CLA | CAC-C3C-C4C | 3.00 | 128.70 | 124.81 |
| 22 | A | 820 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.72 |
| 22 | B | 816 | CLA | CAA-C2A-C3A | -3.00 | 104.56 | 112.78 |
| 22 | B | 834 | CLA | CHC-C1C-C2C | -3.00 | 118.42 | 126.72 |
| 29 | Z | 601 | CHL | CMB-C2B-C3B | 3.00 | 130.29 | 124.68 |
| 22 | B | 803 | CLA | CHB-C4A-NA | 3.00 | 128.66 | 124.51 |
| 22 | A | 835 | CLA | C2A-C1A-CHA | -3.00 | 118.62 | 123.86 |
| 22 | 8 | 601 | CLA | CHC-C1C-C2C | -3.00 | 118.43 | 126.72 |
| 22 | 1 | 614 | CLA | C4-C3-C5 | 3.00 | 120.31 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | 7 | 607 | CHL | C4-C3-C5 | 3.00 | 120.31 | 115.27 |
| 22 | B | 838 | CLA | C3B-C4B-NB | 3.00 | 113.08 | 109.21 |
| 22 | 2 | 609 | CLA | CAC-C3C-C4C | 3.00 | 128.70 | 124.81 |
| 22 | A | 836 | CLA | CMA-C3A-C4A | -2.99 | 103.72 | 111.77 |
| 22 | 7 | 601 | CLA | CHD-C4C-NC | 2.99 | 128.92 | 124.20 |
| 22 | B | 804 | CLA | O2D-CGD-O1D | -2.99 | 117.99 | 123.84 |
| 22 | B | 803 | CLA | C3B-C4B-NB | 2.99 | 113.08 | 109.21 |
| 22 | B | 841 | CLA | O2D-CGD-O1D | -2.99 | 117.99 | 123.84 |
| 22 | F | 303 | CLA | CHD-C4C-NC | 2.99 | 128.92 | 124.20 |
| 29 | Z | 607 | CHL | CAC-C3C-C4C | 2.99 | 128.69 | 124.81 |
| 22 | 6 | 612 | CLA | CHC-C1C-C2C | -2.99 | 118.45 | 126.72 |
| 22 | B | 832 | CLA | CAA-C2A-C3A | -2.99 | 104.59 | 112.78 |
| 22 | 1 | 608 | CLA | O2A-CGA-CBA | 2.99 | 121.29 | 111.91 |
| 22 | A | 814 | CLA | C4-C3-C5 | 2.99 | 120.30 | 115.27 |
| 22 | 3 | 614 | CLA | CAA-C2A-C3A | -2.99 | 104.59 | 112.78 |
| 22 | B | 807 | CLA | O2D-CGD-O1D | -2.99 | 118.00 | 123.84 |
| 22 | A | 838 | CLA | C4C-C3C-C2C | -2.99 | 102.54 | 106.90 |
| 22 | B | 852 | CLA | CHC-C1C-C2C | -2.99 | 118.46 | 126.72 |
| 22 | 7 | 606 | CLA | O2D-CGD-O1D | -2.99 | 118.00 | 123.84 |
| 22 | 4 | 609 | CLA | C1-C2-C3 | -2.99 | 121.92 | 126.75 |
| 22 | F | 301 | CLA | CHD-C4C-NC | 2.99 | 128.91 | 124.20 |
| 22 | 5 | 603 | CLA | CHD-C4C-NC | 2.99 | 128.91 | 124.20 |
| 22 | A | 823 | CLA | CAC-C3C-C4C | 2.98 | 128.68 | 124.81 |
| 22 | 7 | 609 | CLA | CAC-C3C-C4C | 2.98 | 128.68 | 124.81 |
| 21 | A | 801 | CL0 | C4C-C3C-C2C | -2.98 | 102.55 | 106.90 |
| 22 | 2 | 602 | CLA | CHC-C1C-C2C | -2.98 | 118.47 | 126.72 |
| 22 | 9 | 602 | CLA | C4-C3-C5 | 2.98 | 120.29 | 115.27 |
| 22 | Z | 611 | CLA | C4C-C3C-C2C | -2.98 | 102.55 | 106.90 |
| 29 | 1 | 601 | CHL | C3B-C4B-NB | 2.98 | 113.07 | 109.21 |
| 22 | B | 805 | CLA | C1C-C2C-C3C | -2.98 | 103.82 | 106.96 |
| 22 | 1 | 604 | CLA | C4-C3-C5 | 2.98 | 120.29 | 115.27 |
| 22 | B | 827 | CLA | CAC-C3C-C4C | 2.98 | 128.68 | 124.81 |
| 22 | B | 808 | CLA | O2A-CGA-O1A | -2.98 | 116.07 | 123.59 |
| 22 | 7 | 603 | CLA | O2D-CGD-O1D | -2.98 | 118.01 | 123.84 |
| 22 | 5 | 613 | CLA | CHB-C4A-NA | 2.98 | 128.63 | 124.51 |
| 22 | A | 815 | CLA | C2A-C1A-CHA | -2.98 | 118.65 | 123.86 |
| 30 | 9 | 616 | LUT | C7-C8-C9 | -2.98 | 121.73 | 126.23 |
| 22 | A | 829 | CLA | CAC-C3C-C4C | 2.98 | 128.68 | 124.81 |
| 22 | B | 810 | CLA | C4C-C3C-C2C | -2.98 | 102.56 | 106.90 |
| 22 | B | 813 | CLA | CAA-C2A-C3A | -2.98 | 104.62 | 112.78 |
| 22 | B | 813 | CLA | C1-C2-C3 | -2.98 | 120.89 | 126.04 |
| 21 | A | 801 | CL0 | CHD-C4C-NC | 2.98 | 128.90 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 604 | CLA | CAC-C3C-C4C | 2.98 | 128.67 | 124.81 |
| 30 | 5 | 624 | LUT | C15-C14-C13 | -2.98 | 123.06 | 127.31 |
| 22 | B | 820 | CLA | C2A-C1A-CHA | -2.98 | 118.65 | 123.86 |
| 22 | 5 | 616 | CLA | CAC-C3C-C4C | 2.98 | 128.67 | 124.81 |
| 22 | B | 808 | CLA | O2A-CGA-CBA | 2.98 | 121.25 | 111.91 |
| 22 | A | 840 | CLA | CHC-C1C-C2C | -2.98 | 118.49 | 126.72 |
| 22 | 8 | 612 | CLA | CHC-C1C-C2C | -2.98 | 118.49 | 126.72 |
| 22 | B | 817 | CLA | C4C-C3C-C2C | -2.98 | 102.56 | 106.90 |
| 22 | Z | 603 | CLA | C4-C3-C5 | 2.98 | 120.28 | 115.27 |
| 22 | K | 4002 | CLA | CHC-C1C-C2C | -2.98 | 118.49 | 126.72 |
| 22 | 3 | 613 | CLA | C4A-NA-C1A | -2.98 | 105.37 | 106.71 |
| 22 | 7 | 602 | CLA | O2A-CGA-CBA | 2.98 | 121.25 | 111.91 |
| 22 | F | 303 | CLA | C4C-C3C-C2C | -2.98 | 102.56 | 106.90 |
| 25 | 3 | 717 | BCR | C38-C26-C25 | -2.97 | 121.19 | 124.53 |
| 22 | 8 | 610 | CLA | C4C-C3C-C2C | -2.97 | 102.56 | 106.90 |
| 22 | A | 827 | CLA | CHD-C4C-NC | 2.97 | 128.89 | 124.20 |
| 22 | A | 836 | CLA | C1-C2-C3 | -2.97 | 121.94 | 126.75 |
| 22 | 2 | 610 | CLA | CAC-C3C-C4C | 2.97 | 128.67 | 124.81 |
| 22 | G | 203 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.90 |
| 22 | 8 | 611 | CLA | O2D-CGD-O1D | -2.97 | 118.03 | 123.84 |
| 22 | Z | 611 | CLA | CHC-C1C-C2C | -2.97 | 118.50 | 126.72 |
| 22 | B | 812 | CLA | C3B-C4B-NB | 2.97 | 113.05 | 109.21 |
| 22 | 6 | 609 | CLA | CMB-C2B-C3B | 2.97 | 130.23 | 124.68 |
| 22 | B | 806 | CLA | C3B-C4B-NB | 2.97 | 113.05 | 109.21 |
| 22 | B | 817 | CLA | O2A-CGA-CBA | 2.97 | 121.22 | 111.91 |
| 22 | B | 826 | CLA | O2A-CGA-CBA | 2.97 | 121.22 | 111.91 |
| 22 | 5 | 616 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.90 |
| 22 | B | 830 | CLA | C3B-C4B-NB | 2.97 | 113.05 | 109.21 |
| 22 | B | 834 | CLA | CHB-C4A-NA | 2.97 | 128.62 | 124.51 |
| 22 | A | 823 | CLA | CHC-C1C-C2C | -2.97 | 118.51 | 126.72 |
| 22 | A | 823 | CLA | C4C-C3C-C2C | -2.97 | 102.57 | 106.90 |
| 22 | A | 804 | CLA | CHC-C1C-C2C | -2.97 | 118.52 | 126.72 |
| 22 | 3 | 620 | CLA | CAC-C3C-C4C | 2.97 | 128.66 | 124.81 |
| 22 | 8 | 609 | CLA | C4C-C3C-C2C | -2.97 | 102.58 | 106.90 |
| 22 | 8 | 613 | CLA | CHC-C1C-C2C | -2.96 | 118.52 | 126.72 |
| 30 | 7 | 622 | LUT | C15-C14-C13 | -2.96 | 123.08 | 127.31 |
| 22 | 2 | 611 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.72 |
| 22 | 9 | 604 | CLA | C1-C2-C3 | -2.96 | 121.96 | 126.75 |
| 22 | A | 827 | CLA | CAC-C3C-C4C | 2.96 | 128.65 | 124.81 |
| 22 | B | 812 | CLA | CAC-C3C-C4C | 2.96 | 128.65 | 124.81 |
| 22 | 8 | 603 | CLA | CAC-C3C-C4C | 2.96 | 128.65 | 124.81 |
| 22 | 7 | 602 | CLA | CAA-C2A-C3A | -2.96 | 104.67 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 838 | CLA | CAC-C3C-C4C | 2.96 | 128.65 | 124.81 |
| 22 | 8 | 612 | CLA | CHD-C4C-NC | 2.96 | 128.87 | 124.20 |
| 22 | 7 | 606 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.72 |
| 22 | 7 | 614 | CLA | O1D-CGD-CBD | -2.96 | 118.42 | 124.48 |
| 22 | 7 | 604 | CLA | CHC-C1C-C2C | -2.96 | 118.53 | 126.72 |
| 22 | B | 823 | CLA | C1C-C2C-C3C | -2.96 | 103.84 | 106.96 |
| 22 | 3 | 607 | CLA | C4C-C3C-C2C | -2.96 | 102.58 | 106.90 |
| 22 | 9 | 602 | CLA | CHD-C4C-NC | 2.96 | 128.87 | 124.20 |
| 22 | A | 804 | CLA | CMD-C2D-C3D | -2.96 | 120.81 | 127.61 |
| 22 | 1 | 613 | CLA | C4C-C3C-C2C | -2.96 | 102.58 | 106.90 |
| 22 | 3 | 620 | CLA | CBC-CAC-C3C | -2.96 | 104.28 | 112.43 |
| 22 | Z | 603 | CLA | C1-O2A-CGA | 2.96 | 124.20 | 116.44 |
| 22 | B | 840 | CLA | CAA-C2A-C3A | -2.96 | 104.68 | 112.78 |
| 22 | B | 838 | CLA | O2A-CGA-CBA | 2.96 | 121.19 | 111.91 |
| 22 | 1 | 611 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.90 |
| 22 | B | 826 | CLA | O2D-CGD-O1D | -2.96 | 118.06 | 123.84 |
| 22 | Z | 616 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.90 |
| 22 | B | 836 | CLA | C4-C3-C5 | 2.96 | 120.24 | 115.27 |
| 29 | 6 | 608 | CHL | C3B-C4B-NB | 2.96 | 113.03 | 109.21 |
| 22 | A | 824 | CLA | CHC-C1C-C2C | -2.96 | 118.55 | 126.72 |
| 22 | B | 815 | CLA | C4C-C3C-C2C | -2.96 | 102.59 | 106.90 |
| 22 | B | 824 | CLA | CHC-C1C-C2C | -2.95 | 118.55 | 126.72 |
| 22 | 6 | 604 | CLA | C3B-C4B-NB | 2.95 | 113.03 | 109.21 |
| 29 | 4 | 607 | CHL | O2A-CGA-CBA | 2.95 | 121.18 | 111.91 |
| 22 | 8 | 606 | CLA | C3B-C4B-NB | 2.95 | 113.03 | 109.21 |
| 22 | 6 | 614 | CLA | CMD-C2D-C3D | -2.95 | 120.82 | 127.61 |
| 22 | 5 | 602 | CLA | O2A-CGA-CBA | 2.95 | 121.17 | 111.91 |
| 22 | A | 810 | CLA | CHC-C1C-C2C | -2.95 | 118.56 | 126.72 |
| 22 | A | 812 | CLA | CAA-C2A-C3A | -2.95 | 104.70 | 112.78 |
| 22 | B | 827 | CLA | C3B-C4B-NB | 2.95 | 113.03 | 109.21 |
| 22 | A | 814 | CLA | C1C-C2C-C3C | -2.95 | 103.86 | 106.96 |
| 22 | 9 | 610 | CLA | O2A-CGA-CBA | 2.95 | 121.17 | 111.91 |
| 22 | 5 | 609 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.90 |
| 22 | B | 809 | CLA | CAC-C3C-C4C | 2.95 | 128.64 | 124.81 |
| 29 | 3 | 608 | CHL | C3D-C4D-ND | 2.95 | 115.01 | 110.24 |
| 22 | B | 820 | CLA | CHC-C1C-C2C | -2.95 | 118.56 | 126.72 |
| 22 | L | 204 | CLA | CHC-C1C-C2C | -2.95 | 118.56 | 126.72 |
| 22 | B | 805 | CLA | O2D-CGD-O1D | -2.95 | 118.07 | 123.84 |
| 30 | 9 | 617 | LUT | C30-C31-C32 | -2.95 | 114.02 | 123.22 |
| 22 | A | 809 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.90 |
| 22 | A | 840 | CLA | O2A-CGA-CBA | 2.95 | 121.16 | 111.91 |
| 30 | 8 | 617 | LUT | C35-C15-C14 | -2.95 | 117.44 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 3 | 602 | CLA | CAA-C2A-C3A | -2.95 | 104.71 | 112.78 |
| 22 | 4 | 616 | CLA | CMA-C3A-C2A | -2.95 | 109.22 | 116.10 |
| 22 | 5 | 613 | CLA | C4C-C3C-C2C | -2.95 | 102.60 | 106.90 |
| 29 | 1 | 601 | CHL | CAC-C3C-C4C | 2.95 | 128.63 | 124.81 |
| 29 | 6 | 607 | CHL | CAC-C3C-C4C | 2.95 | 128.63 | 124.81 |
| 22 | B | 841 | CLA | C2A-C1A-CHA | -2.95 | 118.71 | 123.86 |
| 25 | 4 | 621 | BCR | C20-C21-C22 | -2.95 | 123.11 | 127.31 |
| 22 | 1 | 608 | CLA | CHD-C4C-NC | 2.95 | 128.85 | 124.20 |
| 22 | 6 | 611 | CLA | C4-C3-C5 | 2.95 | 120.23 | 115.27 |
| 22 | Z | 614 | CLA | CHC-C1C-C2C | -2.95 | 118.57 | 126.72 |
| 25 | 6 | 625 | BCR | C21-C20-C19 | -2.95 | 114.03 | 123.22 |
| 22 | 5 | 610 | CLA | CHD-C4C-NC | 2.95 | 128.84 | 124.20 |
| 22 | 8 | 606 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.90 |
| 22 | 4 | 612 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.90 |
| 22 | 5 | 606 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.72 |
| 22 | 2 | 607 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.72 |
| 25 | I | 172 | BCR | C15-C14-C13 | -2.94 | 123.11 | 127.31 |
| 22 | B | 812 | CLA | C1-O2A-CGA | 2.94 | 124.17 | 116.44 |
| 22 | Z | 613 | CLA | CHD-C4C-NC | 2.94 | 128.84 | 124.20 |
| 22 | A | 818 | CLA | O2D-CGD-O1D | -2.94 | 118.08 | 123.84 |
| 22 | 2 | 612 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.90 |
| 22 | A | 816 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.72 |
| 22 | 4 | 610 | CLA | CAC-C3C-C4C | 2.94 | 128.63 | 124.81 |
| 22 | 3 | 614 | CLA | CHC-C1C-C2C | -2.94 | 118.58 | 126.72 |
| 22 | B | 841 | CLA | CHD-C4C-NC | 2.94 | 128.84 | 124.20 |
| 25 | B | 845 | BCR | C16-C15-C14 | -2.94 | 117.45 | 123.47 |
| 22 | J | 3002 | CLA | CAC-C3C-C4C | 2.94 | 128.63 | 124.81 |
| 22 | 3 | 603 | CLA | CBC-CAC-C3C | -2.94 | 104.32 | 112.43 |
| 22 | 7 | 606 | CLA | C4C-C3C-C2C | -2.94 | 102.61 | 106.90 |
| 22 | F | 304 | CLA | C1-O2A-CGA | 2.94 | 124.16 | 116.44 |
| 22 | A | 818 | CLA | CHC-C1C-C2C | -2.94 | 118.59 | 126.72 |
| 22 | 2 | 610 | CLA | CHC-C1C-C2C | -2.94 | 118.59 | 126.72 |
| 22 | A | 811 | CLA | CHD-C4C-NC | 2.94 | 128.83 | 124.20 |
| 22 | Z | 608 | CLA | CAC-C3C-C4C | 2.94 | 128.62 | 124.81 |
| 22 | 7 | 601 | CLA | C4C-C3C-C2C | -2.94 | 102.62 | 106.90 |
| 29 | 1 | 607 | CHL | C3D-C4D-ND | 2.94 | 114.99 | 110.24 |
| 22 | B | 806 | CLA | CAA-C2A-C3A | -2.94 | 104.73 | 112.78 |
| 22 | B | 837 | CLA | CAC-C3C-C4C | 2.94 | 128.62 | 124.81 |
| 22 | 3 | 617 | CLA | C3B-C4B-NB | 2.94 | 113.01 | 109.21 |
| 22 | 7 | 604 | CLA | CHD-C4C-NC | 2.93 | 128.83 | 124.20 |
| 22 | L | 203 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.90 |
| 22 | B | 814 | CLA | CMC-C2C-C1C | 2.93 | 129.51 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 843 | CLA | CAA-C2A-C3A | -2.93 | 104.74 | 112.78 |
| 22 | A | 837 | CLA | O2D-CGD-O1D | -2.93 | 118.10 | 123.84 |
| 22 | Z | 608 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.90 |
| 22 | 2 | 614 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.90 |
| 22 | A | 839 | CLA | C4C-C3C-C2C | -2.93 | 102.62 | 106.90 |
| 22 | Z | 608 | CLA | O2A-CGA-CBA | 2.93 | 121.11 | 111.91 |
| 22 | B | 833 | CLA | C4-C3-C5 | 2.93 | 120.20 | 115.27 |
| 22 | 8 | 610 | CLA | CHD-C4C-NC | 2.93 | 128.82 | 124.20 |
| 22 | 7 | 620 | CLA | CAC-C3C-C4C | 2.93 | 128.61 | 124.81 |
| 22 | 9 | 610 | CLA | C3B-C4B-NB | 2.93 | 113.00 | 109.21 |
| 22 | A | 832 | CLA | CHC-C1C-C2C | -2.93 | 118.62 | 126.72 |
| 22 | A | 822 | CLA | C4C-C3C-C2C | -2.93 | 102.63 | 106.90 |
| 22 | B | 821 | CLA | C4C-C3C-C2C | -2.93 | 102.63 | 106.90 |
| 22 | 9 | 602 | CLA | C4C-C3C-C2C | -2.93 | 102.63 | 106.90 |
| 22 | A | 822 | CLA | CHC-C1C-C2C | -2.93 | 118.62 | 126.72 |
| 22 | 5 | 612 | CLA | C4-C3-C5 | 2.93 | 120.19 | 115.27 |
| 22 | 1 | 614 | CLA | CAA-C2A-C3A | -2.93 | 104.76 | 112.78 |
| 22 | A | 828 | CLA | C3B-C4B-NB | 2.93 | 112.99 | 109.21 |
| 22 | 9 | 614 | CLA | CHC-C1C-C2C | -2.93 | 118.63 | 126.72 |
| 22 | 7 | 612 | CLA | C4C-C3C-C2C | -2.93 | 102.63 | 106.90 |
| 22 | A | 826 | CLA | C3B-C4B-NB | 2.93 | 112.99 | 109.21 |
| 29 | 6 | 608 | CHL | CHD-C4C-NC | 2.93 | 128.81 | 124.20 |
| 22 | B | 829 | CLA | CHB-C4A-NA | 2.93 | 128.56 | 124.51 |
| 22 | A | 822 | CLA | CAA-C2A-C3A | -2.93 | 104.77 | 112.78 |
| 22 | 5 | 610 | CLA | CAC-C3C-C4C | 2.92 | 128.60 | 124.81 |
| 22 | 1 | 612 | CLA | O2A-CGA-CBA | 2.92 | 121.08 | 111.91 |
| 22 | 3 | 602 | CLA | C4C-C3C-C2C | -2.92 | 102.64 | 106.90 |
| 22 | F | 301 | CLA | CMC-C2C-C1C | 2.92 | 129.49 | 125.04 |
| 22 | 4 | 611 | CLA | CAA-C2A-C3A | -2.92 | 104.77 | 112.78 |
| 22 | 6 | 609 | CLA | C1-C2-C3 | -2.92 | 122.02 | 126.75 |
| 22 | B | 823 | CLA | C3B-C4B-NB | 2.92 | 112.99 | 109.21 |
| 22 | 9 | 610 | CLA | CHD-C4C-NC | 2.92 | 128.81 | 124.20 |
| 29 | 5 | 618 | CHL | C2A-C3A-C4A | -2.92 | 97.15 | 101.87 |
| 22 | 6 | 604 | CLA | CHC-C1C-C2C | -2.92 | 118.64 | 126.72 |
| 29 | 6 | 607 | CHL | CHB-C4A-NA | 2.92 | 128.55 | 124.51 |
| 22 | 3 | 610 | CLA | O2D-CGD-O1D | -2.92 | 118.13 | 123.84 |
| 25 | A | 851 | BCR | C15-C16-C17 | -2.92 | 117.49 | 123.47 |
| 30 | 7 | 621 | LUT | C30-C31-C32 | -2.92 | 114.11 | 123.22 |
| 30 | 7 | 622 | LUT | C38-C25-C24 | -2.92 | 117.31 | 123.56 |
| 25 | G | 205 | BCR | C16-C15-C14 | -2.92 | 117.50 | 123.47 |
| 22 | 7 | 602 | CLA | C1C-C2C-C3C | -2.92 | 103.89 | 106.96 |
| 22 | B | 837 | CLA | CHD-C4C-NC | 2.92 | 128.80 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 1 | 611 | CLA | CMB-C2B-C3B | 2.92 | 130.14 | 124.68 |
| 22 | 2 | 611 | CLA | C4-C3-C5 | 2.92 | 120.18 | 115.27 |
| 22 | 5 | 604 | CLA | C1-C2-C3 | -2.92 | 122.03 | 126.75 |
| 22 | A | 809 | CLA | CMC-C2C-C1C | 2.92 | 129.48 | 125.04 |
| 29 | 4 | 618 | CHL | C1B-CHB-C4A | -2.92 | 124.34 | 130.12 |
| 22 | B | 826 | CLA | CHD-C4C-NC | 2.92 | 128.80 | 124.20 |
| 22 | A | 823 | CLA | O2A-CGA-CBA | 2.91 | 121.06 | 111.91 |
| 24 | 4 | 622 | LHG | C6-C5-C4 | -2.91 | 104.89 | 111.79 |
| 22 | 3 | 606 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.90 |
| 22 | 1 | 603 | CLA | CBC-CAC-C3C | -2.91 | 104.40 | 112.43 |
| 22 | 4 | 604 | CLA | CAC-C3C-C4C | 2.91 | 128.59 | 124.81 |
| 22 | Z | 613 | CLA | CMC-C2C-C1C | 2.91 | 129.48 | 125.04 |
| 22 | B | 835 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.90 |
| 22 | B | 839 | CLA | C4C-C3C-C2C | -2.91 | 102.65 | 106.90 |
| 22 | B | 802 | CLA | C1C-C2C-C3C | -2.91 | 103.89 | 106.96 |
| 22 | G | 203 | CLA | CAA-C2A-C3A | -2.91 | 104.80 | 112.78 |
| 22 | 7 | 601 | CLA | CHC-C1C-C2C | -2.91 | 118.67 | 126.72 |
| 22 | 6 | 613 | CLA | CHC-C1C-C2C | -2.91 | 118.67 | 126.72 |
| 22 | A | 810 | CLA | C11-C12-C13 | -2.91 | 106.52 | 115.92 |
| 22 | A | 828 | CLA | CAC-C3C-C2C | 2.91 | 132.50 | 127.53 |
| 22 | B | 830 | CLA | CHC-C1C-C2C | -2.91 | 118.68 | 126.72 |
| 22 | B | 823 | CLA | O2A-CGA-CBA | 2.91 | 121.03 | 111.91 |
| 22 | A | 842 | CLA | CHD-C4C-NC | 2.91 | 128.79 | 124.20 |
| 30 | 3 | 621 | LUT | C30-C31-C32 | -2.91 | 114.14 | 123.22 |
| 29 | 4 | 608 | CHL | CHD-C4C-NC | 2.91 | 128.78 | 124.20 |
| 22 | A | 815 | CLA | O2D-CGD-O1D | -2.91 | 118.16 | 123.84 |
| 22 | 6 | 603 | CLA | CAA-C2A-C3A | -2.90 | 104.82 | 112.78 |
| 22 | 8 | 609 | CLA | CMB-C2B-C3B | 2.90 | 130.11 | 124.68 |
| 22 | 5 | 617 | CLA | CHC-C1C-C2C | -2.90 | 118.69 | 126.72 |
| 22 | B | 802 | CLA | C1-C2-C3 | -2.90 | 121.02 | 126.04 |
| 22 | 7 | 612 | CLA | CAC-C3C-C4C | 2.90 | 128.57 | 124.81 |
| 22 | A | 827 | CLA | C4C-C3C-C2C | -2.90 | 102.67 | 106.90 |
| 22 | 4 | 614 | CLA | C4C-C3C-C2C | -2.90 | 102.67 | 106.90 |
| 22 | A | 854 | CLA | CAC-C3C-C4C | 2.90 | 128.57 | 124.81 |
| 22 | B | 827 | CLA | CHC-C1C-C2C | -2.90 | 118.70 | 126.72 |
| 22 | 5 | 610 | CLA | CMB-C2B-C3B | 2.90 | 130.10 | 124.68 |
| 22 | 6 | 602 | CLA | C4C-C3C-C2C | -2.90 | 102.67 | 106.90 |
| 22 | 9 | 602 | CLA | CHC-C1C-C2C | -2.90 | 118.71 | 126.72 |
| 25 | F | 305 | BCR | C23-C24-C25 | -2.90 | 119.06 | 127.20 |
| 25 | A | 851 | BCR | C16-C15-C14 | -2.90 | 117.54 | 123.47 |
| 22 | Z | 606 | CLA | CHD-C4C-NC | 2.90 | 128.77 | 124.20 |
| 25 | L | 205 | BCR | C20-C21-C22 | -2.90 | 123.18 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 5 | 602 | CLA | CAC-C3C-C4C | 2.90 | 128.57 | 124.81 |
| 25 | A | 851 | BCR | C10-C11-C12 | -2.90 | 114.18 | 123.22 |
| 22 | 5 | 606 | CLA | CHD-C4C-NC | 2.89 | 128.76 | 124.20 |
| 22 | B | 814 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 22 | 4 | 611 | CLA | C4-C3-C5 | 2.89 | 120.14 | 115.27 |
| 22 | Z | 613 | CLA | CAC-C3C-C4C | 2.89 | 128.56 | 124.81 |
| 22 | A | 814 | CLA | O2A-CGA-CBA | 2.89 | 120.99 | 111.91 |
| 22 | A | 814 | CLA | O2D-CGD-O1D | -2.89 | 118.18 | 123.84 |
| 22 | A | 840 | CLA | CHD-C4C-NC | 2.89 | 128.76 | 124.20 |
| 22 | A | 841 | CLA | CHC-C1C-C2C | -2.89 | 118.72 | 126.72 |
| 22 | B | 829 | CLA | O2A-CGA-CBA | 2.89 | 120.98 | 111.91 |
| 30 | 2 | 616 | LUT | C35-C15-C14 | -2.89 | 117.55 | 123.47 |
| 22 | A | 809 | CLA | CHB-C4A-NA | 2.89 | 128.51 | 124.51 |
| 22 | Z | 614 | CLA | C4-C3-C5 | 2.89 | 120.13 | 115.27 |
| 22 | A | 805 | CLA | C3B-C4B-NB | 2.89 | 112.95 | 109.21 |
| 22 | 7 | 601 | CLA | C4-C3-C5 | 2.89 | 120.13 | 115.27 |
| 22 | B | 822 | CLA | C4C-C3C-C2C | -2.89 | 102.69 | 106.90 |
| 22 | Z | 612 | CLA | C4C-C3C-C2C | -2.89 | 102.69 | 106.90 |
| 22 | Z | 613 | CLA | C4C-C3C-C2C | -2.89 | 102.69 | 106.90 |
| 22 | 4 | 603 | CLA | CBC-CAC-C3C | -2.89 | 104.47 | 112.43 |
| 22 | A | 833 | CLA | C4C-C3C-C2C | -2.89 | 102.69 | 106.90 |
| 22 | A | 819 | CLA | C1C-C2C-C3C | -2.89 | 103.92 | 106.96 |
| 29 | 7 | 607 | CHL | C3D-C4D-ND | 2.89 | 114.91 | 110.24 |
| 22 | A | 842 | CLA | O2D-CGD-O1D | -2.89 | 118.19 | 123.84 |
| 22 | B | 825 | CLA | O2D-CGD-CBD | 2.89 | 116.40 | 111.27 |
| 22 | 7 | 601 | CLA | C4A-NA-C1A | -2.89 | 105.41 | 106.71 |
| 22 | L | 203 | CLA | CHC-C1C-C2C | -2.89 | 118.74 | 126.72 |
| 22 | 5 | 601 | CLA | O2D-CGD-O1D | -2.89 | 118.19 | 123.84 |
| 22 | B | 837 | CLA | C3B-C4B-NB | 2.89 | 112.94 | 109.21 |
| 22 | A | 803 | CLA | C4-C3-C5 | 2.89 | 120.13 | 115.27 |
| 22 | A | 826 | CLA | C4C-C3C-C2C | -2.89 | 102.69 | 106.90 |
| 22 | A | 854 | CLA | CMB-C2B-C3B | 2.89 | 130.08 | 124.68 |
| 22 | A | 835 | CLA | CHD-C4C-NC | 2.89 | 128.75 | 124.20 |
| 22 | Z | 612 | CLA | CHD-C4C-NC | 2.88 | 128.75 | 124.20 |
| 29 | 5 | 607 | CHL | C1B-CHB-C4A | -2.88 | 124.40 | 130.12 |
| 22 | 6 | 603 | CLA | C4C-C3C-C2C | -2.88 | 102.69 | 106.90 |
| 30 | 7 | 622 | LUT | C35-C34-C33 | -2.88 | 123.19 | 127.31 |
| 22 | B | 826 | CLA | C1C-C2C-C3C | -2.88 | 103.92 | 106.96 |
| 22 | A | 808 | CLA | C1-C2-C3 | -2.88 | 121.06 | 126.04 |
| 22 | A | 809 | CLA | C3B-C4B-NB | 2.88 | 112.94 | 109.21 |
| 22 | 5 | 610 | CLA | CMC-C2C-C1C | 2.88 | 129.43 | 125.04 |
| 22 | A | 845 | CLA | CAA-C2A-C3A | -2.88 | 104.89 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 9 | 609 | CLA | C1-C2-C3 | -2.88 | 122.09 | 126.75 |
| 22 | Z | 606 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.90 |
| 22 | B | 814 | CLA | O2D-CGD-O1D | -2.88 | 118.21 | 123.84 |
| 25 | A | 849 | BCR | C34-C9-C8 | 2.88 | 122.61 | 118.08 |
| 22 | 1 | 608 | CLA | CAC-C3C-C4C | 2.88 | 128.55 | 124.81 |
| 22 | B | 815 | CLA | CAA-C2A-C3A | -2.88 | 104.89 | 112.78 |
| 30 | 8 | 617 | LUT | C20-C13-C12 | 2.88 | 122.61 | 118.08 |
| 22 | B | 836 | CLA | O2A-CGA-CBA | 2.88 | 120.94 | 111.91 |
| 22 | F | 301 | CLA | CMB-C2B-C3B | 2.88 | 130.06 | 124.68 |
| 22 | A | 824 | CLA | C1-C2-C3 | -2.88 | 121.07 | 126.04 |
| 22 | 1 | 611 | CLA | CAC-C3C-C4C | 2.88 | 128.54 | 124.81 |
| 22 | A | 808 | CLA | C4C-C3C-C2C | -2.88 | 102.70 | 106.90 |
| 22 | 1 | 602 | CLA | C4C-C3C-C2C | -2.88 | 102.71 | 106.90 |
| 22 | B | 827 | CLA | O2A-CGA-CBA | 2.88 | 120.93 | 111.91 |
| 22 | 4 | 603 | CLA | CAA-C2A-C3A | -2.88 | 104.91 | 112.78 |
| 22 | 7 | 620 | CLA | C4C-C3C-C2C | -2.87 | 102.71 | 106.90 |
| 22 | 5 | 610 | CLA | CHC-C1C-C2C | -2.87 | 118.77 | 126.72 |
| 22 | 5 | 609 | CLA | CHB-C4A-NA | 2.87 | 128.49 | 124.51 |
| 22 | 4 | 612 | CLA | O2D-CGD-O1D | -2.87 | 118.22 | 123.84 |
| 22 | A | 842 | CLA | C4C-C3C-C2C | -2.87 | 102.71 | 106.90 |
| 22 | A | 802 | CLA | CHC-C1C-C2C | -2.87 | 118.77 | 126.72 |
| 22 | 8 | 601 | CLA | O2D-CGD-O1D | -2.87 | 118.22 | 123.84 |
| 30 | 4 | 619 | LUT | C20-C13-C12 | 2.87 | 122.61 | 118.08 |
| 22 | B | 825 | CLA | O2A-CGA-CBA | 2.87 | 120.92 | 111.91 |
| 22 | B | 826 | CLA | CHC-C1C-C2C | -2.87 | 118.78 | 126.72 |
| 22 | 1 | 616 | CLA | C4C-C3C-C2C | -2.87 | 102.71 | 106.90 |
| 30 | 7 | 622 | LUT | C10-C11-C12 | -2.87 | 114.25 | 123.22 |
| 22 | B | 814 | CLA | CHC-C1C-C2C | -2.87 | 118.78 | 126.72 |
| 29 | 5 | 607 | CHL | C1-O2A-CGA | 2.87 | 123.98 | 116.44 |
| 22 | B | 812 | CLA | CHD-C4C-NC | 2.87 | 128.73 | 124.20 |
| 22 | 6 | 612 | CLA | CHD-C4C-NC | 2.87 | 128.73 | 124.20 |
| 22 | 9 | 603 | CLA | C4C-C3C-C2C | -2.87 | 102.72 | 106.90 |
| 22 | A | 807 | CLA | CHD-C4C-NC | 2.87 | 128.72 | 124.20 |
| 22 | 2 | 607 | CLA | C4C-C3C-C2C | -2.87 | 102.72 | 106.90 |
| 29 | Z | 601 | CHL | C3B-C4B-NB | 2.87 | 112.92 | 109.21 |
| 22 | 9 | 611 | CLA | C4C-C3C-C2C | -2.87 | 102.72 | 106.90 |
| 22 | B | 817 | CLA | C1-C2-C3 | -2.87 | 121.09 | 126.04 |
| 22 | B | 833 | CLA | O2A-CGA-CBA | 2.87 | 120.90 | 111.91 |
| 25 | A | 848 | BCR | C15-C14-C13 | -2.87 | 123.22 | 127.31 |
| 25 | 7 | 623 | BCR | C2-C1-C6 | 2.86 | 114.89 | 110.48 |
| 22 | 6 | 614 | CLA | CAC-C3C-C4C | 2.86 | 128.53 | 124.81 |
| 22 | Z | 608 | CLA | CHD-C4C-NC | 2.86 | 128.72 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 829 | CLA | C4-C3-C5 | 2.86 | 120.09 | 115.27 |
| 22 | F | 304 | CLA | CHD-C4C-NC | 2.86 | 128.71 | 124.20 |
| 22 | A | 813 | CLA | C3B-C4B-NB | 2.86 | 112.91 | 109.21 |
| 22 | Z | 606 | CLA | CAC-C3C-C4C | 2.86 | 128.52 | 124.81 |
| 22 | 3 | 609 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.90 |
| 22 | 9 | 610 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.90 |
| 29 | 1 | 601 | CHL | C2A-C1A-CHA | -2.86 | 118.86 | 123.86 |
| 22 | 2 | 610 | CLA | C4-C3-C5 | 2.86 | 120.08 | 115.27 |
| 22 | B | 816 | CLA | C1C-C2C-C3C | -2.86 | 103.95 | 106.96 |
| 22 | 9 | 611 | CLA | CHD-C4C-NC | 2.86 | 128.71 | 124.20 |
| 25 | 3 | 717 | BCR | C16-C15-C14 | -2.86 | 117.62 | 123.47 |
| 29 | 1 | 607 | CHL | CAC-C3C-C4C | 2.86 | 128.52 | 124.81 |
| 22 | 4 | 613 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.90 |
| 25 | 4 | 621 | BCR | C24-C23-C22 | -2.86 | 121.92 | 126.23 |
| 22 | B | 822 | CLA | CAC-C3C-C4C | 2.86 | 128.52 | 124.81 |
| 22 | 3 | 612 | CLA | C4C-C3C-C2C | -2.86 | 102.73 | 106.90 |
| 22 | 6 | 604 | CLA | CAC-C3C-C4C | 2.86 | 128.52 | 124.81 |
| 30 | 3 | 622 | LUT | C20-C13-C12 | 2.86 | 122.58 | 118.08 |
| 22 | F | 301 | CLA | C4C-C3C-C2C | -2.85 | 102.74 | 106.90 |
| 29 | 4 | 608 | CHL | CAC-C3C-C4C | 2.85 | 128.51 | 124.81 |
| 22 | Z | 611 | CLA | CHD-C4C-NC | 2.85 | 128.70 | 124.20 |
| 24 | A | 847 | LHG | O8-C23-C24 | 2.85 | 120.86 | 111.91 |
| 22 | 2 | 613 | CLA | C4C-C3C-C2C | -2.85 | 102.74 | 106.90 |
| 22 | A | 843 | CLA | O2A-CGA-CBA | 2.85 | 120.86 | 111.91 |
| 22 | B | 814 | CLA | C3B-C4B-NB | 2.85 | 112.90 | 109.21 |
| 25 | A | 852 | BCR | C15-C14-C13 | -2.85 | 123.24 | 127.31 |
| 22 | 7 | 601 | CLA | O2D-CGD-O1D | -2.85 | 118.26 | 123.84 |
| 22 | B | 806 | CLA | C4C-C3C-C2C | -2.85 | 102.74 | 106.90 |
| 29 | 4 | 618 | CHL | CMB-C2B-C3B | 2.85 | 130.01 | 124.68 |
| 25 | 5 | 625 | BCR | C40-C30-C25 | 2.85 | 114.92 | 110.30 |
| 25 | K | 4001 | BCR | C2-C1-C6 | 2.85 | 114.87 | 110.48 |
| 29 | 4 | 606 | CHL | C3B-C4B-NB | 2.85 | 112.89 | 109.21 |
| 22 | 8 | 602 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.90 |
| 22 | 1 | 602 | CLA | CMC-C2C-C1C | 2.85 | 129.38 | 125.04 |
| 22 | 7 | 614 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.90 |
| 22 | 3 | 609 | CLA | C1-C2-C3 | -2.85 | 122.14 | 126.75 |
| 30 | 9 | 617 | LUT | C18-C5-C6 | -2.85 | 121.33 | 124.53 |
| 22 | 9 | 604 | CLA | C4C-C3C-C2C | -2.85 | 102.75 | 106.90 |
| 22 | B | 822 | CLA | CAA-C2A-C3A | -2.85 | 104.98 | 112.78 |
| 22 | A | 815 | CLA | CHD-C4C-NC | 2.85 | 128.69 | 124.20 |
| 22 | A | 804 | CLA | CAC-C3C-C4C | 2.85 | 128.50 | 124.81 |
| 22 | F | 301 | CLA | C1-C2-C3 | -2.85 | 121.12 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29 | 4 | 606 | CHL | O2A-CGA-CBA | 2.85 | 120.84 | 111.91 |
| 30 | 3 | 621 | LUT | C35-C34-C33 | -2.85 | 123.25 | 127.31 |
| 22 | 3 | 603 | CLA | C4C-C3C-C2C | -2.84 | 102.75 | 106.90 |
| 22 | B | 835 | CLA | CHD-C4C-NC | 2.84 | 128.69 | 124.20 |
| 22 | 8 | 616 | CLA | CAC-C3C-C4C | 2.84 | 128.50 | 124.81 |
| 22 | 4 | 612 | CLA | CHD-C4C-NC | 2.84 | 128.68 | 124.20 |
| 22 | A | 805 | CLA | C2A-C1A-CHA | -2.84 | 118.89 | 123.86 |
| 22 | 4 | 610 | CLA | CMB-C2B-C3B | 2.84 | 130.00 | 124.68 |
| 29 | 6 | 606 | CHL | C3B-C4B-NB | 2.84 | 112.89 | 109.21 |
| 22 | A | 809 | CLA | CHD-C4C-NC | 2.84 | 128.68 | 124.20 |
| 22 | A | 835 | CLA | CAC-C3C-C4C | 2.84 | 128.50 | 124.81 |
| 22 | 4 | 609 | CLA | CED-O2D-CGD | 2.84 | 122.36 | 115.94 |
| 22 | B | 822 | CLA | CHD-C4C-NC | 2.84 | 128.68 | 124.20 |
| 22 | A | 829 | CLA | C3B-C4B-NB | 2.84 | 112.88 | 109.21 |
| 22 | 3 | 610 | CLA | C4C-C3C-C2C | -2.84 | 102.76 | 106.90 |
| 22 | A | 830 | CLA | CHC-C1C-C2C | -2.84 | 118.87 | 126.72 |
| 22 | B | 822 | CLA | CHC-C1C-C2C | -2.84 | 118.87 | 126.72 |
| 22 | A | 841 | CLA | C1-C2-C3 | -2.84 | 121.13 | 126.04 |
| 29 | 5 | 608 | CHL | C3D-C4D-ND | 2.84 | 114.83 | 110.24 |
| 22 | G | 204 | CLA | C4C-C3C-C2C | -2.84 | 102.76 | 106.90 |
| 22 | 3 | 604 | CLA | CAC-C3C-C4C | 2.84 | 128.49 | 124.81 |
| 22 | 2 | 606 | CLA | CAC-C3C-C4C | 2.84 | 128.49 | 124.81 |
| 22 | B | 806 | CLA | C1-C2-C3 | -2.84 | 121.14 | 126.04 |
| 22 | 3 | 611 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 29 | 5 | 608 | CHL | CMB-C2B-C3B | 2.84 | 129.99 | 124.68 |
| 22 | B | 813 | CLA | O2D-CGD-O1D | -2.84 | 118.29 | 123.84 |
| 22 | 9 | 610 | CLA | CHC-C1C-C2C | -2.84 | 118.88 | 126.72 |
| 22 | A | 832 | CLA | C1-C2-C3 | -2.84 | 122.16 | 126.75 |
| 22 | 6 | 611 | CLA | C4C-C3C-C2C | -2.84 | 102.76 | 106.90 |
| 22 | 1 | 611 | CLA | O2A-CGA-CBA | 2.84 | 120.81 | 111.91 |
| 22 | B | 805 | CLA | C4-C3-C5 | 2.84 | 120.04 | 115.27 |
| 22 | A | 816 | CLA | CAA-C2A-C3A | -2.84 | 105.01 | 112.78 |
| 22 | 2 | 610 | CLA | CHD-C4C-NC | 2.84 | 128.67 | 124.20 |
| 22 | A | 806 | CLA | C4C-C3C-C2C | -2.84 | 102.77 | 106.90 |
| 22 | 7 | 603 | CLA | C4C-C3C-C2C | -2.84 | 102.77 | 106.90 |
| 22 | 7 | 614 | CLA | CHD-C4C-NC | 2.83 | 128.67 | 124.20 |
| 22 | J | 3002 | CLA | C4C-C3C-C2C | -2.83 | 102.77 | 106.90 |
| 22 | 6 | 614 | CLA | CHC-C1C-C2C | -2.83 | 118.88 | 126.72 |
| 22 | 3 | 602 | CLA | CMC-C2C-C1C | 2.83 | 129.35 | 125.04 |
| 22 | K | 4002 | CLA | CAC-C3C-C4C | 2.83 | 128.49 | 124.81 |
| 22 | 2 | 611 | CLA | CAC-C3C-C4C | 2.83 | 128.49 | 124.81 |
| 22 | 7 | 611 | CLA | CMA-C3A-C2A | -2.83 | 109.49 | 116.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 832 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 22 | B | 803 | CLA | O2A-CGA-CBA | 2.83 | 120.80 | 111.91 |
| 22 | 8 | 613 | CLA | CMC-C2C-C1C | 2.83 | 129.35 | 125.04 |
| 22 | A | 815 | CLA | CHC-C1C-C2C | -2.83 | 118.89 | 126.72 |
| 22 | 5 | 606 | CLA | C3B-C4B-NB | 2.83 | 112.87 | 109.21 |
| 22 | 4 | 612 | CLA | CAC-C3C-C4C | 2.83 | 128.48 | 124.81 |
| 30 | 7 | 622 | LUT | C7-C8-C9 | -2.83 | 121.96 | 126.23 |
| 22 | 9 | 601 | CLA | C4C-C3C-C2C | -2.83 | 102.77 | 106.90 |
| 22 | A | 817 | CLA | O2D-CGD-O1D | -2.83 | 118.30 | 123.84 |
| 22 | A | 835 | CLA | CHC-C1C-C2C | -2.83 | 118.89 | 126.72 |
| 22 | B | 837 | CLA | CHB-C4A-NA | 2.83 | 128.43 | 124.51 |
| 22 | A | 835 | CLA | C4C-C3C-C2C | -2.83 | 102.77 | 106.90 |
| 22 | F | 303 | CLA | C3B-C4B-NB | 2.83 | 112.87 | 109.21 |
| 22 | 3 | 617 | CLA | C4C-C3C-C2C | -2.83 | 102.78 | 106.90 |
| 22 | A | 836 | CLA | CHB-C4A-NA | 2.83 | 128.42 | 124.51 |
| 22 | B | 808 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 22 | B | 810 | CLA | O2A-CGA-CBA | 2.83 | 120.78 | 111.91 |
| 22 | B | 841 | CLA | CAC-C3C-C4C | 2.83 | 128.48 | 124.81 |
| 22 | 9 | 613 | CLA | C4C-C3C-C2C | -2.83 | 102.78 | 106.90 |
| 22 | 2 | 609 | CLA | C1-C2-C3 | -2.83 | 122.18 | 126.75 |
| 22 | 7 | 602 | CLA | CAC-C3C-C4C | 2.83 | 128.48 | 124.81 |
| 22 | B | 818 | CLA | CBA-CAA-C2A | 2.83 | 122.20 | 113.86 |
| 22 | 4 | 613 | CLA | O2A-C1-C2 | 2.83 | 116.06 | 108.64 |
| 22 | 4 | 601 | CLA | O2D-CGD-O1D | -2.83 | 118.31 | 123.84 |
| 22 | 4 | 601 | CLA | C4C-C3C-C2C | -2.82 | 102.78 | 106.90 |
| 22 | 5 | 609 | CLA | CAC-C3C-C4C | 2.82 | 128.47 | 124.81 |
| 30 | 1 | 618 | LUT | C38-C25-C24 | -2.82 | 117.52 | 123.56 |
| 22 | 8 | 612 | CLA | O2A-CGA-CBA | 2.82 | 120.77 | 111.91 |
| 22 | A | 813 | CLA | CHC-C1C-C2C | -2.82 | 118.91 | 126.72 |
| 22 | B | 839 | CLA | CMB-C2B-C3B | 2.82 | 129.96 | 124.68 |
| 22 | 8 | 611 | CLA | C4C-C3C-C2C | -2.82 | 102.78 | 106.90 |
| 22 | B | 818 | CLA | O2D-CGD-O1D | -2.82 | 118.32 | 123.84 |
| 22 | B | 834 | CLA | CMA-C3A-C2A | -2.82 | 102.45 | 113.83 |
| 22 | A | 802 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 30 | 1 | 617 | LUT | C21-C26-C27 | -2.82 | 109.14 | 112.70 |
| 22 | A | 818 | CLA | C4-C3-C5 | 2.82 | 120.02 | 115.27 |
| 22 | 9 | 612 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 24 | 7 | 625 | LHG | O8-C23-C24 | 2.82 | 120.76 | 111.91 |
| 22 | 2 | 602 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 22 | B | 838 | CLA | CHD-C4C-NC | 2.82 | 128.65 | 124.20 |
| 22 | 9 | 612 | CLA | CAC-C3C-C4C | 2.82 | 128.47 | 124.81 |
| 22 | A | 842 | CLA | CAA-C2A-C3A | -2.82 | 105.06 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 609 | CLA | CED-O2D-CGD | 2.82 | 122.31 | 115.94 |
| 22 | 6 | 610 | CLA | CHC-C1C-C2C | -2.82 | 118.93 | 126.72 |
| 22 | 1 | 608 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 22 | 2 | 601 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 22 | 6 | 614 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 22 | 6 | 612 | CLA | CAC-C3C-C4C | 2.82 | 128.46 | 124.81 |
| 22 | A | 833 | CLA | CAC-C3C-C4C | 2.82 | 128.46 | 124.81 |
| 22 | 2 | 606 | CLA | C4C-C3C-C2C | -2.82 | 102.79 | 106.90 |
| 25 | 4 | 621 | BCR | C33-C5-C4 | 2.82 | 119.02 | 113.62 |
| 22 | 6 | 612 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.90 |
| 22 | 4 | 613 | CLA | CHD-C4C-NC | 2.81 | 128.64 | 124.20 |
| 21 | A | 801 | CL0 | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 22 | 8 | 616 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 22 | B | 824 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.90 |
| 22 | 8 | 603 | CLA | CHD-C4C-NC | 2.81 | 128.64 | 124.20 |
| 29 | 4 | 608 | CHL | C3B-C4B-NB | 2.81 | 112.85 | 109.21 |
| 22 | 4 | 613 | CLA | CHB-C4A-NA | 2.81 | 128.40 | 124.51 |
| 22 | 8 | 612 | CLA | CAC-C3C-C4C | 2.81 | 128.46 | 124.81 |
| 22 | A | 805 | CLA | CHC-C1C-C2C | -2.81 | 118.94 | 126.72 |
| 30 | Z | 618 | LUT | C38-C25-C24 | -2.81 | 117.54 | 123.56 |
| 22 | K | 4002 | CLA | O2D-CGD-O1D | -2.81 | 118.34 | 123.84 |
| 22 | 3 | 612 | CLA | CAC-C3C-C4C | 2.81 | 128.46 | 124.81 |
| 30 | 7 | 621 | LUT | C20-C13-C12 | 2.81 | 122.50 | 118.08 |
| 30 | 1 | 618 | LUT | C10-C11-C12 | -2.81 | 114.45 | 123.22 |
| 25 | J | 3003 | BCR | C10-C11-C12 | -2.81 | 114.45 | 123.22 |
| 22 | Z | 610 | CLA | C1C-C2C-C3C | -2.81 | 104.00 | 106.96 |
| 22 | B | 806 | CLA | CMC-C2C-C1C | 2.81 | 129.32 | 125.04 |
| 22 | 1 | 614 | CLA | C4C-C3C-C2C | -2.81 | 102.80 | 106.90 |
| 24 | B | 851 | LHG | C5-O7-C7 | -2.81 | 110.88 | 117.79 |
| 30 | 3 | 622 | LUT | C10-C11-C12 | -2.81 | 114.46 | 123.22 |
| 22 | 6 | 614 | CLA | CHD-C4C-NC | 2.81 | 128.63 | 124.20 |
| 29 | 3 | 608 | CHL | O2A-CGA-CBA | 2.81 | 120.72 | 111.91 |
| 22 | 7 | 604 | CLA | C4C-C3C-C2C | -2.81 | 102.81 | 106.90 |
| 22 | 2 | 611 | CLA | C4C-C3C-C2C | -2.81 | 102.81 | 106.90 |
| 22 | 2 | 610 | CLA | C4C-C3C-C2C | -2.81 | 102.81 | 106.90 |
| 25 | B | 845 | BCR | C37-C22-C21 | -2.81 | 118.99 | 122.92 |
| 22 | B | 823 | CLA | C4-C3-C5 | 2.81 | 119.99 | 115.27 |
| 22 | A | 815 | CLA | O2A-CGA-CBA | 2.81 | 120.71 | 111.91 |
| 22 | 8 | 611 | CLA | CHB-C4A-NA | 2.81 | 128.39 | 124.51 |
| 22 | 6 | 622 | CLA | C4C-C3C-C2C | -2.80 | 102.81 | 106.90 |
| 25 | B | 801 | BCR | C2-C1-C6 | 2.80 | 114.80 | 110.48 |
| 30 | 2 | 617 | LUT | C11-C10-C9 | -2.80 | 123.31 | 127.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 5 | 603 | CLA | C4C-C3C-C2C | -2.80 | 102.81 | 106.90 |
| 22 | 1 | 612 | CLA | C4C-C3C-C2C | -2.80 | 102.81 | 106.90 |
| 22 | 8 | 603 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 22 | B | 812 | CLA | C4C-C3C-C2C | -2.80 | 102.81 | 106.90 |
| 22 | 8 | 608 | CLA | C1-C2-C3 | -2.80 | 122.22 | 126.75 |
| 22 | A | 812 | CLA | O2D-CGD-O1D | -2.80 | 118.36 | 123.84 |
| 25 | 8 | 619 | BCR | C37-C22-C23 | 2.80 | 122.49 | 118.08 |
| 25 | L | 201 | BCR | C11-C10-C9 | -2.80 | 123.31 | 127.31 |
| 22 | A | 802 | CLA | CHD-C4C-NC | 2.80 | 128.62 | 124.20 |
| 22 | 6 | 604 | CLA | C4C-C3C-C2C | -2.80 | 102.82 | 106.90 |
| 22 | Z | 602 | CLA | CHC-C1C-C2C | -2.80 | 118.98 | 126.72 |
| 22 | 5 | 612 | CLA | CAC-C3C-C4C | 2.80 | 128.44 | 124.81 |
| 25 | B | 801 | BCR | C15-C14-C13 | -2.80 | 123.31 | 127.31 |
| 25 | L | 205 | BCR | C16-C17-C18 | -2.80 | 123.31 | 127.31 |
| 25 | 4 | 621 | BCR | C3-C4-C5 | -2.80 | 109.08 | 114.08 |
| 22 | 6 | 604 | CLA | CHD-C4C-NC | 2.80 | 128.61 | 124.20 |
| 22 | A | 836 | CLA | C4C-C3C-C2C | -2.80 | 102.82 | 106.90 |
| 22 | B | 830 | CLA | CAC-C3C-C4C | 2.80 | 128.44 | 124.81 |
| 22 | A | 820 | CLA | CHD-C4C-NC | 2.80 | 128.61 | 124.20 |
| 30 | 4 | 619 | LUT | C12-C13-C14 | -2.80 | 114.65 | 118.94 |
| 22 | 5 | 601 | CLA | C4C-C3C-C2C | -2.80 | 102.82 | 106.90 |
| 22 | 1 | 613 | CLA | CAA-C2A-C3A | -2.80 | 105.12 | 112.78 |
| 22 | 2 | 601 | CLA | CHD-C4C-NC | 2.80 | 128.61 | 124.20 |
| 25 | 3 | 718 | BCR | C16-C15-C14 | -2.80 | 117.74 | 123.47 |
| 25 | 3 | 718 | BCR | C21-C20-C19 | -2.80 | 114.49 | 123.22 |
| 22 | B | 829 | CLA | O2D-CGD-O1D | -2.80 | 118.37 | 123.84 |
| 22 | 9 | 613 | CLA | O2D-CGD-O1D | -2.80 | 118.37 | 123.84 |
| 22 | 7 | 608 | CLA | C4C-C3C-C2C | -2.80 | 102.82 | 106.90 |
| 22 | 2 | 607 | CLA | C1-C2-C3 | -2.80 | 122.23 | 126.75 |
| 22 | A | 806 | CLA | CAA-CBA-CGA | -2.79 | 105.09 | 113.25 |
| 22 | A | 826 | CLA | O2D-CGD-O1D | -2.79 | 118.37 | 123.84 |
| 22 | 9 | 602 | CLA | O2D-CGD-O1D | -2.79 | 118.37 | 123.84 |
| 22 | A | 817 | CLA | CHD-C4C-NC | 2.79 | 128.61 | 124.20 |
| 22 | B | 820 | CLA | C4-C3-C5 | 2.79 | 119.97 | 115.27 |
| 22 | Z | 602 | CLA | CMC-C2C-C1C | 2.79 | 129.29 | 125.04 |
| 22 | Z | 610 | CLA | CMB-C2B-C3B | 2.79 | 129.91 | 124.68 |
| 22 | Z | 614 | CLA | CHD-C4C-NC | 2.79 | 128.60 | 124.20 |
| 22 | 5 | 610 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.90 |
| 22 | 5 | 611 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.90 |
| 22 | K | 4003 | CLA | CAA-C2A-C3A | -2.79 | 105.13 | 112.78 |
| 22 | 1 | 606 | CLA | CHC-C1C-C2C | -2.79 | 119.00 | 126.72 |
| 22 | 8 | 608 | CLA | O2A-CGA-CBA | 2.79 | 120.67 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 816 | CLA | C4-C3-C5 | 2.79 | 119.97 | 115.27 |
| 22 | 6 | 609 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 22 | B | 841 | CLA | CHC-C1C-C2C | -2.79 | 119.00 | 126.72 |
| 22 | A | 820 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.90 |
| 22 | K | 4002 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.90 |
| 25 | B | 844 | BCR | C20-C21-C22 | -2.79 | 123.33 | 127.31 |
| 22 | A | 827 | CLA | CMC-C2C-C1C | 2.79 | 129.29 | 125.04 |
| 22 | 3 | 617 | CLA | CAC-C3C-C4C | 2.79 | 128.43 | 124.81 |
| 22 | 4 | 616 | CLA | C4C-C3C-C2C | -2.79 | 102.83 | 106.90 |
| 22 | B | 805 | CLA | CHB-C4A-NA | 2.79 | 128.37 | 124.51 |
| 22 | 7 | 613 | CLA | O2A-CGA-CBA | 2.79 | 120.65 | 111.91 |
| 22 | 8 | 614 | CLA | CHC-C1C-C2C | -2.79 | 119.01 | 126.72 |
| 22 | A | 834 | CLA | C4C-C3C-C2C | -2.79 | 102.84 | 106.90 |
| 22 | 3 | 614 | CLA | C4C-C3C-C2C | -2.79 | 102.84 | 106.90 |
| 22 | 7 | 606 | CLA | CMB-C2B-C3B | 2.79 | 129.89 | 124.68 |
| 22 | 4 | 611 | CLA | CMB-C2B-C3B | 2.79 | 129.89 | 124.68 |
| 22 | B | 837 | CLA | CAA-C2A-C3A | -2.78 | 105.16 | 112.78 |
| 29 | 7 | 607 | CHL | CAC-C3C-C4C | 2.78 | 128.42 | 124.81 |
| 22 | A | 808 | CLA | CHD-C4C-NC | 2.78 | 128.59 | 124.20 |
| 22 | B | 834 | CLA | CHD-C4C-NC | 2.78 | 128.59 | 124.20 |
| 22 | 8 | 601 | CLA | C4C-C3C-C2C | -2.78 | 102.84 | 106.90 |
| 22 | 1 | 602 | CLA | CAA-C2A-C3A | -2.78 | 105.16 | 112.78 |
| 22 | B | 820 | CLA | CAC-C3C-C4C | 2.78 | 128.42 | 124.81 |
| 22 | 3 | 602 | CLA | CHD-C4C-NC | 2.78 | 128.58 | 124.20 |
| 22 | 5 | 621 | CLA | CAA-C2A-C1A | 2.78 | 121.08 | 111.97 |
| 22 | 7 | 609 | CLA | CED-O2D-CGD | 2.78 | 122.22 | 115.94 |
| 22 | B | 837 | CLA | CHC-C1C-C2C | -2.78 | 119.04 | 126.72 |
| 22 | Z | 614 | CLA | O2A-CGA-CBA | 2.78 | 120.62 | 111.91 |
| 22 | 7 | 620 | CLA | CHD-C4C-NC | 2.78 | 128.58 | 124.20 |
| 22 | 3 | 610 | CLA | O2A-CGA-O1A | -2.78 | 116.58 | 123.59 |
| 22 | 4 | 611 | CLA | C4C-C3C-C2C | -2.78 | 102.85 | 106.90 |
| 30 | 3 | 621 | LUT | C15-C14-C13 | -2.78 | 123.35 | 127.31 |
| 22 | 5 | 602 | CLA | CAA-C2A-C3A | -2.78 | 105.18 | 112.78 |
| 22 | 6 | 610 | CLA | CHD-C4C-NC | 2.77 | 128.58 | 124.20 |
| 22 | 5 | 614 | CLA | C4C-C3C-C2C | -2.77 | 102.85 | 106.90 |
| 22 | 5 | 611 | CLA | CHD-C4C-NC | 2.77 | 128.57 | 124.20 |
| 22 | L | 203 | CLA | CAC-C3C-C4C | 2.77 | 128.41 | 124.81 |
| 22 | Z | 602 | CLA | C3B-C4B-NB | 2.77 | 112.80 | 109.21 |
| 22 | 7 | 602 | CLA | CHB-C4A-NA | 2.77 | 128.35 | 124.51 |
| 22 | A | 813 | CLA | CMB-C2B-C3B | 2.77 | 129.87 | 124.68 |
| 22 | B | 807 | CLA | CHB-C4A-NA | 2.77 | 128.35 | 124.51 |
| 25 | A | 849 | BCR | C32-C1-C6 | 2.77 | 114.80 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 9 | 612 | CLA | O2A-CGA-CBA | 2.77 | 120.61 | 111.91 |
| 22 | 1 | 610 | CLA | C1-C2-C3 | -2.77 | 121.25 | 126.04 |
| 22 | 4 | 610 | CLA | C1-C2-C3 | -2.77 | 121.25 | 126.04 |
| 22 | 4 | 609 | CLA | CHD-C4C-NC | 2.77 | 128.57 | 124.20 |
| 22 | 5 | 603 | CLA | CAA-C2A-C3A | -2.77 | 105.19 | 112.78 |
| 22 | B | 819 | CLA | C3B-C4B-NB | 2.77 | 112.79 | 109.21 |
| 22 | J | 3002 | CLA | CHD-C4C-NC | 2.77 | 128.57 | 124.20 |
| 29 | 6 | 608 | CHL | O2A-CGA-CBA | 2.77 | 120.60 | 111.91 |
| 22 | A | 815 | CLA | C4C-C3C-C2C | -2.77 | 102.86 | 106.90 |
| 24 | 4 | 623 | LHG | O8-C23-C24 | 2.77 | 120.60 | 111.91 |
| 30 | Z | 617 | LUT | C15-C14-C13 | -2.77 | 123.36 | 127.31 |
| 25 | K | 4001 | BCR | C35-C13-C12 | 2.77 | 122.44 | 118.08 |
| 22 | 9 | 601 | CLA | CHD-C4C-NC | 2.77 | 128.56 | 124.20 |
| 22 | 8 | 603 | CLA | C4C-C3C-C2C | -2.77 | 102.86 | 106.90 |
| 30 | 4 | 620 | LUT | C10-C11-C12 | -2.77 | 114.58 | 123.22 |
| 22 | 4 | 604 | CLA | CHD-C4C-NC | 2.77 | 128.56 | 124.20 |
| 22 | 1 | 606 | CLA | CAC-C3C-C4C | 2.77 | 128.40 | 124.81 |
| 22 | A | 808 | CLA | C4-C3-C5 | 2.77 | 119.92 | 115.27 |
| 30 | 8 | 618 | LUT | C38-C25-C24 | -2.77 | 117.64 | 123.56 |
| 22 | B | 802 | CLA | CMC-C2C-C1C | 2.77 | 129.25 | 125.04 |
| 27 | B | 850 | DGD | O1G-C1A-C2A | 2.77 | 120.58 | 111.91 |
| 22 | 4 | 609 | CLA | C3B-C4B-NB | 2.76 | 112.78 | 109.21 |
| 22 | B | 819 | CLA | C4C-C3C-C2C | -2.76 | 102.87 | 106.90 |
| 22 | 8 | 604 | CLA | C4C-C3C-C2C | -2.76 | 102.87 | 106.90 |
| 22 | 1 | 612 | CLA | CAC-C3C-C4C | 2.76 | 128.40 | 124.81 |
| 29 | 5 | 608 | CHL | C3B-C4B-NB | 2.76 | 112.78 | 109.21 |
| 22 | 3 | 610 | CLA | CMB-C2B-C3B | 2.76 | 129.85 | 124.68 |
| 22 | 7 | 611 | CLA | C4C-C3C-C2C | -2.76 | 102.87 | 106.90 |
| 22 | A | 828 | CLA | C1C-C2C-C3C | -2.76 | 104.05 | 106.96 |
| 22 | 6 | 612 | CLA | C4-C3-C5 | 2.76 | 119.92 | 115.27 |
| 22 | B | 818 | CLA | CHD-C4C-NC | 2.76 | 128.55 | 124.20 |
| 22 | B | 839 | CLA | CHD-C4C-NC | 2.76 | 128.55 | 124.20 |
| 22 | 2 | 610 | CLA | C1-C2-C3 | -2.76 | 121.27 | 126.04 |
| 30 | 6 | 624 | LUT | C16-C1-C6 | -2.76 | 105.82 | 110.30 |
| 25 | 7 | 623 | BCR | C15-C16-C17 | -2.76 | 117.82 | 123.47 |
| 22 | 2 | 606 | CLA | CHD-C4C-NC | 2.76 | 128.55 | 124.20 |
| 22 | Z | 606 | CLA | O2A-CGA-CBA | 2.76 | 120.57 | 111.91 |
| 30 | 1 | 618 | LUT | C3-C4-C5 | -2.76 | 106.36 | 111.85 |
| 22 | Z | 603 | CLA | C6-C5-C3 | -2.76 | 106.22 | 113.45 |
| 22 | B | 826 | CLA | C1-C2-C3 | -2.76 | 121.27 | 126.04 |
| 30 | 3 | 622 | LUT | C15-C35-C34 | -2.76 | 117.83 | 123.47 |
| 22 | A | 802 | CLA | CAC-C3C-C4C | 2.76 | 128.39 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 805 | CLA | C4C-C3C-C2C | -2.76 | 102.88 | 106.90 |
| 22 | A | 837 | CLA | C4C-C3C-C2C | -2.76 | 102.88 | 106.90 |
| 22 | A | 824 | CLA | CAC-C3C-C4C | 2.76 | 128.39 | 124.81 |
| 23 | A | 844 | PQN | C11-C12-C13 | -2.76 | 122.20 | 126.79 |
| 25 | 3 | 718 | BCR | C11-C12-C13 | -2.76 | 118.67 | 126.42 |
| 22 | 5 | 602 | CLA | C4C-C3C-C2C | -2.76 | 102.88 | 106.90 |
| 22 | B | 805 | CLA | CAC-C3C-C4C | 2.76 | 128.39 | 124.81 |
| 22 | B | 834 | CLA | O2A-CGA-CBA | 2.76 | 120.56 | 111.91 |
| 22 | 5 | 611 | CLA | CHB-C4A-NA | 2.76 | 128.32 | 124.51 |
| 22 | B | 820 | CLA | CHD-C4C-NC | 2.75 | 128.54 | 124.20 |
| 22 | 8 | 606 | CLA | CAC-C3C-C4C | 2.75 | 128.38 | 124.81 |
| 22 | B | 815 | CLA | C4-C3-C5 | 2.75 | 119.90 | 115.27 |
| 22 | 6 | 610 | CLA | C4C-C3C-C2C | -2.75 | 102.88 | 106.90 |
| 22 | 7 | 602 | CLA | CHC-C1C-C2C | -2.75 | 119.11 | 126.72 |
| 22 | 7 | 608 | CLA | C3B-C4B-NB | 2.75 | 112.77 | 109.21 |
| 22 | A | 818 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 22 | B | 815 | CLA | CHB-C4A-NA | 2.75 | 128.32 | 124.51 |
| 22 | B | 820 | CLA | O2D-CGD-O1D | -2.75 | 118.46 | 123.84 |
| 25 | A | 849 | BCR | C24-C23-C22 | -2.75 | 122.08 | 126.23 |
| 22 | B | 806 | CLA | CHC-C1C-C2C | -2.75 | 119.11 | 126.72 |
| 22 | 1 | 612 | CLA | CHD-C4C-NC | 2.75 | 128.54 | 124.20 |
| 22 | 4 | 602 | CLA | CHD-C4C-NC | 2.75 | 128.53 | 124.20 |
| 22 | A | 829 | CLA | C1-C2-C3 | -2.75 | 121.29 | 126.04 |
| 22 | B | 816 | CLA | C3B-C4B-NB | 2.75 | 112.76 | 109.21 |
| 30 | 6 | 621 | LUT | C18-C5-C6 | -2.75 | 121.44 | 124.53 |
| 22 | A | 808 | CLA | CAA-C2A-C3A | -2.75 | 105.25 | 112.78 |
| 22 | B | 816 | CLA | O2A-CGA-CBA | 2.75 | 120.53 | 111.91 |
| 25 | B | 846 | BCR | C29-C30-C25 | 2.75 | 114.71 | 110.48 |
| 22 | 3 | 607 | CLA | CMB-C2B-C3B | 2.75 | 129.82 | 124.68 |
| 22 | A | 805 | CLA | O2A-CGA-CBA | 2.74 | 120.52 | 111.91 |
| 22 | Z | 603 | CLA | CBC-CAC-C3C | -2.74 | 104.86 | 112.43 |
| 22 | 4 | 614 | CLA | CMC-C2C-C1C | 2.74 | 129.22 | 125.04 |
| 22 | A | 825 | CLA | C4C-C3C-C2C | -2.74 | 102.90 | 106.90 |
| 22 | 7 | 608 | CLA | O2A-CGA-CBA | 2.74 | 120.52 | 111.91 |
| 25 | A | 848 | BCR | C20-C21-C22 | -2.74 | 123.40 | 127.31 |
| 22 | B | 814 | CLA | O2A-CGA-CBA | 2.74 | 120.51 | 111.91 |
| 22 | 4 | 612 | CLA | O2A-CGA-CBA | 2.74 | 120.51 | 111.91 |
| 22 | A | 816 | CLA | O2D-CGD-O1D | -2.74 | 118.48 | 123.84 |
| 30 | 2 | 616 | LUT | C18-C5-C4 | 2.74 | 119.43 | 114.36 |
| 22 | Z | 614 | CLA | C4C-C3C-C2C | -2.74 | 102.90 | 106.90 |
| 22 | A | 854 | CLA | O2A-CGA-CBA | 2.74 | 120.51 | 111.91 |
| 22 | B | 820 | CLA | O2A-CGA-CBA | 2.74 | 120.51 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 9 | 610 | CLA | CMC-C2C-C1C | 2.74 | 129.21 | 125.04 |
| 22 | 8 | 616 | CLA | CHD-C4C-NC | 2.74 | 128.52 | 124.20 |
| 22 | 5 | 601 | CLA | CHD-C4C-NC | 2.74 | 128.52 | 124.20 |
| 22 | 5 | 606 | CLA | O2A-CGA-CBA | 2.74 | 120.50 | 111.91 |
| 22 | A | 811 | CLA | CHC-C1C-C2C | -2.74 | 119.14 | 126.72 |
| 22 | 7 | 609 | CLA | CMB-C2B-C3B | 2.74 | 129.80 | 124.68 |
| 22 | A | 833 | CLA | CHD-C4C-NC | 2.74 | 128.52 | 124.20 |
| 22 | A | 806 | CLA | CHB-C4A-NA | 2.74 | 128.30 | 124.51 |
| 22 | Z | 604 | CLA | C4C-C3C-C2C | -2.74 | 102.91 | 106.90 |
| 22 | 8 | 610 | CLA | C4-C3-C5 | 2.74 | 119.88 | 115.27 |
| 25 | A | 850 | BCR | C16-C15-C14 | -2.74 | 117.87 | 123.47 |
| 22 | 3 | 607 | CLA | CHD-C4C-NC | 2.74 | 128.52 | 124.20 |
| 30 | 5 | 624 | LUT | C18-C5-C6 | -2.74 | 121.45 | 124.53 |
| 22 | 8 | 613 | CLA | CHD-C4C-NC | 2.74 | 128.51 | 124.20 |
| 22 | A | 825 | CLA | O2A-CGA-O1A | -2.74 | 116.69 | 123.59 |
| 22 | A | 828 | CLA | CAA-C2A-C3A | -2.74 | 105.29 | 112.78 |
| 22 | 2 | 613 | CLA | CHB-C4A-NA | 2.74 | 128.29 | 124.51 |
| 22 | 4 | 603 | CLA | C4C-C3C-C2C | -2.74 | 102.91 | 106.90 |
| 25 | F | 305 | BCR | C21-C20-C19 | -2.74 | 114.68 | 123.22 |
| 22 | A | 815 | CLA | C4-C3-C5 | 2.74 | 119.87 | 115.27 |
| 29 | 4 | 608 | CHL | C3D-C4D-ND | 2.74 | 114.66 | 110.24 |
| 22 | 4 | 614 | CLA | CHC-C1C-C2C | -2.74 | 119.16 | 126.72 |
| 22 | 3 | 607 | CLA | O2D-CGD-O1D | -2.73 | 118.49 | 123.84 |
| 22 | 1 | 602 | CLA | O2A-CGA-CBA | 2.73 | 120.49 | 111.91 |
| 25 | 6 | 623 | BCR | C16-C15-C14 | -2.73 | 117.87 | 123.47 |
| 22 | 3 | 614 | CLA | CHD-C4C-NC | 2.73 | 128.51 | 124.20 |
| 22 | A | 807 | CLA | CAC-C3C-C4C | 2.73 | 128.36 | 124.81 |
| 22 | B | 831 | CLA | C1C-C2C-C3C | -2.73 | 104.08 | 106.96 |
| 22 | A | 841 | CLA | C3B-C4B-NB | 2.73 | 112.74 | 109.21 |
| 22 | 3 | 611 | CLA | C4C-C3C-C2C | -2.73 | 102.92 | 106.90 |
| 22 | 8 | 601 | CLA | C4-C3-C5 | 2.73 | 119.87 | 115.27 |
| 25 | A | 852 | BCR | C29-C30-C25 | 2.73 | 114.69 | 110.48 |
| 22 | A | 816 | CLA | CHB-C4A-NA | 2.73 | 128.29 | 124.51 |
| 24 | 5 | 623 | LHG | O8-C23-C24 | 2.73 | 120.48 | 111.91 |
| 22 | B | 811 | CLA | CHD-C4C-NC | 2.73 | 128.51 | 124.20 |
| 30 | 6 | 621 | LUT | C30-C31-C32 | -2.73 | 114.69 | 123.22 |
| 22 | 5 | 606 | CLA | CAC-C3C-C4C | 2.73 | 128.35 | 124.81 |
| 29 | 6 | 606 | CHL | C2A-C3A-C4A | -2.73 | 97.46 | 101.87 |
| 22 | 5 | 602 | CLA | C3B-C4B-NB | 2.73 | 112.74 | 109.21 |
| 22 | B | 838 | CLA | O2D-CGD-O1D | -2.73 | 118.50 | 123.84 |
| 22 | A | 823 | CLA | CHD-C4C-NC | 2.73 | 128.50 | 124.20 |
| 22 | B | 820 | CLA | C4C-C3C-C2C | -2.73 | 102.92 | 106.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 804 | CLA | CHD-C4C-NC | 2.73 | 128.50 | 124.20 |
| 22 | Z | 613 | CLA | CHC-C1C-C2C | -2.73 | 119.17 | 126.72 |
| 30 | Z | 617 | LUT | C17-C1-C6 | 2.73 | 114.72 | 110.30 |
| 22 | B | 829 | CLA | CHD-C4C-NC | 2.73 | 128.50 | 124.20 |
| 30 | 6 | 621 | LUT | C20-C13-C12 | 2.73 | 122.38 | 118.08 |
| 25 | B | 845 | BCR | C2-C1-C6 | 2.73 | 114.68 | 110.48 |
| 30 | 7 | 622 | LUT | C35-C15-C14 | -2.73 | 117.89 | 123.47 |
| 22 | A | 828 | CLA | O2A-CGA-CBA | 2.73 | 120.47 | 111.91 |
| 22 | A | 817 | CLA | CMD-C2D-C3D | -2.73 | 121.34 | 127.61 |
| 22 | 1 | 610 | CLA | C1C-C2C-C3C | -2.73 | 104.09 | 106.96 |
| 22 | Z | 616 | CLA | O2D-CGD-O1D | -2.73 | 118.51 | 123.84 |
| 25 | 3 | 718 | BCR | C2-C1-C6 | 2.73 | 114.68 | 110.48 |
| 22 | B | 813 | CLA | CMB-C2B-C3B | 2.73 | 129.78 | 124.68 |
| 22 | A | 829 | CLA | C4-C3-C5 | 2.72 | 119.86 | 115.27 |
| 22 | 1 | 614 | CLA | O2A-CGA-CBA | 2.72 | 120.46 | 111.91 |
| 25 | B | 843 | BCR | C11-C12-C13 | -2.72 | 118.76 | 126.42 |
| 22 | 5 | 614 | CLA | CMC-C2C-C1C | 2.72 | 129.19 | 125.04 |
| 22 | 5 | 614 | CLA | CHD-C4C-NC | 2.72 | 128.50 | 124.20 |
| 22 | 6 | 601 | CLA | CHD-C4C-NC | 2.72 | 128.50 | 124.20 |
| 22 | B | 804 | CLA | CMC-C2C-C1C | 2.72 | 129.19 | 125.04 |
| 22 | A | 820 | CLA | C2A-C3A-C4A | -2.72 | 97.47 | 101.87 |
| 22 | B | 840 | CLA | O2A-CGA-CBA | 2.72 | 120.45 | 111.91 |
| 22 | B | 830 | CLA | CHD-C4C-NC | 2.72 | 128.49 | 124.20 |
| 22 | 2 | 603 | CLA | CHD-C4C-NC | 2.72 | 128.49 | 124.20 |
| 30 | 4 | 619 | LUT | C39-C29-C28 | 2.72 | 122.37 | 118.08 |
| 30 | 1 | 618 | LUT | C35-C15-C14 | -2.72 | 117.90 | 123.47 |
| 30 | 6 | 624 | LUT | C10-C11-C12 | -2.72 | 114.72 | 123.22 |
| 22 | 4 | 609 | CLA | C4C-C3C-C2C | -2.72 | 102.93 | 106.90 |
| 22 | A | 819 | CLA | CHC-C1C-C2C | -2.72 | 119.19 | 126.72 |
| 22 | 5 | 601 | CLA | CAA-C2A-C3A | -2.72 | 105.33 | 112.78 |
| 22 | 6 | 610 | CLA | C1-C2-C3 | -2.72 | 121.34 | 126.04 |
| 22 | 2 | 603 | CLA | C4C-C3C-C2C | -2.72 | 102.93 | 106.90 |
| 25 | 5 | 622 | BCR | C2-C1-C6 | 2.72 | 114.67 | 110.48 |
| 22 | 4 | 609 | CLA | CMB-C2B-C3B | 2.72 | 129.77 | 124.68 |
| 22 | 1 | 609 | CLA | CHD-C4C-NC | 2.72 | 128.49 | 124.20 |
| 29 | 5 | 618 | CHL | CMB-C2B-C3B | 2.72 | 129.76 | 124.68 |
| 22 | A | 809 | CLA | CBA-CAA-C2A | 2.72 | 121.89 | 113.86 |
| 22 | 7 | 614 | CLA | CAA-C2A-C3A | -2.72 | 105.34 | 112.78 |
| 30 | Z | 618 | LUT | C35-C34-C33 | -2.72 | 123.43 | 127.31 |
| 22 | 2 | 606 | CLA | CMB-C2B-C3B | 2.72 | 129.76 | 124.68 |
| 22 | 8 | 609 | CLA | CHD-C4C-NC | 2.71 | 128.48 | 124.20 |
| 30 | 1 | 619 | LUT | C15-C35-C34 | -2.71 | 117.91 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 852 | CLA | O2A-CGA-CBA | 2.71 | 120.42 | 111.91 |
| 22 | 9 | 602 | CLA | CMC-C2C-C1C | 2.71 | 129.17 | 125.04 |
| 25 | 4 | 621 | BCR | C16-C17-C18 | -2.71 | 123.44 | 127.31 |
| 22 | K | 4003 | CLA | CAC-C3C-C4C | 2.71 | 128.33 | 124.81 |
| 22 | 2 | 607 | CLA | CHD-C4C-NC | 2.71 | 128.48 | 124.20 |
| 22 | 6 | 602 | CLA | CAC-C3C-C4C | 2.71 | 128.33 | 124.81 |
| 29 | 5 | 618 | CHL | O2D-CGD-O1D | -2.71 | 118.54 | 123.84 |
| 22 | A | 803 | CLA | CHC-C1C-C2C | -2.71 | 119.22 | 126.72 |
| 22 | A | 815 | CLA | CAC-C3C-C4C | 2.71 | 128.33 | 124.81 |
| 22 | A | 827 | CLA | C3B-C4B-NB | 2.71 | 112.71 | 109.21 |
| 22 | B | 822 | CLA | O2A-CGA-CBA | 2.71 | 120.41 | 111.91 |
| 22 | 1 | 616 | CLA | CHD-C4C-NC | 2.71 | 128.47 | 124.20 |
| 22 | L | 204 | CLA | C1-C2-C3 | -2.71 | 122.37 | 126.75 |
| 25 | A | 851 | BCR | C34-C9-C8 | 2.71 | 122.35 | 118.08 |
| 25 | A | 849 | BCR | C16-C15-C14 | -2.71 | 117.92 | 123.47 |
| 29 | 1 | 601 | CHL | CMB-C2B-C3B | 2.71 | 129.75 | 124.68 |
| 22 | A | 810 | CLA | C4-C3-C5 | 2.71 | 119.83 | 115.27 |
| 22 | K | 4002 | CLA | CHD-C4C-NC | 2.71 | 128.47 | 124.20 |
| 29 | Z | 607 | CHL | O2A-CGA-CBA | 2.71 | 120.41 | 111.91 |
| 22 | B | 834 | CLA | CMB-C2B-C3B | 2.71 | 129.74 | 124.68 |
| 22 | 4 | 609 | CLA | CAC-C3C-C4C | 2.71 | 128.32 | 124.81 |
| 22 | A | 845 | CLA | O2A-CGA-CBA | 2.71 | 120.40 | 111.91 |
| 22 | F | 301 | CLA | CHC-C1C-C2C | -2.71 | 119.24 | 126.72 |
| 22 | A | 822 | CLA | CHD-C4C-NC | 2.71 | 128.47 | 124.20 |
| 22 | 1 | 604 | CLA | CMA-C3A-C4A | -2.70 | 104.50 | 111.77 |
| 22 | A | 829 | CLA | CHB-C4A-NA | 2.70 | 128.25 | 124.51 |
| 22 | Z | 609 | CLA | O2A-CGA-CBA | 2.70 | 120.39 | 111.91 |
| 22 | Z | 610 | CLA | C4-C3-C5 | 2.70 | 119.82 | 115.27 |
| 22 | 4 | 602 | CLA | O2A-CGA-CBA | 2.70 | 120.39 | 111.91 |
| 22 | B | 805 | CLA | CHD-C4C-NC | 2.70 | 128.46 | 124.20 |
| 22 | 9 | 614 | CLA | CHD-C4C-NC | 2.70 | 128.46 | 124.20 |
| 22 | 9 | 609 | CLA | CHA-C1A-NA | -2.70 | 120.21 | 126.40 |
| 30 | 9 | 617 | LUT | C35-C34-C33 | -2.70 | 123.46 | 127.31 |
| 22 | A | 838 | CLA | O2D-CGD-O1D | -2.70 | 118.56 | 123.84 |
| 22 | 3 | 603 | CLA | CHD-C4C-NC | 2.70 | 128.46 | 124.20 |
| 22 | B | 814 | CLA | CAC-C3C-C4C | 2.70 | 128.31 | 124.81 |
| 22 | A | 854 | CLA | CHA-C1A-NA | -2.70 | 120.22 | 126.40 |
| 23 | B | 842 | PQN | C11-C12-C13 | -2.70 | 122.30 | 126.79 |
| 22 | 1 | 606 | CLA | C3B-C4B-NB | 2.70 | 112.70 | 109.21 |
| 22 | B | 838 | CLA | CHC-C1C-C2C | -2.70 | 119.26 | 126.72 |
| 22 | A | 806 | CLA | CMC-C2C-C1C | 2.70 | 129.15 | 125.04 |
| 25 | 5 | 625 | BCR | C21-C20-C19 | -2.70 | 114.80 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 5 | 606 | CLA | C4C-C3C-C2C | -2.70 | 102.97 | 106.90 |
| 22 | B | 819 | CLA | CHB-C4A-NA | 2.70 | 128.24 | 124.51 |
| 30 | 3 | 621 | LUT | C35-C15-C14 | -2.70 | 117.95 | 123.47 |
| 22 | B | 821 | CLA | CHD-C4C-NC | 2.70 | 128.45 | 124.20 |
| 22 | 3 | 602 | CLA | CHC-C1C-C2C | -2.70 | 119.27 | 126.72 |
| 22 | 5 | 614 | CLA | CHC-C1C-C2C | -2.69 | 119.27 | 126.72 |
| 22 | 7 | 608 | CLA | C1-C2-C3 | -2.69 | 122.39 | 126.75 |
| 25 | B | 844 | BCR | C29-C30-C25 | 2.69 | 114.63 | 110.48 |
| 22 | 7 | 601 | CLA | CMB-C2B-C3B | 2.69 | 129.72 | 124.68 |
| 22 | Z | 608 | CLA | C4-C3-C5 | 2.69 | 119.80 | 115.27 |
| 24 | A | 847 | LHG | C5-O7-C7 | -2.69 | 111.16 | 117.79 |
| 22 | B | 832 | CLA | C4C-C3C-C2C | -2.69 | 102.98 | 106.90 |
| 25 | A | 848 | BCR | C29-C30-C25 | 2.69 | 114.62 | 110.48 |
| 22 | 5 | 601 | CLA | CBC-CAC-C3C | -2.69 | 105.02 | 112.43 |
| 22 | 9 | 602 | CLA | O2A-CGA-CBA | 2.69 | 120.34 | 111.91 |
| 22 | B | 828 | CLA | O2A-CGA-CBA | 2.69 | 120.34 | 111.91 |
| 30 | 5 | 624 | LUT | C15-C35-C34 | -2.69 | 117.97 | 123.47 |
| 22 | A | 822 | CLA | CMB-C2B-C3B | 2.69 | 129.70 | 124.68 |
| 22 | 2 | 611 | CLA | CHD-C4C-NC | 2.69 | 128.44 | 124.20 |
| 22 | 6 | 617 | CLA | CHD-C4C-NC | 2.68 | 128.43 | 124.20 |
| 22 | Z | 610 | CLA | O2A-CGA-O1A | -2.68 | 116.82 | 123.59 |
| 22 | Z | 614 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 22 | 1 | 613 | CLA | C1-O2A-CGA | 2.68 | 123.48 | 116.44 |
| 29 | 6 | 618 | CHL | CMB-C2B-C3B | 2.68 | 129.70 | 124.68 |
| 22 | B | 808 | CLA | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 22 | A | 818 | CLA | O2A-CGA-CBA | 2.68 | 120.33 | 111.91 |
| 22 | Z | 613 | CLA | CAA-C2A-C3A | -2.68 | 105.43 | 112.78 |
| 22 | 1 | 602 | CLA | CHC-C1C-C2C | -2.68 | 119.30 | 126.72 |
| 22 | 5 | 611 | CLA | CAC-C3C-C4C | 2.68 | 128.29 | 124.81 |
| 29 | 5 | 608 | CHL | O2A-CGA-CBA | 2.68 | 120.32 | 111.91 |
| 22 | A | 808 | CLA | CHC-C1C-C2C | -2.68 | 119.31 | 126.72 |
| 22 | B | 819 | CLA | CHD-C4C-NC | 2.68 | 128.43 | 124.20 |
| 22 | 2 | 601 | CLA | CED-O2D-CGD | 2.68 | 122.00 | 115.94 |
| 22 | A | 835 | CLA | C4-C3-C5 | 2.68 | 119.78 | 115.27 |
| 22 | A | 803 | CLA | CHA-C1A-NA | -2.68 | 120.26 | 126.40 |
| 22 | A | 822 | CLA | C3B-C4B-NB | 2.68 | 112.67 | 109.21 |
| 21 | A | 801 | CL0 | CHB-C4A-NA | 2.68 | 128.22 | 124.51 |
| 22 | 7 | 620 | CLA | CMB-C2B-C3B | 2.68 | 129.69 | 124.68 |
| 25 | 8 | 619 | BCR | C23-C24-C25 | -2.68 | 119.68 | 127.20 |
| 22 | 6 | 602 | CLA | O2A-CGA-CBA | 2.68 | 120.31 | 111.91 |
| 22 | 9 | 611 | CLA | CMB-C2B-C3B | 2.68 | 129.69 | 124.68 |
| 22 | A | 803 | CLA | CHD-C4C-NC | 2.68 | 128.42 | 124.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29 | 7 | 607 | CHL | O2A-CGA-CBA | 2.68 | 120.31 | 111.91 |
| 22 | 6 | 612 | CLA | CMC-C2C-C1C | 2.68 | 129.12 | 125.04 |
| 22 | A | 843 | CLA | CBC-CAC-C3C | -2.68 | 105.05 | 112.43 |
| 22 | B | 812 | CLA | CBC-CAC-C3C | -2.68 | 105.05 | 112.43 |
| 22 | 8 | 614 | CLA | CMB-C2B-C3B | 2.68 | 129.69 | 124.68 |
| 22 | B | 815 | CLA | CAC-C3C-C4C | 2.68 | 128.28 | 124.81 |
| 22 | A | 827 | CLA | CMB-C2B-C3B | 2.68 | 129.68 | 124.68 |
| 22 | 7 | 612 | CLA | CHD-C4C-NC | 2.67 | 128.42 | 124.20 |
| 22 | 4 | 614 | CLA | CAC-C3C-C4C | 2.67 | 128.28 | 124.81 |
| 22 | 7 | 613 | CLA | C4A-NA-C1A | -2.67 | 105.50 | 106.71 |
| 22 | B | 827 | CLA | C1-C2-C3 | -2.67 | 121.42 | 126.04 |
| 29 | 1 | 601 | CHL | C4-C3-C2 | -2.67 | 116.82 | 123.68 |
| 25 | B | 846 | BCR | C28-C27-C26 | -2.67 | 109.31 | 114.08 |
| 22 | 9 | 609 | CLA | O2A-CGA-CBA | 2.67 | 120.29 | 111.91 |
| 24 | 1 | 620 | LHG | O8-C23-C24 | 2.67 | 120.29 | 111.91 |
| 22 | A | 821 | CLA | CHD-C4C-NC | 2.67 | 128.41 | 124.20 |
| 22 | 4 | 609 | CLA | O2A-CGA-CBA | 2.67 | 120.29 | 111.91 |
| 22 | 6 | 616 | CLA | CHD-C4C-NC | 2.67 | 128.41 | 124.20 |
| 22 | 8 | 614 | CLA | CMA-C3A-C4A | -2.67 | 104.59 | 111.77 |
| 30 | 2 | 616 | LUT | C3-C4-C5 | -2.67 | 106.53 | 111.85 |
| 22 | Z | 603 | CLA | C4C-C3C-C2C | -2.67 | 103.00 | 106.90 |
| 22 | A | 810 | CLA | O2A-CGA-O1A | -2.67 | 116.85 | 123.59 |
| 22 | B | 834 | CLA | C4C-C3C-C2C | -2.67 | 103.01 | 106.90 |
| 22 | 5 | 604 | CLA | O2A-CGA-CBA | 2.67 | 120.28 | 111.91 |
| 22 | 6 | 602 | CLA | C1-C2-C3 | -2.67 | 121.43 | 126.04 |
| 22 | 8 | 604 | CLA | CMA-C3A-C2A | -2.67 | 103.07 | 113.83 |
| 22 | B | 810 | CLA | CHD-C4C-NC | 2.67 | 128.41 | 124.20 |
| 22 | 7 | 608 | CLA | CHC-C1C-C2C | -2.67 | 119.35 | 126.72 |
| 22 | A | 819 | CLA | C1-O2A-CGA | 2.67 | 123.44 | 116.44 |
| 22 | 6 | 602 | CLA | CHC-C1C-C2C | -2.67 | 119.35 | 126.72 |
| 22 | F | 301 | CLA | CAC-C3C-C4C | 2.67 | 128.27 | 124.81 |
| 30 | 2 | 617 | LUT | C18-C5-C6 | -2.67 | 121.53 | 124.53 |
| 22 | 3 | 604 | CLA | C4C-C3C-C2C | -2.66 | 103.01 | 106.90 |
| 22 | Z | 611 | CLA | C1-C2-C3 | -2.66 | 121.44 | 126.04 |
| 22 | A | 803 | CLA | O2A-CGA-O1A | -2.66 | 116.87 | 123.59 |
| 22 | 3 | 604 | CLA | CHD-C4C-NC | 2.66 | 128.40 | 124.20 |
| 25 | 3 | 718 | BCR | C29-C30-C25 | 2.66 | 114.58 | 110.48 |
| 30 | 3 | 622 | LUT | C15-C14-C13 | -2.66 | 123.51 | 127.31 |
| 22 | 8 | 608 | CLA | CMB-C2B-C3B | 2.66 | 129.66 | 124.68 |
| 25 | 8 | 619 | BCR | C32-C1-C6 | 2.66 | 114.62 | 110.30 |
| 22 | 5 | 603 | CLA | CBC-CAC-C3C | -2.66 | 105.09 | 112.43 |
| 22 | A | 827 | CLA | C1-C2-C3 | -2.66 | 121.44 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25 | G | 205 | BCR | C10-C11-C12 | -2.66 | 114.91 | 123.22 |
| 22 | B | 825 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 22 | 8 | 614 | CLA | CAC-C3C-C4C | 2.66 | 128.26 | 124.81 |
| 29 | 4 | 607 | CHL | CHD-C4C-NC | 2.66 | 128.39 | 124.20 |
| 22 | 1 | 604 | CLA | CHB-C4A-NA | 2.66 | 128.19 | 124.51 |
| 22 | G | 203 | CLA | O2D-CGD-O1D | -2.66 | 118.64 | 123.84 |
| 30 | 3 | 622 | LUT | C30-C31-C32 | -2.66 | 114.92 | 123.22 |
| 22 | B | 831 | CLA | CMB-C2B-C3B | 2.66 | 129.65 | 124.68 |
| 22 | 7 | 610 | CLA | CMB-C2B-C3B | 2.66 | 129.65 | 124.68 |
| 22 | 3 | 620 | CLA | C4C-C3C-C2C | -2.66 | 103.02 | 106.90 |
| 22 | Z | 614 | CLA | CAA-C2A-C3A | -2.66 | 105.50 | 112.78 |
| 22 | 1 | 603 | CLA | C4C-C3C-C2C | -2.66 | 103.03 | 106.90 |
| 22 | 2 | 602 | CLA | CMB-C2B-C3B | 2.66 | 129.65 | 124.68 |
| 25 | A | 848 | BCR | C31-C1-C6 | -2.65 | 105.99 | 110.30 |
| 25 | 8 | 619 | BCR | C3-C4-C5 | -2.65 | 109.34 | 114.08 |
| 22 | 9 | 614 | CLA | C4C-C3C-C2C | -2.65 | 103.03 | 106.90 |
| 22 | B | 824 | CLA | O2A-CGA-O1A | -2.65 | 116.89 | 123.59 |
| 22 | 3 | 613 | CLA | O2A-CGA-CBA | 2.65 | 120.23 | 111.91 |
| 22 | A | 819 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 22 | B | 811 | CLA | CAA-C2A-C3A | -2.65 | 105.51 | 112.78 |
| 30 | 7 | 621 | LUT | C38-C25-C24 | -2.65 | 117.88 | 123.56 |
| 22 | 9 | 601 | CLA | CMB-C2B-C3B | 2.65 | 129.64 | 124.68 |
| 22 | 3 | 617 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 22 | 3 | 603 | CLA | O2A-CGA-CBA | 2.65 | 120.23 | 111.91 |
| 22 | B | 804 | CLA | CHC-C1C-C2C | -2.65 | 119.39 | 126.72 |
| 25 | 7 | 623 | BCR | C20-C21-C22 | -2.65 | 123.53 | 127.31 |
| 25 | A | 852 | BCR | C34-C9-C10 | -2.65 | 119.21 | 122.92 |
| 22 | A | 840 | CLA | CHB-C4A-NA | 2.65 | 128.18 | 124.51 |
| 22 | 2 | 609 | CLA | CMB-C2B-C3B | 2.65 | 129.64 | 124.68 |
| 25 | B | 847 | BCR | C20-C21-C22 | -2.65 | 123.53 | 127.31 |
| 22 | B | 809 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 22 | 3 | 609 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 22 | Z | 616 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 25 | 5 | 622 | BCR | C21-C20-C19 | -2.65 | 114.95 | 123.22 |
| 22 | 2 | 602 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 22 | B | 852 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 22 | B | 815 | CLA | CHD-C4C-NC | 2.65 | 128.38 | 124.20 |
| 22 | 4 | 610 | CLA | O2A-CGA-O1A | -2.65 | 116.91 | 123.59 |
| 22 | B | 833 | CLA | CHD-C4C-NC | 2.65 | 128.37 | 124.20 |
| 22 | 8 | 608 | CLA | CHC-C1C-C2C | -2.65 | 119.40 | 126.72 |
| 22 | 6 | 622 | CLA | O2D-CGD-O1D | -2.65 | 118.67 | 123.84 |
| 22 | 4 | 602 | CLA | C4C-C3C-C2C | -2.65 | 103.04 | 106.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 5 | 604 | CLA | CAA-C2A-C3A | -2.64 | 105.53 | 112.78 |
| 22 | 1 | 603 | CLA | CHD-C4C-NC | 2.64 | 128.37 | 124.20 |
| 22 | 2 | 609 | CLA | CBC-CAC-C3C | -2.64 | 105.14 | 112.43 |
| 22 | 2 | 609 | CLA | C4C-C3C-C2C | -2.64 | 103.04 | 106.90 |
| 22 | 9 | 601 | CLA | CAC-C3C-C4C | 2.64 | 128.24 | 124.81 |
| 22 | A | 830 | CLA | CHD-C4C-NC | 2.64 | 128.37 | 124.20 |
| 22 | 2 | 601 | CLA | CGD-CBD-CAD | -2.64 | 102.17 | 110.73 |
| 25 | 5 | 622 | BCR | C37-C22-C23 | 2.64 | 122.24 | 118.08 |
| 22 | B | 817 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 22 | B | 841 | CLA | C4C-C3C-C2C | -2.64 | 103.05 | 106.90 |
| 22 | B | 811 | CLA | CAB-C3B-C2B | 2.64 | 129.86 | 124.69 |
| 22 | B | 803 | CLA | O2D-CGD-O1D | -2.64 | 118.67 | 123.84 |
| 24 | A | 846 | LHG | O8-C23-C24 | 2.64 | 120.20 | 111.91 |
| 29 | 4 | 607 | CHL | C1-C2-C3 | -2.64 | 122.48 | 126.75 |
| 30 | 9 | 617 | LUT | C21-C26-C27 | -2.64 | 109.36 | 112.70 |
| 22 | 1 | 613 | CLA | CHD-C4C-NC | 2.64 | 128.37 | 124.20 |
| 22 | A | 804 | CLA | CMA-C3A-C4A | -2.64 | 104.68 | 111.77 |
| 22 | B | 811 | CLA | O2A-CGA-CBA | 2.64 | 120.19 | 111.91 |
| 22 | B | 802 | CLA | O2A-CGA-CBA | 2.64 | 120.19 | 111.91 |
| 22 | A | 839 | CLA | CHD-C4C-NC | 2.64 | 128.36 | 124.20 |
| 22 | A | 805 | CLA | C4-C3-C5 | 2.64 | 119.71 | 115.27 |
| 22 | Z | 609 | CLA | CHB-C4A-NA | 2.64 | 128.16 | 124.51 |
| 22 | A | 836 | CLA | O2A-CGA-CBA | 2.64 | 120.19 | 111.91 |
| 22 | B | 803 | CLA | CMB-C2B-C3B | 2.64 | 129.61 | 124.68 |
| 22 | B | 832 | CLA | O2D-CGD-O1D | -2.64 | 118.68 | 123.84 |
| 22 | A | 829 | CLA | C1-O2A-CGA | 2.64 | 123.36 | 116.44 |
| 22 | A | 832 | CLA | CMC-C2C-C1C | 2.64 | 129.06 | 125.04 |
| 22 | B | 825 | CLA | C4-C3-C5 | 2.64 | 119.71 | 115.27 |
| 22 | 5 | 604 | CLA | C4C-C3C-C2C | -2.64 | 103.05 | 106.90 |
| 29 | 1 | 607 | CHL | O2A-CGA-CBA | 2.64 | 120.18 | 111.91 |
| 22 | 1 | 604 | CLA | CHD-C4C-NC | 2.64 | 128.36 | 124.20 |
| 22 | 8 | 602 | CLA | CAA-C2A-C3A | -2.64 | 105.56 | 112.78 |
| 22 | A | 825 | CLA | C1-C2-C3 | -2.64 | 121.48 | 126.04 |
| 22 | A | 838 | CLA | CBA-CAA-C2A | -2.64 | 106.08 | 113.86 |
| 22 | 5 | 610 | CLA | O2D-CGD-O1D | -2.64 | 118.69 | 123.84 |
| 22 | 3 | 606 | CLA | CHD-C4C-NC | 2.63 | 128.35 | 124.20 |
| 22 | 8 | 606 | CLA | CHD-C4C-NC | 2.63 | 128.35 | 124.20 |
| 22 | 8 | 614 | CLA | CAA-C2A-C3A | -2.63 | 105.57 | 112.78 |
| 22 | B | 827 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 25 | K | 4004 | BCR | C2-C1-C6 | 2.63 | 114.53 | 110.48 |
| 22 | A | 816 | CLA | C3B-C4B-NB | 2.63 | 112.61 | 109.21 |
| 22 | B | 814 | CLA | C4C-C3C-C2C | -2.63 | 103.06 | 106.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 8 | 614 | CLA | CHD-C4C-NC | 2.63 | 128.35 | 124.20 |
| 22 | A | 805 | CLA | CMB-C2B-C3B | 2.63 | 129.60 | 124.68 |
| 25 | 3 | 717 | BCR | C7-C8-C9 | -2.63 | 122.26 | 126.23 |
| 25 | I | 172 | BCR | C10-C11-C12 | -2.63 | 115.01 | 123.22 |
| 25 | A | 856 | BCR | C31-C1-C6 | -2.63 | 106.03 | 110.30 |
| 22 | 8 | 604 | CLA | CHB-C4A-NA | 2.63 | 128.15 | 124.51 |
| 22 | 7 | 604 | CLA | C1-C2-C3 | -2.63 | 121.50 | 126.04 |
| 22 | Z | 609 | CLA | CMB-C2B-C3B | 2.63 | 129.60 | 124.68 |
| 25 | 3 | 717 | BCR | C32-C1-C6 | 2.63 | 114.56 | 110.30 |
| 22 | B | 819 | CLA | C4-C3-C5 | 2.63 | 119.69 | 115.27 |
| 29 | 8 | 607 | CHL | C2A-C1A-CHA | -2.63 | 119.26 | 123.86 |
| 22 | B | 807 | CLA | CAA-C2A-C3A | -2.63 | 105.58 | 112.78 |
| 30 | 1 | 619 | LUT | C8-C9-C10 | -2.63 | 114.91 | 118.94 |
| 22 | A | 821 | CLA | O2D-CGD-O1D | -2.63 | 118.70 | 123.84 |
| 22 | 7 | 610 | CLA | O2A-CGA-O1A | -2.63 | 116.97 | 123.59 |
| 22 | 6 | 622 | CLA | CHB-C4A-NA | 2.63 | 128.14 | 124.51 |
| 22 | B | 827 | CLA | O1D-CGD-CBD | -2.63 | 119.11 | 124.48 |
| 22 | B | 827 | CLA | CMB-C2B-C3B | 2.63 | 129.59 | 124.68 |
| 22 | 4 | 603 | CLA | CHD-C4C-NC | 2.62 | 128.34 | 124.20 |
| 22 | 5 | 610 | CLA | CMA-C3A-C2A | -2.62 | 103.24 | 113.83 |
| 30 | 5 | 620 | LUT | C31-C30-C29 | -2.62 | 123.57 | 127.31 |
| 30 | 3 | 622 | LUT | C38-C25-C24 | -2.62 | 117.95 | 123.56 |
| 22 | B | 811 | CLA | CAC-C3C-C4C | 2.62 | 128.21 | 124.81 |
| 22 | B | 802 | CLA | O2D-CGD-O1D | -2.62 | 118.71 | 123.84 |
| 30 | 7 | 621 | LUT | C35-C34-C33 | -2.62 | 123.57 | 127.31 |
| 22 | Z | 611 | CLA | CMB-C2B-C3B | 2.62 | 129.58 | 124.68 |
| 22 | G | 204 | CLA | CHD-C4C-NC | 2.62 | 128.33 | 124.20 |
| 30 | 5 | 620 | LUT | C7-C8-C9 | -2.62 | 122.28 | 126.23 |
| 29 | 4 | 608 | CHL | C1-C2-C3 | -2.62 | 122.52 | 126.75 |
| 22 | 8 | 602 | CLA | CHB-C4A-NA | 2.62 | 128.13 | 124.51 |
| 25 | 4 | 621 | BCR | C11-C12-C13 | -2.62 | 119.06 | 126.42 |
| 22 | 3 | 609 | CLA | O2A-CGA-CBA | 2.62 | 120.12 | 111.91 |
| 22 | 8 | 614 | CLA | CHB-C4A-NA | 2.62 | 128.13 | 124.51 |
| 22 | A | 838 | CLA | CMB-C2B-C3B | 2.62 | 129.57 | 124.68 |
| 22 | 6 | 604 | CLA | C4-C3-C5 | 2.62 | 119.67 | 115.27 |
| 22 | J | 3002 | CLA | O2D-CGD-O1D | -2.62 | 118.72 | 123.84 |
| 22 | 5 | 606 | CLA | C1-C2-C3 | -2.62 | 121.52 | 126.04 |
| 22 | 4 | 601 | CLA | O2A-CGA-CBA | 2.62 | 120.12 | 111.91 |
| 22 | B | 805 | CLA | C3B-C4B-NB | 2.62 | 112.59 | 109.21 |
| 22 | B | 805 | CLA | O1D-CGD-CBD | -2.62 | 119.13 | 124.48 |
| 30 | Z | 617 | LUT | C20-C13-C12 | 2.61 | 122.20 | 118.08 |
| 22 | 6 | 602 | CLA | CMB-C2B-C3B | 2.61 | 129.57 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 21 | A | 801 | CL0 | CMA-C3A-C2A | -2.61 | 103.28 | 113.83 |
| 22 | B | 836 | CLA | CHD-C4C-NC | 2.61 | 128.32 | 124.20 |
| 22 | B | 811 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 22 | 6 | 604 | CLA | O2A-CGA-CBA | 2.61 | 120.11 | 111.91 |
| 30 | 1 | 618 | LUT | C7-C8-C9 | -2.61 | 122.29 | 126.23 |
| 22 | B | 825 | CLA | CHC-C1C-C2C | -2.61 | 119.50 | 126.72 |
| 22 | 5 | 601 | CLA | CAC-C3C-C4C | 2.61 | 128.20 | 124.81 |
| 22 | 8 | 602 | CLA | O2A-CGA-CBA | 2.61 | 120.10 | 111.91 |
| 22 | Z | 613 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 22 | 5 | 603 | CLA | O2D-CGD-O1D | -2.61 | 118.73 | 123.84 |
| 22 | 7 | 604 | CLA | O2A-CGA-CBA | 2.61 | 120.10 | 111.91 |
| 22 | 8 | 610 | CLA | CAC-C3C-C4C | 2.61 | 128.20 | 124.81 |
| 22 | A | 829 | CLA | CAA-C2A-C3A | -2.61 | 105.63 | 112.78 |
| 30 | 1 | 617 | LUT | C20-C13-C12 | 2.61 | 122.19 | 118.08 |
| 22 | 3 | 620 | CLA | O2A-CGA-CBA | 2.61 | 120.10 | 111.91 |
| 22 | 2 | 613 | CLA | C1-C2-C3 | -2.61 | 122.53 | 126.75 |
| 22 | 6 | 603 | CLA | CHD-C4C-NC | 2.61 | 128.31 | 124.20 |
| 30 | Z | 617 | LUT | C21-C26-C27 | -2.61 | 109.40 | 112.70 |
| 22 | 3 | 620 | CLA | CAA-C2A-C3A | -2.61 | 105.63 | 112.78 |
| 22 | A | 816 | CLA | CHD-C4C-NC | 2.61 | 128.31 | 124.20 |
| 22 | Z | 603 | CLA | CHD-C4C-NC | 2.61 | 128.31 | 124.20 |
| 22 | A | 813 | CLA | CHD-C4C-NC | 2.61 | 128.31 | 124.20 |
| 25 | 6 | 625 | BCR | C37-C22-C23 | 2.61 | 122.18 | 118.08 |
| 25 | L | 201 | BCR | C33-C5-C6 | -2.61 | 121.60 | 124.53 |
| 22 | 1 | 610 | CLA | C4-C3-C5 | 2.61 | 119.66 | 115.27 |
| 22 | A | 810 | CLA | CHD-C4C-NC | 2.61 | 128.31 | 124.20 |
| 22 | Z | 610 | CLA | O1D-CGD-CBD | -2.61 | 119.15 | 124.48 |
| 22 | 9 | 604 | CLA | CHB-C4A-NA | 2.61 | 128.12 | 124.51 |
| 30 | 3 | 621 | LUT | C10-C11-C12 | -2.61 | 115.09 | 123.22 |
| 22 | 1 | 614 | CLA | CMB-C2B-C3B | 2.61 | 129.55 | 124.68 |
| 25 | K | 4001 | BCR | C29-C30-C25 | 2.60 | 114.49 | 110.48 |
| 28 | J | 3001 | LMG | O6-C1-O1 | -2.60 | 103.81 | 109.97 |
| 30 | 1 | 618 | LUT | C15-C14-C13 | -2.60 | 123.59 | 127.31 |
| 22 | 8 | 603 | CLA | CAA-C2A-C3A | -2.60 | 105.65 | 112.78 |
| 30 | Z | 617 | LUT | C39-C29-C28 | 2.60 | 122.18 | 118.08 |
| 22 | 2 | 610 | CLA | O2D-CGD-O1D | -2.60 | 118.75 | 123.84 |
| 22 | 4 | 616 | CLA | CHD-C4C-NC | 2.60 | 128.31 | 124.20 |
| 22 | 8 | 610 | CLA | CMB-C2B-C3B | 2.60 | 129.55 | 124.68 |
| 22 | 9 | 612 | CLA | CHD-C4C-NC | 2.60 | 128.30 | 124.20 |
| 22 | 7 | 609 | CLA | O2A-CGA-CBA | 2.60 | 120.07 | 111.91 |
| 29 | 5 | 607 | CHL | O2A-CGA-CBA | 2.60 | 120.07 | 111.91 |
| 22 | 5 | 612 | CLA | O2A-CGA-CBA | 2.60 | 120.07 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 821 | CLA | CAA-C2A-C3A | -2.60 | 105.66 | 112.78 |
| 30 | 9 | 617 | LUT | C15-C14-C13 | -2.60 | 123.60 | 127.31 |
| 22 | 4 | 604 | CLA | C4C-C3C-C2C | -2.60 | 103.11 | 106.90 |
| 25 | B | 848 | BCR | C21-C20-C19 | -2.60 | 115.11 | 123.22 |
| 22 | B | 803 | CLA | CHC-C1C-NC | 2.60 | 128.14 | 124.20 |
| 22 | A | 845 | CLA | CHD-C4C-NC | 2.60 | 128.30 | 124.20 |
| 25 | 5 | 625 | BCR | C23-C24-C25 | -2.60 | 119.91 | 127.20 |
| 22 | 3 | 602 | CLA | CHB-C4A-NA | 2.60 | 128.10 | 124.51 |
| 22 | A | 824 | CLA | O2A-CGA-CBA | 2.60 | 120.06 | 111.91 |
| 22 | 5 | 610 | CLA | CHB-C4A-NA | 2.60 | 128.10 | 124.51 |
| 22 | B | 818 | CLA | CMB-C2B-C3B | 2.60 | 129.53 | 124.68 |
| 22 | A | 829 | CLA | CMB-C2B-C3B | 2.60 | 129.53 | 124.68 |
| 22 | 6 | 604 | CLA | CMC-C2C-C1C | 2.59 | 128.99 | 125.04 |
| 22 | 6 | 616 | CLA | CBC-CAC-C3C | -2.59 | 105.28 | 112.43 |
| 22 | B | 831 | CLA | CHB-C4A-NA | 2.59 | 128.10 | 124.51 |
| 22 | B | 802 | CLA | CHC-C1C-C2C | -2.59 | 119.55 | 126.72 |
| 22 | 4 | 611 | CLA | CHB-C4A-NA | 2.59 | 128.10 | 124.51 |
| 22 | 1 | 609 | CLA | CMB-C2B-C3B | 2.59 | 129.53 | 124.68 |
| 22 | A | 804 | CLA | O2A-CGA-CBA | 2.59 | 120.04 | 111.91 |
| 30 | 5 | 620 | LUT | C11-C10-C9 | -2.59 | 123.61 | 127.31 |
| 22 | 1 | 602 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 22 | 7 | 616 | CLA | CHD-C4C-NC | 2.59 | 128.29 | 124.20 |
| 22 | 9 | 613 | CLA | CAA-C2A-C3A | -2.59 | 105.68 | 112.78 |
| 22 | A | 833 | CLA | O2D-CGD-O1D | -2.59 | 118.77 | 123.84 |
| 22 | 2 | 614 | CLA | CHD-C4C-NC | 2.59 | 128.28 | 124.20 |
| 25 | B | 847 | BCR | C32-C1-C6 | 2.59 | 114.50 | 110.30 |
| 22 | A | 827 | CLA | CHC-C1C-C2C | -2.59 | 119.56 | 126.72 |
| 22 | B | 813 | CLA | CHD-C4C-NC | 2.59 | 128.28 | 124.20 |
| 22 | A | 830 | CLA | O2A-CGA-CBA | 2.59 | 120.03 | 111.91 |
| 22 | 1 | 610 | CLA | CHB-C4A-NA | 2.59 | 128.09 | 124.51 |
| 22 | 6 | 602 | CLA | C3B-C4B-NB | 2.59 | 112.56 | 109.21 |
| 22 | 6 | 601 | CLA | C4C-C3C-C2C | -2.59 | 103.12 | 106.90 |
| 22 | 5 | 613 | CLA | O2A-CGA-CBA | 2.59 | 120.03 | 111.91 |
| 22 | 2 | 607 | CLA | CMB-C2B-C3B | 2.59 | 129.52 | 124.68 |
| 22 | B | 816 | CLA | CMB-C2B-C3B | 2.59 | 129.52 | 124.68 |
| 22 | 7 | 603 | CLA | CAC-C3C-C4C | 2.59 | 128.16 | 124.81 |
| 22 | 7 | 611 | CLA | CHD-C4C-NC | 2.59 | 128.28 | 124.20 |
| 22 | A | 819 | CLA | C3B-C4B-NB | 2.59 | 112.55 | 109.21 |
| 25 | J | 3003 | BCR | C11-C10-C9 | -2.58 | 123.62 | 127.31 |
| 22 | 9 | 611 | CLA | CAC-C3C-C4C | 2.58 | 128.16 | 124.81 |
| 22 | A | 819 | CLA | O2D-CGD-O1D | -2.58 | 118.79 | 123.84 |
| 22 | 8 | 611 | CLA | CBC-CAC-C3C | -2.58 | 105.31 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 7 | 601 | CLA | CAA-C2A-C3A | -2.58 | 105.70 | 112.78 |
| 22 | 6 | 617 | CLA | CMB-C2B-C3B | 2.58 | 129.51 | 124.68 |
| 25 | B | 846 | BCR | C20-C21-C22 | -2.58 | 123.62 | 127.31 |
| 22 | A | 806 | CLA | CHD-C4C-NC | 2.58 | 128.27 | 124.20 |
| 22 | 2 | 610 | CLA | O2A-CGA-CBA | 2.58 | 120.01 | 111.91 |
| 22 | B | 829 | CLA | CHC-C1C-C2C | -2.58 | 119.58 | 126.72 |
| 22 | 2 | 603 | CLA | CBC-CAC-C3C | -2.58 | 105.32 | 112.43 |
| 25 | 3 | 718 | BCR | C37-C22-C23 | 2.58 | 122.14 | 118.08 |
| 24 | A | 855 | LHG | O8-C23-C24 | 2.58 | 120.01 | 111.91 |
| 22 | A | 812 | CLA | CHB-C4A-NA | 2.58 | 128.08 | 124.51 |
| 22 | 2 | 610 | CLA | CAA-C2A-C3A | -2.58 | 105.71 | 112.78 |
| 22 | B | 852 | CLA | C4-C3-C5 | 2.58 | 119.61 | 115.27 |
| 22 | B | 839 | CLA | C1-C2-C3 | -2.58 | 121.58 | 126.04 |
| 22 | 3 | 603 | CLA | C1-C2-C3 | -2.58 | 121.58 | 126.04 |
| 22 | A | 805 | CLA | CAC-C3C-C4C | 2.58 | 128.16 | 124.81 |
| 29 | 9 | 606 | CHL | CHD-C4C-NC | 2.58 | 128.27 | 124.20 |
| 22 | B | 830 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 29 | 6 | 607 | CHL | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 22 | A | 821 | CLA | C4C-C3C-C2C | -2.58 | 103.14 | 106.90 |
| 22 | 3 | 614 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 30 | 8 | 617 | LUT | C38-C25-C24 | -2.58 | 118.04 | 123.56 |
| 25 | 6 | 623 | BCR | C21-C20-C19 | -2.58 | 115.17 | 123.22 |
| 22 | 9 | 604 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 22 | 6 | 614 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 22 | A | 819 | CLA | CHD-C4C-NC | 2.58 | 128.26 | 124.20 |
| 22 | 9 | 609 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 22 | A | 845 | CLA | C4-C3-C5 | 2.58 | 119.60 | 115.27 |
| 22 | 1 | 603 | CLA | C4-C3-C5 | 2.58 | 119.60 | 115.27 |
| 22 | 1 | 608 | CLA | C4-C3-C5 | 2.58 | 119.60 | 115.27 |
| 22 | 5 | 602 | CLA | CBC-CAC-C3C | -2.58 | 105.33 | 112.43 |
| 30 | 1 | 619 | LUT | C8-C7-C6 | -2.58 | 119.97 | 127.20 |
| 22 | 9 | 614 | CLA | CMB-C2B-C3B | 2.58 | 129.50 | 124.68 |
| 22 | 3 | 620 | CLA | CHD-C4C-NC | 2.58 | 128.26 | 124.20 |
| 22 | 6 | 613 | CLA | CHD-C4C-NC | 2.58 | 128.26 | 124.20 |
| 22 | B | 831 | CLA | O2D-CGD-O1D | -2.58 | 118.80 | 123.84 |
| 22 | 1 | 616 | CLA | CAA-C2A-C3A | -2.58 | 105.73 | 112.78 |
| 29 | 4 | 607 | CHL | C2A-C3A-C4A | -2.58 | 97.71 | 101.87 |
| 25 | B | 848 | BCR | C16-C15-C14 | -2.57 | 118.20 | 123.47 |
| 22 | B | 824 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 22 | B | 809 | CLA | CBC-CAC-C3C | -2.57 | 105.33 | 112.43 |
| 22 | 7 | 612 | CLA | O2D-CGD-O1D | -2.57 | 118.81 | 123.84 |
| 22 | A | 832 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 834 | CLA | O2A-CGA-CBA | 2.57 | 119.98 | 111.91 |
| 22 | 7 | 614 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 25 | 4 | 621 | BCR | C8-C7-C6 | -2.57 | 119.98 | 127.20 |
| 22 | B | 804 | CLA | CAC-C3C-C4C | 2.57 | 128.15 | 124.81 |
| 22 | 6 | 611 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 22 | 8 | 602 | CLA | CHC-C1C-C2C | -2.57 | 119.61 | 126.72 |
| 22 | Z | 604 | CLA | CHB-C4A-NA | 2.57 | 128.07 | 124.51 |
| 22 | 3 | 611 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 22 | 5 | 611 | CLA | CMB-C2B-C3B | 2.57 | 129.49 | 124.68 |
| 29 | 5 | 618 | CHL | CBC-CAC-C3C | -2.57 | 105.35 | 112.43 |
| 29 | 5 | 608 | CHL | CHD-C4C-NC | 2.57 | 128.25 | 124.20 |
| 22 | A | 809 | CLA | CHC-C1C-C2C | -2.57 | 119.61 | 126.72 |
| 29 | 4 | 606 | CHL | C2A-C3A-C4A | -2.57 | 97.72 | 101.87 |
| 22 | Z | 609 | CLA | C4C-C3C-C2C | -2.57 | 103.15 | 106.90 |
| 24 | 6 | 619 | LHG | O8-C23-C24 | 2.57 | 119.97 | 111.91 |
| 22 | A | 811 | CLA | CMB-C2B-C3B | 2.57 | 129.48 | 124.68 |
| 22 | 1 | 604 | CLA | O2A-CGA-CBA | 2.57 | 119.97 | 111.91 |
| 22 | B | 840 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 22 | 5 | 613 | CLA | C1-O2A-CGA | 2.57 | 123.18 | 116.44 |
| 22 | 2 | 602 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 22 | A | 824 | CLA | CHD-C4C-NC | 2.57 | 128.25 | 124.20 |
| 30 | 6 | 621 | LUT | C1-C2-C3 | 2.57 | 119.44 | 113.64 |
| 22 | 7 | 612 | CLA | C4-C3-C5 | 2.57 | 119.59 | 115.27 |
| 28 | 9 | 620 | LMG | O6-C1-O1 | -2.57 | 103.90 | 109.97 |
| 22 | 9 | 613 | CLA | C1-O2A-CGA | 2.57 | 123.17 | 116.44 |
| 22 | A | 808 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 22 | 7 | 604 | CLA | CHB-C4A-NA | 2.57 | 128.06 | 124.51 |
| 22 | 5 | 617 | CLA | CMB-C2B-C3B | 2.56 | 129.48 | 124.68 |
| 22 | B | 841 | CLA | CMB-C2B-C3B | 2.56 | 129.47 | 124.68 |
| 22 | 4 | 602 | CLA | CMB-C2B-C3B | 2.56 | 129.47 | 124.68 |
| 25 | 5 | 622 | BCR | C29-C30-C25 | 2.56 | 114.43 | 110.48 |
| 22 | 5 | 616 | CLA | CHB-C4A-NA | 2.56 | 128.06 | 124.51 |
| 22 | A | 832 | CLA | O2A-CGA-CBA | 2.56 | 119.95 | 111.91 |
| 22 | 4 | 610 | CLA | CHD-C4C-NC | 2.56 | 128.24 | 124.20 |
| 22 | 2 | 612 | CLA | CHD-C4C-NC | 2.56 | 128.24 | 124.20 |
| 29 | 6 | 618 | CHL | C2A-C1A-CHA | -2.56 | 119.38 | 123.86 |
| 22 | A | 803 | CLA | O2D-CGD-O1D | -2.56 | 118.83 | 123.84 |
| 22 | B | 823 | CLA | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 22 | G | 204 | CLA | CAA-C2A-C3A | -2.56 | 105.76 | 112.78 |
| 22 | Z | 612 | CLA | C1-C2-C3 | -2.56 | 121.61 | 126.04 |
| 22 | Z | 604 | CLA | O2A-CGA-CBA | 2.56 | 119.94 | 111.91 |
| 25 | F | 305 | BCR | C11-C12-C13 | -2.56 | 119.22 | 126.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 833 | CLA | CAA-C2A-C1A | -2.56 | 103.59 | 111.97 |
| 22 | B | 836 | CLA | CAA-C2A-C3A | -2.56 | 105.77 | 112.78 |
| 22 | 4 | 609 | CLA | O2D-CGD-O1D | -2.56 | 118.83 | 123.84 |
| 22 | 9 | 613 | CLA | CHB-C4A-NA | 2.56 | 128.05 | 124.51 |
| 30 | 4 | 619 | LUT | C10-C11-C12 | -2.56 | 115.23 | 123.22 |
| 25 | 5 | 625 | BCR | C20-C19-C18 | -2.56 | 119.23 | 126.42 |
| 22 | L | 204 | CLA | O2A-CGA-CBA | 2.56 | 119.93 | 111.91 |
| 22 | B | 829 | CLA | CMD-C2D-C3D | -2.56 | 121.73 | 127.61 |
| 22 | A | 842 | CLA | CAC-C3C-C4C | 2.56 | 128.13 | 124.81 |
| 22 | A | 827 | CLA | O2A-CGA-CBA | 2.56 | 119.93 | 111.91 |
| 22 | A | 807 | CLA | O2D-CGD-O1D | -2.56 | 118.84 | 123.84 |
| 25 | 3 | 718 | BCR | C11-C10-C9 | -2.56 | 123.66 | 127.31 |
| 22 | 6 | 612 | CLA | O2A-CGA-CBA | 2.56 | 119.93 | 111.91 |
| 22 | B | 806 | CLA | CMB-C2B-C3B | 2.56 | 129.46 | 124.68 |
| 22 | 1 | 604 | CLA | C4C-C3C-C2C | -2.56 | 103.17 | 106.90 |
| 22 | 2 | 613 | CLA | CMB-C2B-C3B | 2.55 | 129.46 | 124.68 |
| 29 | 6 | 618 | CHL | O2D-CGD-O1D | -2.55 | 118.85 | 123.84 |
| 22 | B | 823 | CLA | CAA-C2A-C3A | -2.55 | 105.79 | 112.78 |
| 22 | A | 836 | CLA | CBC-CAC-C3C | -2.55 | 105.39 | 112.43 |
| 22 | B | 840 | CLA | C1-C2-C3 | -2.55 | 121.63 | 126.04 |
| 22 | 1 | 603 | CLA | O2A-CGA-CBA | 2.55 | 119.91 | 111.91 |
| 22 | Z | 613 | CLA | CMB-C2B-C3B | 2.55 | 129.45 | 124.68 |
| 22 | 9 | 609 | CLA | CAC-C3C-C4C | 2.55 | 128.12 | 124.81 |
| 22 | B | 830 | CLA | O2A-CGA-CBA | 2.55 | 119.91 | 111.91 |
| 30 | 5 | 620 | LUT | C35-C15-C14 | -2.55 | 118.25 | 123.47 |
| 22 | 8 | 614 | CLA | C4-C3-C5 | 2.55 | 119.56 | 115.27 |
| 29 | Z | 601 | CHL | C4-C3-C5 | 2.55 | 119.56 | 115.27 |
| 22 | 5 | 621 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 22 | Z | 611 | CLA | O2A-CGA-CBA | 2.55 | 119.90 | 111.91 |
| 25 | A | 851 | BCR | C23-C24-C25 | -2.55 | 120.05 | 127.20 |
| 22 | A | 854 | CLA | CMC-C2C-C1C | 2.55 | 128.92 | 125.04 |
| 22 | 6 | 613 | CLA | C1-C2-C3 | -2.55 | 121.64 | 126.04 |
| 22 | A | 820 | CLA | CAC-C3C-C4C | 2.55 | 128.11 | 124.81 |
| 30 | Z | 619 | LUT | C10-C11-C12 | -2.55 | 115.27 | 123.22 |
| 22 | 5 | 609 | CLA | O2D-CGD-O1D | -2.55 | 118.86 | 123.84 |
| 22 | A | 823 | CLA | O2D-CGD-O1D | -2.54 | 118.86 | 123.84 |
| 22 | 3 | 611 | CLA | CMA-C3A-C2A | -2.54 | 110.16 | 116.10 |
| 22 | 6 | 611 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 22 | Z | 610 | CLA | C3B-C4B-NB | 2.54 | 112.50 | 109.21 |
| 22 | A | 812 | CLA | CHD-C4C-NC | 2.54 | 128.21 | 124.20 |
| 29 | 4 | 606 | CHL | CBC-CAC-C3C | -2.54 | 105.43 | 112.43 |
| 30 | 7 | 622 | LUT | C30-C31-C32 | -2.54 | 115.29 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | B | 846 | BCR | C2-C1-C6 | 2.54 | 114.39 | 110.48 |
| 22 | 7 | 613 | CLA | CHB-C4A-NA | 2.54 | 128.03 | 124.51 |
| 30 | 1 | 619 | LUT | C38-C25-C24 | -2.54 | 118.12 | 123.56 |
| 22 | 8 | 611 | CLA | CMB-C2B-C3B | 2.54 | 129.43 | 124.68 |
| 22 | 7 | 602 | CLA | C4-C3-C5 | 2.54 | 119.54 | 115.27 |
| 22 | K | 4003 | CLA | CHD-C4C-NC | 2.54 | 128.21 | 124.20 |
| 22 | A | 804 | CLA | C2A-C1A-CHA | -2.54 | 119.42 | 123.86 |
| 30 | Z | 618 | LUT | C30-C31-C32 | -2.54 | 115.29 | 123.22 |
| 22 | A | 837 | CLA | CHD-C4C-NC | 2.54 | 128.20 | 124.20 |
| 22 | 8 | 608 | CLA | CAC-C3C-C4C | 2.54 | 128.10 | 124.81 |
| 22 | 4 | 602 | CLA | CBC-CAC-C3C | -2.54 | 105.43 | 112.43 |
| 22 | B | 852 | CLA | CMB-C2B-C3B | 2.54 | 129.43 | 124.68 |
| 22 | B | 838 | CLA | CAA-C2A-C3A | -2.54 | 105.83 | 112.78 |
| 22 | G | 203 | CLA | CHD-C4C-NC | 2.54 | 128.20 | 124.20 |
| 22 | 4 | 614 | CLA | CAA-C2A-C3A | -2.54 | 105.83 | 112.78 |
| 22 | 8 | 613 | CLA | C1-O2A-CGA | 2.54 | 123.10 | 116.44 |
| 22 | A | 841 | CLA | CHD-C4C-NC | 2.54 | 128.20 | 124.20 |
| 25 | F | 305 | BCR | C35-C13-C14 | -2.54 | 119.37 | 122.92 |
| 22 | 6 | 609 | CLA | CAC-C3C-C4C | 2.54 | 128.10 | 124.81 |
| 22 | B | 807 | CLA | C1-C2-C3 | -2.54 | 121.66 | 126.04 |
| 22 | 8 | 614 | CLA | O2D-CGD-O1D | -2.54 | 118.88 | 123.84 |
| 22 | B | 822 | CLA | CMC-C2C-C1C | 2.54 | 128.90 | 125.04 |
| 22 | 6 | 601 | CLA | O2A-CGA-CBA | 2.53 | 119.86 | 111.91 |
| 22 | Z | 602 | CLA | CAA-C2A-C3A | -2.53 | 105.84 | 112.78 |
| 25 | L | 201 | BCR | C20-C21-C22 | -2.53 | 123.69 | 127.31 |
| 22 | 8 | 602 | CLA | C4-C3-C5 | 2.53 | 119.53 | 115.27 |
| 22 | 1 | 602 | CLA | CAC-C3C-C4C | 2.53 | 128.10 | 124.81 |
| 22 | 2 | 611 | CLA | CHB-C4A-NA | 2.53 | 128.02 | 124.51 |
| 25 | F | 305 | BCR | C24-C23-C22 | -2.53 | 122.41 | 126.23 |
| 22 | B | 809 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 22 | 7 | 609 | CLA | CMA-C3A-C2A | -2.53 | 103.61 | 113.83 |
| 22 | B | 829 | CLA | CMC-C2C-C1C | 2.53 | 128.90 | 125.04 |
| 22 | 5 | 604 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 22 | 5 | 614 | CLA | CMB-C2B-C3B | 2.53 | 129.42 | 124.68 |
| 22 | 9 | 614 | CLA | O2D-CGD-O1D | -2.53 | 118.89 | 123.84 |
| 22 | 6 | 616 | CLA | CHC-C1C-NC | 2.53 | 128.04 | 124.20 |
| 22 | B | 812 | CLA | CAA-C2A-C3A | -2.53 | 105.85 | 112.78 |
| 22 | Z | 616 | CLA | CMB-C2B-C3B | 2.53 | 129.41 | 124.68 |
| 22 | 9 | 611 | CLA | O2A-CGA-CBA | 2.53 | 119.85 | 111.91 |
| 22 | 5 | 616 | CLA | CHD-C4C-NC | 2.53 | 128.19 | 124.20 |
| 22 | 6 | 611 | CLA | CHD-C4C-NC | 2.53 | 128.19 | 124.20 |
| 22 | 5 | 603 | CLA | CAC-C3C-C4C | 2.53 | 128.09 | 124.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 1 | 602 | CLA | C3B-C4B-NB | 2.53 | 112.48 | 109.21 |
| 22 | B | 827 | CLA | CHD-C4C-NC | 2.53 | 128.19 | 124.20 |
| 22 | 1 | 611 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 22 | B | 806 | CLA | O2A-CGA-CBA | 2.53 | 119.85 | 111.91 |
| 30 | Z | 619 | LUT | C15-C35-C34 | -2.53 | 118.29 | 123.47 |
| 22 | 9 | 611 | CLA | CHB-C4A-NA | 2.53 | 128.01 | 124.51 |
| 22 | B | 830 | CLA | O1D-CGD-CBD | -2.53 | 119.31 | 124.48 |
| 22 | B | 803 | CLA | C4-C3-C5 | 2.53 | 119.52 | 115.27 |
| 30 | 1 | 617 | LUT | C39-C29-C28 | 2.53 | 122.06 | 118.08 |
| 25 | 7 | 623 | BCR | C11-C10-C9 | -2.53 | 123.70 | 127.31 |
| 22 | 7 | 613 | CLA | CHD-C4C-NC | 2.53 | 128.19 | 124.20 |
| 22 | 4 | 601 | CLA | CBC-CAC-C3C | -2.53 | 105.47 | 112.43 |
| 30 | 9 | 616 | LUT | C35-C15-C14 | -2.53 | 118.30 | 123.47 |
| 22 | A | 809 | CLA | CMB-C2B-C3B | 2.53 | 129.41 | 124.68 |
| 22 | 5 | 611 | CLA | O2A-CGA-CBA | 2.53 | 119.84 | 111.91 |
| 22 | 6 | 614 | CLA | CHB-C4A-NA | 2.53 | 128.00 | 124.51 |
| 22 | A | 812 | CLA | O2A-CGA-CBA | 2.53 | 119.83 | 111.91 |
| 22 | 1 | 614 | CLA | CAC-C3C-C4C | 2.52 | 128.09 | 124.81 |
| 22 | 1 | 614 | CLA | O2D-CGD-O1D | -2.52 | 118.90 | 123.84 |
| 22 | 4 | 614 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 22 | A | 814 | CLA | CMB-C2B-C3B | 2.52 | 129.40 | 124.68 |
| 22 | 1 | 608 | CLA | CAA-CBA-CGA | -2.52 | 105.88 | 113.25 |
| 22 | 1 | 614 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 22 | 3 | 617 | CLA | CMB-C2B-C3B | 2.52 | 129.39 | 124.68 |
| 22 | 5 | 617 | CLA | O2D-CGD-O1D | -2.52 | 118.91 | 123.84 |
| 22 | A | 822 | CLA | CHB-C4A-NA | 2.52 | 128.00 | 124.51 |
| 22 | 3 | 611 | CLA | CHD-C4C-NC | 2.52 | 128.17 | 124.20 |
| 22 | 6 | 610 | CLA | CMC-C2C-C1C | 2.52 | 128.88 | 125.04 |
| 29 | 4 | 607 | CHL | CAC-C3C-C4C | 2.52 | 128.08 | 124.81 |
| 22 | L | 203 | CLA | CAA-C2A-C3A | -2.52 | 105.88 | 112.78 |
| 22 | 9 | 614 | CLA | CMC-C2C-C1C | 2.52 | 128.87 | 125.04 |
| 29 | 6 | 606 | CHL | O2D-CGD-O1D | -2.52 | 118.92 | 123.84 |
| 22 | 3 | 607 | CLA | C1-O2A-CGA | 2.52 | 123.05 | 116.44 |
| 22 | A | 842 | CLA | CHB-C4A-NA | 2.52 | 127.99 | 124.51 |
| 22 | Z | 604 | CLA | CHD-C4C-NC | 2.52 | 128.17 | 124.20 |
| 22 | 5 | 616 | CLA | CMB-C2B-C3B | 2.52 | 129.39 | 124.68 |
| 30 | 9 | 616 | LUT | C3-C4-C5 | -2.52 | 106.84 | 111.85 |
| 25 | 3 | 719 | BCR | C10-C11-C12 | -2.52 | 115.36 | 123.22 |
| 22 | 9 | 610 | CLA | CMB-C2B-C3B | 2.52 | 129.39 | 124.68 |
| 22 | 5 | 613 | CLA | CAA-C2A-C3A | -2.52 | 105.89 | 112.78 |
| 22 | A | 835 | CLA | CMB-C2B-C3B | 2.52 | 129.38 | 124.68 |
| 22 | A | 841 | CLA | CMB-C2B-C3B | 2.52 | 129.38 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | Z | 608 | CLA | CMB-C2B-C3B | 2.52 | 129.38 | 124.68 |
| 22 | 7 | 616 | CLA | C4C-C3C-C2C | -2.51 | 103.23 | 106.90 |
| 22 | 5 | 612 | CLA | CHD-C4C-NC | 2.51 | 128.17 | 124.20 |
| 30 | 2 | 617 | LUT | C31-C30-C29 | -2.51 | 123.72 | 127.31 |
| 22 | 2 | 609 | CLA | CHD-C4C-NC | 2.51 | 128.16 | 124.20 |
| 22 | B | 835 | CLA | CAC-C3C-C4C | 2.51 | 128.07 | 124.81 |
| 22 | Z | 614 | CLA | CAC-C3C-C4C | 2.51 | 128.07 | 124.81 |
| 22 | 4 | 601 | CLA | CAA-C2A-C3A | -2.51 | 105.90 | 112.78 |
| 22 | 7 | 616 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 22 | 3 | 611 | CLA | CMC-C2C-C1C | 2.51 | 128.86 | 125.04 |
| 22 | 1 | 613 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 25 | I | 172 | BCR | C28-C27-C26 | -2.51 | 109.59 | 114.08 |
| 25 | B | 847 | BCR | C34-C9-C8 | 2.51 | 122.03 | 118.08 |
| 22 | B | 804 | CLA | O1D-CGD-CBD | -2.51 | 119.35 | 124.48 |
| 22 | A | 834 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 22 | B | 811 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 22 | J | 3002 | CLA | CMB-C2B-C3B | 2.51 | 129.37 | 124.68 |
| 28 | J | 3001 | LMG | C1-C2-C3 | -2.51 | 104.77 | 110.00 |
| 30 | Z | 619 | LUT | C38-C25-C24 | -2.51 | 118.19 | 123.56 |
| 22 | B | 840 | CLA | CHD-C4C-NC | 2.51 | 128.16 | 124.20 |
| 22 | A | 832 | CLA | CMB-C2B-C3B | 2.51 | 129.37 | 124.68 |
| 30 | 3 | 621 | LUT | C18-C5-C6 | -2.51 | 121.71 | 124.53 |
| 22 | B | 815 | CLA | CMB-C2B-C3B | 2.51 | 129.37 | 124.68 |
| 22 | 9 | 601 | CLA | O2D-CGD-O1D | -2.51 | 118.93 | 123.84 |
| 22 | B | 813 | CLA | C4-C3-C5 | 2.51 | 119.49 | 115.27 |
| 22 | 9 | 611 | CLA | CBC-CAC-C3C | -2.51 | 105.52 | 112.43 |
| 22 | B | 817 | CLA | CHB-C4A-NA | 2.51 | 127.98 | 124.51 |
| 30 | Z | 618 | LUT | C3-C4-C5 | -2.51 | 106.86 | 111.85 |
| 22 | B | 826 | CLA | C4-C3-C5 | 2.51 | 119.49 | 115.27 |
| 22 | B | 831 | CLA | CAC-C3C-C4C | 2.51 | 128.06 | 124.81 |
| 22 | A | 843 | CLA | CMC-C2C-C1C | 2.51 | 128.86 | 125.04 |
| 29 | 7 | 607 | CHL | CMB-C2B-C3B | 2.51 | 129.37 | 124.68 |
| 22 | Z | 614 | CLA | CMB-C2B-C3B | 2.51 | 129.37 | 124.68 |
| 22 | 5 | 602 | CLA | CHC-C1C-C2C | -2.51 | 119.79 | 126.72 |
| 22 | A | 840 | CLA | C4-C3-C5 | 2.51 | 119.48 | 115.27 |
| 29 | 4 | 606 | CHL | CHD-C4C-NC | 2.50 | 128.15 | 124.20 |
| 22 | A | 802 | CLA | C4-C3-C5 | 2.50 | 119.48 | 115.27 |
| 22 | A | 854 | CLA | CMA-C3A-C4A | -2.50 | 105.04 | 111.77 |
| 22 | A | 813 | CLA | CMC-C2C-C1C | 2.50 | 128.85 | 125.04 |
| 22 | 7 | 610 | CLA | C1-C2-C3 | -2.50 | 121.71 | 126.04 |
| 22 | 9 | 602 | CLA | CHB-C4A-NA | 2.50 | 127.97 | 124.51 |
| 25 | A | 852 | BCR | C10-C11-C12 | -2.50 | 115.41 | 123.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 1 | 611 | CLA | CHD-C4C-NC | 2.50 | 128.15 | 124.20 |
| 22 | B | 802 | CLA | CAC-C3C-C4C | 2.50 | 128.06 | 124.81 |
| 22 | 2 | 601 | CLA | CBC-CAC-C3C | -2.50 | 105.53 | 112.43 |
| 22 | K | 4002 | CLA | CMB-C2B-C3B | 2.50 | 129.36 | 124.68 |
| 22 | 5 | 613 | CLA | C4A-NA-C1A | -2.50 | 105.58 | 106.71 |
| 22 | 1 | 609 | CLA | C4C-C3C-C2C | -2.50 | 103.25 | 106.90 |
| 22 | B | 824 | CLA | CAA-C2A-C3A | -2.50 | 105.93 | 112.78 |
| 22 | 4 | 616 | CLA | CMB-C2B-C3B | 2.50 | 129.36 | 124.68 |
| 22 | 8 | 601 | CLA | CMC-C2C-C1C | 2.50 | 128.85 | 125.04 |
| 22 | A | 817 | CLA | O2A-CGA-CBA | 2.50 | 119.76 | 111.91 |
| 22 | 5 | 604 | CLA | CHD-C4C-NC | 2.50 | 128.15 | 124.20 |
| 22 | 3 | 604 | CLA | CBC-CAC-C3C | -2.50 | 105.54 | 112.43 |
| 22 | 1 | 614 | CLA | CHD-C4C-NC | 2.50 | 128.14 | 124.20 |
| 22 | 9 | 613 | CLA | CHD-C4C-NC | 2.50 | 128.14 | 124.20 |
| 22 | 2 | 611 | CLA | O2A-CGA-CBA | 2.50 | 119.75 | 111.91 |
| 22 | B | 807 | CLA | CBC-CAC-C3C | -2.50 | 105.54 | 112.43 |
| 22 | 9 | 603 | CLA | CHD-C4C-NC | 2.50 | 128.14 | 124.20 |
| 22 | 9 | 612 | CLA | C4-C3-C5 | 2.50 | 119.47 | 115.27 |
| 22 | Z | 603 | CLA | O1D-CGD-CBD | -2.50 | 119.37 | 124.48 |
| 22 | B | 812 | CLA | CMC-C2C-C1C | 2.50 | 128.84 | 125.04 |
| 22 | A | 807 | CLA | C1-C2-C3 | -2.50 | 121.72 | 126.04 |
| 22 | 4 | 616 | CLA | CBC-CAC-C3C | -2.50 | 105.55 | 112.43 |
| 22 | B | 802 | CLA | CHB-C4A-NA | 2.50 | 127.97 | 124.51 |
| 25 | 6 | 625 | BCR | C29-C30-C25 | 2.50 | 114.33 | 110.48 |
| 30 | 1 | 619 | LUT | C18-C5-C6 | -2.50 | 121.72 | 124.53 |
| 22 | 9 | 614 | CLA | CAA-C2A-C3A | -2.50 | 105.94 | 112.78 |
| 22 | A | 830 | CLA | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 29 | 1 | 607 | CHL | CMB-C2B-C3B | 2.50 | 129.35 | 124.68 |
| 29 | 4 | 618 | CHL | O2D-CGD-O1D | -2.50 | 118.96 | 123.84 |
| 22 | A | 821 | CLA | CAC-C3C-C4C | 2.50 | 128.05 | 124.81 |
| 22 | 1 | 613 | CLA | CHB-C4A-NA | 2.50 | 127.96 | 124.51 |
| 22 | 7 | 620 | CLA | CHB-C4A-NA | 2.50 | 127.96 | 124.51 |
| 25 | A | 848 | BCR | C32-C1-C6 | 2.50 | 114.35 | 110.30 |
| 22 | 1 | 603 | CLA | O2D-CGD-O1D | -2.50 | 118.96 | 123.84 |
| 22 | 3 | 602 | CLA | O2D-CGD-O1D | -2.50 | 118.96 | 123.84 |
| 22 | 5 | 610 | CLA | C1-C2-C3 | -2.50 | 121.73 | 126.04 |
| 22 | 7 | 616 | CLA | CMC-C2C-C1C | 2.50 | 128.84 | 125.04 |
| 22 | F | 303 | CLA | CMB-C2B-C3B | 2.49 | 129.35 | 124.68 |
| 22 | Z | 609 | CLA | C1-C2-C3 | -2.49 | 121.73 | 126.04 |
| 22 | 6 | 622 | CLA | CMC-C2C-C1C | 2.49 | 128.84 | 125.04 |
| 22 | B | 825 | CLA | CAC-C3C-C4C | 2.49 | 128.05 | 124.81 |
| 25 | 4 | 621 | BCR | C38-C26-C27 | 2.49 | 118.41 | 113.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 806 | CLA | CAA-C2A-C3A | -2.49 | 105.95 | 112.78 |
| 22 | 9 | 612 | CLA | CAA-C2A-C3A | -2.49 | 105.95 | 112.78 |
| 22 | Z | 606 | CLA | C1-C2-C3 | -2.49 | 121.73 | 126.04 |
| 22 | 8 | 608 | CLA | C4C-C3C-C2C | -2.49 | 103.27 | 106.90 |
| 22 | B | 841 | CLA | C4-C3-C5 | 2.49 | 119.46 | 115.27 |
| 25 | B | 845 | BCR | C11-C10-C9 | -2.49 | 123.75 | 127.31 |
| 22 | 3 | 603 | CLA | CMC-C2C-C1C | 2.49 | 128.83 | 125.04 |
| 22 | 3 | 609 | CLA | CMB-C2B-C3B | 2.49 | 129.34 | 124.68 |
| 22 | 8 | 608 | CLA | O2D-CGD-O1D | -2.49 | 118.97 | 123.84 |
| 22 | 3 | 604 | CLA | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 22 | A | 838 | CLA | O2A-CGA-CBA | 2.49 | 119.72 | 111.91 |
| 22 | A | 822 | CLA | CAC-C3C-C4C | 2.49 | 128.04 | 124.81 |
| 25 | 5 | 622 | BCR | C11-C12-C13 | -2.49 | 119.42 | 126.42 |
| 22 | 3 | 607 | CLA | CAC-C3C-C4C | 2.49 | 128.04 | 124.81 |
| 22 | Z | 602 | CLA | O2A-CGA-CBA | 2.49 | 119.72 | 111.91 |
| 25 | 3 | 719 | BCR | C2-C1-C6 | 2.49 | 114.31 | 110.48 |
| 22 | B | 816 | CLA | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 22 | 6 | 622 | CLA | CHD-C4C-NC | 2.49 | 128.12 | 124.20 |
| 22 | 5 | 601 | CLA | CMB-C2B-C3B | 2.49 | 129.33 | 124.68 |
| 30 | 6 | 624 | LUT | C38-C25-C24 | -2.49 | 118.24 | 123.56 |
| 22 | 7 | 612 | CLA | CHB-C4A-NA | 2.49 | 127.95 | 124.51 |
| 22 | L | 203 | CLA | CHD-C4C-NC | 2.49 | 128.12 | 124.20 |
| 22 | 6 | 601 | CLA | CAC-C3C-C4C | 2.49 | 128.03 | 124.81 |
| 22 | 1 | 608 | CLA | CMC-C2C-C1C | 2.49 | 128.82 | 125.04 |
| 25 | B | 801 | BCR | C16-C17-C18 | -2.49 | 123.76 | 127.31 |
| 22 | 1 | 608 | CLA | CBC-CAC-C3C | -2.49 | 105.58 | 112.43 |
| 22 | B | 829 | CLA | CAC-C3C-C4C | 2.48 | 128.03 | 124.81 |
| 22 | 8 | 616 | CLA | CMB-C2B-C3B | 2.48 | 129.32 | 124.68 |
| 22 | 6 | 604 | CLA | CAA-C2A-C3A | -2.48 | 105.98 | 112.78 |
| 25 | 8 | 619 | BCR | C31-C1-C6 | -2.48 | 106.27 | 110.30 |
| 22 | 8 | 604 | CLA | CHD-C4C-NC | 2.48 | 128.12 | 124.20 |
| 22 | A | 841 | CLA | O2A-CGA-O1A | -2.48 | 117.33 | 123.59 |
| 22 | 6 | 602 | CLA | CAA-C2A-C3A | -2.48 | 105.98 | 112.78 |
| 22 | 4 | 602 | CLA | C1-C2-C3 | -2.48 | 121.75 | 126.04 |
| 25 | B | 845 | BCR | C21-C20-C19 | -2.48 | 115.47 | 123.22 |
| 22 | A | 815 | CLA | CMB-C2B-C3B | 2.48 | 129.32 | 124.68 |
| 22 | 9 | 602 | CLA | CAA-C2A-C3A | -2.48 | 105.99 | 112.78 |
| 22 | 7 | 610 | CLA | O1D-CGD-CBD | -2.48 | 119.41 | 124.48 |
| 30 | 8 | 618 | LUT | C7-C8-C9 | -2.48 | 122.49 | 126.23 |
| 22 | 6 | 622 | CLA | CAA-C2A-C3A | -2.48 | 105.99 | 112.78 |
| 22 | Z | 614 | CLA | CBC-CAC-C3C | -2.48 | 105.60 | 112.43 |
| 29 | 6 | 618 | CHL | CBC-CAC-C3C | -2.48 | 105.60 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 839 | CLA | CAA-C2A-C3A | -2.48 | 106.00 | 112.78 |
| 22 | 8 | 609 | CLA | CAA-C2A-C3A | -2.48 | 106.00 | 112.78 |
| 22 | 2 | 607 | CLA | CAA-C2A-C3A | -2.48 | 106.00 | 112.78 |
| 22 | 7 | 614 | CLA | CHB-C4A-NA | 2.48 | 127.94 | 124.51 |
| 22 | F | 301 | CLA | CMD-C2D-C3D | -2.48 | 121.92 | 127.61 |
| 22 | 6 | 603 | CLA | CBC-CAC-C3C | -2.48 | 105.61 | 112.43 |
| 30 | 2 | 616 | LUT | C21-C26-C27 | -2.48 | 109.57 | 112.70 |
| 29 | 4 | 607 | CHL | C2A-C1A-CHA | -2.48 | 119.53 | 123.86 |
| 29 | 4 | 608 | CHL | O2A-CGA-CBA | 2.47 | 119.67 | 111.91 |
| 22 | A | 834 | CLA | CMB-C2B-C3B | 2.47 | 129.31 | 124.68 |
| 22 | 4 | 601 | CLA | CHB-C4A-NA | 2.47 | 127.93 | 124.51 |
| 22 | 6 | 616 | CLA | CAA-CBA-CGA | -2.47 | 106.03 | 113.25 |
| 22 | 1 | 604 | CLA | CBC-CAC-C3C | -2.47 | 105.61 | 112.43 |
| 22 | A | 817 | CLA | C4C-C3C-C2C | -2.47 | 103.29 | 106.90 |
| 22 | 7 | 604 | CLA | CED-O2D-CGD | 2.47 | 121.53 | 115.94 |
| 22 | 7 | 613 | CLA | CAA-C2A-C3A | -2.47 | 106.01 | 112.78 |
| 22 | 6 | 601 | CLA | CBC-CAC-C3C | -2.47 | 105.62 | 112.43 |
| 22 | 7 | 602 | CLA | O2D-CGD-O1D | -2.47 | 119.01 | 123.84 |
| 22 | B | 821 | CLA | O2D-CGD-O1D | -2.47 | 119.01 | 123.84 |
| 22 | Z | 602 | CLA | CBC-CAC-C3C | -2.47 | 105.63 | 112.43 |
| 22 | B | 812 | CLA | O2D-CGD-O1D | -2.47 | 119.02 | 123.84 |
| 22 | F | 301 | CLA | C3B-C4B-NB | 2.47 | 112.40 | 109.21 |
| 22 | A | 825 | CLA | CHD-C4C-NC | 2.47 | 128.09 | 124.20 |
| 22 | Z | 611 | CLA | CAC-C3C-C4C | 2.47 | 128.01 | 124.81 |
| 22 | A | 822 | CLA | C1-C2-C3 | -2.47 | 121.78 | 126.04 |
| 22 | 2 | 613 | CLA | CAA-C2A-C1A | 2.47 | 120.05 | 111.97 |
| 22 | 3 | 604 | CLA | C4-C3-C5 | 2.47 | 119.42 | 115.27 |
| 22 | A | 828 | CLA | CHC-C1C-C2C | -2.46 | 119.91 | 126.72 |
| 30 | 4 | 620 | LUT | C19-C9-C8 | 2.46 | 121.96 | 118.08 |
| 29 | 5 | 607 | CHL | CMB-C2B-C3B | 2.46 | 129.29 | 124.68 |
| 22 | B | 816 | CLA | O2D-CGD-O1D | -2.46 | 119.02 | 123.84 |
| 22 | 8 | 601 | CLA | CHD-C4C-NC | 2.46 | 128.09 | 124.20 |
| 30 | 4 | 619 | LUT | C28-C29-C30 | -2.46 | 115.16 | 118.94 |
| 22 | 2 | 609 | CLA | O2A-CGA-CBA | 2.46 | 119.64 | 111.91 |
| 25 | B | 801 | BCR | C34-C9-C10 | -2.46 | 119.47 | 122.92 |
| 22 | A | 802 | CLA | C1-O2A-CGA | 2.46 | 122.90 | 116.44 |
| 22 | 2 | 614 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 22 | A | 826 | CLA | CHA-C1A-NA | -2.46 | 120.76 | 126.40 |
| 22 | G | 203 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 22 | 1 | 604 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 22 | A | 821 | CLA | CMB-C2B-C3B | 2.46 | 129.28 | 124.68 |
| 22 | 3 | 613 | CLA | CHB-C4A-NA | 2.46 | 127.91 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 837 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 22 | A | 836 | CLA | CAA-C2A-C3A | -2.46 | 106.05 | 112.78 |
| 25 | I | 172 | BCR | C29-C30-C25 | 2.46 | 114.26 | 110.48 |
| 22 | 1 | 609 | CLA | CMC-C2C-C1C | 2.46 | 128.78 | 125.04 |
| 22 | A | 819 | CLA | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 29 | Z | 601 | CHL | O2A-CGA-CBA | 2.46 | 119.62 | 111.91 |
| 22 | 7 | 608 | CLA | CAA-C2A-C3A | -2.46 | 106.05 | 112.78 |
| 25 | 7 | 624 | BCR | C2-C1-C6 | 2.46 | 114.26 | 110.48 |
| 22 | B | 834 | CLA | CMC-C2C-C1C | 2.46 | 128.78 | 125.04 |
| 22 | F | 304 | CLA | O2D-CGD-O1D | -2.46 | 119.04 | 123.84 |
| 30 | 9 | 616 | LUT | C18-C5-C6 | -2.46 | 121.77 | 124.53 |
| 22 | 6 | 601 | CLA | C1-C2-C3 | -2.46 | 121.80 | 126.04 |
| 22 | 3 | 612 | CLA | O2D-CGD-O1D | -2.46 | 119.04 | 123.84 |
| 22 | G | 204 | CLA | CMB-C2B-C3B | 2.46 | 129.27 | 124.68 |
| 25 | L | 205 | BCR | C11-C10-C9 | -2.46 | 123.81 | 127.31 |
| 22 | 1 | 609 | CLA | CHB-C4A-NA | 2.46 | 127.91 | 124.51 |
| 22 | Z | 612 | CLA | O2D-CGD-O1D | -2.45 | 119.04 | 123.84 |
| 22 | 1 | 616 | CLA | CHB-C4A-NA | 2.45 | 127.91 | 124.51 |
| 25 | A | 848 | BCR | C3-C4-C5 | -2.45 | 109.70 | 114.08 |
| 25 | A | 850 | BCR | C7-C8-C9 | -2.45 | 122.53 | 126.23 |
| 22 | A | 803 | CLA | C1B-CHB-C4A | -2.45 | 125.26 | 130.12 |
| 22 | A | 845 | CLA | CHB-C4A-NA | 2.45 | 127.90 | 124.51 |
| 29 | 4 | 608 | CHL | CMB-C2B-C3B | 2.45 | 129.27 | 124.68 |
| 22 | 4 | 610 | CLA | CHC-C1C-NC | 2.45 | 127.92 | 124.20 |
| 22 | 2 | 611 | CLA | CMB-C2B-C3B | 2.45 | 129.26 | 124.68 |
| 22 | L | 203 | CLA | C4-C3-C5 | 2.45 | 119.39 | 115.27 |
| 22 | L | 203 | CLA | CMC-C2C-C1C | 2.45 | 128.77 | 125.04 |
| 22 | Z | 613 | CLA | C1-O2A-CGA | 2.45 | 122.88 | 116.44 |
| 22 | B | 824 | CLA | CMB-C2B-C3B | 2.45 | 129.26 | 124.68 |
| 22 | 9 | 613 | CLA | O2A-CGA-CBA | 2.45 | 119.59 | 111.91 |
| 22 | 9 | 610 | CLA | CBC-CAC-C3C | -2.45 | 105.68 | 112.43 |
| 22 | 7 | 620 | CLA | CAA-C2A-C3A | -2.45 | 106.07 | 112.78 |
| 22 | 7 | 608 | CLA | CMC-C2C-C1C | 2.45 | 128.77 | 125.04 |
| 22 | A | 807 | CLA | CHB-C4A-NA | 2.45 | 127.90 | 124.51 |
| 21 | A | 801 | CL0 | CAC-C3C-C4C | 2.45 | 127.99 | 124.81 |
| 22 | 2 | 607 | CLA | O2A-CGA-CBA | 2.45 | 119.59 | 111.91 |
| 25 | 5 | 622 | BCR | C8-C7-C6 | -2.45 | 120.33 | 127.20 |
| 22 | B | 830 | CLA | CHB-C4A-NA | 2.45 | 127.90 | 124.51 |
| 22 | 4 | 612 | CLA | C4-C3-C5 | 2.45 | 119.39 | 115.27 |
| 22 | B | 817 | CLA | CHD-C4C-NC | 2.45 | 128.06 | 124.20 |
| 22 | B | 816 | CLA | CHC-C1C-C2C | -2.45 | 119.95 | 126.72 |
| 22 | 3 | 607 | CLA | CHB-C4A-NA | 2.45 | 127.89 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 9 | 602 | CLA | CMB-C2B-C3B | 2.45 | 129.25 | 124.68 |
| 22 | B | 809 | CLA | C4C-C3C-C2C | -2.45 | 103.33 | 106.90 |
| 30 | 2 | 617 | LUT | C15-C14-C13 | -2.44 | 123.82 | 127.31 |
| 29 | 5 | 618 | CHL | C1B-CHB-C4A | -2.44 | 125.28 | 130.12 |
| 29 | 8 | 607 | CHL | O2A-CGA-CBA | 2.44 | 119.58 | 111.91 |
| 22 | A | 804 | CLA | C4-C3-C5 | 2.44 | 119.38 | 115.27 |
| 22 | A | 820 | CLA | O2D-CGD-O1D | -2.44 | 119.06 | 123.84 |
| 22 | 4 | 604 | CLA | CHB-C4A-NA | 2.44 | 127.89 | 124.51 |
| 22 | 2 | 603 | CLA | CAA-C2A-C3A | -2.44 | 106.09 | 112.78 |
| 22 | 5 | 609 | CLA | CHD-C4C-NC | 2.44 | 128.05 | 124.20 |
| 22 | B | 820 | CLA | CMB-C2B-C3B | 2.44 | 129.25 | 124.68 |
| 22 | 7 | 614 | CLA | CBC-CAC-C3C | -2.44 | 105.70 | 112.43 |
| 30 | 5 | 620 | LUT | C10-C11-C12 | -2.44 | 115.60 | 123.22 |
| 22 | 5 | 603 | CLA | CMC-C2C-C1C | 2.44 | 128.76 | 125.04 |
| 29 | 9 | 607 | CHL | O2D-CGD-O1D | -2.44 | 119.07 | 123.84 |
| 22 | B | 805 | CLA | C4A-NA-C1A | -2.44 | 105.61 | 106.71 |
| 22 | 3 | 606 | CLA | O2D-CGD-O1D | -2.44 | 119.07 | 123.84 |
| 30 | 1 | 618 | LUT | C30-C31-C32 | -2.44 | 115.61 | 123.22 |
| 22 | 3 | 612 | CLA | CBC-CAC-C3C | -2.44 | 105.71 | 112.43 |
| 22 | 6 | 609 | CLA | O2D-CGD-O1D | -2.44 | 119.07 | 123.84 |
| 22 | A | 840 | CLA | CMC-C2C-C1C | 2.44 | 128.75 | 125.04 |
| 22 | A | 821 | CLA | CHB-C4A-NA | 2.44 | 127.88 | 124.51 |
| 22 | 9 | 609 | CLA | CHB-C4A-NA | 2.44 | 127.88 | 124.51 |
| 22 | L | 204 | CLA | CAA-C2A-C3A | -2.44 | 106.10 | 112.78 |
| 22 | 2 | 601 | CLA | CMB-C2B-C3B | 2.44 | 129.24 | 124.68 |
| 22 | B | 839 | CLA | O2A-CGA-CBA | 2.44 | 119.56 | 111.91 |
| 29 | 6 | 607 | CHL | C1-C2-C3 | -2.44 | 121.83 | 126.04 |
| 22 | 8 | 616 | CLA | CMC-C2C-C1C | 2.44 | 128.75 | 125.04 |
| 22 | B | 814 | CLA | CBC-CAC-C3C | -2.44 | 105.72 | 112.43 |
| 22 | A | 824 | CLA | C4-C3-C5 | 2.44 | 118.77 | 115.98 |
| 22 | B | 828 | CLA | C1-C2-C3 | -2.44 | 121.83 | 126.04 |
| 22 | 3 | 617 | CLA | O2D-CGD-O1D | -2.44 | 119.08 | 123.84 |
| 22 | K | 4002 | CLA | CHB-C4A-NA | 2.44 | 127.88 | 124.51 |
| 22 | Z | 603 | CLA | CHB-C4A-NA | 2.44 | 127.88 | 124.51 |
| 22 | B | 835 | CLA | CBC-CAC-C3C | -2.44 | 105.72 | 112.43 |
| 22 | B | 809 | CLA | C4-C3-C5 | 2.43 | 119.36 | 115.27 |
| 22 | B | 819 | CLA | CBC-CAC-C3C | -2.43 | 105.72 | 112.43 |
| 22 | 4 | 616 | CLA | CHB-C4A-NA | 2.43 | 127.88 | 124.51 |
| 22 | 9 | 612 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 22 | A | 833 | CLA | CMC-C2C-C1C | 2.43 | 128.74 | 125.04 |
| 22 | B | 841 | CLA | CMC-C2C-C1C | 2.43 | 128.74 | 125.04 |
| 22 | 7 | 603 | CLA | CMC-C2C-C1C | 2.43 | 128.74 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 1 | 612 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 22 | 6 | 609 | CLA | CAA-C2A-C3A | -2.43 | 106.12 | 112.78 |
| 22 | B | 810 | CLA | C4-C3-C5 | 2.43 | 119.36 | 115.27 |
| 29 | 9 | 606 | CHL | C2A-C1A-CHA | -2.43 | 119.61 | 123.85 |
| 22 | 6 | 611 | CLA | O2D-CGD-O1D | -2.43 | 119.08 | 123.84 |
| 22 | 4 | 604 | CLA | CBC-CAC-C3C | -2.43 | 105.73 | 112.43 |
| 22 | 3 | 604 | CLA | C1-C2-C3 | -2.43 | 121.84 | 126.04 |
| 25 | 4 | 621 | BCR | C28-C27-C26 | -2.43 | 109.74 | 114.08 |
| 30 | 7 | 621 | LUT | C10-C11-C12 | -2.43 | 115.63 | 123.22 |
| 22 | 5 | 613 | CLA | CHD-C4C-NC | 2.43 | 128.03 | 124.20 |
| 22 | 3 | 612 | CLA | CHD-C4C-NC | 2.43 | 128.03 | 124.20 |
| 30 | 8 | 617 | LUT | C10-C11-C12 | -2.43 | 115.64 | 123.22 |
| 22 | K | 4003 | CLA | O2D-CGD-O1D | -2.43 | 119.09 | 123.84 |
| 22 | 5 | 601 | CLA | C1-C2-C3 | -2.43 | 121.84 | 126.04 |
| 25 | 5 | 622 | BCR | C34-C9-C8 | 2.43 | 121.90 | 118.08 |
| 25 | I | 172 | BCR | C7-C8-C9 | -2.43 | 122.57 | 126.23 |
| 22 | 2 | 603 | CLA | CMB-C2B-C3B | 2.43 | 129.22 | 124.68 |
| 22 | 3 | 614 | CLA | CMC-C2C-C1C | 2.42 | 128.73 | 125.04 |
| 22 | 8 | 610 | CLA | CMA-C3A-C2A | -2.42 | 104.05 | 113.83 |
| 22 | 1 | 612 | CLA | C4-C3-C5 | 2.42 | 119.35 | 115.27 |
| 22 | 6 | 622 | CLA | CMB-C2B-C3B | 2.42 | 129.21 | 124.68 |
| 22 | 2 | 613 | CLA | CHA-C1A-NA | -2.42 | 120.85 | 126.40 |
| 29 | 6 | 608 | CHL | CAA-CBA-CGA | -2.42 | 106.17 | 113.25 |
| 22 | 6 | 610 | CLA | CMA-C3A-C2A | -2.42 | 104.06 | 113.83 |
| 22 | 1 | 616 | CLA | CBC-CAC-C3C | -2.42 | 105.76 | 112.43 |
| 22 | 4 | 602 | CLA | CAA-C2A-C3A | -2.42 | 106.15 | 112.78 |
| 22 | A | 834 | CLA | CAC-C3C-C4C | 2.42 | 127.95 | 124.81 |
| 22 | B | 807 | CLA | CMB-C2B-C3B | 2.42 | 129.20 | 124.68 |
| 22 | B | 832 | CLA | CHB-C4A-NA | 2.42 | 127.86 | 124.51 |
| 22 | Z | 611 | CLA | CHB-C4A-NA | 2.42 | 127.86 | 124.51 |
| 22 | Z | 613 | CLA | CHB-C4A-NA | 2.42 | 127.86 | 124.51 |
| 22 | 6 | 611 | CLA | O2A-CGA-CBA | 2.42 | 119.50 | 111.91 |
| 22 | 4 | 612 | CLA | CBC-CAC-C3C | -2.42 | 105.77 | 112.43 |
| 22 | 5 | 616 | CLA | CBC-CAC-C3C | -2.42 | 105.77 | 112.43 |
| 22 | 2 | 610 | CLA | CMC-C2C-C1C | 2.42 | 128.72 | 125.04 |
| 22 | A | 833 | CLA | CBC-CAC-C3C | -2.42 | 105.77 | 112.43 |
| 22 | Z | 612 | CLA | CAC-C3C-C4C | 2.42 | 127.94 | 124.81 |
| 22 | 4 | 611 | CLA | O2D-CGD-O1D | -2.42 | 119.11 | 123.84 |
| 22 | 2 | 613 | CLA | CMC-C2C-C1C | 2.42 | 128.72 | 125.04 |
| 22 | 4 | 611 | CLA | CHD-C4C-NC | 2.42 | 128.01 | 124.20 |
| 22 | B | 835 | CLA | CHB-C4A-NA | 2.42 | 127.85 | 124.51 |
| 22 | 4 | 602 | CLA | CHB-C4A-NA | 2.42 | 127.85 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 5 | 602 | CLA | CHB-C4A-NA | 2.42 | 127.85 | 124.51 |
| 22 | A | 824 | CLA | O2D-CGD-O1D | -2.42 | 119.12 | 123.84 |
| 22 | 6 | 610 | CLA | C4-C3-C5 | 2.41 | 119.33 | 115.27 |
| 22 | A | 829 | CLA | CHC-C1C-C2C | -2.41 | 120.04 | 126.72 |
| 22 | 1 | 606 | CLA | O2A-CGA-CBA | 2.41 | 119.48 | 111.91 |
| 22 | B | 810 | CLA | CMB-C2B-C3B | 2.41 | 129.19 | 124.68 |
| 30 | 1 | 618 | LUT | C20-C13-C12 | 2.41 | 121.88 | 118.08 |
| 22 | L | 203 | CLA | O2D-CGD-O1D | -2.41 | 119.12 | 123.84 |
| 22 | 1 | 602 | CLA | C4-C3-C5 | 2.41 | 119.33 | 115.27 |
| 22 | 7 | 602 | CLA | C3B-C4B-NB | 2.41 | 112.33 | 109.21 |
| 25 | B | 844 | BCR | C33-C5-C6 | -2.41 | 121.82 | 124.53 |
| 22 | A | 819 | CLA | CMC-C2C-C1C | 2.41 | 128.71 | 125.04 |
| 22 | 6 | 604 | CLA | O2D-CGD-O1D | -2.41 | 119.12 | 123.84 |
| 22 | B | 852 | CLA | CAA-C2A-C3A | -2.41 | 106.17 | 112.78 |
| 22 | 1 | 610 | CLA | C3B-C4B-NB | 2.41 | 112.33 | 109.21 |
| 22 | 2 | 602 | CLA | CMC-C2C-C1C | 2.41 | 128.71 | 125.04 |
| 22 | 9 | 611 | CLA | CAA-C2A-C3A | -2.41 | 106.17 | 112.78 |
| 25 | G | 205 | BCR | C7-C8-C9 | -2.41 | 122.59 | 126.23 |
| 22 | B | 809 | CLA | O2A-CGA-CBA | 2.41 | 119.48 | 111.91 |
| 22 | K | 4003 | CLA | CMB-C2B-C3B | 2.41 | 129.19 | 124.68 |
| 22 | B | 833 | CLA | C1-C2-C3 | -2.41 | 121.87 | 126.04 |
| 25 | B | 848 | BCR | C33-C5-C6 | -2.41 | 121.82 | 124.53 |
| 22 | A | 839 | CLA | CMB-C2B-C3B | 2.41 | 129.19 | 124.68 |
| 25 | J | 3003 | BCR | C15-C16-C17 | -2.41 | 118.54 | 123.47 |
| 22 | 9 | 604 | CLA | O2A-CGA-CBA | 2.41 | 119.47 | 111.91 |
| 22 | 2 | 613 | CLA | CHD-C4C-NC | 2.41 | 128.00 | 124.20 |
| 22 | 5 | 606 | CLA | CMC-C2C-C1C | 2.41 | 128.71 | 125.04 |
| 25 | B | 843 | BCR | C16-C17-C18 | -2.41 | 123.87 | 127.31 |
| 22 | B | 808 | CLA | CHD-C4C-NC | 2.41 | 128.00 | 124.20 |
| 22 | 8 | 601 | CLA | O2A-CGA-CBA | 2.41 | 119.46 | 111.91 |
| 28 | 9 | 620 | LMG | O3-C3-C2 | -2.41 | 104.78 | 110.35 |
| 22 | 8 | 616 | CLA | CHB-C4A-NA | 2.41 | 127.84 | 124.51 |
| 22 | B | 831 | CLA | CHC-C1C-C2C | -2.41 | 120.06 | 126.72 |
| 24 | Z | 620 | LHG | O8-C23-C24 | 2.41 | 119.46 | 111.91 |
| 22 | B | 805 | CLA | O2A-CGA-O1A | -2.41 | 117.52 | 123.59 |
| 22 | B | 823 | CLA | C1-C2-C3 | -2.41 | 121.88 | 126.04 |
| 23 | B | 842 | PQN | C14-C13-C15 | 2.41 | 119.32 | 115.27 |
| 22 | A | 832 | CLA | CHD-C4C-NC | 2.41 | 127.99 | 124.20 |
| 22 | A | 843 | CLA | CHD-C4C-NC | 2.40 | 127.99 | 124.20 |
| 22 | B | 812 | CLA | CHB-C4A-NA | 2.40 | 127.84 | 124.51 |
| 22 | B | 819 | CLA | C1-C2-C3 | -2.40 | 121.89 | 126.04 |
| 22 | A | 842 | CLA | O2A-CGA-CBA | 2.40 | 119.45 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 845 | CLA | O2D-CGD-O1D | -2.40 | 119.14 | 123.84 |
| 22 | B | 834 | CLA | CED-O2D-CGD | 2.40 | 121.37 | 115.94 |
| 22 | B | 812 | CLA | CMB-C2B-C3B | 2.40 | 129.17 | 124.68 |
| 22 | A | 811 | CLA | CMA-C3A-C2A | -2.40 | 104.14 | 113.83 |
| 25 | A | 849 | BCR | C15-C16-C17 | -2.40 | 118.56 | 123.47 |
| 22 | 8 | 602 | CLA | CBC-CAC-C3C | -2.40 | 105.81 | 112.43 |
| 22 | A | 827 | CLA | CHB-C4A-NA | 2.40 | 127.83 | 124.51 |
| 22 | 6 | 601 | CLA | CHB-C4A-NA | 2.40 | 127.83 | 124.51 |
| 29 | Z | 601 | CHL | O2D-CGD-O1D | -2.40 | 119.14 | 123.84 |
| 22 | B | 813 | CLA | CMC-C2C-C1C | 2.40 | 128.69 | 125.04 |
| 22 | 3 | 620 | CLA | C1-C2-C3 | -2.40 | 121.89 | 126.04 |
| 22 | 5 | 602 | CLA | C4-C3-C5 | 2.40 | 119.31 | 115.27 |
| 22 | Z | 609 | CLA | CHD-C4C-NC | 2.40 | 127.98 | 124.20 |
| 22 | 4 | 613 | CLA | CAA-C2A-C3A | -2.40 | 106.21 | 112.78 |
| 22 | 7 | 616 | CLA | CMB-C2B-C3B | 2.40 | 129.17 | 124.68 |
| 22 | 4 | 609 | CLA | CAA-C2A-C3A | -2.40 | 106.21 | 112.78 |
| 22 | 2 | 603 | CLA | O2D-CGD-O1D | -2.40 | 119.15 | 123.84 |
| 22 | A | 814 | CLA | C1-C2-C3 | -2.40 | 121.90 | 126.04 |
| 22 | 8 | 602 | CLA | O2D-CGD-O1D | -2.40 | 119.15 | 123.84 |
| 22 | A | 818 | CLA | CAA-C2A-C3A | -2.40 | 106.22 | 112.78 |
| 22 | 2 | 612 | CLA | O2A-CGA-CBA | 2.40 | 119.43 | 111.91 |
| 22 | A | 809 | CLA | CAC-C3C-C4C | 2.40 | 127.92 | 124.81 |
| 22 | A | 835 | CLA | O2A-CGA-CBA | 2.40 | 119.43 | 111.91 |
| 30 | 9 | 616 | LUT | C30-C31-C32 | -2.40 | 115.74 | 123.22 |
| 22 | L | 203 | CLA | CHB-C4A-NA | 2.40 | 127.82 | 124.51 |
| 29 | Z | 607 | CHL | CHB-C4A-NA | 2.40 | 127.82 | 124.51 |
| 22 | 8 | 602 | CLA | CMC-C2C-C1C | 2.39 | 128.69 | 125.04 |
| 22 | 9 | 604 | CLA | O2D-CGD-O1D | -2.39 | 119.16 | 123.84 |
| 29 | 6 | 618 | CHL | C2A-C3A-C4A | -2.39 | 98.00 | 101.87 |
| 30 | 3 | 621 | LUT | C38-C25-C24 | -2.39 | 118.44 | 123.56 |
| 22 | 8 | 612 | CLA | CMA-C3A-C4A | -2.39 | 105.34 | 111.77 |
| 22 | B | 811 | CLA | CMB-C2B-C3B | 2.39 | 129.37 | 124.69 |
| 30 | 2 | 616 | LUT | C18-C5-C6 | -2.39 | 121.84 | 124.53 |
| 22 | B | 808 | CLA | CMB-C2B-C3B | 2.39 | 129.15 | 124.68 |
| 22 | B | 838 | CLA | CAC-C3C-C4C | 2.39 | 127.91 | 124.81 |
| 22 | A | 854 | CLA | CHD-C4C-NC | 2.39 | 127.97 | 124.20 |
| 22 | 8 | 601 | CLA | CMB-C2B-C3B | 2.39 | 129.15 | 124.68 |
| 22 | 1 | 610 | CLA | CMA-C3A-C2A | -2.39 | 104.18 | 113.83 |
| 22 | B | 822 | CLA | C4-C3-C5 | 2.39 | 119.29 | 115.27 |
| 22 | B | 824 | CLA | O1D-CGD-CBD | -2.39 | 119.59 | 124.48 |
| 22 | 5 | 612 | CLA | CMB-C2B-C3B | 2.39 | 129.15 | 124.68 |
| 22 | 3 | 610 | CLA | C3B-C4B-NB | 2.39 | 112.30 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 854 | CLA | C1C-C2C-C3C | -2.39 | 104.45 | 106.96 |
| 22 | 2 | 612 | CLA | O2D-CGD-O1D | -2.39 | 119.17 | 123.84 |
| 25 | K | 4001 | BCR | C7-C6-C5 | 2.39 | 127.24 | 121.46 |
| 22 | 2 | 607 | CLA | CHB-C4A-NA | 2.39 | 127.81 | 124.51 |
| 22 | B | 824 | CLA | C1-C2-C3 | -2.39 | 121.92 | 126.04 |
| 22 | 4 | 614 | CLA | CMB-C2B-C3B | 2.39 | 129.14 | 124.68 |
| 22 | 8 | 611 | CLA | CHD-C4C-NC | 2.39 | 127.96 | 124.20 |
| 22 | A | 816 | CLA | CMB-C2B-C3B | 2.38 | 129.14 | 124.68 |
| 30 | 8 | 618 | LUT | C15-C35-C34 | -2.38 | 118.59 | 123.47 |
| 22 | A | 838 | CLA | CAA-C2A-C3A | -2.38 | 106.25 | 112.78 |
| 22 | F | 304 | CLA | C1-C2-C3 | -2.38 | 121.92 | 126.04 |
| 22 | 3 | 617 | CLA | CMC-C2C-C1C | 2.38 | 128.67 | 125.04 |
| 22 | 7 | 620 | CLA | C4-C3-C5 | 2.38 | 119.28 | 115.27 |
| 22 | 9 | 611 | CLA | CMC-C2C-C1C | 2.38 | 128.67 | 125.04 |
| 22 | 9 | 610 | CLA | CHB-C4A-NA | 2.38 | 127.81 | 124.51 |
| 25 | 7 | 624 | BCR | C29-C30-C25 | 2.38 | 114.15 | 110.48 |
| 22 | 9 | 603 | CLA | O2D-CGD-O1D | -2.38 | 119.18 | 123.84 |
| 22 | Z | 612 | CLA | C4-C3-C5 | 2.38 | 119.28 | 115.27 |
| 22 | 6 | 622 | CLA | CBC-CAC-C3C | -2.38 | 105.86 | 112.43 |
| 22 | Z | 602 | CLA | CHB-C4A-NA | 2.38 | 127.81 | 124.51 |
| 22 | 7 | 609 | CLA | CHD-C4C-NC | 2.38 | 127.95 | 124.20 |
| 25 | 6 | 623 | BCR | C24-C23-C22 | -2.38 | 122.64 | 126.23 |
| 22 | B | 822 | CLA | C1-C2-C3 | -2.38 | 121.93 | 126.04 |
| 22 | Z | 612 | CLA | CMB-C2B-C3B | 2.38 | 129.13 | 124.68 |
| 22 | B | 806 | CLA | CHB-C4A-NA | 2.38 | 127.80 | 124.51 |
| 22 | 2 | 609 | CLA | CHB-C4A-NA | 2.38 | 127.80 | 124.51 |
| 22 | 1 | 612 | CLA | CHB-C4A-NA | 2.38 | 127.80 | 124.51 |
| 22 | 7 | 610 | CLA | C1C-C2C-C3C | -2.38 | 104.45 | 106.96 |
| 29 | 5 | 618 | CHL | C2A-C1A-CHA | -2.38 | 119.70 | 123.86 |
| 22 | B | 813 | CLA | C1C-C2C-C3C | -2.38 | 104.46 | 106.96 |
| 23 | A | 844 | PQN | C14-C13-C15 | 2.38 | 119.27 | 115.27 |
| 22 | B | 809 | CLA | CMC-C2C-C1C | 2.38 | 128.66 | 125.04 |
| 22 | 2 | 611 | CLA | O2D-CGD-O1D | -2.38 | 119.19 | 123.84 |
| 22 | B | 817 | CLA | CBC-CAC-C3C | -2.38 | 105.88 | 112.43 |
| 22 | 8 | 603 | CLA | CBC-CAC-C3C | -2.38 | 105.88 | 112.43 |
| 22 | 3 | 602 | CLA | C1-C2-C3 | -2.38 | 121.93 | 126.04 |
| 22 | 1 | 613 | CLA | CMC-C2C-C1C | 2.38 | 128.66 | 125.04 |
| 22 | 4 | 604 | CLA | CAA-C2A-C3A | -2.38 | 106.27 | 112.78 |
| 22 | 3 | 620 | CLA | CMC-C2C-C1C | 2.38 | 128.66 | 125.04 |
| 22 | A | 819 | CLA | CBA-CAA-C2A | 2.38 | 120.88 | 113.86 |
| 25 | L | 201 | BCR | C24-C23-C22 | -2.38 | 122.65 | 126.23 |
| 25 | 8 | 619 | BCR | C29-C30-C25 | 2.37 | 114.14 | 110.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | J | 3003 | BCR | C16-C15-C14 | -2.37 | 118.61 | 123.47 |
| 22 | 4 | 601 | CLA | CHD-C4C-NC | 2.37 | 127.94 | 124.20 |
| 25 | 3 | 719 | BCR | C24-C23-C22 | -2.37 | 122.65 | 126.23 |
| 22 | L | 204 | CLA | CHD-C4C-NC | 2.37 | 127.94 | 124.20 |
| 25 | 7 | 623 | BCR | C31-C1-C6 | -2.37 | 106.45 | 110.30 |
| 22 | A | 854 | CLA | O2A-C1-C2 | 2.37 | 114.87 | 108.64 |
| 22 | 6 | 602 | CLA | CBC-CAC-C3C | -2.37 | 105.89 | 112.43 |
| 22 | Z | 606 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 22 | A | 811 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 22 | 1 | 613 | CLA | O2A-CGA-CBA | 2.37 | 119.35 | 111.91 |
| 22 | 3 | 617 | CLA | CHB-C4A-NA | 2.37 | 127.79 | 124.51 |
| 22 | B | 823 | CLA | CED-O2D-CGD | 2.37 | 121.30 | 115.94 |
| 22 | A | 831 | CLA | O2A-CGA-CBA | 2.37 | 119.34 | 111.91 |
| 22 | Z | 609 | CLA | CAA-CBA-CGA | -2.37 | 106.33 | 113.25 |
| 25 | L | 205 | BCR | C38-C26-C25 | -2.37 | 121.87 | 124.53 |
| 25 | B | 847 | BCR | C36-C18-C19 | 2.37 | 121.81 | 118.08 |
| 22 | 7 | 602 | CLA | CMC-C2C-C1C | 2.37 | 128.65 | 125.04 |
| 30 | Z | 619 | LUT | C11-C10-C9 | -2.37 | 123.93 | 127.31 |
| 22 | 8 | 612 | CLA | CMC-C2C-C1C | 2.37 | 128.64 | 125.04 |
| 22 | A | 837 | CLA | CHB-C4A-NA | 2.37 | 127.78 | 124.51 |
| 30 | Z | 619 | LUT | C19-C9-C8 | 2.37 | 121.81 | 118.08 |
| 25 | K | 4001 | BCR | C20-C21-C22 | -2.37 | 123.93 | 127.31 |
| 29 | 6 | 606 | CHL | CBC-CAC-C3C | -2.37 | 105.91 | 112.43 |
| 22 | B | 819 | CLA | O2A-CGA-CBA | 2.37 | 119.33 | 111.91 |
| 22 | 1 | 612 | CLA | CBC-CAC-C3C | -2.36 | 105.91 | 112.43 |
| 22 | 1 | 608 | CLA | CMB-C2B-C3B | 2.36 | 129.10 | 124.68 |
| 22 | B | 818 | CLA | CHB-C4A-NA | 2.36 | 127.78 | 124.51 |
| 29 | 6 | 606 | CHL | O2A-CGA-CBA | 2.36 | 119.32 | 111.91 |
| 29 | 9 | 607 | CHL | O2A-CGA-CBA | 2.36 | 119.32 | 111.91 |
| 22 | Z | 606 | CLA | CBC-CAC-C3C | -2.36 | 105.92 | 112.43 |
| 22 | 9 | 609 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 22 | A | 837 | CLA | CBC-CAC-C3C | -2.36 | 105.92 | 112.43 |
| 22 | 7 | 614 | CLA | CMC-C2C-C1C | 2.36 | 128.63 | 125.04 |
| 22 | B | 803 | CLA | C11-C12-C13 | -2.36 | 108.29 | 115.92 |
| 22 | J | 3002 | CLA | CHB-C4A-NA | 2.36 | 127.78 | 124.51 |
| 22 | B | 839 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 25 | J | 3003 | BCR | C2-C1-C6 | 2.36 | 114.11 | 110.48 |
| 22 | 3 | 614 | CLA | O2D-CGD-O1D | -2.36 | 119.22 | 123.84 |
| 22 | B | 814 | CLA | CAA-C2A-C3A | -2.36 | 106.31 | 112.78 |
| 22 | Z | 608 | CLA | CAA-CBA-CGA | -2.36 | 106.36 | 113.25 |
| 30 | 9 | 617 | LUT | C19-C9-C8 | 2.36 | 121.80 | 118.08 |
| 22 | 8 | 610 | CLA | CHB-C4A-NA | 2.36 | 127.78 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 810 | CLA | CBC-CAC-C3C | -2.36 | 105.93 | 112.43 |
| 22 | 4 | 609 | CLA | CMC-C2C-C1C | 2.36 | 128.63 | 125.04 |
| 25 | F | 305 | BCR | C16-C17-C18 | -2.36 | 123.94 | 127.31 |
| 22 | B | 809 | CLA | CHB-C4A-NA | 2.36 | 127.77 | 124.51 |
| 25 | 5 | 622 | BCR | C31-C1-C6 | -2.36 | 106.47 | 110.30 |
| 22 | 4 | 611 | CLA | O2A-CGA-CBA | 2.36 | 119.31 | 111.91 |
| 22 | 2 | 601 | CLA | CHB-C4A-NA | 2.36 | 127.77 | 124.51 |
| 29 | 6 | 607 | CHL | OMC-CMC-C2C | -2.36 | 120.36 | 125.69 |
| 22 | 2 | 602 | CLA | CBC-CAC-C3C | -2.36 | 105.93 | 112.43 |
| 25 | 6 | 623 | BCR | C38-C26-C25 | -2.36 | 121.88 | 124.53 |
| 22 | A | 833 | CLA | CAA-C2A-C3A | -2.36 | 106.32 | 112.78 |
| 22 | 6 | 613 | CLA | O2A-CGA-CBA | 2.36 | 119.31 | 111.91 |
| 22 | 3 | 607 | CLA | C4-C3-C5 | 2.36 | 119.24 | 115.27 |
| 22 | 5 | 621 | CLA | CHA-C1A-NA | -2.36 | 121.00 | 126.40 |
| 22 | A | 809 | CLA | CBC-CAC-C3C | -2.36 | 105.93 | 112.43 |
| 22 | 4 | 610 | CLA | O2D-CGD-O1D | -2.36 | 119.23 | 123.84 |
| 22 | A | 802 | CLA | CMB-C2B-C3B | 2.36 | 129.09 | 124.68 |
| 22 | G | 204 | CLA | O2D-CGD-O1D | -2.36 | 119.23 | 123.84 |
| 22 | 7 | 616 | CLA | CHB-C4A-NA | 2.36 | 127.77 | 124.51 |
| 22 | A | 836 | CLA | CHD-C4C-NC | 2.36 | 127.92 | 124.20 |
| 25 | K | 4004 | BCR | C38-C26-C25 | -2.36 | 121.88 | 124.53 |
| 22 | 7 | 620 | CLA | O2D-CGD-O1D | -2.36 | 119.23 | 123.84 |
| 22 | 8 | 616 | CLA | CBC-CAC-C3C | -2.36 | 105.94 | 112.43 |
| 22 | 7 | 604 | CLA | CAA-C2A-C3A | -2.35 | 106.33 | 112.78 |
| 22 | 1 | 606 | CLA | CMB-C2B-C3B | 2.35 | 129.08 | 124.68 |
| 25 | 7 | 623 | BCR | C37-C22-C23 | 2.35 | 121.79 | 118.08 |
| 30 | 6 | 621 | LUT | C10-C11-C12 | -2.35 | 115.87 | 123.22 |
| 22 | 4 | 616 | CLA | CMC-C2C-C1C | 2.35 | 128.62 | 125.04 |
| 22 | 4 | 613 | CLA | O2D-CGD-O1D | -2.35 | 119.24 | 123.84 |
| 30 | 1 | 619 | LUT | C2-C3-C4 | 2.35 | 113.53 | 110.30 |
| 22 | 8 | 612 | CLA | CHB-C4A-NA | 2.35 | 127.77 | 124.51 |
| 29 | 7 | 607 | CHL | CHB-C4A-NA | 2.35 | 127.77 | 124.51 |
| 22 | 7 | 602 | CLA | CMB-C2B-C3B | 2.35 | 129.08 | 124.68 |
| 22 | 2 | 603 | CLA | CMC-C2C-C1C | 2.35 | 128.62 | 125.04 |
| 22 | 8 | 610 | CLA | CHC-C1C-C2C | -2.35 | 120.22 | 126.72 |
| 29 | Z | 607 | CHL | CMB-C2B-C3B | 2.35 | 129.08 | 124.68 |
| 30 | 6 | 621 | LUT | C39-C29-C28 | 2.35 | 121.78 | 118.08 |
| 22 | B | 803 | CLA | C4A-NA-C1A | -2.35 | 105.65 | 106.71 |
| 22 | A | 815 | CLA | CMC-C2C-C1C | 2.35 | 128.62 | 125.04 |
| 22 | 6 | 610 | CLA | O1D-CGD-CBD | -2.35 | 119.67 | 124.48 |
| 22 | B | 818 | CLA | CAC-C3C-C4C | 2.35 | 127.86 | 124.81 |
| 22 | B | 840 | CLA | C4-C3-C5 | 2.35 | 119.22 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 838 | CLA | CHB-C4A-NA | 2.35 | 127.76 | 124.51 |
| 30 | 1 | 619 | LUT | C22-C23-C24 | -2.35 | 109.07 | 111.74 |
| 25 | G | 205 | BCR | C37-C22-C23 | 2.35 | 121.78 | 118.08 |
| 22 | B | 841 | CLA | CBC-CAC-C3C | -2.35 | 105.96 | 112.43 |
| 22 | 4 | 603 | CLA | O2D-CGD-O1D | -2.35 | 119.25 | 123.84 |
| 22 | 3 | 611 | CLA | CBC-CAC-C3C | -2.35 | 105.96 | 112.43 |
| 22 | 3 | 609 | CLA | CMC-C2C-C1C | 2.35 | 128.61 | 125.04 |
| 22 | 8 | 612 | CLA | CAA-C2A-C3A | -2.35 | 106.35 | 112.78 |
| 22 | Z | 606 | CLA | CMC-C2C-C1C | 2.35 | 128.61 | 125.04 |
| 29 | 5 | 608 | CHL | CHA-C1A-NA | -2.35 | 121.03 | 126.40 |
| 22 | A | 841 | CLA | CMA-C3A-C2A | -2.35 | 104.37 | 113.83 |
| 22 | 4 | 613 | CLA | CMC-C2C-C1C | 2.35 | 128.61 | 125.04 |
| 22 | 1 | 613 | CLA | C6-C7-C8 | -2.35 | 108.34 | 115.92 |
| 30 | 5 | 624 | LUT | C20-C13-C12 | 2.34 | 121.77 | 118.08 |
| 30 | 4 | 620 | LUT | C35-C15-C14 | -2.34 | 118.67 | 123.47 |
| 22 | 3 | 613 | CLA | C1-C2-C3 | -2.34 | 121.99 | 126.04 |
| 22 | A | 805 | CLA | CMC-C2C-C1C | 2.34 | 128.61 | 125.04 |
| 22 | 5 | 617 | CLA | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 22 | A | 839 | CLA | CHB-C4A-NA | 2.34 | 127.75 | 124.51 |
| 25 | 5 | 622 | BCR | C16-C15-C14 | -2.34 | 118.68 | 123.47 |
| 30 | 4 | 619 | LUT | C38-C25-C24 | -2.34 | 118.55 | 123.56 |
| 22 | F | 304 | CLA | C4-C3-C5 | 2.34 | 119.21 | 115.27 |
| 22 | A | 838 | CLA | CHD-C4C-NC | 2.34 | 127.89 | 124.20 |
| 22 | 8 | 610 | CLA | O2A-CGA-O1A | -2.34 | 117.68 | 123.59 |
| 22 | 2 | 607 | CLA | O2D-CGD-O1D | -2.34 | 119.26 | 123.84 |
| 22 | 5 | 610 | CLA | CBC-CAC-C3C | -2.34 | 105.98 | 112.43 |
| 25 | B | 848 | BCR | C34-C9-C8 | 2.34 | 121.77 | 118.08 |
| 22 | A | 818 | CLA | O1D-CGD-CBD | -2.34 | 119.70 | 124.48 |
| 22 | 8 | 604 | CLA | O2D-CGD-O1D | -2.34 | 119.26 | 123.84 |
| 25 | 6 | 625 | BCR | C23-C22-C21 | -2.34 | 115.35 | 118.94 |
| 22 | 6 | 617 | CLA | O2D-CGD-O1D | -2.34 | 119.27 | 123.84 |
| 22 | 3 | 610 | CLA | CHC-C1C-C2C | -2.34 | 120.25 | 126.72 |
| 25 | A | 852 | BCR | C16-C15-C14 | -2.34 | 118.69 | 123.47 |
| 22 | 6 | 610 | CLA | CHB-C4A-NA | 2.34 | 127.74 | 124.51 |
| 29 | 6 | 608 | CHL | CHB-C4A-NA | 2.34 | 127.74 | 124.51 |
| 22 | 2 | 607 | CLA | CMC-C2C-C1C | 2.34 | 128.59 | 125.04 |
| 29 | 4 | 608 | CHL | C2A-C3A-C4A | -2.33 | 98.10 | 101.87 |
| 22 | B | 807 | CLA | CHD-C4C-NC | 2.33 | 127.88 | 124.20 |
| 22 | 7 | 608 | CLA | O2D-CGD-O1D | -2.33 | 119.27 | 123.84 |
| 29 | Z | 607 | CHL | O2D-CGD-O1D | -2.33 | 119.27 | 123.84 |
| 29 | 1 | 607 | CHL | CHD-C4C-NC | 2.33 | 127.88 | 124.20 |
| 22 | 4 | 604 | CLA | CMC-C2C-C1C | 2.33 | 128.59 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30 | 2 | 616 | LUT | C38-C25-C24 | -2.33 | 118.57 | 123.56 |
| 22 | F | 304 | CLA | CHB-C4A-NA | 2.33 | 127.74 | 124.51 |
| 22 | A | 805 | CLA | CBC-CAC-C3C | -2.33 | 106.00 | 112.43 |
| 30 | 4 | 620 | LUT | C3-C4-C5 | -2.33 | 107.21 | 111.85 |
| 22 | 7 | 601 | CLA | CHB-C4A-NA | 2.33 | 127.74 | 124.51 |
| 22 | 8 | 601 | CLA | CHB-C4A-NA | 2.33 | 127.74 | 124.51 |
| 22 | 8 | 601 | CLA | O1D-CGD-CBD | -2.33 | 119.71 | 124.48 |
| 22 | A | 802 | CLA | CBC-CAC-C3C | -2.33 | 106.00 | 112.43 |
| 22 | Z | 602 | CLA | CMB-C2B-C3B | 2.33 | 129.04 | 124.68 |
| 22 | 6 | 603 | CLA | O2D-CGD-O1D | -2.33 | 119.28 | 123.84 |
| 22 | 5 | 610 | CLA | CMA-C3A-C4A | -2.33 | 105.51 | 111.77 |
| 22 | B | 838 | CLA | CHB-C4A-NA | 2.33 | 127.73 | 124.51 |
| 22 | 9 | 601 | CLA | CHB-C4A-NA | 2.33 | 127.73 | 124.51 |
| 29 | 6 | 607 | CHL | O2A-CGA-CBA | 2.33 | 119.22 | 111.91 |
| 22 | B | 819 | CLA | O2D-CGD-O1D | -2.33 | 119.28 | 123.84 |
| 22 | A | 829 | CLA | CHA-C1A-NA | -2.33 | 121.06 | 126.40 |
| 22 | 8 | 602 | CLA | C1-C2-C3 | -2.33 | 122.01 | 126.04 |
| 22 | B | 832 | CLA | O2A-CGA-O1A | -2.33 | 117.71 | 123.59 |
| 22 | B | 839 | CLA | CMC-C2C-C1C | 2.33 | 128.59 | 125.04 |
| 22 | 6 | 603 | CLA | CMC-C2C-C1C | 2.33 | 128.59 | 125.04 |
| 22 | 7 | 611 | CLA | CMB-C2B-C3B | 2.33 | 129.03 | 124.68 |
| 22 | L | 203 | CLA | O2A-CGA-CBA | 2.33 | 119.21 | 111.91 |
| 22 | A | 842 | CLA | CMC-C2C-C1C | 2.33 | 128.58 | 125.04 |
| 22 | Z | 606 | CLA | O2D-CGD-O1D | -2.33 | 119.29 | 123.84 |
| 22 | 3 | 602 | CLA | CBC-CAC-C3C | -2.33 | 106.02 | 112.43 |
| 25 | L | 205 | BCR | C33-C5-C6 | -2.33 | 121.92 | 124.53 |
| 22 | B | 818 | CLA | C4C-C3C-C2C | -2.33 | 103.51 | 106.90 |
| 29 | 6 | 607 | CHL | C1B-CHB-C4A | -2.33 | 125.51 | 130.12 |
| 22 | 6 | 609 | CLA | O2A-CGA-CBA | 2.33 | 119.21 | 111.91 |
| 22 | A | 815 | CLA | CBC-CAC-C3C | -2.33 | 106.02 | 112.43 |
| 30 | 4 | 620 | LUT | C38-C25-C24 | -2.33 | 118.58 | 123.56 |
| 22 | 9 | 602 | CLA | CBC-CAC-C3C | -2.33 | 106.02 | 112.43 |
| 22 | 8 | 613 | CLA | CHB-C4A-NA | 2.33 | 127.73 | 124.51 |
| 22 | L | 204 | CLA | O2D-CGD-O1D | -2.33 | 119.29 | 123.84 |
| 29 | 6 | 607 | CHL | CED-O2D-CGD | 2.33 | 121.20 | 115.94 |
| 22 | B | 834 | CLA | CBC-CAC-C3C | -2.32 | 106.02 | 112.43 |
| 25 | A | 849 | BCR | C31-C1-C6 | -2.32 | 106.53 | 110.30 |
| 22 | 3 | 611 | CLA | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 28 | J | 3001 | LMG | O1-C7-C8 | -2.32 | 105.29 | 110.90 |
| 29 | Z | 607 | CHL | CBC-CAC-C3C | -2.32 | 106.03 | 112.43 |
| 22 | B | 837 | CLA | O2A-CGA-O1A | -2.32 | 117.73 | 123.59 |
| 30 | Z | 617 | LUT | C19-C9-C8 | 2.32 | 121.74 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 806 | CLA | CAC-C3C-C4C | 2.32 | 127.82 | 124.81 |
| 22 | 1 | 608 | CLA | O2D-CGD-O1D | -2.32 | 119.30 | 123.84 |
| 22 | B | 822 | CLA | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 22 | 9 | 612 | CLA | CMB-C2B-C3B | 2.32 | 129.02 | 124.68 |
| 22 | Z | 614 | CLA | CED-O2D-CGD | 2.32 | 121.19 | 115.94 |
| 29 | 5 | 607 | CHL | OMC-CMC-C2C | -2.32 | 120.44 | 125.69 |
| 22 | 8 | 608 | CLA | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 29 | 9 | 607 | CHL | C2A-C1A-CHA | -2.32 | 119.80 | 123.86 |
| 22 | 5 | 606 | CLA | CBC-CAC-C3C | -2.32 | 106.04 | 112.43 |
| 22 | 7 | 604 | CLA | CBC-CAC-C3C | -2.32 | 106.04 | 112.43 |
| 22 | 4 | 612 | CLA | C1-C2-C3 | -2.32 | 122.03 | 126.04 |
| 29 | 5 | 607 | CHL | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 22 | A | 804 | CLA | CMA-C3A-C2A | -2.32 | 104.48 | 113.83 |
| 25 | 5 | 625 | BCR | C35-C13-C14 | -2.32 | 119.68 | 122.92 |
| 22 | K | 4003 | CLA | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 22 | L | 204 | CLA | CHB-C4A-NA | 2.32 | 127.72 | 124.51 |
| 22 | A | 820 | CLA | C11-C10-C8 | -2.32 | 108.43 | 115.92 |
| 22 | A | 834 | CLA | CBC-CAC-C3C | -2.32 | 106.05 | 112.43 |
| 22 | B | 811 | CLA | CMA-C3A-C2A | -2.32 | 104.49 | 113.83 |
| 29 | 6 | 606 | CHL | CHD-C4C-NC | 2.32 | 127.85 | 124.20 |
| 22 | B | 840 | CLA | O2D-CGD-O1D | -2.31 | 119.31 | 123.84 |
| 22 | A | 835 | CLA | CMC-C2C-C1C | 2.31 | 128.56 | 125.04 |
| 22 | 1 | 604 | CLA | O2D-CGD-O1D | -2.31 | 119.31 | 123.84 |
| 22 | A | 812 | CLA | CMB-C2B-C3B | 2.31 | 129.01 | 124.68 |
| 22 | 6 | 602 | CLA | CHB-C4A-NA | 2.31 | 127.71 | 124.51 |
| 30 | 8 | 617 | LUT | C30-C31-C32 | -2.31 | 116.00 | 123.22 |
| 30 | 7 | 621 | LUT | C16-C1-C6 | -2.31 | 106.55 | 110.30 |
| 22 | B | 832 | CLA | CHA-C1A-NA | -2.31 | 121.10 | 126.40 |
| 22 | 9 | 604 | CLA | CHD-C4C-NC | 2.31 | 127.85 | 124.20 |
| 22 | 6 | 616 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 22 | 5 | 603 | CLA | OBD-CAD-C3D | -2.31 | 122.95 | 128.52 |
| 22 | B | 837 | CLA | CMC-C2C-C1C | 2.31 | 128.56 | 125.04 |
| 22 | 7 | 603 | CLA | CBC-CAC-C3C | -2.31 | 106.06 | 112.43 |
| 22 | 7 | 603 | CLA | CMB-C2B-C3B | 2.31 | 129.00 | 124.68 |
| 22 | A | 830 | CLA | CED-O2D-CGD | 2.31 | 121.17 | 115.94 |
| 22 | 1 | 610 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 22 | Z | 604 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 22 | A | 810 | CLA | CMC-C2C-C1C | 2.31 | 128.56 | 125.04 |
| 22 | A | 826 | CLA | CBC-CAC-C3C | -2.31 | 106.06 | 112.43 |
| 22 | 9 | 610 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 22 | A | 835 | CLA | CBC-CAC-C3C | -2.31 | 106.06 | 112.43 |
| 22 | 6 | 612 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 8 | 602 | CLA | CAC-C3C-C2C | 2.31 | 131.48 | 127.53 |
| 22 | A | 811 | CLA | O2D-CGD-O1D | -2.31 | 119.32 | 123.84 |
| 22 | B | 818 | CLA | CBC-CAC-C3C | -2.31 | 106.07 | 112.43 |
| 30 | 8 | 617 | LUT | C18-C5-C6 | -2.31 | 121.94 | 124.53 |
| 22 | B | 806 | CLA | CMA-C3A-C4A | -2.31 | 105.57 | 111.77 |
| 22 | F | 301 | CLA | O1D-CGD-CBD | -2.31 | 119.76 | 124.48 |
| 22 | Z | 613 | CLA | O2A-CGA-CBA | 2.31 | 119.15 | 111.91 |
| 22 | B | 822 | CLA | O1D-CGD-CBD | -2.31 | 119.77 | 124.48 |
| 22 | 4 | 611 | CLA | C1-C2-C3 | -2.31 | 122.06 | 126.04 |
| 22 | 5 | 617 | CLA | CHD-C4C-NC | 2.31 | 127.84 | 124.20 |
| 29 | 5 | 608 | CHL | CBC-CAC-C3C | -2.31 | 106.08 | 112.43 |
| 22 | Z | 610 | CLA | CHB-C4A-NA | 2.31 | 127.70 | 124.51 |
| 22 | B | 816 | CLA | C4-C3-C5 | 2.31 | 119.15 | 115.27 |
| 22 | 1 | 609 | CLA | CBC-CAC-C3C | -2.30 | 106.08 | 112.43 |
| 29 | 4 | 606 | CHL | C1-C2-C3 | -2.30 | 122.06 | 126.04 |
| 29 | 5 | 608 | CHL | C1-C2-C3 | -2.30 | 123.02 | 126.75 |
| 22 | A | 825 | CLA | CHB-C4A-NA | 2.30 | 127.70 | 124.51 |
| 22 | 5 | 606 | CLA | CHB-C4A-NA | 2.30 | 127.70 | 124.51 |
| 25 | 3 | 717 | BCR | C34-C9-C10 | -2.30 | 119.70 | 122.92 |
| 22 | 3 | 612 | CLA | CMB-C2B-C3B | 2.30 | 128.99 | 124.68 |
| 22 | 2 | 606 | CLA | CMC-C2C-C1C | 2.30 | 128.54 | 125.04 |
| 22 | B | 829 | CLA | CAA-C2A-C3A | -2.30 | 106.48 | 112.78 |
| 22 | B | 832 | CLA | C4-C3-C5 | 2.30 | 119.14 | 115.27 |
| 29 | 4 | 606 | CHL | C4-C3-C5 | 2.30 | 119.14 | 115.27 |
| 30 | 9 | 616 | LUT | C38-C25-C24 | -2.30 | 118.64 | 123.56 |
| 22 | A | 803 | CLA | CHB-C4A-NA | 2.30 | 127.69 | 124.51 |
| 22 | 5 | 601 | CLA | O2A-C1-C2 | 2.30 | 114.68 | 108.64 |
| 22 | B | 811 | CLA | C4-C3-C5 | 2.30 | 119.14 | 115.27 |
| 22 | 8 | 604 | CLA | CBC-CAC-C3C | -2.30 | 106.09 | 112.43 |
| 22 | 3 | 613 | CLA | CMC-C2C-C1C | 2.30 | 128.54 | 125.04 |
| 22 | B | 814 | CLA | CMB-C2B-C3B | 2.30 | 128.98 | 124.68 |
| 22 | A | 843 | CLA | CHB-C4A-NA | 2.30 | 127.69 | 124.51 |
| 22 | B | 824 | CLA | C4-C3-C5 | 2.30 | 119.14 | 115.27 |
| 22 | 8 | 608 | CLA | C5-C3-C4 | 2.30 | 119.68 | 114.60 |
| 22 | B | 813 | CLA | O2A-CGA-O1A | -2.30 | 117.80 | 123.59 |
| 22 | A | 831 | CLA | CHD-C4C-NC | 2.30 | 127.82 | 124.20 |
| 22 | Z | 616 | CLA | CHB-C4A-NA | 2.30 | 127.69 | 124.51 |
| 29 | 3 | 608 | CHL | CHB-C4A-NA | 2.30 | 127.69 | 124.51 |
| 22 | B | 832 | CLA | C6-C7-C8 | -2.30 | 108.50 | 115.92 |
| 24 | 4 | 622 | LHG | O8-C23-C24 | 2.30 | 119.11 | 111.91 |
| 22 | 7 | 608 | CLA | CHB-C4A-NA | 2.30 | 127.69 | 124.51 |
| 22 | 9 | 611 | CLA | O2D-CGD-O1D | -2.30 | 119.35 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 825 | CLA | CAA-C2A-C3A | -2.30 | 106.49 | 112.78 |
| 22 | 6 | 614 | CLA | C1B-CHB-C4A | -2.30 | 125.57 | 130.12 |
| 22 | 5 | 603 | CLA | CHA-C1A-NA | -2.30 | 121.14 | 126.40 |
| 22 | A | 832 | CLA | CMA-C3A-C4A | -2.29 | 105.61 | 111.77 |
| 25 | 7 | 624 | BCR | C39-C30-C25 | -2.29 | 106.58 | 110.30 |
| 22 | 5 | 610 | CLA | C4-C3-C5 | 2.29 | 119.13 | 115.27 |
| 30 | 6 | 621 | LUT | C38-C25-C24 | -2.29 | 118.65 | 123.56 |
| 22 | 7 | 613 | CLA | CBC-CAC-C3C | -2.29 | 106.11 | 112.43 |
| 22 | G | 204 | CLA | CHB-C4A-NA | 2.29 | 127.68 | 124.51 |
| 29 | 4 | 607 | CHL | O2D-CGD-O1D | -2.29 | 119.36 | 123.84 |
| 25 | I | 172 | BCR | C11-C10-C9 | -2.29 | 124.04 | 127.31 |
| 22 | 5 | 614 | CLA | O1D-CGD-CBD | -2.29 | 119.80 | 124.48 |
| 29 | 8 | 607 | CHL | CHD-C4C-NC | 2.29 | 127.81 | 124.20 |
| 22 | A | 808 | CLA | CMB-C2B-C3B | 2.29 | 128.96 | 124.68 |
| 22 | 4 | 614 | CLA | O2D-CGD-O1D | -2.29 | 119.36 | 123.84 |
| 22 | A | 810 | CLA | CAA-CBA-CGA | -2.29 | 106.57 | 113.25 |
| 22 | 5 | 609 | CLA | CHA-C1A-NA | -2.29 | 121.16 | 126.40 |
| 22 | 6 | 617 | CLA | CHB-C4A-NA | 2.29 | 127.68 | 124.51 |
| 22 | 2 | 610 | CLA | CBC-CAC-C3C | -2.29 | 106.12 | 112.43 |
| 25 | L | 201 | BCR | C38-C26-C25 | -2.29 | 121.96 | 124.53 |
| 25 | 3 | 717 | BCR | C36-C18-C19 | 2.29 | 121.68 | 118.08 |
| 22 | A | 831 | CLA | C1-C2-C3 | -2.29 | 122.09 | 126.04 |
| 25 | K | 4004 | BCR | C16-C15-C14 | -2.29 | 118.79 | 123.47 |
| 25 | 8 | 619 | BCR | C16-C15-C14 | -2.29 | 118.79 | 123.47 |
| 22 | B | 818 | CLA | C2A-C3A-C4A | -2.29 | 98.18 | 101.87 |
| 22 | 9 | 609 | CLA | CAA-C2A-C3A | -2.29 | 106.52 | 112.78 |
| 22 | 6 | 604 | CLA | CHB-C4A-NA | 2.29 | 127.67 | 124.51 |
| 22 | Z | 609 | CLA | O2D-CGD-O1D | -2.29 | 119.37 | 123.84 |
| 22 | 2 | 602 | CLA | CAA-C2A-C3A | -2.29 | 106.52 | 112.78 |
| 22 | 1 | 606 | CLA | O2D-CGD-O1D | -2.29 | 119.37 | 123.84 |
| 22 | B | 826 | CLA | CHB-C4A-NA | 2.28 | 127.67 | 124.51 |
| 22 | 2 | 606 | CLA | O2D-CGD-O1D | -2.28 | 119.37 | 123.84 |
| 25 | A | 856 | BCR | C20-C19-C18 | -2.28 | 120.00 | 126.42 |
| 22 | B | 816 | CLA | O2A-CGA-O1A | -2.28 | 117.83 | 123.59 |
| 22 | B | 839 | CLA | CAA-C2A-C3A | -2.28 | 106.53 | 112.78 |
| 30 | Z | 619 | LUT | C18-C5-C6 | -2.28 | 121.96 | 124.53 |
| 22 | 9 | 609 | CLA | CAA-C2A-C1A | 2.28 | 119.46 | 111.97 |
| 29 | 6 | 608 | CHL | O2D-CGD-O1D | -2.28 | 119.38 | 123.84 |
| 22 | 1 | 602 | CLA | CBC-CAC-C3C | -2.28 | 106.14 | 112.43 |
| 22 | K | 4002 | CLA | CMC-C2C-C1C | 2.28 | 128.51 | 125.04 |
| 22 | 6 | 612 | CLA | CBC-CAC-C3C | -2.28 | 106.14 | 112.43 |
| 22 | B | 826 | CLA | CMB-C2B-C3B | 2.28 | 128.95 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27 | B | 850 | DGD | O2G-C1B-O1B | -2.28 | 118.19 | 123.70 |
| 22 | 2 | 609 | CLA | CMC-C2C-C1C | 2.28 | 128.51 | 125.04 |
| 22 | 7 | 612 | CLA | O2A-CGA-O1A | -2.28 | 117.83 | 123.59 |
| 22 | 7 | 608 | CLA | CMB-C2B-C3B | 2.28 | 128.94 | 124.68 |
| 22 | 8 | 613 | CLA | CMB-C2B-C3B | 2.28 | 128.94 | 124.68 |
| 25 | K | 4004 | BCR | C10-C11-C12 | -2.28 | 116.10 | 123.22 |
| 22 | B | 818 | CLA | CMC-C2C-C1C | 2.28 | 128.51 | 125.04 |
| 22 | 1 | 616 | CLA | O2D-CGD-O1D | -2.28 | 119.38 | 123.84 |
| 22 | 3 | 614 | CLA | CHB-C4A-NA | 2.28 | 127.67 | 124.51 |
| 22 | B | 836 | CLA | C1-C2-C3 | -2.28 | 122.10 | 126.04 |
| 30 | Z | 619 | LUT | C31-C32-C33 | -2.28 | 120.01 | 126.42 |
| 22 | 5 | 621 | CLA | CMC-C2C-C1C | 2.28 | 128.51 | 125.04 |
| 22 | 9 | 612 | CLA | CBC-CAC-C3C | -2.28 | 106.15 | 112.43 |
| 22 | 9 | 613 | CLA | CMC-C2C-C1C | 2.28 | 128.51 | 125.04 |
| 22 | A | 845 | CLA | CMB-C2B-C3B | 2.28 | 128.94 | 124.68 |
| 29 | 5 | 608 | CHL | O2D-CGD-O1D | -2.28 | 119.39 | 123.84 |
| 22 | 1 | 610 | CLA | CBC-CAC-C3C | -2.28 | 106.16 | 112.43 |
| 29 | 6 | 607 | CHL | O1D-CGD-CBD | -2.28 | 119.83 | 124.48 |
| 25 | A | 848 | BCR | C35-C13-C12 | 2.28 | 121.66 | 118.08 |
| 25 | 7 | 624 | BCR | C20-C21-C22 | -2.28 | 124.06 | 127.31 |
| 22 | 6 | 610 | CLA | CBC-CAC-C3C | -2.28 | 106.16 | 112.43 |
| 30 | 3 | 621 | LUT | C16-C1-C6 | -2.28 | 106.61 | 110.30 |
| 30 | 3 | 621 | LUT | C39-C29-C28 | 2.28 | 121.66 | 118.08 |
| 22 | A | 807 | CLA | CMC-C2C-C1C | 2.28 | 128.50 | 125.04 |
| 22 | 4 | 604 | CLA | CMB-C2B-C3B | 2.28 | 128.94 | 124.68 |
| 22 | 6 | 601 | CLA | O1D-CGD-CBD | -2.28 | 119.83 | 124.48 |
| 25 | 3 | 719 | BCR | C11-C10-C9 | -2.27 | 124.06 | 127.31 |
| 22 | 1 | 612 | CLA | CMB-C2B-C3B | 2.27 | 128.93 | 124.68 |
| 29 | 4 | 607 | CHL | CMB-C2B-C3B | 2.27 | 128.93 | 124.68 |
| 22 | 8 | 610 | CLA | O2D-CGD-O1D | -2.27 | 119.39 | 123.84 |
| 22 | 5 | 612 | CLA | O2D-CGD-O1D | -2.27 | 119.39 | 123.84 |
| 22 | 6 | 613 | CLA | CMC-C2C-C1C | 2.27 | 128.50 | 125.04 |
| 22 | 3 | 606 | CLA | CMB-C2B-C3B | 2.27 | 128.93 | 124.68 |
| 22 | 8 | 609 | CLA | O2A-CGA-CBA | 2.27 | 121.21 | 112.23 |
| 22 | 1 | 602 | CLA | C1-C2-C3 | -2.27 | 122.11 | 126.04 |
| 22 | B | 838 | CLA | CMC-C2C-C1C | 2.27 | 128.50 | 125.04 |
| 22 | 2 | 602 | CLA | O2D-CGD-O1D | -2.27 | 119.40 | 123.84 |
| 22 | B | 815 | CLA | CMA-C3A-C4A | -2.27 | 105.67 | 111.77 |
| 22 | Z | 604 | CLA | CBC-CAC-C3C | -2.27 | 106.17 | 112.43 |
| 30 | 7 | 621 | LUT | C31-C30-C29 | -2.27 | 124.07 | 127.31 |
| 22 | Z | 614 | CLA | CMC-C2C-C1C | 2.27 | 128.50 | 125.04 |
| 22 | B | 821 | CLA | CMB-C2B-C3B | 2.27 | 128.93 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 3 | 603 | CLA | CED-O2D-CGD | 2.27 | 121.07 | 115.94 |
| 22 | 3 | 610 | CLA | C4-C3-C5 | 2.27 | 119.09 | 115.27 |
| 22 | 9 | 604 | CLA | C5-C3-C4 | 2.27 | 119.62 | 114.60 |
| 22 | K | 4002 | CLA | O1D-CGD-CBD | -2.27 | 119.84 | 124.48 |
| 22 | A | 814 | CLA | CHD-C4C-NC | 2.27 | 127.78 | 124.20 |
| 25 | 6 | 623 | BCR | C33-C5-C6 | -2.27 | 121.98 | 124.53 |
| 25 | A | 850 | BCR | C1-C6-C7 | 2.27 | 122.20 | 115.78 |
| 30 | 9 | 617 | LUT | C16-C1-C6 | -2.27 | 106.62 | 110.30 |
| 22 | A | 831 | CLA | CAA-C2A-C3A | -2.27 | 106.57 | 112.78 |
| 22 | 4 | 610 | CLA | CHB-C4A-NA | 2.27 | 127.65 | 124.51 |
| 22 | B | 826 | CLA | CAA-CBA-CGA | -2.27 | 106.63 | 113.25 |
| 25 | 3 | 719 | BCR | C29-C30-C25 | 2.27 | 113.97 | 110.48 |
| 22 | 1 | 612 | CLA | C1-C2-C3 | -2.27 | 122.12 | 126.04 |
| 22 | 4 | 601 | CLA | C1-C2-C3 | -2.27 | 122.12 | 126.04 |
| 30 | 8 | 617 | LUT | C28-C29-C30 | -2.27 | 115.46 | 118.94 |
| 22 | L | 203 | CLA | CBC-CAC-C3C | -2.27 | 106.18 | 112.43 |
| 22 | 7 | 612 | CLA | CBC-CAC-C3C | -2.27 | 106.18 | 112.43 |
| 25 | K | 4004 | BCR | C7-C8-C9 | -2.27 | 122.81 | 126.23 |
| 30 | 5 | 624 | LUT | C39-C29-C28 | 2.27 | 121.65 | 118.08 |
| 22 | 1 | 612 | CLA | CBA-CAA-C2A | -2.27 | 107.17 | 113.86 |
| 22 | 5 | 621 | CLA | CHB-C4A-NA | 2.27 | 127.64 | 124.51 |
| 22 | 5 | 611 | CLA | C1-C2-C3 | -2.27 | 122.12 | 126.04 |
| 22 | B | 837 | CLA | CBA-CAA-C2A | 2.26 | 120.55 | 113.86 |
| 22 | F | 304 | CLA | CMB-C2B-C3B | 2.26 | 128.91 | 124.68 |
| 22 | B | 831 | CLA | C3B-C4B-NB | 2.26 | 112.14 | 109.21 |
| 25 | 5 | 625 | BCR | C28-C27-C26 | -2.26 | 110.03 | 114.08 |
| 21 | A | 801 | CL0 | CGD-CBD-CAD | -2.26 | 103.40 | 110.73 |
| 22 | 4 | 612 | CLA | CMB-C2B-C3B | 2.26 | 128.91 | 124.68 |
| 22 | B | 818 | CLA | O2A-CGA-CBA | 2.26 | 119.01 | 111.91 |
| 22 | A | 809 | CLA | C6-C5-C3 | -2.26 | 107.52 | 113.45 |
| 22 | 1 | 606 | CLA | CMC-C2C-C1C | 2.26 | 128.48 | 125.04 |
| 22 | 5 | 601 | CLA | CMC-C2C-C1C | 2.26 | 128.48 | 125.04 |
| 22 | 6 | 609 | CLA | CHD-C4C-NC | 2.26 | 127.77 | 124.20 |
| 22 | 7 | 611 | CLA | CHB-C4A-NA | 2.26 | 127.64 | 124.51 |
| 22 | 5 | 612 | CLA | CHB-C4A-NA | 2.26 | 127.64 | 124.51 |
| 29 | 8 | 607 | CHL | C4-C3-C5 | 2.26 | 119.07 | 115.27 |
| 30 | 1 | 619 | LUT | C1-C2-C3 | 2.26 | 118.75 | 113.64 |
| 22 | A | 826 | CLA | CHD-C4C-NC | 2.26 | 127.76 | 124.20 |
| 22 | 8 | 612 | CLA | CMB-C2B-C3B | 2.26 | 128.91 | 124.68 |
| 22 | 6 | 601 | CLA | C4-C3-C5 | 2.26 | 119.07 | 115.27 |
| 22 | Z | 602 | CLA | C1-C2-C3 | -2.26 | 122.14 | 126.04 |
| 30 | 2 | 616 | LUT | C20-C13-C12 | 2.26 | 121.63 | 118.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | B | 808 | CLA | C1-C2-C3 | -2.26 | 122.14 | 126.04 |
| 30 | 5 | 620 | LUT | C21-C26-C27 | -2.26 | 109.85 | 112.70 |
| 22 | A | 826 | CLA | C1-O2A-CGA | 2.26 | 122.36 | 116.44 |
| 22 | B | 821 | CLA | CHB-C4A-NA | 2.26 | 127.63 | 124.51 |
| 22 | 7 | 616 | CLA | CBC-CAC-C3C | -2.26 | 106.21 | 112.43 |
| 25 | B | 844 | BCR | C29-C28-C27 | -2.25 | 106.34 | 111.38 |
| 22 | 1 | 606 | CLA | CBC-CAC-C3C | -2.25 | 106.22 | 112.43 |
| 22 | A | 820 | CLA | CMC-C2C-C1C | 2.25 | 128.47 | 125.04 |
| 25 | A | 856 | BCR | C11-C12-C13 | -2.25 | 120.08 | 126.42 |
| 22 | A | 854 | CLA | C1-C2-C3 | -2.25 | 122.15 | 126.04 |
| 30 | Z | 617 | LUT | C38-C25-C24 | -2.25 | 118.74 | 123.56 |
| 22 | B | 828 | CLA | CBC-CAC-C3C | -2.25 | 106.22 | 112.43 |
| 29 | 6 | 608 | CHL | CBC-CAC-C3C | -2.25 | 106.22 | 112.43 |
| 22 | 3 | 613 | CLA | CHD-C4C-NC | 2.25 | 127.75 | 124.20 |
| 22 | 1 | 616 | CLA | CMC-C2C-C1C | 2.25 | 128.47 | 125.04 |
| 30 | 9 | 617 | LUT | C20-C13-C12 | 2.25 | 121.62 | 118.08 |
| 22 | 6 | 610 | CLA | CED-O2D-CGD | 2.25 | 121.03 | 115.94 |
| 22 | 7 | 606 | CLA | CHB-C4A-NA | 2.25 | 127.62 | 124.51 |
| 30 | 7 | 622 | LUT | C39-C29-C28 | 2.25 | 121.62 | 118.08 |
| 22 | 2 | 609 | CLA | CHA-C1A-NA | -2.25 | 121.25 | 126.40 |
| 22 | B | 814 | CLA | CMD-C2D-C3D | -2.25 | 122.44 | 127.61 |
| 22 | A | 810 | CLA | C16-C15-C13 | -2.25 | 108.65 | 115.92 |
| 25 | 3 | 717 | BCR | C37-C22-C23 | 2.25 | 121.62 | 118.08 |
| 25 | 3 | 717 | BCR | C38-C26-C27 | 2.25 | 117.93 | 113.62 |
| 25 | B | 845 | BCR | C36-C18-C19 | 2.25 | 121.62 | 118.08 |
| 22 | A | 815 | CLA | O1D-CGD-CBD | -2.25 | 119.89 | 124.48 |
| 22 | 3 | 604 | CLA | CMC-C2C-C1C | 2.25 | 128.46 | 125.04 |
| 22 | F | 303 | CLA | CHA-C1A-NA | -2.25 | 121.25 | 126.40 |
| 29 | 1 | 601 | CHL | C4-C3-C5 | 2.25 | 119.05 | 115.27 |
| 22 | Z | 603 | CLA | CMA-C3A-C4A | -2.25 | 105.74 | 111.77 |
| 24 | 5 | 623 | LHG | C6-C5-C4 | -2.25 | 106.48 | 111.79 |
| 22 | B | 828 | CLA | CHD-C4C-NC | 2.25 | 127.74 | 124.20 |
| 22 | A | 833 | CLA | CHB-C4A-NA | 2.25 | 127.62 | 124.51 |
| 22 | 4 | 602 | CLA | O2D-CGD-O1D | -2.25 | 119.45 | 123.84 |
| 22 | A | 823 | CLA | CMC-C2C-C1C | 2.25 | 128.46 | 125.04 |
| 22 | Z | 608 | CLA | CMC-C2C-C1C | 2.25 | 128.46 | 125.04 |
| 22 | A | 813 | CLA | CHB-C4A-NA | 2.24 | 127.62 | 124.51 |
| 22 | 4 | 602 | CLA | C4-C3-C5 | 2.24 | 119.05 | 115.27 |
| 22 | A | 822 | CLA | CED-O2D-CGD | 2.24 | 121.01 | 115.94 |
| 22 | A | 832 | CLA | C5-C3-C4 | 2.24 | 119.56 | 114.60 |
| 29 | Z | 601 | CHL | C1B-CHB-C4A | -2.24 | 125.67 | 130.12 |
| 22 | 5 | 601 | CLA | CHB-C4A-NA | 2.24 | 127.61 | 124.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 9 | 614 | CLA | CHB-C4A-NA | 2.24 | 127.61 | 124.51 |
| 22 | 7 | 612 | CLA | CMB-C2B-C3B | 2.24 | 128.87 | 124.68 |
| 22 | 6 | 613 | CLA | CAA-C2A-C3A | -2.24 | 106.64 | 112.78 |
| 22 | 1 | 604 | CLA | CMC-C2C-C1C | 2.24 | 128.45 | 125.04 |
| 22 | 6 | 617 | CLA | CMC-C2C-C1C | 2.24 | 128.45 | 125.04 |
| 22 | B | 804 | CLA | CAA-C2A-C3A | -2.24 | 106.64 | 112.78 |
| 22 | 2 | 606 | CLA | CBC-CAC-C3C | -2.24 | 106.25 | 112.43 |
| 22 | A | 809 | CLA | O1D-CGD-CBD | -2.24 | 119.90 | 124.48 |
| 22 | 5 | 602 | CLA | O2D-CGD-O1D | -2.24 | 119.46 | 123.84 |
| 22 | 3 | 612 | CLA | CHA-C1A-NA | -2.24 | 121.27 | 126.40 |
| 22 | B | 821 | CLA | CAA-C2A-C3A | -2.24 | 106.64 | 112.78 |
| 22 | A | 827 | CLA | C4-C3-C5 | 2.24 | 119.04 | 115.27 |
| 22 | B | 823 | CLA | CHD-C4C-NC | 2.24 | 127.73 | 124.20 |
| 22 | A | 818 | CLA | CAC-C3C-C4C | 2.24 | 127.72 | 124.81 |
| 25 | K | 4001 | BCR | C1-C6-C5 | -2.24 | 119.46 | 122.61 |
| 25 | B | 847 | BCR | C11-C12-C13 | -2.24 | 120.13 | 126.42 |
| 22 | 6 | 616 | CLA | CHB-C4A-NA | 2.24 | 127.61 | 124.51 |
| 22 | 9 | 603 | CLA | CAA-C2A-C3A | -2.24 | 106.65 | 112.78 |
| 22 | B | 820 | CLA | CBC-CAC-C3C | -2.24 | 106.26 | 112.43 |
| 22 | Z | 603 | CLA | O2D-CGD-O1D | -2.24 | 119.46 | 123.84 |
| 25 | B | 801 | BCR | C29-C30-C25 | 2.24 | 113.92 | 110.48 |
| 25 | K | 4004 | BCR | C11-C10-C9 | -2.24 | 124.12 | 127.31 |
| 22 | A | 816 | CLA | C1-C2-C3 | -2.24 | 122.17 | 126.04 |
| 30 | Z | 619 | LUT | C8-C7-C6 | -2.24 | 120.92 | 127.20 |
| 22 | B | 823 | CLA | CAA-CBA-CGA | -2.24 | 106.72 | 113.25 |
| 22 | 5 | 616 | CLA | O2D-CGD-O1D | -2.24 | 119.47 | 123.84 |
| 29 | 4 | 618 | CHL | C2A-C1A-CHA | -2.24 | 119.95 | 123.86 |
| 22 | 5 | 613 | CLA | CMC-C2C-C1C | 2.24 | 128.44 | 125.04 |
| 22 | A | 804 | CLA | CMB-C2B-C3B | 2.24 | 128.86 | 124.68 |
| 22 | 6 | 616 | CLA | CAA-C2A-C1A | -2.24 | 104.65 | 111.97 |
| 22 | 4 | 612 | CLA | CMC-C2C-C1C | 2.24 | 128.44 | 125.04 |
| 22 | A | 828 | CLA | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 22 | 1 | 614 | CLA | CBC-CAC-C3C | -2.23 | 106.27 | 112.43 |
| 21 | A | 801 | CL0 | CMC-C2C-C1C | 2.23 | 128.44 | 125.04 |
| 29 | 1 | 607 | CHL | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 22 | A | 836 | CLA | O2D-CGD-O1D | -2.23 | 119.47 | 123.84 |
| 22 | 6 | 613 | CLA | CMB-C2B-C3B | 2.23 | 128.85 | 124.68 |
| 29 | 4 | 608 | CHL | O2D-CGD-O1D | -2.23 | 119.47 | 123.84 |
| 22 | B | 828 | CLA | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 30 | 5 | 620 | LUT | C20-C13-C12 | 2.23 | 121.59 | 118.08 |
| 30 | 6 | 624 | LUT | C3-C4-C5 | -2.23 | 107.41 | 111.85 |
| 22 | A | 836 | CLA | CMA-C3A-C2A | -2.23 | 104.83 | 113.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30 | Z | 617 | LUT | C16-C1-C6 | -2.23 | 106.68 | 110.30 |
| 30 | 4 | 620 | LUT | C20-C13-C12 | 2.23 | 121.59 | 118.08 |
| 22 | 3 | 610 | CLA | CHB-C4A-NA | 2.23 | 127.60 | 124.51 |
| 22 | A | 809 | CLA | C1-O2A-CGA | 2.23 | 122.30 | 116.44 |
| 29 | 5 | 618 | CHL | O1D-CGD-CBD | -2.23 | 119.92 | 124.48 |
| 22 | 3 | 604 | CLA | O2D-CGD-O1D | -2.23 | 119.48 | 123.84 |
| 22 | Z | 602 | CLA | O2D-CGD-O1D | -2.23 | 119.48 | 123.84 |
| 22 | 5 | 612 | CLA | CAA-C2A-C3A | -2.23 | 106.67 | 112.78 |
| 22 | 5 | 604 | CLA | CMC-C2C-C1C | 2.23 | 128.43 | 125.04 |
| 29 | 9 | 606 | CHL | O2D-CGD-O1D | -2.23 | 119.48 | 123.84 |
| 22 | B | 836 | CLA | CHA-C1A-NA | -2.23 | 121.30 | 126.40 |
| 22 | A | 854 | CLA | CHB-C4A-NA | 2.23 | 127.59 | 124.51 |
| 22 | 3 | 606 | CLA | CHB-C4A-NA | 2.23 | 127.59 | 124.51 |
| 22 | Z | 612 | CLA | CHB-C4A-NA | 2.23 | 127.59 | 124.51 |
| 25 | A | 848 | BCR | C24-C23-C22 | -2.23 | 122.87 | 126.23 |
| 22 | 4 | 610 | CLA | CMA-C3A-C2A | -2.23 | 104.85 | 113.83 |
| 25 | A | 849 | BCR | C35-C13-C12 | 2.23 | 121.58 | 118.08 |
| 30 | 3 | 621 | LUT | C1-C2-C3 | 2.22 | 118.67 | 113.64 |
| 22 | 7 | 620 | CLA | CBC-CAC-C3C | -2.22 | 106.30 | 112.43 |
| 24 | A | 855 | LHG | C5-O7-C7 | -2.22 | 112.32 | 117.79 |
| 22 | A | 822 | CLA | CAA-CBA-CGA | 2.22 | 119.75 | 113.25 |
| 22 | A | 811 | CLA | CBC-CAC-C3C | -2.22 | 106.30 | 112.43 |
| 22 | Z | 616 | CLA | CMC-C2C-C1C | 2.22 | 128.42 | 125.04 |
| 22 | 7 | 610 | CLA | C4-C3-C5 | 2.22 | 119.01 | 115.27 |
| 22 | 8 | 613 | CLA | O2D-CGD-O1D | -2.22 | 119.49 | 123.84 |
| 25 | A | 856 | BCR | C23-C24-C25 | -2.22 | 120.96 | 127.20 |
| 25 | 8 | 619 | BCR | C7-C8-C9 | -2.22 | 122.88 | 126.23 |
| 22 | Z | 604 | CLA | CMC-C2C-C1C | 2.22 | 128.42 | 125.04 |
| 22 | Z | 606 | CLA | CMB-C2B-C3B | 2.22 | 128.83 | 124.68 |
| 22 | B | 825 | CLA | CMA-C3A-C2A | -2.22 | 104.87 | 113.83 |
| 22 | 3 | 602 | CLA | C4-C3-C5 | 2.22 | 119.00 | 115.27 |
| 22 | B | 832 | CLA | CMC-C2C-C1C | 2.22 | 128.42 | 125.04 |
| 22 | 3 | 607 | CLA | CBC-CAC-C3C | -2.22 | 106.31 | 112.43 |
| 29 | 1 | 607 | CHL | CBC-CAC-C3C | -2.22 | 106.31 | 112.43 |
| 22 | 2 | 613 | CLA | C5-C3-C4 | 2.22 | 119.50 | 114.60 |
| 25 | B | 845 | BCR | C10-C11-C12 | -2.22 | 116.29 | 123.22 |
| 22 | Z | 612 | CLA | CBC-CAC-C3C | -2.22 | 106.32 | 112.43 |
| 22 | 5 | 612 | CLA | CBC-CAC-C3C | -2.22 | 106.32 | 112.43 |
| 22 | A | 839 | CLA | O1D-CGD-CBD | -2.22 | 119.95 | 124.48 |
| 22 | 8 | 601 | CLA | C6-C7-C8 | -2.22 | 108.75 | 115.92 |
| 22 | 5 | 611 | CLA | CBC-CAC-C3C | -2.22 | 106.32 | 112.43 |
| 22 | 7 | 610 | CLA | C2A-C3A-C4A | -2.22 | 98.29 | 101.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | A | 807 | CLA | CMB-C2B-C3B | 2.22 | 128.82 | 124.68 |
| 25 | 3 | 719 | BCR | C34-C9-C8 | 2.22 | 121.57 | 118.08 |
| 22 | 6 | 612 | CLA | CMB-C2B-C3B | 2.21 | 128.82 | 124.68 |
| 25 | A | 849 | BCR | C21-C20-C19 | -2.21 | 116.31 | 123.22 |
| 22 | 8 | 612 | CLA | O2D-CGD-O1D | -2.21 | 119.51 | 123.84 |
| 29 | 4 | 606 | CHL | C1B-CHB-C4A | -2.21 | 125.73 | 130.12 |
| 22 | A | 823 | CLA | CMB-C2B-C3B | 2.21 | 128.82 | 124.68 |
| 22 | 3 | 613 | CLA | CAA-C2A-C3A | -2.21 | 106.72 | 112.78 |
| 22 | A | 802 | CLA | O2D-CGD-O1D | -2.21 | 119.51 | 123.84 |
| 22 | 6 | 610 | CLA | O2A-CGA-O1A | -2.21 | 118.01 | 123.59 |
| 30 | 3 | 621 | LUT | C20-C13-C12 | 2.21 | 121.56 | 118.08 |
| 22 | B | 818 | CLA | CAA-C2A-C3A | -2.21 | 106.72 | 112.78 |
| 22 | A | 854 | CLA | CHC-C1C-C2C | -2.21 | 120.61 | 126.72 |
| 22 | 4 | 602 | CLA | CMC-C2C-C1C | 2.21 | 128.41 | 125.04 |
| 30 | 8 | 618 | LUT | C16-C1-C6 | -2.21 | 106.71 | 110.30 |
| 30 | 2 | 617 | LUT | C3-C4-C5 | -2.21 | 107.45 | 111.85 |
| 22 | B | 852 | CLA | O2D-CGD-O1D | -2.21 | 119.52 | 123.84 |
| 22 | 5 | 606 | CLA | O2D-CGD-O1D | -2.21 | 119.52 | 123.84 |
| 22 | B | 815 | CLA | C1-C2-C3 | -2.21 | 122.22 | 126.04 |
| 22 | K | 4002 | CLA | CAA-C2A-C3A | -2.21 | 106.72 | 112.78 |
| 22 | Z | 603 | CLA | O2A-CGA-CBA | 2.21 | 118.84 | 111.91 |
| 22 | A | 802 | CLA | CED-O2D-CGD | 2.21 | 120.94 | 115.94 |
| 22 | 9 | 609 | CLA | CHD-C4C-NC | 2.21 | 127.69 | 124.20 |
| 22 | B | 836 | CLA | CMC-C2C-C1C | 2.21 | 128.40 | 125.04 |
| 22 | 3 | 620 | CLA | CHB-C4A-NA | 2.21 | 127.56 | 124.51 |
| 22 | A | 802 | CLA | O2A-CGA-CBA | 2.21 | 118.83 | 111.91 |
| 30 | Z | 617 | LUT | C28-C29-C30 | -2.21 | 115.55 | 118.94 |
| 22 | 7 | 620 | CLA | CMC-C2C-C1C | 2.21 | 128.40 | 125.04 |
| 22 | A | 836 | CLA | CMB-C2B-C3B | 2.21 | 128.81 | 124.68 |
| 22 | B | 825 | CLA | CAA-C2A-C1A | -2.21 | 104.74 | 111.97 |
| 22 | 2 | 609 | CLA | C5-C3-C4 | 2.21 | 119.47 | 114.60 |
| 22 | 8 | 606 | CLA | CHB-C4A-NA | 2.21 | 127.56 | 124.51 |
| 22 | A | 830 | CLA | CHB-C4A-NA | 2.20 | 127.56 | 124.51 |
| 25 | K | 4004 | BCR | C35-C13-C12 | 2.20 | 121.55 | 118.08 |
| 25 | 5 | 625 | BCR | C2-C1-C6 | 2.20 | 113.87 | 110.48 |
| 22 | A | 834 | CLA | C11-C10-C8 | -2.20 | 108.80 | 115.92 |
| 29 | 9 | 607 | CHL | CMB-C2B-C3B | 2.20 | 128.80 | 124.68 |
| 22 | A | 808 | CLA | O2A-CGA-CBA | 2.20 | 118.82 | 111.91 |
| 22 | B | 852 | CLA | CHB-C4A-NA | 2.20 | 127.56 | 124.51 |
| 22 | 1 | 606 | CLA | CHB-C4A-NA | 2.20 | 127.56 | 124.51 |
| 29 | 9 | 606 | CHL | CMB-C2B-C3B | 2.20 | 128.80 | 124.68 |
| 22 | Z | 604 | CLA | C1-C2-C3 | -2.20 | 122.23 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 827 | CLA | CHA-C1A-NA | -2.20 | 121.36 | 126.40 |
| 22 | B | 821 | CLA | CMC-C2C-C1C | 2.20 | 128.39 | 125.04 |
| 21 | A | 801 | CL0 | O2A-CGA-O1A | -2.20 | 118.04 | 123.59 |
| 22 | 5 | 606 | CLA | CMB-C2B-C3B | 2.20 | 128.80 | 124.68 |
| 22 | B | 830 | CLA | C5-C3-C4 | 2.20 | 119.46 | 114.60 |
| 25 | 4 | 621 | BCR | C21-C20-C19 | -2.20 | 116.35 | 123.22 |
| 22 | A | 834 | CLA | O2D-CGD-O1D | -2.20 | 119.54 | 123.84 |
| 25 | 3 | 718 | BCR | C23-C22-C21 | -2.20 | 115.57 | 118.94 |
| 22 | 4 | 603 | CLA | CMB-C2B-C3B | 2.20 | 128.79 | 124.68 |
| 29 | 5 | 607 | CHL | CBC-CAC-C3C | -2.20 | 106.37 | 112.43 |
| 22 | 7 | 609 | CLA | CBA-CAA-C2A | 2.20 | 120.35 | 113.86 |
| 22 | A | 826 | CLA | C1-C2-C3 | -2.20 | 122.24 | 126.04 |
| 22 | A | 831 | CLA | CMA-C3A-C2A | -2.20 | 104.96 | 113.83 |
| 22 | B | 805 | CLA | CHA-C1A-NA | -2.20 | 121.36 | 126.40 |
| 22 | B | 826 | CLA | CAC-C3C-C4C | 2.20 | 127.66 | 124.81 |
| 22 | 1 | 603 | CLA | O1D-CGD-CBD | -2.20 | 119.99 | 124.48 |
| 29 | 5 | 607 | CHL | CHD-C4C-NC | 2.20 | 127.67 | 124.20 |
| 22 | G | 204 | CLA | CBC-CAC-C3C | -2.20 | 106.37 | 112.43 |
| 22 | 2 | 612 | CLA | CBC-CAC-C3C | -2.20 | 106.37 | 112.43 |
| 22 | J | 3002 | CLA | CMC-C2C-C1C | 2.20 | 128.38 | 125.04 |
| 29 | 1 | 601 | CHL | C2A-C3A-C4A | -2.20 | 98.32 | 101.87 |
| 22 | 6 | 603 | CLA | CMB-C2B-C3B | 2.20 | 128.79 | 124.68 |
| 29 | Z | 601 | CHL | C2A-C3A-C4A | -2.20 | 98.32 | 101.87 |
| 22 | 8 | 614 | CLA | C1-C2-C3 | -2.19 | 122.25 | 126.04 |
| 30 | 8 | 617 | LUT | C16-C1-C6 | -2.19 | 106.74 | 110.30 |
| 22 | B | 810 | CLA | O2D-CGD-O1D | -2.19 | 119.55 | 123.84 |
| 29 | 6 | 608 | CHL | C1-C2-C3 | -2.19 | 123.20 | 126.75 |
| 22 | B | 813 | CLA | CHB-C4A-NA | 2.19 | 127.55 | 124.51 |
| 22 | 4 | 601 | CLA | CMB-C2B-C3B | 2.19 | 128.78 | 124.68 |
| 22 | B | 831 | CLA | CAA-C2A-C3A | -2.19 | 106.78 | 112.78 |
| 22 | 7 | 609 | CLA | C5-C3-C4 | 2.19 | 119.44 | 114.60 |
| 22 | 9 | 609 | CLA | C5-C3-C4 | 2.19 | 119.44 | 114.60 |
| 30 | 8 | 618 | LUT | C30-C31-C32 | -2.19 | 116.38 | 123.22 |
| 22 | 7 | 601 | CLA | C4-C3-C2 | -2.19 | 118.06 | 123.68 |
| 22 | 2 | 606 | CLA | CHB-C4A-NA | 2.19 | 127.54 | 124.51 |
| 25 | L | 201 | BCR | C21-C20-C19 | -2.19 | 116.38 | 123.22 |
| 22 | B | 826 | CLA | O1D-CGD-CBD | -2.19 | 120.00 | 124.48 |
| 22 | B | 825 | CLA | CMC-C2C-C1C | 2.19 | 128.37 | 125.04 |
| 25 | I | 172 | BCR | C2-C1-C6 | 2.19 | 113.85 | 110.48 |
| 22 | 3 | 612 | CLA | CHB-C4A-NA | 2.19 | 127.54 | 124.51 |
| 22 | 1 | 602 | CLA | O2D-CGD-O1D | -2.19 | 119.56 | 123.84 |
| 25 | B | 848 | BCR | C8-C9-C10 | -2.19 | 115.58 | 118.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 834 | CLA | C4-C3-C5 | 2.19 | 118.95 | 115.27 |
| 25 | B | 847 | BCR | C31-C1-C6 | -2.19 | 106.75 | 110.30 |
| 22 | 3 | 602 | CLA | O1D-CGD-CBD | -2.19 | 120.01 | 124.48 |
| 22 | 2 | 611 | CLA | CBC-CAC-C3C | -2.19 | 106.40 | 112.43 |
| 22 | F | 301 | CLA | O2A-CGA-O1A | -2.19 | 118.08 | 123.59 |
| 22 | B | 812 | CLA | O2A-CGA-CBA | 2.19 | 118.77 | 111.91 |
| 29 | 4 | 608 | CHL | C5-C3-C4 | 2.18 | 119.43 | 114.60 |
| 22 | 5 | 603 | CLA | CHB-C4A-NA | 2.18 | 127.53 | 124.51 |
| 21 | A | 801 | CL0 | CMB-C2B-C1B | 2.18 | 131.82 | 128.46 |
| 22 | 5 | 602 | CLA | CMB-C2B-C3B | 2.18 | 128.76 | 124.68 |
| 30 | 2 | 616 | LUT | C16-C1-C6 | -2.18 | 106.76 | 110.30 |
| 25 | A | 849 | BCR | C3-C4-C5 | -2.18 | 110.18 | 114.08 |
| 22 | 7 | 604 | CLA | C4-C3-C5 | 2.18 | 118.94 | 115.27 |
| 22 | Z | 612 | CLA | CMC-C2C-C1C | 2.18 | 128.36 | 125.04 |
| 30 | 1 | 618 | LUT | C39-C29-C28 | 2.18 | 121.52 | 118.08 |
| 22 | A | 821 | CLA | O1D-CGD-CBD | -2.18 | 120.02 | 124.48 |
| 30 | 8 | 618 | LUT | C19-C9-C8 | 2.18 | 121.52 | 118.08 |
| 29 | 8 | 607 | CHL | O2D-CGD-O1D | -2.18 | 119.57 | 123.84 |
| 25 | 6 | 623 | BCR | C1-C6-C7 | 2.18 | 121.95 | 115.78 |
| 22 | B | 828 | CLA | CMA-C3A-C2A | -2.18 | 105.03 | 113.83 |
| 25 | 3 | 717 | BCR | C29-C28-C27 | -2.18 | 106.50 | 111.38 |
| 29 | 6 | 608 | CHL | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 22 | 9 | 614 | CLA | CBC-CAC-C3C | -2.18 | 106.42 | 112.43 |
| 30 | Z | 618 | LUT | C20-C13-C12 | 2.18 | 121.51 | 118.08 |
| 22 | A | 802 | CLA | CMC-C2C-C1C | 2.18 | 128.36 | 125.04 |
| 22 | G | 203 | CLA | O2A-CGA-O1A | -2.18 | 118.09 | 123.59 |
| 22 | A | 820 | CLA | C1B-CHB-C4A | -2.18 | 125.80 | 130.12 |
| 22 | 4 | 601 | CLA | C4-C3-C5 | 2.18 | 118.94 | 115.27 |
| 22 | A | 809 | CLA | CAA-C2A-C3A | -2.18 | 106.81 | 112.78 |
| 22 | 5 | 616 | CLA | O2A-CGA-CBA | 2.18 | 120.84 | 112.23 |
| 25 | J | 3003 | BCR | C34-C9-C8 | 2.18 | 121.51 | 118.08 |
| 28 | J | 3001 | LMG | O3-C3-C2 | -2.18 | 105.31 | 110.35 |
| 25 | I | 172 | BCR | C16-C15-C14 | -2.18 | 119.01 | 123.47 |
| 22 | Z | 608 | CLA | CHB-C4A-NA | 2.18 | 127.52 | 124.51 |
| 22 | B | 813 | CLA | O1D-CGD-CBD | -2.18 | 120.03 | 124.48 |
| 30 | 5 | 624 | LUT | C1-C2-C3 | 2.18 | 118.56 | 113.64 |
| 22 | B | 807 | CLA | CMC-C2C-C1C | 2.18 | 128.35 | 125.04 |
| 29 | 6 | 607 | CHL | CMA-C3A-C4A | -2.18 | 105.92 | 111.77 |
| 30 | 6 | 624 | LUT | C39-C29-C28 | 2.18 | 121.51 | 118.08 |
| 25 | 8 | 619 | BCR | C2-C1-C6 | 2.18 | 113.83 | 110.48 |
| 22 | 6 | 612 | CLA | CHB-C4A-NA | 2.18 | 127.52 | 124.51 |
| 22 | 9 | 604 | CLA | CAA-C2A-C3A | -2.18 | 106.82 | 112.78 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 7 | 610 | CLA | CHC-C1C-C2C | -2.18 | 120.70 | 126.72 |
| 22 | 9 | 612 | CLA | CMC-C2C-C1C | 2.17 | 128.35 | 125.04 |
| 22 | A | 804 | CLA | CBC-CAC-C3C | -2.17 | 106.44 | 112.43 |
| 22 | A | 813 | CLA | CAA-C2A-C3A | -2.17 | 106.82 | 112.78 |
| 22 | Z | 610 | CLA | CHC-C1C-C2C | -2.17 | 120.71 | 126.72 |
| 25 | 3 | 717 | BCR | C11-C12-C13 | -2.17 | 120.31 | 126.42 |
| 22 | 7 | 606 | CLA | CMC-C2C-C1C | 2.17 | 128.35 | 125.04 |
| 29 | 6 | 608 | CHL | C5-C3-C4 | 2.17 | 119.41 | 114.60 |
| 29 | 9 | 606 | CHL | CAA-C2A-C3A | -2.17 | 111.03 | 116.10 |
| 29 | 4 | 618 | CHL | CHD-C4C-NC | 2.17 | 127.63 | 124.20 |
| 25 | 6 | 623 | BCR | C2-C1-C6 | 2.17 | 113.83 | 110.48 |
| 30 | 5 | 620 | LUT | C39-C29-C28 | 2.17 | 121.50 | 118.08 |
| 22 | 6 | 613 | CLA | CHB-C4A-NA | 2.17 | 127.52 | 124.51 |
| 22 | A | 817 | CLA | CHB-C4A-NA | 2.17 | 127.52 | 124.51 |
| 29 | 8 | 607 | CHL | CHB-C4A-NA | 2.17 | 127.52 | 124.51 |
| 22 | A | 831 | CLA | CMA-C3A-C4A | -2.17 | 105.94 | 111.77 |
| 30 | 8 | 618 | LUT | C20-C13-C12 | 2.17 | 121.50 | 118.08 |
| 22 | 9 | 603 | CLA | CMC-C2C-C1C | 2.17 | 128.35 | 125.04 |
| 22 | A | 825 | CLA | O2D-CGD-O1D | -2.17 | 119.59 | 123.84 |
| 22 | 7 | 602 | CLA | O1D-CGD-CBD | -2.17 | 120.04 | 124.48 |
| 22 | 9 | 602 | CLA | O1D-CGD-CBD | -2.17 | 120.04 | 124.48 |
| 22 | B | 832 | CLA | C1-C2-C3 | -2.17 | 122.29 | 126.04 |
| 22 | 5 | 612 | CLA | C1-C2-C3 | -2.17 | 122.29 | 126.04 |
| 22 | A | 816 | CLA | O2A-CGA-CBA | 2.17 | 118.72 | 111.91 |
| 22 | 2 | 614 | CLA | CMC-C2C-C1C | 2.17 | 128.34 | 125.04 |
| 22 | B | 802 | CLA | C4-C3-C5 | 2.17 | 118.92 | 115.27 |
| 22 | 4 | 609 | CLA | CBA-CAA-C2A | 2.17 | 120.27 | 113.86 |
| 22 | 5 | 621 | CLA | O2A-CGA-CBA | 2.17 | 120.80 | 112.23 |
| 22 | 7 | 611 | CLA | CBC-CAC-C3C | -2.17 | 106.45 | 112.43 |
| 22 | A | 840 | CLA | C1-O2A-CGA | 2.17 | 122.13 | 116.44 |
| 22 | J | 3002 | CLA | CBC-CAC-C3C | -2.17 | 106.45 | 112.43 |
| 22 | 8 | 603 | CLA | CMC-C2C-C1C | 2.17 | 128.34 | 125.04 |
| 25 | A | 849 | BCR | C8-C7-C6 | -2.17 | 121.11 | 127.20 |
| 25 | 3 | 719 | BCR | C16-C15-C14 | -2.17 | 119.03 | 123.47 |
| 30 | 2 | 617 | LUT | C18-C5-C4 | 2.17 | 118.37 | 114.36 |
| 22 | 6 | 614 | CLA | O2D-CGD-O1D | -2.17 | 119.60 | 123.84 |
| 22 | B | 820 | CLA | CMC-C2C-C1C | 2.17 | 128.34 | 125.04 |
| 22 | A | 830 | CLA | CMC-C2C-C1C | 2.17 | 128.34 | 125.04 |
| 29 | 7 | 607 | CHL | CHC-C1C-C2C | -2.17 | 118.25 | 126.11 |
| 24 | 8 | 620 | LHG | O8-C23-C24 | 2.17 | 118.71 | 111.91 |
| 22 | 2 | 607 | CLA | C5-C3-C4 | 2.17 | 119.39 | 114.60 |
| 22 | B | 809 | CLA | CMB-C2B-C3B | 2.17 | 128.73 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 29 | 9 | 607 | CHL | O1D-CGD-CBD | -2.17 | 120.05 | 124.48 |
| 22 | A | 824 | CLA | CHB-C4A-NA | 2.17 | 127.51 | 124.51 |
| 30 | 5 | 620 | LUT | C30-C31-C32 | -2.17 | 116.46 | 123.22 |
| 25 | F | 305 | BCR | C36-C18-C19 | 2.16 | 121.49 | 118.08 |
| 24 | A | 846 | LHG | C6-C5-C4 | -2.16 | 106.67 | 111.79 |
| 22 | A | 808 | CLA | C1-O2A-CGA | 2.16 | 122.12 | 116.44 |
| 22 | 1 | 609 | CLA | C4-C3-C5 | 2.16 | 118.91 | 115.27 |
| 30 | 1 | 617 | LUT | C38-C25-C24 | -2.16 | 118.93 | 123.56 |
| 24 | 8 | 620 | LHG | C6-C5-C4 | -2.16 | 106.67 | 111.79 |
| 22 | 6 | 611 | CLA | CMC-C2C-C1C | 2.16 | 128.33 | 125.04 |
| 29 | 1 | 601 | CHL | CHD-C4C-NC | 2.16 | 127.61 | 124.20 |
| 22 | A | 814 | CLA | O1D-CGD-CBD | -2.16 | 120.06 | 124.48 |
| 22 | Z | 604 | CLA | CMB-C2B-C3B | 2.16 | 128.72 | 124.68 |
| 25 | 5 | 622 | BCR | C23-C24-C25 | -2.16 | 121.13 | 127.20 |
| 25 | 6 | 625 | BCR | C23-C24-C25 | -2.16 | 121.13 | 127.20 |
| 25 | G | 205 | BCR | C15-C14-C13 | -2.16 | 124.22 | 127.31 |
| 22 | G | 203 | CLA | CHB-C4A-NA | 2.16 | 127.50 | 124.51 |
| 22 | 6 | 602 | CLA | O2D-CGD-O1D | -2.16 | 119.61 | 123.84 |
| 22 | 7 | 601 | CLA | C1-C2-C3 | -2.16 | 122.30 | 126.04 |
| 22 | A | 819 | CLA | CHA-C1A-NA | -2.16 | 121.45 | 126.40 |
| 22 | A | 833 | CLA | C1-C2-C3 | -2.16 | 122.31 | 126.04 |
| 22 | Z | 616 | CLA | CBC-CAC-C3C | -2.16 | 106.47 | 112.43 |
| 25 | A | 848 | BCR | C10-C11-C12 | -2.16 | 116.47 | 123.22 |
| 25 | K | 4004 | BCR | C20-C19-C18 | -2.16 | 120.35 | 126.42 |
| 22 | 2 | 607 | CLA | CBC-CAC-C3C | -2.16 | 106.48 | 112.43 |
| 22 | B | 837 | CLA | O1D-CGD-CBD | -2.16 | 120.06 | 124.48 |
| 22 | A | 840 | CLA | CHA-C1A-NA | -2.16 | 121.45 | 126.40 |
| 30 | Z | 618 | LUT | C35-C15-C14 | -2.16 | 119.05 | 123.47 |
| 25 | A | 850 | BCR | C32-C1-C6 | 2.16 | 113.80 | 110.30 |
| 22 | 5 | 611 | CLA | CMC-C2C-C1C | 2.16 | 128.33 | 125.04 |
| 22 | 8 | 613 | CLA | CAA-C2A-C3A | -2.16 | 106.87 | 112.78 |
| 22 | 2 | 609 | CLA | O2D-CGD-O1D | -2.16 | 119.62 | 123.84 |
| 22 | B | 822 | CLA | CBC-CAC-C3C | -2.16 | 106.48 | 112.43 |
| 22 | B | 833 | CLA | CAA-CBA-CGA | -2.16 | 106.95 | 113.25 |
| 22 | 6 | 604 | CLA | C1-C2-C3 | -2.16 | 122.31 | 126.04 |
| 22 | B | 828 | CLA | O2D-CGD-O1D | -2.15 | 119.62 | 123.84 |
| 22 | 6 | 609 | CLA | C5-C3-C4 | 2.15 | 119.36 | 114.60 |
| 22 | A | 818 | CLA | C4-C3-C2 | -2.15 | 118.15 | 123.68 |
| 25 | L | 201 | BCR | C15-C16-C17 | -2.15 | 119.06 | 123.47 |
| 25 | 7 | 624 | BCR | C37-C22-C23 | 2.15 | 121.47 | 118.08 |
| 22 | B | 833 | CLA | O1D-CGD-CBD | -2.15 | 120.08 | 124.48 |
| 22 | 5 | 604 | CLA | O2D-CGD-O1D | -2.15 | 119.63 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | L | 204 | CLA | C5-C3-C4 | 2.15 | 119.36 | 114.60 |
| 22 | 8 | 611 | CLA | CMC-C2C-C1C | 2.15 | 128.32 | 125.04 |
| 22 | 9 | 613 | CLA | CMB-C2B-C3B | 2.15 | 128.71 | 124.68 |
| 22 | 8 | 614 | CLA | CMC-C2C-C1C | 2.15 | 128.32 | 125.04 |
| 22 | Z | 603 | CLA | CMB-C2B-C3B | 2.15 | 128.70 | 124.68 |
| 22 | A | 828 | CLA | OBD-CAD-C3D | -2.15 | 123.34 | 128.52 |
| 22 | 9 | 602 | CLA | C1-C2-C3 | -2.15 | 122.32 | 126.04 |
| 22 | B | 839 | CLA | CHB-C4A-NA | 2.15 | 127.49 | 124.51 |
| 22 | 2 | 601 | CLA | CMC-C2C-C1C | 2.15 | 128.31 | 125.04 |
| 25 | 3 | 718 | BCR | C4-C5-C6 | -2.15 | 119.61 | 122.73 |
| 22 | 3 | 617 | CLA | O1D-CGD-CBD | -2.15 | 120.08 | 124.48 |
| 29 | 3 | 608 | CHL | C2A-C3A-C4A | -2.15 | 98.40 | 101.87 |
| 29 | 9 | 607 | CHL | C5-C3-C4 | 2.15 | 119.35 | 114.60 |
| 22 | Z | 613 | CLA | CBC-CAC-C3C | -2.15 | 106.50 | 112.43 |
| 22 | 1 | 609 | CLA | O2A-CGA-O1A | -2.15 | 118.17 | 123.59 |
| 22 | 9 | 604 | CLA | CBC-CAC-C3C | -2.15 | 106.51 | 112.43 |
| 22 | B | 852 | CLA | C1-C2-C3 | -2.15 | 122.33 | 126.04 |
| 22 | B | 811 | CLA | CBC-CAC-C3C | -2.15 | 106.51 | 112.43 |
| 22 | 8 | 614 | CLA | O2A-CGA-O1A | -2.15 | 118.17 | 123.59 |
| 22 | B | 818 | CLA | O1D-CGD-CBD | -2.15 | 120.09 | 124.48 |
| 22 | A | 811 | CLA | C1-O2A-CGA | 2.15 | 122.08 | 116.44 |
| 22 | Z | 603 | CLA | CHA-C1A-NA | -2.15 | 121.48 | 126.40 |
| 29 | 9 | 607 | CHL | C1-C2-C3 | -2.15 | 123.28 | 126.75 |
| 30 | 9 | 616 | LUT | C21-C26-C27 | -2.15 | 109.99 | 112.70 |
| 25 | 6 | 625 | BCR | C2-C1-C6 | 2.15 | 113.79 | 110.48 |
| 22 | B | 852 | CLA | O2A-CGA-O1A | -2.15 | 118.17 | 123.59 |
| 22 | A | 823 | CLA | CHB-C4A-NA | 2.15 | 127.48 | 124.51 |
| 22 | 9 | 603 | CLA | CHA-C1A-NA | -2.15 | 121.48 | 126.40 |
| 22 | Z | 603 | CLA | CAA-C2A-C3A | -2.15 | 106.90 | 112.78 |
| 30 | Z | 618 | LUT | C40-C33-C32 | 2.15 | 121.46 | 118.08 |
| 22 | B | 834 | CLA | O2D-CGD-O1D | -2.15 | 119.64 | 123.84 |
| 22 | 8 | 611 | CLA | CED-O2D-CGD | 2.14 | 120.79 | 115.94 |
| 29 | 6 | 606 | CHL | C2A-C1A-CHA | -2.14 | 120.11 | 123.86 |
| 22 | 2 | 614 | CLA | CHB-C4A-NA | 2.14 | 127.48 | 124.51 |
| 22 | 5 | 614 | CLA | CAA-C2A-C3A | -2.14 | 106.91 | 112.78 |
| 22 | B | 818 | CLA | C1B-CHB-C4A | -2.14 | 125.87 | 130.12 |
| 22 | B | 823 | CLA | O2D-CGD-O1D | -2.14 | 119.65 | 123.84 |
| 25 | 6 | 625 | BCR | C33-C5-C6 | -2.14 | 122.12 | 124.53 |
| 29 | 6 | 618 | CHL | CHB-C4A-NA | 2.14 | 127.48 | 124.51 |
| 22 | 2 | 613 | CLA | CBC-CAC-C3C | -2.14 | 106.52 | 112.43 |
| 22 | 9 | 610 | CLA | C6-C7-C8 | -2.14 | 108.99 | 115.92 |
| 22 | F | 303 | CLA | CMC-C2C-C1C | 2.14 | 128.30 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | B | 803 | CLA | C1C-C2C-C3C | -2.14 | 104.70 | 106.96 |
| 22 | B | 810 | CLA | C1-C2-C3 | -2.14 | 122.34 | 126.04 |
| 22 | A | 838 | CLA | O1D-CGD-CBD | -2.14 | 120.10 | 124.48 |
| 22 | 3 | 603 | CLA | CHA-C1A-NA | -2.14 | 121.49 | 126.40 |
| 22 | A | 837 | CLA | CMC-C2C-C1C | 2.14 | 128.30 | 125.04 |
| 29 | 6 | 606 | CHL | CMB-C2B-C3B | 2.14 | 128.68 | 124.68 |
| 24 | 8 | 620 | LHG | C5-O7-C7 | -2.14 | 112.52 | 117.79 |
| 22 | Z | 611 | CLA | C4-C3-C5 | 2.14 | 118.87 | 115.27 |
| 22 | 6 | 609 | CLA | CHA-C1A-NA | -2.14 | 121.50 | 126.40 |
| 22 | 1 | 611 | CLA | C1-C2-C3 | -2.14 | 122.34 | 126.04 |
| 22 | B | 830 | CLA | CMC-C2C-C1C | 2.14 | 128.30 | 125.04 |
| 30 | 9 | 617 | LUT | C38-C25-C24 | -2.14 | 118.98 | 123.56 |
| 22 | G | 203 | CLA | C5-C3-C4 | 2.14 | 119.33 | 114.60 |
| 22 | A | 817 | CLA | CAA-C2A-C3A | -2.14 | 106.92 | 112.78 |
| 22 | 6 | 616 | CLA | O2A-CGA-CBA | 2.14 | 120.68 | 112.23 |
| 22 | A | 834 | CLA | CMC-C2C-C1C | 2.14 | 128.29 | 125.04 |
| 25 | B | 848 | BCR | C37-C22-C23 | 2.14 | 121.44 | 118.08 |
| 22 | 4 | 611 | CLA | CMC-C2C-C1C | 2.14 | 128.29 | 125.04 |
| 22 | 3 | 614 | CLA | CBC-CAC-C3C | -2.14 | 106.54 | 112.43 |
| 22 | A | 817 | CLA | C1-C2-C3 | -2.14 | 122.35 | 126.04 |
| 28 | J | 3001 | LMG | O2-C2-C1 | -2.14 | 104.86 | 110.05 |
| 22 | B | 803 | CLA | C1B-CHB-C4A | -2.14 | 125.89 | 130.12 |
| 22 | 4 | 601 | CLA | O1D-CGD-CBD | -2.13 | 120.12 | 124.48 |
| 25 | L | 201 | BCR | C37-C22-C23 | 2.13 | 121.44 | 118.08 |
| 22 | 6 | 604 | CLA | CBC-CAC-C3C | -2.13 | 106.55 | 112.43 |
| 24 | 8 | 620 | LHG | C25-C24-C23 | -2.13 | 105.86 | 113.62 |
| 22 | 7 | 608 | CLA | C5-C3-C4 | 2.13 | 119.31 | 114.60 |
| 22 | 2 | 613 | CLA | O1D-CGD-CBD | -2.13 | 120.12 | 124.48 |
| 22 | B | 838 | CLA | O2A-CGA-O1A | -2.13 | 118.21 | 123.59 |
| 22 | 5 | 604 | CLA | CBC-CAC-C3C | -2.13 | 106.55 | 112.43 |
| 22 | 9 | 601 | CLA | CMC-C2C-C1C | 2.13 | 128.29 | 125.04 |
| 25 | 6 | 623 | BCR | C29-C30-C25 | 2.13 | 113.76 | 110.48 |
| 22 | A | 810 | CLA | O2D-CGD-O1D | -2.13 | 119.67 | 123.84 |
| 22 | 4 | 610 | CLA | C4-C3-C5 | 2.13 | 118.86 | 115.27 |
| 22 | Z | 608 | CLA | CBC-CAC-C3C | -2.13 | 106.56 | 112.43 |
| 22 | B | 839 | CLA | C1-O2A-CGA | 2.13 | 122.03 | 116.44 |
| 22 | 3 | 612 | CLA | O2A-CGA-CBA | 2.13 | 120.65 | 112.23 |
| 22 | 3 | 609 | CLA | CMA-C3A-C4A | -2.13 | 106.05 | 111.77 |
| 30 | 6 | 624 | LUT | C19-C9-C8 | 2.13 | 121.43 | 118.08 |
| 22 | 8 | 601 | CLA | CHA-C1A-NA | -2.13 | 121.52 | 126.40 |
| 22 | B | 827 | CLA | C6-C7-C8 | -2.13 | 109.03 | 115.92 |
| 25 | J | 3003 | BCR | C31-C1-C6 | -2.13 | 106.84 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 4 | 610 | CLA | O1D-CGD-CBD | -2.13 | 120.13 | 124.48 |
| 22 | 5 | 613 | CLA | CMB-C2B-C3B | 2.13 | 128.66 | 124.68 |
| 30 | 4 | 619 | LUT | C21-C26-C27 | -2.13 | 110.01 | 112.70 |
| 30 | 1 | 617 | LUT | C19-C9-C8 | 2.13 | 121.43 | 118.08 |
| 30 | 7 | 622 | LUT | C20-C13-C12 | 2.13 | 121.43 | 118.08 |
| 22 | A | 818 | CLA | CMB-C2B-C3B | 2.13 | 128.66 | 124.68 |
| 22 | B | 809 | CLA | C1-C2-C3 | -2.13 | 122.36 | 126.04 |
| 22 | A | 817 | CLA | C4-C3-C5 | 2.13 | 118.85 | 115.27 |
| 22 | L | 204 | CLA | CMB-C2B-C3B | 2.13 | 128.66 | 124.68 |
| 22 | 5 | 601 | CLA | O1D-CGD-CBD | -2.13 | 120.13 | 124.48 |
| 22 | A | 838 | CLA | CBC-CAC-C3C | -2.13 | 106.57 | 112.43 |
| 22 | B | 818 | CLA | CHA-C1A-NA | -2.13 | 121.53 | 126.40 |
| 22 | A | 824 | CLA | O1D-CGD-CBD | -2.12 | 120.14 | 124.48 |
| 22 | 9 | 603 | CLA | CHB-C4A-NA | 2.12 | 127.45 | 124.51 |
| 22 | B | 829 | CLA | C2A-C1A-CHA | -2.12 | 120.14 | 123.86 |
| 22 | 4 | 612 | CLA | O2A-CGA-O1A | -2.12 | 118.23 | 123.59 |
| 22 | K | 4002 | CLA | CBC-CAC-C3C | -2.12 | 106.57 | 112.43 |
| 22 | A | 824 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 24 | 1 | 620 | LHG | C5-O7-C7 | -2.12 | 112.56 | 117.79 |
| 25 | A | 850 | BCR | C21-C20-C19 | -2.12 | 116.59 | 123.22 |
| 22 | A | 840 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 22 | 7 | 612 | CLA | CAA-C2A-C3A | -2.12 | 106.96 | 112.78 |
| 29 | 6 | 618 | CHL | C1B-CHB-C4A | -2.12 | 125.91 | 130.12 |
| 29 | 8 | 607 | CHL | C1-C2-C3 | -2.12 | 122.37 | 126.04 |
| 22 | 5 | 614 | CLA | CHA-C1A-NA | -2.12 | 121.54 | 126.40 |
| 22 | A | 820 | CLA | O1D-CGD-CBD | -2.12 | 120.14 | 124.48 |
| 22 | 6 | 601 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 22 | A | 808 | CLA | CBC-CAC-C3C | -2.12 | 106.58 | 112.43 |
| 22 | A | 827 | CLA | CGD-CBD-CAD | -2.12 | 103.86 | 110.73 |
| 22 | 7 | 611 | CLA | C2A-C3A-C4A | -2.12 | 99.08 | 101.78 |
| 22 | Z | 614 | CLA | CMA-C3A-C4A | -2.12 | 106.07 | 111.77 |
| 25 | A | 856 | BCR | C34-C9-C8 | 2.12 | 121.42 | 118.08 |
| 22 | B | 805 | CLA | CMB-C2B-C3B | 2.12 | 128.65 | 124.68 |
| 22 | L | 203 | CLA | C1-C2-C3 | -2.12 | 122.38 | 126.04 |
| 22 | 5 | 614 | CLA | CGD-CBD-CAD | -2.12 | 103.87 | 110.73 |
| 29 | Z | 607 | CHL | C2A-C1A-CHA | -2.12 | 120.15 | 123.86 |
| 22 | 2 | 603 | CLA | O2A-CGA-CBA | 2.12 | 120.61 | 112.23 |
| 25 | L | 205 | BCR | C35-C13-C12 | 2.12 | 121.42 | 118.08 |
| 22 | 2 | 612 | CLA | CAA-C2A-C3A | -2.12 | 106.97 | 112.78 |
| 22 | 8 | 603 | CLA | CMB-C2B-C3B | 2.12 | 128.64 | 124.68 |
| 22 | 6 | 603 | CLA | CHB-C4A-NA | 2.12 | 127.44 | 124.51 |
| 22 | 9 | 603 | CLA | CMB-C2B-C3B | 2.12 | 128.64 | 124.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | A | 813 | CLA | CHA-C1A-NA | -2.12 | 121.55 | 126.40 |
| 25 | 8 | 619 | BCR | C23-C22-C21 | -2.12 | 115.69 | 118.94 |
| 30 | 1 | 617 | LUT | C18-C5-C6 | -2.12 | 122.15 | 124.53 |
| 22 | 2 | 614 | CLA | O2D-CGD-O1D | -2.12 | 119.70 | 123.84 |
| 30 | 5 | 624 | LUT | C7-C8-C9 | -2.12 | 123.03 | 126.23 |
| 22 | 7 | 602 | CLA | CBC-CAC-C3C | -2.12 | 106.59 | 112.43 |
| 22 | A | 830 | CLA | O2D-CGD-O1D | -2.12 | 119.70 | 123.84 |
| 22 | A | 829 | CLA | CMA-C3A-C2A | -2.12 | 105.28 | 113.83 |
| 22 | 1 | 603 | CLA | C1-C2-C3 | -2.12 | 122.38 | 126.04 |
| 30 | 4 | 620 | LUT | C21-C26-C27 | -2.12 | 110.03 | 112.70 |
| 22 | 3 | 602 | CLA | C1B-CHB-C4A | -2.12 | 125.92 | 130.12 |
| 25 | 7 | 624 | BCR | C21-C20-C19 | -2.12 | 116.61 | 123.22 |
| 22 | B | 825 | CLA | C1-C2-C3 | -2.12 | 122.38 | 126.04 |
| 25 | B | 843 | BCR | C36-C18-C19 | 2.12 | 121.41 | 118.08 |
| 22 | Z | 610 | CLA | CBC-CAC-C3C | -2.12 | 106.60 | 112.43 |
| 22 | B | 819 | CLA | CMC-C2C-C1C | 2.12 | 128.26 | 125.04 |
| 22 | 4 | 604 | CLA | C5-C3-C4 | 2.12 | 119.28 | 114.60 |
| 22 | 7 | 611 | CLA | CMC-C2C-C1C | 2.12 | 128.26 | 125.04 |
| 22 | 3 | 620 | CLA | O2D-CGD-O1D | -2.11 | 119.70 | 123.84 |
| 22 | 1 | 616 | CLA | CMB-C2B-C3B | 2.11 | 128.63 | 124.68 |
| 22 | Z | 606 | CLA | O1D-CGD-CBD | -2.11 | 120.16 | 124.48 |
| 29 | 6 | 607 | CHL | CHD-C4C-NC | 2.11 | 127.53 | 124.20 |
| 22 | 3 | 609 | CLA | O2D-CGD-O1D | -2.11 | 119.70 | 123.84 |
| 22 | 6 | 613 | CLA | O2D-CGD-O1D | -2.11 | 119.70 | 123.84 |
| 22 | 9 | 611 | CLA | C1-C2-C3 | -2.11 | 122.39 | 126.04 |
| 22 | 6 | 614 | CLA | CMC-C2C-C1C | 2.11 | 128.26 | 125.04 |
| 30 | 8 | 617 | LUT | C1-C2-C3 | 2.11 | 118.41 | 113.64 |
| 22 | 1 | 608 | CLA | CHB-C4A-NA | 2.11 | 127.43 | 124.51 |
| 22 | 1 | 608 | CLA | C1-C2-C3 | -2.11 | 122.39 | 126.04 |
| 22 | 1 | 604 | CLA | CMD-C2D-C3D | -2.11 | 122.76 | 127.61 |
| 30 | 2 | 617 | LUT | C16-C1-C6 | -2.11 | 106.88 | 110.30 |
| 25 | B | 845 | BCR | C23-C22-C21 | 2.11 | 122.18 | 118.94 |
| 22 | B | 804 | CLA | O2A-CGA-CBA | 2.11 | 120.81 | 114.03 |
| 22 | 8 | 606 | CLA | CMB-C2B-C3B | 2.11 | 128.62 | 124.68 |
| 30 | 2 | 616 | LUT | C10-C11-C12 | -2.11 | 116.64 | 123.22 |
| 29 | 4 | 606 | CHL | O2D-CGD-O1D | -2.11 | 119.72 | 123.84 |
| 22 | A | 831 | CLA | O1D-CGD-CBD | -2.11 | 120.17 | 124.48 |
| 22 | B | 829 | CLA | CMA-C3A-C4A | -2.11 | 106.11 | 111.77 |
| 22 | A | 832 | CLA | CAA-C2A-C3A | -2.11 | 107.01 | 112.78 |
| 22 | B | 833 | CLA | CHB-C4A-NA | 2.11 | 127.42 | 124.51 |
| 22 | B | 835 | CLA | CMC-C2C-C1C | 2.11 | 128.25 | 125.04 |
| 22 | B | 841 | CLA | O2A-CGA-O1A | -2.10 | 118.28 | 123.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | B | 847 | BCR | C8-C9-C10 | -2.10 | 115.71 | 118.94 |
| 29 | 4 | 608 | CHL | C1B-CHB-C4A | -2.10 | 125.95 | 130.12 |
| 22 | A | 841 | CLA | O2D-CGD-O1D | -2.10 | 119.72 | 123.84 |
| 22 | 7 | 613 | CLA | CMC-C2C-C1C | 2.10 | 128.24 | 125.04 |
| 25 | A | 851 | BCR | C7-C8-C9 | -2.10 | 123.06 | 126.23 |
| 22 | B | 814 | CLA | C4-C3-C5 | 2.10 | 118.81 | 115.27 |
| 22 | 5 | 609 | CLA | CBC-CAC-C3C | -2.10 | 106.63 | 112.43 |
| 22 | 7 | 610 | CLA | CHB-C4A-NA | 2.10 | 127.42 | 124.51 |
| 22 | 6 | 617 | CLA | CHA-C1A-NA | -2.10 | 121.58 | 126.40 |
| 22 | 6 | 614 | CLA | CBC-CAC-C3C | -2.10 | 106.63 | 112.43 |
| 22 | B | 822 | CLA | O2D-CGD-O1D | -2.10 | 119.73 | 123.84 |
| 22 | A | 825 | CLA | CBC-CAC-C3C | -2.10 | 106.64 | 112.43 |
| 22 | 9 | 613 | CLA | C5-C3-C4 | 2.10 | 119.25 | 114.60 |
| 22 | 4 | 604 | CLA | CED-O2D-CGD | 2.10 | 120.69 | 115.94 |
| 22 | A | 829 | CLA | O2A-CGA-CBA | 2.10 | 118.50 | 111.91 |
| 22 | B | 806 | CLA | CBC-CAC-C3C | -2.10 | 106.64 | 112.43 |
| 22 | B | 815 | CLA | C1-O2A-CGA | 2.10 | 121.96 | 116.44 |
| 22 | 9 | 604 | CLA | CMC-C2C-C1C | 2.10 | 128.24 | 125.04 |
| 25 | A | 852 | BCR | C37-C22-C23 | 2.10 | 121.39 | 118.08 |
| 22 | B | 825 | CLA | O2D-CGD-O1D | -2.10 | 119.73 | 123.84 |
| 22 | 6 | 617 | CLA | CBC-CAC-C3C | -2.10 | 106.65 | 112.43 |
| 29 | 3 | 608 | CHL | C1B-CHB-C4A | -2.10 | 125.96 | 130.12 |
| 30 | 5 | 620 | LUT | C18-C5-C4 | 2.10 | 118.24 | 114.36 |
| 30 | Z | 617 | LUT | C8-C9-C10 | -2.10 | 115.72 | 118.94 |
| 30 | 7 | 622 | LUT | C16-C1-C6 | -2.10 | 106.90 | 110.30 |
| 22 | 6 | 616 | CLA | C2A-C3A-C4A | -2.10 | 98.48 | 101.87 |
| 29 | 9 | 606 | CHL | CHB-C4A-NA | 2.10 | 127.41 | 124.51 |
| 22 | 9 | 614 | CLA | O2A-CGA-CBA | 2.10 | 120.76 | 114.03 |
| 22 | 4 | 604 | CLA | O2A-CGA-CBA | 2.09 | 118.48 | 111.91 |
| 29 | 5 | 608 | CHL | C5-C3-C4 | 2.09 | 119.23 | 114.60 |
| 22 | 8 | 603 | CLA | CHA-C1A-NA | -2.09 | 121.60 | 126.40 |
| 25 | 3 | 718 | BCR | C15-C16-C17 | -2.09 | 119.19 | 123.47 |
| 29 | 4 | 607 | CHL | C5-C3-C4 | 2.09 | 119.22 | 114.60 |
| 22 | 2 | 606 | CLA | C2A-C3A-C4A | -2.09 | 99.11 | 101.78 |
| 29 | 4 | 608 | CHL | CBC-CAC-C3C | -2.09 | 106.66 | 112.43 |
| 22 | 9 | 601 | CLA | CBC-CAC-C3C | -2.09 | 106.67 | 112.43 |
| 22 | Z | 614 | CLA | O2D-CGD-O1D | -2.09 | 119.75 | 123.84 |
| 22 | 2 | 610 | CLA | CHB-C4A-NA | 2.09 | 127.40 | 124.51 |
| 25 | K | 4001 | BCR | C4-C5-C6 | -2.09 | 119.69 | 122.73 |
| 25 | A | 849 | BCR | C11-C12-C13 | -2.09 | 120.54 | 126.42 |
| 30 | 2 | 617 | LUT | C1-C2-C3 | 2.09 | 118.36 | 113.64 |
| 25 | B | 846 | BCR | C16-C15-C14 | -2.09 | 119.19 | 123.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 6 | 604 | CLA | CMB-C2B-C3B | 2.09 | 128.59 | 124.68 |
| 22 | 4 | 614 | CLA | CMA-C3A-C4A | -2.09 | 106.16 | 111.77 |
| 29 | 3 | 608 | CHL | C1-C2-C3 | -2.09 | 122.43 | 126.04 |
| 22 | A | 822 | CLA | CBC-CAC-C3C | -2.09 | 106.68 | 112.43 |
| 29 | 6 | 618 | CHL | CHD-C4C-NC | 2.09 | 127.49 | 124.20 |
| 22 | F | 301 | CLA | CHA-C1A-NA | -2.09 | 121.62 | 126.40 |
| 22 | B | 827 | CLA | C4-C3-C5 | 2.09 | 118.78 | 115.27 |
| 22 | 7 | 603 | CLA | CAA-CBA-CGA | -2.09 | 107.15 | 113.25 |
| 22 | A | 826 | CLA | CMB-C2B-C1B | 2.09 | 131.67 | 128.46 |
| 22 | 2 | 603 | CLA | CHA-C1A-NA | -2.09 | 121.62 | 126.40 |
| 30 | 9 | 617 | LUT | C3-C4-C5 | -2.09 | 107.70 | 111.85 |
| 22 | 9 | 603 | CLA | O2A-CGA-CBA | 2.09 | 120.47 | 112.23 |
| 25 | 3 | 718 | BCR | C20-C21-C22 | -2.09 | 124.33 | 127.31 |
| 25 | B | 844 | BCR | C11-C12-C13 | -2.08 | 120.56 | 126.42 |
| 22 | A | 826 | CLA | CMC-C2C-C1C | 2.08 | 128.21 | 125.04 |
| 29 | 3 | 608 | CHL | CMB-C2B-C3B | 2.08 | 128.58 | 124.68 |
| 22 | A | 816 | CLA | O1D-CGD-CBD | -2.08 | 120.22 | 124.48 |
| 22 | 8 | 609 | CLA | CHA-C1A-NA | -2.08 | 121.63 | 126.40 |
| 30 | 6 | 624 | LUT | C20-C13-C12 | 2.08 | 121.36 | 118.08 |
| 30 | Z | 619 | LUT | C1-C2-C3 | 2.08 | 118.35 | 113.64 |
| 22 | 3 | 610 | CLA | C2A-C1A-CHA | -2.08 | 120.22 | 123.86 |
| 25 | A | 848 | BCR | C21-C20-C19 | -2.08 | 116.72 | 123.22 |
| 22 | 4 | 613 | CLA | CMB-C2B-C3B | 2.08 | 128.57 | 124.68 |
| 29 | 8 | 607 | CHL | CMB-C2B-C3B | 2.08 | 128.57 | 124.68 |
| 22 | G | 204 | CLA | CMC-C2C-C1C | 2.08 | 128.21 | 125.04 |
| 22 | 8 | 609 | CLA | CMA-C3A-C2A | -2.08 | 105.43 | 113.83 |
| 22 | B | 820 | CLA | O1D-CGD-CBD | -2.08 | 120.23 | 124.48 |
| 22 | B | 811 | CLA | C1-C2-C3 | -2.08 | 122.44 | 126.04 |
| 29 | 6 | 608 | CHL | CAA-C2A-C1A | -2.08 | 105.16 | 111.97 |
| 30 | Z | 617 | LUT | C12-C13-C14 | -2.08 | 115.75 | 118.94 |
| 22 | A | 841 | CLA | C11-C10-C8 | -2.08 | 109.20 | 115.92 |
| 22 | A | 836 | CLA | C5-C3-C4 | 2.08 | 119.20 | 114.60 |
| 22 | 1 | 612 | CLA | C1-O2A-CGA | 2.08 | 121.90 | 116.44 |
| 22 | 2 | 614 | CLA | CHA-C1A-NA | -2.08 | 121.64 | 126.40 |
| 25 | K | 4004 | BCR | C35-C13-C14 | -2.08 | 120.01 | 122.92 |
| 22 | A | 843 | CLA | O2D-CGD-O1D | -2.08 | 119.77 | 123.84 |
| 22 | A | 843 | CLA | CED-O2D-CGD | 2.08 | 120.64 | 115.94 |
| 22 | 4 | 616 | CLA | O2D-CGD-O1D | -2.08 | 119.78 | 123.84 |
| 29 | 9 | 607 | CHL | CHB-C4A-NA | 2.08 | 127.39 | 124.51 |
| 22 | 3 | 604 | CLA | CMB-C2B-C3B | 2.08 | 128.56 | 124.68 |
| 22 | 8 | 602 | CLA | CMB-C2B-C3B | 2.08 | 128.56 | 124.68 |
| 22 | A | 836 | CLA | CMC-C2C-C1C | 2.08 | 128.20 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22 | 5 | 621 | CLA | CHD-C4C-NC | 2.08 | 127.48 | 124.20 |
| 25 | A | 849 | BCR | C20-C19-C18 | -2.08 | 120.58 | 126.42 |
| 30 | 4 | 620 | LUT | C30-C31-C32 | -2.08 | 116.74 | 123.22 |
| 22 | 8 | 612 | CLA | C4-C3-C2 | -2.08 | 118.35 | 123.68 |
| 22 | 1 | 604 | CLA | CAA-C2A-C3A | -2.08 | 107.09 | 112.78 |
| 30 | 1 | 618 | LUT | C11-C10-C9 | -2.08 | 124.35 | 127.31 |
| 25 | 7 | 623 | BCR | C10-C11-C12 | -2.08 | 116.74 | 123.22 |
| 22 | 3 | 613 | CLA | O1D-CGD-CBD | -2.08 | 120.24 | 124.48 |
| 22 | 6 | 603 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 22 | 8 | 601 | CLA | C16-C15-C13 | -2.07 | 109.21 | 115.92 |
| 22 | B | 811 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 22 | 1 | 616 | CLA | O2A-CGA-CBA | 2.07 | 120.43 | 112.23 |
| 22 | 8 | 612 | CLA | CED-O2D-CGD | 2.07 | 120.63 | 115.94 |
| 22 | A | 812 | CLA | CMC-C2C-C1C | 2.07 | 128.20 | 125.04 |
| 22 | 8 | 610 | CLA | O1D-CGD-CBD | -2.07 | 120.24 | 124.48 |
| 22 | B | 833 | CLA | CMB-C2B-C3B | 2.07 | 128.56 | 124.68 |
| 29 | 6 | 607 | CHL | O2D-CGD-O1D | -2.07 | 119.78 | 123.84 |
| 24 | A | 847 | LHG | C6-C5-C4 | -2.07 | 106.88 | 111.79 |
| 22 | 2 | 612 | CLA | CHB-C4A-NA | 2.07 | 127.38 | 124.51 |
| 22 | 5 | 609 | CLA | CAA-C2A-C3A | -2.07 | 107.10 | 112.78 |
| 22 | K | 4003 | CLA | CHC-C1C-NC | 2.07 | 127.35 | 124.20 |
| 22 | Z | 609 | CLA | CHA-C1A-NA | -2.07 | 121.65 | 126.40 |
| 22 | B | 835 | CLA | O2D-CGD-O1D | -2.07 | 119.79 | 123.84 |
| 29 | 9 | 607 | CHL | C1B-CHB-C4A | -2.07 | 126.01 | 130.12 |
| 22 | 3 | 603 | CLA | CHB-C4A-NA | 2.07 | 127.38 | 124.51 |
| 22 | 2 | 606 | CLA | CMA-C3A-C2A | -2.07 | 111.27 | 116.10 |
| 22 | 4 | 612 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 25 | 5 | 622 | BCR | C11-C10-C9 | -2.07 | 124.36 | 127.31 |
| 29 | 3 | 608 | CHL | C2A-C1A-CHA | -2.07 | 120.24 | 123.86 |
| 22 | 1 | 604 | CLA | C1-C2-C3 | -2.07 | 122.46 | 126.04 |
| 25 | I | 172 | BCR | C15-C16-C17 | -2.07 | 119.23 | 123.47 |
| 22 | Z | 602 | CLA | CMA-C3A-C2A | -2.07 | 105.48 | 113.83 |
| 22 | 1 | 611 | CLA | CED-O2D-CGD | 2.07 | 120.62 | 115.94 |
| 22 | 7 | 610 | CLA | CBC-CAC-C3C | -2.07 | 106.73 | 112.43 |
| 22 | 4 | 611 | CLA | C1-O2A-CGA | 2.07 | 121.87 | 116.44 |
| 22 | A | 831 | CLA | O2A-CGA-O1A | -2.07 | 118.37 | 123.59 |
| 29 | 7 | 607 | CHL | C2A-C1A-CHA | -2.07 | 120.24 | 123.86 |
| 22 | 9 | 614 | CLA | O1D-CGD-CBD | -2.07 | 120.25 | 124.48 |
| 22 | B | 809 | CLA | CHA-C1A-NA | -2.07 | 121.66 | 126.40 |
| 25 | 6 | 623 | BCR | C34-C9-C10 | -2.07 | 120.03 | 122.92 |
| 22 | B | 804 | CLA | CBC-CAC-C3C | -2.07 | 106.73 | 112.43 |
| 22 | 3 | 610 | CLA | CBC-CAC-C3C | -2.07 | 106.73 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30 | 1 | 618 | LUT | C16-C1-C6 | -2.07 | 106.95 | 110.30 |
| 22 | 3 | 607 | CLA | O2A-CGA-O1A | -2.07 | 118.38 | 123.59 |
| 22 | B | 818 | CLA | C1-C2-C3 | -2.06 | 122.47 | 126.04 |
| 22 | 2 | 614 | CLA | CBC-CAC-C3C | -2.06 | 106.74 | 112.43 |
| 22 | B | 828 | CLA | CMB-C2B-C3B | 2.06 | 128.54 | 124.68 |
| 29 | 3 | 608 | CHL | C4-C3-C5 | 2.06 | 118.74 | 115.27 |
| 22 | 5 | 616 | CLA | CHA-C1A-NA | -2.06 | 121.67 | 126.40 |
| 25 | 6 | 625 | BCR | C34-C9-C10 | -2.06 | 120.03 | 122.92 |
| 22 | 3 | 610 | CLA | CMA-C3A-C4A | -2.06 | 106.23 | 111.77 |
| 22 | 9 | 603 | CLA | C1B-CHB-C4A | -2.06 | 126.03 | 130.12 |
| 22 | 8 | 614 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 30 | 1 | 619 | LUT | C30-C31-C32 | -2.06 | 116.78 | 123.22 |
| 30 | Z | 618 | LUT | C15-C35-C34 | -2.06 | 119.25 | 123.47 |
| 22 | 4 | 613 | CLA | C1B-CHB-C4A | -2.06 | 126.03 | 130.12 |
| 22 | B | 835 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 25 | L | 205 | BCR | C21-C20-C19 | -2.06 | 116.79 | 123.22 |
| 30 | Z | 618 | LUT | C16-C1-C6 | -2.06 | 106.96 | 110.30 |
| 22 | A | 802 | CLA | CHB-C4A-NA | 2.06 | 127.36 | 124.51 |
| 22 | 4 | 603 | CLA | CHA-C1A-NA | -2.06 | 121.68 | 126.40 |
| 22 | A | 838 | CLA | CMD-C2D-C3D | -2.06 | 122.88 | 127.61 |
| 22 | 6 | 613 | CLA | CMD-C2D-C3D | -2.06 | 122.88 | 127.61 |
| 22 | 3 | 617 | CLA | CBC-CAC-C3C | -2.06 | 106.76 | 112.43 |
| 22 | Z | 609 | CLA | C11-C10-C8 | -2.06 | 109.27 | 115.92 |
| 25 | 6 | 623 | BCR | C37-C22-C23 | 2.06 | 121.32 | 118.08 |
| 22 | 8 | 602 | CLA | O1D-CGD-CBD | -2.06 | 120.27 | 124.48 |
| 22 | B | 837 | CLA | CMB-C2B-C3B | 2.06 | 128.53 | 124.68 |
| 25 | B | 848 | BCR | C23-C24-C25 | -2.06 | 121.42 | 127.20 |
| 22 | 2 | 611 | CLA | CED-O2D-CGD | 2.06 | 120.59 | 115.94 |
| 25 | B | 801 | BCR | C10-C11-C12 | -2.06 | 116.80 | 123.22 |
| 22 | B | 834 | CLA | CMD-C2D-C3D | -2.06 | 122.88 | 127.61 |
| 22 | B | 807 | CLA | C4-C3-C5 | 2.06 | 118.73 | 115.27 |
| 30 | 5 | 624 | LUT | C30-C31-C32 | -2.06 | 116.80 | 123.22 |
| 22 | 4 | 611 | CLA | CBC-CAC-C3C | -2.06 | 106.76 | 112.43 |
| 25 | B | 845 | BCR | C8-C9-C10 | 2.06 | 122.10 | 118.94 |
| 30 | 1 | 617 | LUT | C31-C30-C29 | -2.06 | 124.38 | 127.31 |
| 30 | 2 | 616 | LUT | C11-C10-C9 | -2.06 | 124.38 | 127.31 |
| 22 | 8 | 613 | CLA | O2A-CGA-CBA | 2.06 | 118.36 | 111.91 |
| 22 | A | 821 | CLA | CMC-C2C-C1C | 2.06 | 128.17 | 125.04 |
| 22 | Z | 611 | CLA | CMC-C2C-C1C | 2.06 | 128.17 | 125.04 |
| 22 | B | 836 | CLA | CHB-C4A-NA | 2.06 | 127.35 | 124.51 |
| 22 | B | 822 | CLA | CMB-C2B-C3B | 2.06 | 128.52 | 124.68 |
| 22 | 2 | 611 | CLA | C1-C2-C3 | -2.05 | 122.49 | 126.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 2 | 609 | CLA | CED-O2D-CGD | 2.05 | 120.58 | 115.94 |
| 25 | I | 172 | BCR | C29-C28-C27 | -2.05 | 106.79 | 111.38 |
| 22 | A | 813 | CLA | C4-C3-C5 | 2.05 | 118.73 | 115.27 |
| 25 | B | 801 | BCR | C34-C9-C8 | 2.05 | 121.31 | 118.08 |
| 30 | 5 | 624 | LUT | C19-C9-C8 | 2.05 | 121.31 | 118.08 |
| 29 | 6 | 607 | CHL | CHC-C1C-C2C | -2.05 | 118.66 | 126.11 |
| 25 | A | 852 | BCR | C40-C30-C25 | -2.05 | 106.97 | 110.30 |
| 22 | 2 | 612 | CLA | CHA-C1A-NA | -2.05 | 121.69 | 126.40 |
| 22 | A | 840 | CLA | CAA-C2A-C3A | -2.05 | 107.16 | 112.78 |
| 22 | 2 | 611 | CLA | CMC-C2C-C1C | 2.05 | 128.16 | 125.04 |
| 30 | 9 | 617 | LUT | C39-C29-C28 | 2.05 | 121.31 | 118.08 |
| 22 | B | 813 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 25 | 3 | 719 | BCR | C29-C28-C27 | -2.05 | 106.79 | 111.38 |
| 24 | 7 | 625 | LHG | O8-C23-O10 | -2.05 | 118.41 | 123.59 |
| 22 | 7 | 620 | CLA | C1-C2-C3 | -2.05 | 122.49 | 126.04 |
| 30 | 6 | 621 | LUT | C28-C29-C30 | -2.05 | 115.79 | 118.94 |
| 22 | A | 837 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 22 | 3 | 602 | CLA | CBA-CAA-C2A | 2.05 | 119.92 | 113.86 |
| 22 | B | 811 | CLA | CMA-C3A-C4A | -2.05 | 106.26 | 111.77 |
| 22 | 4 | 609 | CLA | CHA-C1A-NA | -2.05 | 121.70 | 126.40 |
| 22 | 1 | 610 | CLA | CMA-C3A-C4A | -2.05 | 106.26 | 111.77 |
| 22 | 8 | 604 | CLA | CMC-C2C-C1C | 2.05 | 128.16 | 125.04 |
| 22 | Z | 611 | CLA | O1D-CGD-CBD | -2.05 | 120.29 | 124.48 |
| 29 | 6 | 606 | CHL | C1B-CHB-C4A | -2.05 | 126.06 | 130.12 |
| 30 | 9 | 616 | LUT | C8-C7-C6 | -2.05 | 121.44 | 127.20 |
| 22 | 5 | 610 | CLA | C11-C10-C8 | -2.05 | 109.29 | 115.92 |
| 30 | 9 | 616 | LUT | C39-C29-C28 | 2.05 | 121.31 | 118.08 |
| 22 | B | 829 | CLA | O2A-CGA-O1A | -2.05 | 118.42 | 123.59 |
| 22 | A | 825 | CLA | CMC-C2C-C1C | 2.05 | 128.16 | 125.04 |
| 29 | 1 | 601 | CHL | OBD-CAD-C3D | -2.05 | 123.59 | 128.52 |
| 22 | B | 806 | CLA | CHA-C1A-NA | -2.05 | 121.71 | 126.40 |
| 22 | B | 836 | CLA | O2A-CGA-O1A | -2.05 | 118.42 | 123.59 |
| 22 | 5 | 601 | CLA | O2A-CGA-O1A | -2.05 | 118.42 | 123.59 |
| 22 | B | 814 | CLA | C1-C2-C3 | -2.05 | 122.50 | 126.04 |
| 22 | 4 | 614 | CLA | CBC-CAC-C3C | -2.05 | 106.79 | 112.43 |
| 25 | 4 | 621 | BCR | C36-C18-C19 | 2.05 | 121.30 | 118.08 |
| 29 | Z | 607 | CHL | CHD-C4C-NC | 2.05 | 127.43 | 124.20 |
| 30 | 3 | 621 | LUT | C19-C9-C8 | 2.05 | 121.30 | 118.08 |
| 22 | 9 | 613 | CLA | CBC-CAC-C3C | -2.05 | 106.79 | 112.43 |
| 22 | A | 811 | CLA | C4-C3-C5 | 2.05 | 118.71 | 115.27 |
| 22 | 5 | 616 | CLA | CMC-C2C-C1C | 2.05 | 128.16 | 125.04 |
| 22 | B | 826 | CLA | OBD-CAD-C3D | -2.05 | 123.60 | 128.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 4 | 610 | CLA | CMA-C3A-C4A | -2.05 | 106.28 | 111.77 |
| 25 | 6 | 623 | BCR | C7-C6-C5 | -2.05 | 116.51 | 121.46 |
| 22 | 5 | 609 | CLA | C5-C3-C4 | 2.04 | 119.12 | 114.60 |
| 22 | 7 | 602 | CLA | CMA-C3A-C2A | -2.04 | 105.58 | 113.83 |
| 22 | 7 | 606 | CLA | CAC-C3C-C4C | 2.04 | 127.46 | 124.81 |
| 25 | B | 843 | BCR | C23-C24-C25 | -2.04 | 121.46 | 127.20 |
| 22 | 8 | 606 | CLA | CBC-CAC-C3C | -2.04 | 106.80 | 112.43 |
| 30 | 3 | 621 | LUT | C40-C33-C32 | 2.04 | 121.29 | 118.08 |
| 22 | A | 804 | CLA | CHB-C4A-NA | 2.04 | 127.33 | 124.51 |
| 22 | 7 | 620 | CLA | O2A-CGA-O1A | -2.04 | 118.44 | 123.59 |
| 22 | 1 | 603 | CLA | CMC-C2C-C1C | 2.04 | 128.15 | 125.04 |
| 25 | A | 856 | BCR | C32-C1-C6 | 2.04 | 113.61 | 110.30 |
| 30 | 2 | 616 | LUT | C30-C31-C32 | -2.04 | 116.85 | 123.22 |
| 22 | 9 | 614 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 22 | A | 837 | CLA | CHC-C1C-NC | 2.04 | 127.30 | 124.20 |
| 22 | 1 | 606 | CLA | C1-C2-C3 | -2.04 | 122.52 | 126.04 |
| 22 | 5 | 614 | CLA | CBC-CAC-C3C | -2.04 | 106.81 | 112.43 |
| 29 | 6 | 607 | CHL | C2A-C3A-C4A | -2.04 | 98.58 | 101.87 |
| 22 | A | 820 | CLA | CED-O2D-CGD | 2.04 | 120.55 | 115.94 |
| 22 | B | 815 | CLA | CBC-CAC-C3C | -2.04 | 106.81 | 112.43 |
| 22 | B | 810 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 22 | B | 834 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 22 | B | 841 | CLA | O1D-CGD-CBD | -2.04 | 120.31 | 124.48 |
| 22 | A | 831 | CLA | CHB-C4A-NA | 2.04 | 127.33 | 124.51 |
| 22 | 7 | 614 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 22 | F | 301 | CLA | CBC-CAC-C3C | -2.04 | 106.81 | 112.43 |
| 22 | A | 838 | CLA | CHA-C1A-NA | -2.04 | 121.73 | 126.40 |
| 30 | 2 | 616 | LUT | C39-C29-C28 | 2.04 | 121.29 | 118.08 |
| 22 | B | 813 | CLA | CHC-C1C-NC | 2.04 | 127.29 | 124.20 |
| 30 | 7 | 621 | LUT | C39-C29-C28 | 2.04 | 121.28 | 118.08 |
| 22 | A | 827 | CLA | CMD-C2D-C3D | -2.04 | 122.93 | 127.61 |
| 30 | 3 | 622 | LUT | C40-C33-C32 | 2.03 | 121.28 | 118.08 |
| 30 | 2 | 617 | LUT | C20-C13-C12 | 2.03 | 121.28 | 118.08 |
| 22 | 1 | 610 | CLA | O1D-CGD-CBD | -2.03 | 120.32 | 124.48 |
| 29 | 6 | 606 | CHL | O1D-CGD-CBD | -2.03 | 120.32 | 124.48 |
| 22 | 1 | 603 | CLA | CHA-C1A-NA | -2.03 | 121.74 | 126.40 |
| 29 | 7 | 607 | CHL | C1-C2-C3 | -2.03 | 122.53 | 126.04 |
| 22 | B | 823 | CLA | CMA-C3A-C4A | -2.03 | 106.31 | 111.77 |
| 29 | 4 | 606 | CHL | CBA-CAA-C2A | -2.03 | 107.86 | 113.86 |
| 22 | A | 841 | CLA | CMC-C2C-C1C | 2.03 | 128.14 | 125.04 |
| 22 | B | 836 | CLA | O1D-CGD-CBD | -2.03 | 120.32 | 124.48 |
| 22 | 5 | 604 | CLA | C5-C3-C4 | 2.03 | 119.09 | 114.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22 | 4 | 603 | CLA | CMC-C2C-C1C | 2.03 | 128.13 | 125.04 |
| 25 | B | 847 | BCR | C3-C4-C5 | -2.03 | 110.45 | 114.08 |
| 29 | 8 | 607 | CHL | CHC-C1C-C2C | -2.03 | 118.74 | 126.11 |
| 22 | A | 842 | CLA | CBC-CAC-C3C | -2.03 | 106.83 | 112.43 |
| 25 | B | 801 | BCR | C7-C8-C9 | -2.03 | 123.16 | 126.23 |
| 22 | B | 852 | CLA | CHA-C1A-NA | -2.03 | 121.74 | 126.40 |
| 22 | G | 203 | CLA | O1D-CGD-CBD | -2.03 | 120.33 | 124.48 |
| 29 | 4 | 607 | CHL | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 22 | 4 | 613 | CLA | O2A-CGA-O1A | -2.03 | 118.46 | 123.59 |
| 22 | 1 | 611 | CLA | C4-C3-C5 | 2.03 | 118.69 | 115.27 |
| 29 | 1 | 601 | CHL | CHB-C4A-NA | 2.03 | 127.32 | 124.51 |
| 22 | F | 301 | CLA | CGD-CBD-CAD | -2.03 | 104.16 | 110.73 |
| 25 | 3 | 719 | BCR | C35-C13-C12 | 2.03 | 121.28 | 118.08 |
| 22 | 4 | 609 | CLA | C5-C3-C4 | 2.03 | 119.09 | 114.60 |
| 22 | 2 | 613 | CLA | O2A-CGA-O1A | -2.03 | 118.47 | 123.59 |
| 22 | A | 810 | CLA | CHA-C1A-NA | -2.03 | 121.75 | 126.40 |
| 22 | B | 828 | CLA | CBA-CAA-C2A | 2.03 | 119.84 | 113.86 |
| 22 | Z | 613 | CLA | C4-C3-C5 | 2.03 | 118.68 | 115.27 |
| 22 | B | 817 | CLA | CHA-C1A-NA | -2.03 | 121.76 | 126.40 |
| 22 | A | 803 | CLA | O1D-CGD-CBD | -2.03 | 120.34 | 124.48 |
| 22 | A | 843 | CLA | C1-C2-C3 | -2.03 | 122.54 | 126.04 |
| 22 | 3 | 602 | CLA | C2A-C3A-C4A | -2.03 | 98.60 | 101.87 |
| 22 | 3 | 607 | CLA | C1-C2-C3 | -2.03 | 122.54 | 126.04 |
| 22 | A | 841 | CLA | CAA-C2A-C3A | -2.02 | 107.23 | 112.78 |
| 22 | 6 | 611 | CLA | C1-C2-C3 | -2.02 | 122.54 | 126.04 |
| 22 | 2 | 612 | CLA | CMB-C2B-C3B | 2.02 | 128.46 | 124.68 |
| 22 | B | 817 | CLA | CMB-C2B-C3B | 2.02 | 128.46 | 124.68 |
| 22 | 1 | 602 | CLA | CMB-C2B-C3B | 2.02 | 128.46 | 124.68 |
| 22 | A | 839 | CLA | CBC-CAC-C3C | -2.02 | 106.86 | 112.43 |
| 22 | B | 827 | CLA | O2D-CGD-O1D | -2.02 | 119.89 | 123.84 |
| 22 | G | 203 | CLA | CMC-C2C-C1C | 2.02 | 128.12 | 125.04 |
| 30 | 8 | 618 | LUT | C39-C29-C28 | 2.02 | 121.26 | 118.08 |
| 29 | 5 | 607 | CHL | CGD-CBD-CAD | -2.02 | 104.19 | 110.73 |
| 22 | 3 | 606 | CLA | CED-O2D-CGD | 2.02 | 120.51 | 115.94 |
| 22 | 8 | 610 | CLA | CED-O2D-CGD | 2.02 | 120.51 | 115.94 |
| 29 | Z | 607 | CHL | CHC-C1C-C2C | -2.02 | 118.79 | 126.11 |
| 22 | 3 | 620 | CLA | CED-O2D-CGD | 2.02 | 120.50 | 115.94 |
| 22 | A | 830 | CLA | CAA-C2A-C3A | -2.02 | 107.25 | 112.78 |
| 29 | 7 | 607 | CHL | CED-O2D-CGD | 2.02 | 120.50 | 115.94 |
| 22 | A | 837 | CLA | C2A-C3A-C4A | -2.02 | 98.61 | 101.87 |
| 22 | B | 828 | CLA | CED-O2D-CGD | 2.02 | 120.50 | 115.94 |
| 22 | 8 | 609 | CLA | O2D-CGD-O1D | -2.02 | 119.89 | 123.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 25 | A | 849 | BCR | C28-C27-C26 | -2.02 | 110.48 | 114.08 |
| 22 | 6 | 613 | CLA | C1-O2A-CGA | 2.02 | 121.73 | 116.44 |
| 22 | 1 | 610 | CLA | CHC-C1C-C2C | -2.02 | 121.14 | 126.72 |
| 25 | 3 | 718 | BCR | C35-C13-C12 | 2.02 | 121.25 | 118.08 |
| 22 | 5 | 612 | CLA | CHA-C1A-NA | -2.02 | 121.78 | 126.40 |
| 25 | B | 846 | BCR | C15-C16-C17 | -2.02 | 119.35 | 123.47 |
| 25 | L | 205 | BCR | C10-C11-C12 | -2.01 | 116.93 | 123.22 |
| 22 | B | 826 | CLA | O2A-CGA-O1A | -2.01 | 118.51 | 123.59 |
| 25 | A | 852 | BCR | C11-C10-C9 | -2.01 | 124.44 | 127.31 |
| 22 | 4 | 613 | CLA | C4-C3-C5 | 2.01 | 118.66 | 115.27 |
| 22 | 4 | 603 | CLA | CHB-C4A-NA | 2.01 | 127.30 | 124.51 |
| 22 | A | 839 | CLA | CMC-C2C-C1C | 2.01 | 128.10 | 125.04 |
| 22 | B | 835 | CLA | CAA-C2A-C3A | -2.01 | 107.27 | 112.78 |
| 25 | 7 | 623 | BCR | C34-C9-C8 | 2.01 | 121.24 | 118.08 |
| 22 | 1 | 602 | CLA | CMA-C3A-C2A | -2.01 | 105.72 | 113.83 |
| 22 | K | 4002 | CLA | O2A-CGA-CBA | 2.01 | 120.48 | 114.03 |
| 24 | 4 | 623 | LHG | O8-C23-O10 | -2.01 | 118.52 | 123.59 |
| 22 | B | 806 | CLA | C4-C3-C5 | 2.01 | 118.65 | 115.27 |
| 30 | 1 | 617 | LUT | C8-C7-C6 | -2.01 | 121.56 | 127.20 |
| 22 | 9 | 612 | CLA | CHB-C4A-NA | 2.01 | 127.29 | 124.51 |
| 22 | 1 | 612 | CLA | CMC-C2C-C1C | 2.01 | 128.09 | 125.04 |
| 22 | 8 | 611 | CLA | O2A-CGA-CBA | 2.01 | 120.16 | 112.23 |
| 22 | 2 | 613 | CLA | CAA-C2A-C3A | -2.01 | 107.28 | 112.78 |
| 22 | B | 811 | CLA | CMC-C2C-C1C | 2.01 | 128.09 | 125.04 |
| 22 | 8 | 612 | CLA | CBC-CAC-C3C | -2.01 | 106.90 | 112.43 |
| 22 | A | 833 | CLA | CHA-C1A-NA | -2.01 | 121.81 | 126.40 |
| 25 | A | 852 | BCR | C28-C27-C26 | -2.01 | 110.50 | 114.08 |
| 22 | 5 | 604 | CLA | CMB-C2B-C3B | 2.01 | 128.43 | 124.68 |
| 22 | A | 834 | CLA | CMA-C3A-C4A | -2.01 | 106.38 | 111.77 |
| 22 | B | 806 | CLA | O2D-CGD-O1D | -2.00 | 119.92 | 123.84 |
| 22 | 8 | 610 | CLA | C1B-CHB-C4A | -2.00 | 126.15 | 130.12 |
| 22 | A | 829 | CLA | C1B-CHB-C4A | -2.00 | 126.15 | 130.12 |
| 22 | 6 | 603 | CLA | O2A-CGA-CBA | 2.00 | 120.15 | 112.23 |
| 22 | B | 819 | CLA | CHC-C1C-NC | 2.00 | 127.24 | 124.20 |
| 22 | A | 820 | CLA | CAA-C2A-C3A | -2.00 | 107.29 | 112.78 |
| 22 | 6 | 622 | CLA | CHA-C1A-NA | -2.00 | 121.81 | 126.40 |
| 22 | A | 838 | CLA | C1-C2-C3 | -2.00 | 122.58 | 126.04 |
| 22 | A | 806 | CLA | O1D-CGD-CBD | -2.00 | 120.39 | 124.48 |
| 22 | 9 | 612 | CLA | O2A-CGA-O1A | -2.00 | 118.54 | 123.59 |
| 22 | A | 810 | CLA | CHB-C4A-NA | 2.00 | 127.28 | 124.51 |
| 22 | Z | 608 | CLA | CHA-C1A-NA | -2.00 | 121.81 | 126.40 |

All (246) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 21 | A | 801 | CL0 | ND |
| 21 | A | 801 | CL0 | NC |
| 22 | A | 802 | CLA | ND |
| 22 | A | 803 | CLA | ND |
| 22 | A | 804 | CLA | ND |
| 22 | A | 805 | CLA | ND |
| 22 | A | 806 | CLA | ND |
| 22 | A | 807 | CLA | ND |
| 22 | A | 808 | CLA | ND |
| 22 | A | 809 | CLA | ND |
| 22 | A | 811 | CLA | ND |
| 22 | A | 812 | CLA | ND |
| 22 | A | 813 | CLA | ND |
| 22 | A | 814 | CLA | ND |
| 22 | A | 815 | CLA | ND |
| 22 | A | 816 | CLA | ND |
| 22 | A | 817 | CLA | ND |
| 22 | A | 819 | CLA | ND |
| 22 | A | 820 | CLA | ND |
| 22 | A | 821 | CLA | ND |
| 22 | A | 822 | CLA | ND |
| 22 | A | 824 | CLA | ND |
| 22 | A | 826 | CLA | ND |
| 22 | A | 827 | CLA | ND |
| 22 | A | 828 | CLA | ND |
| 22 | A | 829 | CLA | ND |
| 22 | A | 830 | CLA | ND |
| 22 | A | 831 | CLA | ND |
| 22 | A | 832 | CLA | ND |
| 22 | A | 833 | CLA | ND |
| 22 | A | 834 | CLA | ND |
| 22 | A | 835 | CLA | ND |
| 22 | A | 837 | CLA | ND |
| 22 | A | 838 | CLA | ND |
| 22 | A | 839 | CLA | ND |
| 22 | A | 840 | CLA | ND |
| 22 | A | 841 | CLA | ND |
| 22 | A | 842 | CLA | ND |
| 22 | A | 843 | CLA | ND |
| 22 | A | 845 | CLA | ND |
| 22 | A | 854 | CLA | ND |
| 22 | B | 802 | CLA | ND |
| 22 | B | 803 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|------------|--------------|------------|-------------|-------------|
| 22 | B | 804 | CLA | ND |
| 22 | B | 805 | CLA | ND |
| 22 | B | 806 | CLA | ND |
| 22 | B | 807 | CLA | ND |
| 22 | B | 808 | CLA | ND |
| 22 | B | 809 | CLA | ND |
| 22 | B | 810 | CLA | ND |
| 22 | B | 811 | CLA | ND |
| 22 | B | 812 | CLA | ND |
| 22 | B | 813 | CLA | ND |
| 22 | B | 814 | CLA | ND |
| 22 | B | 815 | CLA | ND |
| 22 | B | 816 | CLA | ND |
| 22 | B | 817 | CLA | ND |
| 22 | B | 818 | CLA | ND |
| 22 | B | 819 | CLA | ND |
| 22 | B | 820 | CLA | ND |
| 22 | B | 823 | CLA | ND |
| 22 | B | 824 | CLA | ND |
| 22 | B | 825 | CLA | ND |
| 22 | B | 826 | CLA | ND |
| 22 | B | 827 | CLA | ND |
| 22 | B | 828 | CLA | ND |
| 22 | B | 829 | CLA | ND |
| 22 | B | 831 | CLA | ND |
| 22 | B | 832 | CLA | ND |
| 22 | B | 833 | CLA | ND |
| 22 | B | 834 | CLA | ND |
| 22 | B | 835 | CLA | ND |
| 22 | B | 836 | CLA | ND |
| 22 | B | 837 | CLA | ND |
| 22 | B | 838 | CLA | ND |
| 22 | B | 839 | CLA | ND |
| 22 | B | 841 | CLA | ND |
| 22 | B | 852 | CLA | ND |
| 22 | F | 301 | CLA | ND |
| 22 | F | 303 | CLA | ND |
| 22 | F | 304 | CLA | ND |
| 22 | G | 203 | CLA | ND |
| 22 | G | 204 | CLA | ND |
| 22 | J | 3002 | CLA | ND |
| 22 | K | 4003 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|------------|--------------|------------|-------------|-------------|
| 22 | 1 | 602 | CLA | ND |
| 22 | 1 | 603 | CLA | ND |
| 22 | 1 | 604 | CLA | ND |
| 22 | 1 | 606 | CLA | ND |
| 22 | 1 | 608 | CLA | ND |
| 22 | 1 | 609 | CLA | ND |
| 22 | 1 | 610 | CLA | ND |
| 22 | 1 | 611 | CLA | ND |
| 22 | 1 | 612 | CLA | ND |
| 22 | 1 | 613 | CLA | ND |
| 22 | 1 | 614 | CLA | ND |
| 22 | 1 | 616 | CLA | ND |
| 22 | 3 | 602 | CLA | ND |
| 22 | 3 | 603 | CLA | ND |
| 22 | 3 | 604 | CLA | ND |
| 22 | 3 | 606 | CLA | ND |
| 22 | 3 | 607 | CLA | ND |
| 22 | 3 | 609 | CLA | ND |
| 22 | 3 | 610 | CLA | ND |
| 22 | 3 | 611 | CLA | ND |
| 22 | 3 | 612 | CLA | ND |
| 22 | 3 | 617 | CLA | ND |
| 22 | 3 | 620 | CLA | ND |
| 22 | 7 | 601 | CLA | ND |
| 22 | 7 | 602 | CLA | ND |
| 22 | 7 | 603 | CLA | ND |
| 22 | 7 | 604 | CLA | ND |
| 22 | 7 | 606 | CLA | ND |
| 22 | 7 | 609 | CLA | ND |
| 22 | 7 | 610 | CLA | ND |
| 22 | 7 | 611 | CLA | ND |
| 22 | 7 | 612 | CLA | ND |
| 22 | 7 | 614 | CLA | ND |
| 22 | 7 | 616 | CLA | ND |
| 22 | 7 | 620 | CLA | ND |
| 22 | 8 | 601 | CLA | ND |
| 22 | 8 | 602 | CLA | ND |
| 22 | 8 | 603 | CLA | ND |
| 22 | 8 | 604 | CLA | ND |
| 22 | 8 | 606 | CLA | ND |
| 22 | 8 | 608 | CLA | ND |
| 22 | 8 | 609 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|------------|--------------|------------|-------------|-------------|
| 22 | 8 | 610 | CLA | ND |
| 22 | 8 | 611 | CLA | ND |
| 22 | 8 | 612 | CLA | ND |
| 22 | 8 | 614 | CLA | ND |
| 22 | 8 | 616 | CLA | ND |
| 22 | Z | 603 | CLA | ND |
| 22 | Z | 604 | CLA | ND |
| 22 | Z | 606 | CLA | ND |
| 22 | Z | 608 | CLA | ND |
| 22 | Z | 609 | CLA | ND |
| 22 | Z | 610 | CLA | ND |
| 22 | Z | 611 | CLA | ND |
| 22 | Z | 612 | CLA | ND |
| 22 | Z | 613 | CLA | ND |
| 22 | Z | 614 | CLA | ND |
| 22 | Z | 616 | CLA | ND |
| 22 | 4 | 601 | CLA | ND |
| 22 | 4 | 603 | CLA | ND |
| 22 | 4 | 609 | CLA | ND |
| 22 | 4 | 610 | CLA | ND |
| 22 | 4 | 611 | CLA | ND |
| 22 | 4 | 612 | CLA | ND |
| 22 | 4 | 614 | CLA | ND |
| 22 | 4 | 616 | CLA | ND |
| 22 | 5 | 601 | CLA | ND |
| 22 | 5 | 603 | CLA | ND |
| 22 | 5 | 606 | CLA | ND |
| 22 | 5 | 609 | CLA | ND |
| 22 | 5 | 610 | CLA | ND |
| 22 | 5 | 611 | CLA | ND |
| 22 | 5 | 612 | CLA | ND |
| 22 | 5 | 613 | CLA | ND |
| 22 | 5 | 616 | CLA | ND |
| 22 | 5 | 617 | CLA | ND |
| 22 | 5 | 621 | CLA | ND |
| 22 | 6 | 601 | CLA | ND |
| 22 | 6 | 602 | CLA | ND |
| 22 | 6 | 603 | CLA | ND |
| 22 | 6 | 604 | CLA | ND |
| 22 | 6 | 609 | CLA | ND |
| 22 | 6 | 610 | CLA | ND |
| 22 | 6 | 611 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|------------|--------------|------------|-------------|-------------|
| 22 | 6 | 612 | CLA | ND |
| 22 | 6 | 613 | CLA | ND |
| 22 | 6 | 614 | CLA | ND |
| 22 | 6 | 616 | CLA | ND |
| 22 | 6 | 617 | CLA | ND |
| 22 | 6 | 622 | CLA | ND |
| 22 | 2 | 601 | CLA | ND |
| 22 | 2 | 603 | CLA | ND |
| 22 | 2 | 606 | CLA | ND |
| 22 | 2 | 609 | CLA | ND |
| 22 | 2 | 612 | CLA | ND |
| 22 | 9 | 601 | CLA | ND |
| 22 | 9 | 602 | CLA | ND |
| 22 | 9 | 603 | CLA | ND |
| 22 | 9 | 609 | CLA | ND |
| 22 | 9 | 611 | CLA | ND |
| 22 | 9 | 612 | CLA | ND |
| 22 | 9 | 613 | CLA | ND |
| 29 | 1 | 601 | CHL | ND |
| 29 | 1 | 601 | CHL | NC |
| 29 | 1 | 601 | CHL | NA |
| 29 | 1 | 607 | CHL | ND |
| 29 | 1 | 607 | CHL | NC |
| 29 | 1 | 607 | CHL | NA |
| 29 | 3 | 608 | CHL | ND |
| 29 | 3 | 608 | CHL | NC |
| 29 | 3 | 608 | CHL | NA |
| 29 | 7 | 607 | CHL | ND |
| 29 | 7 | 607 | CHL | NC |
| 29 | 7 | 607 | CHL | NA |
| 29 | 8 | 607 | CHL | ND |
| 29 | 8 | 607 | CHL | NC |
| 29 | 8 | 607 | CHL | NA |
| 29 | Z | 601 | CHL | ND |
| 29 | Z | 601 | CHL | NC |
| 29 | Z | 601 | CHL | NA |
| 29 | Z | 607 | CHL | ND |
| 29 | Z | 607 | CHL | NC |
| 29 | Z | 607 | CHL | NA |
| 29 | 4 | 606 | CHL | ND |
| 29 | 4 | 606 | CHL | NC |
| 29 | 4 | 606 | CHL | NA |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 29 | 4 | 607 | CHL | ND |
| 29 | 4 | 607 | CHL | NC |
| 29 | 4 | 607 | CHL | NA |
| 29 | 4 | 608 | CHL | ND |
| 29 | 4 | 608 | CHL | NC |
| 29 | 4 | 608 | CHL | NA |
| 29 | 4 | 618 | CHL | ND |
| 29 | 4 | 618 | CHL | NC |
| 29 | 4 | 618 | CHL | NA |
| 29 | 5 | 607 | CHL | ND |
| 29 | 5 | 607 | CHL | NC |
| 29 | 5 | 607 | CHL | NA |
| 29 | 5 | 608 | CHL | ND |
| 29 | 5 | 608 | CHL | NC |
| 29 | 5 | 608 | CHL | NA |
| 29 | 5 | 618 | CHL | ND |
| 29 | 5 | 618 | CHL | NC |
| 29 | 5 | 618 | CHL | NA |
| 29 | 6 | 606 | CHL | ND |
| 29 | 6 | 606 | CHL | NC |
| 29 | 6 | 606 | CHL | NA |
| 29 | 6 | 607 | CHL | ND |
| 29 | 6 | 607 | CHL | NC |
| 29 | 6 | 608 | CHL | ND |
| 29 | 6 | 608 | CHL | NC |
| 29 | 6 | 608 | CHL | NA |
| 29 | 6 | 618 | CHL | ND |
| 29 | 6 | 618 | CHL | NC |
| 29 | 6 | 618 | CHL | NA |
| 29 | 9 | 606 | CHL | ND |
| 29 | 9 | 606 | CHL | NC |
| 29 | 9 | 606 | CHL | NA |
| 29 | 9 | 607 | CHL | ND |
| 29 | 9 | 607 | CHL | NC |
| 29 | 9 | 607 | CHL | NA |

All (2298) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 804 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 804 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 804 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 809 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 809 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 812 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 814 | CLA | C2-C3-C5-C6 |
| 22 | A | 814 | CLA | C4-C3-C5-C6 |
| 22 | A | 815 | CLA | C2-C3-C5-C6 |
| 22 | A | 815 | CLA | C4-C3-C5-C6 |
| 22 | A | 816 | CLA | C2-C3-C5-C6 |
| 22 | A | 816 | CLA | C4-C3-C5-C6 |
| 22 | A | 818 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 818 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 818 | CLA | C2-C3-C5-C6 |
| 22 | A | 818 | CLA | C4-C3-C5-C6 |
| 22 | A | 819 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 819 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 820 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 820 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 823 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 823 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 829 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 831 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 831 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 831 | CLA | C4-C3-C5-C6 |
| 22 | A | 834 | CLA | C2-C3-C5-C6 |
| 22 | A | 834 | CLA | C4-C3-C5-C6 |
| 22 | A | 835 | CLA | C4-C3-C5-C6 |
| 22 | A | 837 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 837 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 837 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 843 | CLA | C4-C3-C5-C6 |
| 22 | B | 802 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 802 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 805 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 805 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 806 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 808 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 808 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 810 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 813 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 813 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 818 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 818 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | B | 818 | CLA | C2-C3-C5-C6 |
| 22 | B | 818 | CLA | C4-C3-C5-C6 |
| 22 | B | 823 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 823 | CLA | C2-C3-C5-C6 |
| 22 | B | 823 | CLA | C4-C3-C5-C6 |
| 22 | B | 824 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 828 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 828 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 829 | CLA | C4-C3-C5-C6 |
| 22 | B | 833 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 833 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 836 | CLA | C2-C3-C5-C6 |
| 22 | B | 836 | CLA | C4-C3-C5-C6 |
| 22 | B | 837 | CLA | C2-C3-C5-C6 |
| 22 | B | 837 | CLA | C4-C3-C5-C6 |
| 22 | F | 301 | CLA | CHA-CBD-CGD-O1D |
| 22 | F | 304 | CLA | CHA-CBD-CGD-O1D |
| 22 | F | 304 | CLA | CHA-CBD-CGD-O2D |
| 22 | G | 203 | CLA | CHA-CBD-CGD-O1D |
| 22 | G | 203 | CLA | CHA-CBD-CGD-O2D |
| 22 | J | 3002 | CLA | CHA-CBD-CGD-O2D |
| 22 | L | 204 | CLA | CHA-CBD-CGD-O1D |
| 22 | L | 204 | CLA | CHA-CBD-CGD-O2D |
| 22 | 1 | 603 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 603 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 604 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 604 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 610 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 610 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 613 | CLA | CHA-CBD-CGD-O1D |
| 22 | 1 | 613 | CLA | CHA-CBD-CGD-O2D |
| 22 | 3 | 607 | CLA | C1A-C2A-CAA-CBA |
| 22 | 3 | 607 | CLA | C2-C1-O2A-CGA |
| 22 | 3 | 607 | CLA | C11-C10-C8-C9 |
| 22 | 3 | 611 | CLA | CHA-CBD-CGD-O1D |
| 22 | 3 | 611 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | 7 | 601 | CLA | C2-C3-C5-C6 |
| 22 | 7 | 601 | CLA | C4-C3-C5-C6 |
| 22 | 7 | 603 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 603 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 606 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 7 | 606 | CLA | C3A-C2A-CAA-CBA |
| 22 | 7 | 606 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 606 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 609 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 609 | CLA | C3A-C2A-CAA-CBA |
| 22 | 8 | 606 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 602 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 608 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 610 | CLA | C2-C3-C5-C6 |
| 22 | Z | 610 | CLA | C4-C3-C5-C6 |
| 22 | Z | 613 | CLA | CHA-CBD-CGD-O1D |
| 22 | Z | 613 | CLA | CHA-CBD-CGD-O2D |
| 22 | 4 | 609 | CLA | C1A-C2A-CAA-CBA |
| 22 | 4 | 609 | CLA | C3A-C2A-CAA-CBA |
| 22 | 5 | 609 | CLA | C1A-C2A-CAA-CBA |
| 22 | 5 | 609 | CLA | C3A-C2A-CAA-CBA |
| 22 | 5 | 609 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 611 | CLA | C2-C3-C5-C6 |
| 22 | 5 | 611 | CLA | C4-C3-C5-C6 |
| 22 | 5 | 612 | CLA | C2-C3-C5-C6 |
| 22 | 5 | 612 | CLA | C4-C3-C5-C6 |
| 22 | 5 | 617 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 617 | CLA | CHA-CBD-CGD-O1D |
| 22 | 5 | 617 | CLA | CHA-CBD-CGD-O2D |
| 22 | 5 | 621 | CLA | CHA-CBD-CGD-O1D |
| 22 | 6 | 611 | CLA | C2-C3-C5-C6 |
| 22 | 6 | 611 | CLA | C4-C3-C5-C6 |
| 22 | 6 | 614 | CLA | CBD-CGD-O2D-CED |
| 22 | 2 | 610 | CLA | C2-C3-C5-C6 |
| 22 | 2 | 610 | CLA | C4-C3-C5-C6 |
| 22 | 2 | 611 | CLA | C2-C3-C5-C6 |
| 22 | 2 | 611 | CLA | C4-C3-C5-C6 |
| 22 | 2 | 612 | CLA | C2-C3-C5-C6 |
| 22 | 2 | 612 | CLA | C4-C3-C5-C6 |
| 22 | 2 | 613 | CLA | C1A-C2A-CAA-CBA |
| 22 | 9 | 602 | CLA | C2-C3-C5-C6 |
| 22 | 9 | 602 | CLA | C4-C3-C5-C6 |
| 22 | 9 | 611 | CLA | C4-C3-C5-C6 |
| 22 | 9 | 612 | CLA | C3-C5-C6-C7 |
| 24 | A | 846 | LHG | C3-O3-P-O5 |
| 24 | A | 847 | LHG | C4-O6-P-O4 |
| 24 | A | 855 | LHG | C4-O6-P-O4 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 24 | B | 851 | LHG | C3-O3-P-O5 |
| 24 | B | 851 | LHG | C4-O6-P-O5 |
| 24 | B | 851 | LHG | O9-C7-O7-C5 |
| 24 | 1 | 620 | LHG | O2-C2-C3-O3 |
| 24 | 1 | 620 | LHG | C24-C23-O8-C6 |
| 24 | Z | 620 | LHG | O2-C2-C3-O3 |
| 24 | Z | 620 | LHG | C4-O6-P-O5 |
| 24 | 4 | 622 | LHG | C3-O3-P-O4 |
| 24 | 5 | 623 | LHG | C4-O6-P-O5 |
| 24 | 6 | 619 | LHG | C3-O3-P-O6 |
| 25 | A | 848 | BCR | C1-C6-C7-C8 |
| 25 | A | 850 | BCR | C1-C6-C7-C8 |
| 25 | A | 850 | BCR | C23-C24-C25-C30 |
| 25 | B | 801 | BCR | C21-C22-C23-C24 |
| 25 | B | 801 | BCR | C37-C22-C23-C24 |
| 25 | B | 843 | BCR | C7-C8-C9-C10 |
| 25 | B | 843 | BCR | C7-C8-C9-C34 |
| 25 | B | 843 | BCR | C21-C22-C23-C24 |
| 25 | B | 843 | BCR | C37-C22-C23-C24 |
| 25 | B | 844 | BCR | C1-C6-C7-C8 |
| 25 | B | 844 | BCR | C7-C8-C9-C10 |
| 25 | B | 844 | BCR | C7-C8-C9-C34 |
| 25 | B | 845 | BCR | C7-C8-C9-C10 |
| 25 | B | 845 | BCR | C7-C8-C9-C34 |
| 25 | B | 845 | BCR | C37-C22-C23-C24 |
| 25 | B | 846 | BCR | C1-C6-C7-C8 |
| 25 | B | 846 | BCR | C23-C24-C25-C30 |
| 25 | G | 205 | BCR | C1-C6-C7-C8 |
| 25 | I | 172 | BCR | C1-C6-C7-C8 |
| 25 | I | 172 | BCR | C17-C18-C19-C20 |
| 25 | I | 172 | BCR | C36-C18-C19-C20 |
| 25 | I | 172 | BCR | C21-C22-C23-C24 |
| 25 | I | 172 | BCR | C37-C22-C23-C24 |
| 25 | J | 3003 | BCR | C7-C8-C9-C34 |
| 25 | J | 3003 | BCR | C17-C18-C19-C20 |
| 25 | J | 3003 | BCR | C36-C18-C19-C20 |
| 25 | K | 4001 | BCR | C21-C22-C23-C24 |
| 25 | K | 4001 | BCR | C37-C22-C23-C24 |
| 25 | K | 4004 | BCR | C1-C6-C7-C8 |
| 25 | K | 4004 | BCR | C23-C24-C25-C30 |
| 25 | 3 | 717 | BCR | C1-C6-C7-C8 |
| 25 | 3 | 718 | BCR | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | 3 | 719 | BCR | C1-C6-C7-C8 |
| 25 | 3 | 719 | BCR | C7-C8-C9-C34 |
| 25 | 7 | 623 | BCR | C1-C6-C7-C8 |
| 25 | 7 | 623 | BCR | C17-C18-C19-C20 |
| 25 | 7 | 623 | BCR | C23-C24-C25-C26 |
| 25 | 7 | 624 | BCR | C1-C6-C7-C8 |
| 25 | 7 | 624 | BCR | C23-C24-C25-C30 |
| 25 | 8 | 619 | BCR | C1-C6-C7-C8 |
| 25 | 8 | 619 | BCR | C36-C18-C19-C20 |
| 25 | 5 | 622 | BCR | C11-C12-C13-C14 |
| 25 | 5 | 622 | BCR | C11-C12-C13-C35 |
| 25 | 5 | 625 | BCR | C1-C6-C7-C8 |
| 25 | 5 | 625 | BCR | C7-C8-C9-C10 |
| 25 | 5 | 625 | BCR | C7-C8-C9-C34 |
| 25 | 6 | 623 | BCR | C5-C6-C7-C8 |
| 25 | 6 | 623 | BCR | C7-C8-C9-C10 |
| 25 | 6 | 623 | BCR | C7-C8-C9-C34 |
| 25 | 6 | 623 | BCR | C11-C12-C13-C14 |
| 25 | 6 | 623 | BCR | C11-C12-C13-C35 |
| 25 | 6 | 625 | BCR | C7-C8-C9-C10 |
| 25 | 6 | 625 | BCR | C7-C8-C9-C34 |
| 27 | B | 850 | DGD | O2G-C2G-C3G-O3G |
| 27 | B | 850 | DGD | O6D-C1D-O3G-C3G |
| 29 | 1 | 601 | CHL | C1C-C2C-CMC-OMC |
| 29 | 1 | 601 | CHL | C3C-C2C-CMC-OMC |
| 29 | 1 | 601 | CHL | CHA-CBD-CGD-O1D |
| 29 | 1 | 601 | CHL | CHA-CBD-CGD-O2D |
| 29 | 1 | 601 | CHL | CAD-CBD-CGD-O1D |
| 29 | 1 | 601 | CHL | CAD-CBD-CGD-O2D |
| 29 | 1 | 601 | CHL | O2A-C1-C2-C3 |
| 29 | 1 | 601 | CHL | C2-C3-C5-C6 |
| 29 | 1 | 601 | CHL | C4-C3-C5-C6 |
| 29 | 1 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 3 | 608 | CHL | C14-C13-C15-C16 |
| 29 | 7 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | 7 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 8 | 607 | CHL | C1A-C2A-CAA-CBA |
| 29 | 8 | 607 | CHL | C2A-CAA-CBA-CGA |
| 29 | 8 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | 8 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | Z | 601 | CHL | C1C-C2C-CMC-OMC |
| 29 | Z | 601 | CHL | C3C-C2C-CMC-OMC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | Z | 601 | CHL | CHA-CBD-CGD-O1D |
| 29 | Z | 601 | CHL | CHA-CBD-CGD-O2D |
| 29 | Z | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | Z | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 4 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | 4 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 4 | 608 | CHL | CBD-CGD-O2D-CED |
| 29 | 4 | 618 | CHL | C3C-C2C-CMC-OMC |
| 29 | 5 | 607 | CHL | C1A-C2A-CAA-CBA |
| 29 | 5 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | 5 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 5 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 5 | 608 | CHL | C1A-C2A-CAA-CBA |
| 29 | 5 | 608 | CHL | C3A-C2A-CAA-CBA |
| 29 | 5 | 608 | CHL | C1C-C2C-CMC-OMC |
| 29 | 5 | 608 | CHL | C3C-C2C-CMC-OMC |
| 29 | 5 | 608 | CHL | CBD-CGD-O2D-CED |
| 29 | 5 | 618 | CHL | C3C-C2C-CMC-OMC |
| 29 | 6 | 607 | CHL | C1A-C2A-CAA-CBA |
| 29 | 6 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | 6 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 6 | 608 | CHL | C1A-C2A-CAA-CBA |
| 29 | 6 | 618 | CHL | C1A-C2A-CAA-CBA |
| 29 | 6 | 618 | CHL | C3A-C2A-CAA-CBA |
| 29 | 9 | 607 | CHL | C3C-C2C-CMC-OMC |
| 29 | 9 | 607 | CHL | CHA-CBD-CGD-O1D |
| 29 | 9 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 1 | 619 | LUT | C1-C6-C7-C8 |
| 30 | 8 | 617 | LUT | C1-C6-C7-C8 |
| 30 | 4 | 620 | LUT | C1-C6-C7-C8 |
| 30 | 9 | 616 | LUT | C1-C6-C7-C8 |
| 22 | Z | 611 | CLA | O1D-CGD-O2D-CED |
| 29 | 1 | 607 | CHL | O1D-CGD-O2D-CED |
| 22 | 1 | 611 | CLA | O1D-CGD-O2D-CED |
| 22 | 5 | 616 | CLA | O1D-CGD-O2D-CED |
| 29 | 5 | 607 | CHL | O1D-CGD-O2D-CED |
| 22 | A | 825 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 841 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 803 | CLA | CBD-CGD-O2D-CED |
| 22 | 1 | 602 | CLA | CBD-CGD-O2D-CED |
| 22 | 1 | 608 | CLA | CBD-CGD-O2D-CED |
| 22 | 1 | 611 | CLA | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 7 | 608 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 611 | CLA | CBD-CGD-O2D-CED |
| 22 | 5 | 606 | CLA | CBD-CGD-O2D-CED |
| 22 | 5 | 616 | CLA | CBD-CGD-O2D-CED |
| 22 | 6 | 602 | CLA | CBD-CGD-O2D-CED |
| 22 | 2 | 601 | CLA | CBD-CGD-O2D-CED |
| 29 | 1 | 607 | CHL | CBD-CGD-O2D-CED |
| 29 | 3 | 608 | CHL | CBD-CGD-O2D-CED |
| 29 | 6 | 608 | CHL | CBD-CGD-O2D-CED |
| 24 | 1 | 620 | LHG | O10-C23-O8-C6 |
| 24 | Z | 620 | LHG | O10-C23-O8-C6 |
| 22 | 7 | 608 | CLA | O1D-CGD-O2D-CED |
| 29 | 6 | 608 | CHL | O1D-CGD-O2D-CED |
| 22 | B | 840 | CLA | C4C-C3C-CAC-CBC |
| 22 | B | 803 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 806 | CLA | O1D-CGD-O2D-CED |
| 22 | 8 | 606 | CLA | O1D-CGD-O2D-CED |
| 22 | 6 | 614 | CLA | O1D-CGD-O2D-CED |
| 29 | 3 | 608 | CHL | O1D-CGD-O2D-CED |
| 29 | 5 | 608 | CHL | O1D-CGD-O2D-CED |
| 24 | Z | 620 | LHG | C24-C23-O8-C6 |
| 22 | A | 810 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 811 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 824 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 823 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 835 | CLA | CBD-CGD-O2D-CED |
| 22 | F | 301 | CLA | CBD-CGD-O2D-CED |
| 22 | K | 4002 | CLA | CBD-CGD-O2D-CED |
| 22 | 3 | 603 | CLA | CBD-CGD-O2D-CED |
| 22 | 3 | 613 | CLA | CBD-CGD-O2D-CED |
| 22 | 7 | 604 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 613 | CLA | CBD-CGD-O2D-CED |
| 22 | 4 | 602 | CLA | CBD-CGD-O2D-CED |
| 22 | 4 | 611 | CLA | CBD-CGD-O2D-CED |
| 22 | 6 | 616 | CLA | CBD-CGD-O2D-CED |
| 29 | 4 | 607 | CHL | CBD-CGD-O2D-CED |
| 22 | B | 840 | CLA | C2C-C3C-CAC-CBC |
| 22 | A | 806 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 818 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 822 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 611 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 829 | CLA | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | 4 | 608 | CHL | O1D-CGD-O2D-CED |
| 22 | 3 | 620 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 603 | CLA | CBD-CGD-O2D-CED |
| 29 | 6 | 618 | CHL | CBD-CGD-O2D-CED |
| 22 | Z | 602 | CLA | O1D-CGD-O2D-CED |
| 22 | Z | 608 | CLA | O1D-CGD-O2D-CED |
| 22 | 5 | 617 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 802 | CLA | C3-C5-C6-C7 |
| 22 | A | 806 | CLA | C3-C5-C6-C7 |
| 22 | A | 808 | CLA | C3-C5-C6-C7 |
| 22 | A | 816 | CLA | C3-C5-C6-C7 |
| 22 | A | 817 | CLA | C3-C5-C6-C7 |
| 22 | A | 818 | CLA | C3-C5-C6-C7 |
| 22 | A | 819 | CLA | C3-C5-C6-C7 |
| 22 | A | 825 | CLA | C3-C5-C6-C7 |
| 22 | A | 826 | CLA | C3-C5-C6-C7 |
| 22 | A | 833 | CLA | C3-C5-C6-C7 |
| 22 | A | 840 | CLA | C3-C5-C6-C7 |
| 22 | A | 843 | CLA | C3-C5-C6-C7 |
| 22 | A | 854 | CLA | C3-C5-C6-C7 |
| 22 | B | 807 | CLA | C3-C5-C6-C7 |
| 22 | B | 808 | CLA | C3-C5-C6-C7 |
| 22 | B | 809 | CLA | C3-C5-C6-C7 |
| 22 | B | 818 | CLA | C3-C5-C6-C7 |
| 22 | B | 822 | CLA | C3-C5-C6-C7 |
| 22 | B | 824 | CLA | C3-C5-C6-C7 |
| 22 | B | 827 | CLA | C3-C5-C6-C7 |
| 22 | B | 833 | CLA | C3-C5-C6-C7 |
| 22 | B | 841 | CLA | C3-C5-C6-C7 |
| 22 | F | 301 | CLA | C3-C5-C6-C7 |
| 22 | 1 | 608 | CLA | C3-C5-C6-C7 |
| 22 | 1 | 611 | CLA | C3-C5-C6-C7 |
| 22 | 3 | 607 | CLA | C3-C5-C6-C7 |
| 22 | 3 | 620 | CLA | C3-C5-C6-C7 |
| 22 | 7 | 604 | CLA | C3-C5-C6-C7 |
| 22 | 7 | 620 | CLA | C3-C5-C6-C7 |
| 22 | 8 | 614 | CLA | C3-C5-C6-C7 |
| 22 | 4 | 611 | CLA | C3-C5-C6-C7 |
| 22 | 5 | 613 | CLA | C3-C5-C6-C7 |
| 22 | 2 | 610 | CLA | C3-C5-C6-C7 |
| 22 | 2 | 611 | CLA | C3-C5-C6-C7 |
| 22 | 9 | 610 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 9 | 611 | CLA | C3-C5-C6-C7 |
| 29 | 8 | 607 | CHL | C3-C5-C6-C7 |
| 22 | A | 845 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 822 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | 5 | 601 | CLA | CBA-CGA-O2A-C1 |
| 24 | B | 851 | LHG | C8-C7-O7-C5 |
| 22 | B | 810 | CLA | CBD-CGD-O2D-CED |
| 22 | 7 | 606 | CLA | CBD-CGD-O2D-CED |
| 29 | 9 | 606 | CHL | CBD-CGD-O2D-CED |
| 22 | B | 834 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 845 | CLA | C3-C5-C6-C7 |
| 22 | 7 | 612 | CLA | C3-C5-C6-C7 |
| 22 | 8 | 612 | CLA | C3-C5-C6-C7 |
| 22 | 5 | 612 | CLA | C3-C5-C6-C7 |
| 22 | 6 | 612 | CLA | C3-C5-C6-C7 |
| 22 | 2 | 612 | CLA | C3-C5-C6-C7 |
| 22 | 6 | 604 | CLA | C4-C3-C5-C6 |
| 22 | 6 | 610 | CLA | C4-C3-C5-C6 |
| 22 | A | 831 | CLA | C2-C3-C5-C6 |
| 22 | A | 835 | CLA | C2-C3-C5-C6 |
| 22 | B | 829 | CLA | C2-C3-C5-C6 |
| 22 | 9 | 611 | CLA | C2-C3-C5-C6 |
| 22 | F | 303 | CLA | CBD-CGD-O2D-CED |
| 22 | 2 | 602 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 825 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 837 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 845 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 824 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 839 | CLA | C2A-CAA-CBA-CGA |
| 22 | 3 | 607 | CLA | C2A-CAA-CBA-CGA |
| 22 | Z | 609 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 614 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 621 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 9 | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | 9 | 614 | CLA | C2A-CAA-CBA-CGA |
| 29 | 1 | 607 | CHL | C2A-CAA-CBA-CGA |
| 29 | 4 | 608 | CHL | C2A-CAA-CBA-CGA |
| 29 | 5 | 608 | CHL | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 804 | CLA | C3-C5-C6-C7 |
| 22 | A | 807 | CLA | C3-C5-C6-C7 |
| 22 | B | 802 | CLA | C3-C5-C6-C7 |
| 22 | B | 806 | CLA | C3-C5-C6-C7 |
| 22 | B | 820 | CLA | C3-C5-C6-C7 |
| 22 | 1 | 602 | CLA | C3-C5-C6-C7 |
| 22 | 3 | 610 | CLA | C3-C5-C6-C7 |
| 22 | Z | 608 | CLA | C3-C5-C6-C7 |
| 22 | Z | 611 | CLA | C3-C5-C6-C7 |
| 22 | 4 | 613 | CLA | C3-C5-C6-C7 |
| 22 | A | 806 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 815 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 824 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 829 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 842 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 818 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 825 | CLA | CBA-CGA-O2A-C1 |
| 22 | 3 | 607 | CLA | CBA-CGA-O2A-C1 |
| 22 | 5 | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | 6 | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | 9 | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 602 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 822 | CLA | CBD-CGD-O2D-CED |
| 22 | 1 | 608 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 842 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 845 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 833 | CLA | O1A-CGA-O2A-C1 |
| 22 | Z | 611 | CLA | O1A-CGA-O2A-C1 |
| 22 | 5 | 601 | CLA | O1A-CGA-O2A-C1 |
| 22 | 2 | 601 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 818 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 837 | CLA | CBD-CGD-O2D-CED |
| 22 | 8 | 604 | CLA | CBD-CGD-O2D-CED |
| 22 | 5 | 602 | CLA | CBD-CGD-O2D-CED |
| 29 | 4 | 618 | CHL | CBD-CGD-O2D-CED |
| 29 | 5 | 618 | CHL | CBD-CGD-O2D-CED |
| 22 | 5 | 606 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 809 | CLA | C3-C5-C6-C7 |
| 22 | A | 831 | CLA | C3-C5-C6-C7 |
| 22 | A | 839 | CLA | C3-C5-C6-C7 |
| 22 | B | 819 | CLA | C3-C5-C6-C7 |
| 22 | B | 852 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 6 | 602 | CLA | C3-C5-C6-C7 |
| 29 | 3 | 608 | CHL | C3-C5-C6-C7 |
| 22 | A | 805 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 812 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 820 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 833 | CLA | CBA-CGA-O2A-C1 |
| 22 | 7 | 620 | CLA | CBA-CGA-O2A-C1 |
| 22 | 4 | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | 9 | 602 | CLA | CBA-CGA-O2A-C1 |
| 29 | 6 | 607 | CHL | CBA-CGA-O2A-C1 |
| 22 | A | 812 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 815 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 829 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 825 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 607 | CLA | O1A-CGA-O2A-C1 |
| 22 | Z | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 809 | CLA | CBD-CGD-O2D-CED |
| 22 | G | 204 | CLA | CBD-CGD-O2D-CED |
| 22 | 8 | 609 | CLA | CBD-CGD-O2D-CED |
| 22 | Z | 610 | CLA | CBD-CGD-O2D-CED |
| 22 | 6 | 610 | CLA | CBD-CGD-O2D-CED |
| 22 | 6 | 611 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 805 | CLA | C3-C5-C6-C7 |
| 22 | B | 812 | CLA | C3-C5-C6-C7 |
| 22 | B | 815 | CLA | C3-C5-C6-C7 |
| 22 | 3 | 604 | CLA | C3-C5-C6-C7 |
| 22 | B | 834 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | 6 | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 805 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 620 | CLA | O1A-CGA-O2A-C1 |
| 22 | 4 | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | 5 | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | 9 | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | 9 | 611 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 606 | CLA | C3-C5-C6-C7 |
| 22 | Z | 606 | CLA | C3-C5-C6-C7 |
| 22 | A | 808 | CLA | C4-C3-C5-C6 |
| 22 | A | 833 | CLA | C4-C3-C5-C6 |
| 22 | A | 839 | CLA | C4-C3-C5-C6 |
| 22 | A | 842 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 602 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 1 | 606 | CLA | C4-C3-C5-C6 |
| 22 | 8 | 610 | CLA | C4-C3-C5-C6 |
| 22 | 8 | 612 | CLA | C4-C3-C5-C6 |
| 22 | Z | 602 | CLA | C4-C3-C5-C6 |
| 22 | Z | 604 | CLA | C4-C3-C5-C6 |
| 22 | Z | 606 | CLA | C4-C3-C5-C6 |
| 22 | 4 | 611 | CLA | C4-C3-C5-C6 |
| 22 | A | 808 | CLA | C2-C3-C5-C6 |
| 22 | A | 833 | CLA | C2-C3-C5-C6 |
| 22 | A | 839 | CLA | C2-C3-C5-C6 |
| 22 | A | 842 | CLA | C2-C3-C5-C6 |
| 22 | A | 843 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 602 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 606 | CLA | C2-C3-C5-C6 |
| 22 | 8 | 610 | CLA | C2-C3-C5-C6 |
| 22 | 8 | 612 | CLA | C2-C3-C5-C6 |
| 22 | Z | 602 | CLA | C2-C3-C5-C6 |
| 22 | Z | 604 | CLA | C2-C3-C5-C6 |
| 22 | Z | 606 | CLA | C2-C3-C5-C6 |
| 22 | 4 | 611 | CLA | C2-C3-C5-C6 |
| 22 | A | 854 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 827 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 852 | CLA | C2A-CAA-CBA-CGA |
| 29 | Z | 607 | CHL | C2A-CAA-CBA-CGA |
| 22 | A | 824 | CLA | O1A-CGA-O2A-C1 |
| 29 | 6 | 607 | CHL | O1A-CGA-O2A-C1 |
| 22 | 4 | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | 5 | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | 8 | 614 | CLA | CBD-CGD-O2D-CED |
| 22 | 9 | 613 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 810 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 825 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 820 | CLA | O1A-CGA-O2A-C1 |
| 22 | 6 | 602 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 808 | CLA | CBD-CGD-O2D-CED |
| 22 | 1 | 614 | CLA | CBD-CGD-O2D-CED |
| 22 | 4 | 602 | CLA | O1D-CGD-O2D-CED |
| 24 | 1 | 620 | LHG | C1-C2-C3-O3 |
| 24 | Z | 620 | LHG | C1-C2-C3-O3 |
| 28 | 9 | 620 | LMG | O9-C10-O7-C8 |
| 22 | 5 | 611 | CLA | O1A-CGA-O2A-C1 |
| 22 | 6 | 602 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 3 | 603 | CLA | C3-C5-C6-C7 |
| 22 | 7 | 604 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 807 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 809 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 843 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 810 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 814 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 829 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 831 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | 3 | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | 3 | 620 | CLA | CBA-CGA-O2A-C1 |
| 22 | 7 | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | 8 | 602 | CLA | CBA-CGA-O2A-C1 |
| 22 | 8 | 612 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | 6 | 609 | CLA | CBA-CGA-O2A-C1 |
| 22 | 6 | 612 | CLA | CBA-CGA-O2A-C1 |
| 22 | 9 | 613 | CLA | CBA-CGA-O2A-C1 |
| 22 | 5 | 604 | CLA | CBD-CGD-O2D-CED |
| 22 | 6 | 604 | CLA | CBD-CGD-O2D-CED |
| 22 | 9 | 614 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 841 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 803 | CLA | C10-C11-C12-C13 |
| 22 | 1 | 610 | CLA | C5-C6-C7-C8 |
| 22 | Z | 611 | CLA | C10-C11-C12-C13 |
| 22 | 5 | 610 | CLA | C10-C11-C12-C13 |
| 22 | 6 | 601 | CLA | C10-C11-C12-C13 |
| 22 | 4 | 612 | CLA | C3-C5-C6-C7 |
| 29 | Z | 601 | CHL | C3-C5-C6-C7 |
| 28 | 9 | 620 | LMG | O1-C7-C8-O7 |
| 22 | 7 | 612 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 807 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 810 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 604 | CLA | O1A-CGA-O2A-C1 |
| 22 | 8 | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | 6 | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 819 | CLA | C4-C3-C5-C6 |
| 22 | 3 | 610 | CLA | C4-C3-C5-C6 |
| 22 | 6 | 604 | CLA | C2-C3-C5-C6 |
| 22 | A | 827 | CLA | C6-C7-C8-C9 |
| 22 | A | 828 | CLA | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 839 | CLA | C14-C13-C15-C16 |
| 22 | B | 805 | CLA | C6-C7-C8-C9 |
| 22 | B | 818 | CLA | C6-C7-C8-C9 |
| 22 | 1 | 610 | CLA | C6-C7-C8-C9 |
| 22 | 7 | 601 | CLA | C11-C12-C13-C14 |
| 22 | Z | 610 | CLA | C6-C7-C8-C9 |
| 23 | A | 844 | PQN | C24-C23-C25-C26 |
| 22 | 3 | 603 | CLA | O1D-CGD-O2D-CED |
| 22 | 4 | 613 | CLA | CBD-CGD-O2D-CED |
| 22 | 7 | 620 | CLA | C5-C6-C7-C8 |
| 22 | A | 815 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 852 | BCR | C7-C8-C9-C34 |
| 25 | A | 856 | BCR | C37-C22-C23-C24 |
| 25 | B | 844 | BCR | C37-C22-C23-C24 |
| 25 | L | 205 | BCR | C7-C8-C9-C34 |
| 25 | L | 205 | BCR | C37-C22-C23-C24 |
| 25 | 3 | 718 | BCR | C11-C12-C13-C35 |
| 25 | 7 | 623 | BCR | C36-C18-C19-C20 |
| 25 | 4 | 621 | BCR | C7-C8-C9-C34 |
| 25 | 6 | 625 | BCR | C11-C12-C13-C35 |
| 25 | A | 856 | BCR | C21-C22-C23-C24 |
| 25 | B | 844 | BCR | C21-C22-C23-C24 |
| 25 | L | 205 | BCR | C21-C22-C23-C24 |
| 25 | 4 | 621 | BCR | C7-C8-C9-C10 |
| 25 | 6 | 625 | BCR | C11-C12-C13-C14 |
| 28 | 9 | 620 | LMG | C11-C10-O7-C8 |
| 22 | A | 843 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 831 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 620 | CLA | O1A-CGA-O2A-C1 |
| 22 | 8 | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | Z | 604 | CLA | O1A-CGA-O2A-C1 |
| 22 | 6 | 609 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 812 | CLA | C10-C11-C12-C13 |
| 22 | B | 818 | CLA | C8-C10-C11-C12 |
| 22 | B | 839 | CLA | C15-C16-C17-C18 |
| 22 | 6 | 601 | CLA | C8-C10-C11-C12 |
| 23 | B | 842 | PQN | C20-C21-C22-C23 |
| 22 | 1 | 603 | CLA | C3-C5-C6-C7 |
| 22 | Z | 602 | CLA | C3-C5-C6-C7 |
| 22 | A | 817 | CLA | C8-C10-C11-C12 |
| 22 | A | 814 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 826 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | A | 830 | CLA | C13-C15-C16-C17 |
| 22 | B | 805 | CLA | C15-C16-C17-C18 |
| 22 | B | 812 | CLA | C5-C6-C7-C8 |
| 22 | B | 834 | CLA | C10-C11-C12-C13 |
| 22 | B | 837 | CLA | C8-C10-C11-C12 |
| 22 | B | 837 | CLA | C15-C16-C17-C18 |
| 22 | 1 | 611 | CLA | C8-C10-C11-C12 |
| 22 | 3 | 610 | CLA | C13-C15-C16-C17 |
| 22 | 8 | 613 | CLA | C5-C6-C7-C8 |
| 22 | Z | 608 | CLA | C5-C6-C7-C8 |
| 22 | K | 4002 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 845 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 809 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 808 | CLA | C10-C11-C12-C13 |
| 22 | A | 814 | CLA | C8-C10-C11-C12 |
| 22 | B | 802 | CLA | C10-C11-C12-C13 |
| 22 | B | 825 | CLA | C13-C15-C16-C17 |
| 22 | B | 834 | CLA | C5-C6-C7-C8 |
| 22 | 8 | 601 | CLA | C13-C15-C16-C17 |
| 22 | 8 | 613 | CLA | C15-C16-C17-C18 |
| 22 | Z | 608 | CLA | C8-C10-C11-C12 |
| 22 | Z | 608 | CLA | C15-C16-C17-C18 |
| 22 | Z | 611 | CLA | C5-C6-C7-C8 |
| 24 | A | 847 | LHG | C7-C8-C9-C10 |
| 28 | J | 3001 | LMG | C28-C29-C30-C31 |
| 28 | 9 | 620 | LMG | C10-C11-C12-C13 |
| 29 | 4 | 607 | CHL | O1D-CGD-O2D-CED |
| 22 | A | 826 | CLA | C13-C15-C16-C17 |
| 22 | B | 810 | CLA | C5-C6-C7-C8 |
| 22 | B | 837 | CLA | C13-C15-C16-C17 |
| 22 | 3 | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 806 | CLA | C2-C1-O2A-CGA |
| 22 | B | 810 | CLA | C10-C11-C12-C13 |
| 22 | B | 829 | CLA | C10-C11-C12-C13 |
| 24 | 1 | 620 | LHG | C7-C8-C9-C10 |
| 22 | A | 838 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 832 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 833 | CLA | CBD-CGD-O2D-CED |
| 22 | 8 | 602 | CLA | C13-C15-C16-C17 |
| 22 | A | 814 | CLA | C10-C11-C12-C13 |
| 22 | A | 809 | CLA | C12-C13-C15-C16 |
| 22 | A | 842 | CLA | C6-C7-C8-C10 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 822 | CLA | C3-C5-C6-C7 |
| 22 | Z | 613 | CLA | C3-C5-C6-C7 |
| 22 | A | 814 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 814 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 818 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 812 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 814 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 803 | CLA | C2A-CAA-CBA-CGA |
| 22 | G | 203 | CLA | C2A-CAA-CBA-CGA |
| 22 | 1 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | Z | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 835 | CLA | O1D-CGD-O2D-CED |
| 22 | F | 301 | CLA | O1D-CGD-O2D-CED |
| 22 | 3 | 620 | CLA | O1D-CGD-O2D-CED |
| 22 | 4 | 611 | CLA | O1D-CGD-O2D-CED |
| 22 | 6 | 616 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 834 | CLA | C5-C6-C7-C8 |
| 22 | B | 827 | CLA | C10-C11-C12-C13 |
| 22 | B | 821 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 609 | CLA | CBD-CGD-O2D-CED |
| 22 | 8 | 602 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 831 | CLA | C8-C10-C11-C12 |
| 22 | A | 839 | CLA | C13-C15-C16-C17 |
| 22 | 4 | 602 | CLA | C10-C11-C12-C13 |
| 22 | A | 824 | CLA | O1D-CGD-O2D-CED |
| 29 | 6 | 618 | CHL | O1D-CGD-O2D-CED |
| 24 | Z | 620 | LHG | C7-C8-C9-C10 |
| 22 | B | 808 | CLA | C15-C16-C17-C18 |
| 22 | 1 | 604 | CLA | C5-C6-C7-C8 |
| 22 | A | 809 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 829 | CLA | O1A-CGA-O2A-C1 |
| 22 | 4 | 611 | CLA | O1A-CGA-O2A-C1 |
| 22 | 9 | 613 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 825 | CLA | C15-C16-C17-C18 |
| 22 | 7 | 601 | CLA | C8-C10-C11-C12 |
| 29 | 3 | 608 | CHL | C8-C10-C11-C12 |
| 22 | B | 817 | CLA | C5-C6-C7-C8 |
| 22 | 3 | 604 | CLA | C10-C11-C12-C13 |
| 22 | 4 | 601 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 6 | 610 | CLA | C5-C6-C7-C8 |
| 29 | 3 | 608 | CHL | C10-C11-C12-C13 |
| 24 | A | 855 | LHG | C4-O6-P-O3 |
| 24 | B | 851 | LHG | C3-O3-P-O6 |
| 24 | 7 | 625 | LHG | C4-O6-P-O3 |
| 24 | 8 | 620 | LHG | C3-O3-P-O6 |
| 24 | 8 | 620 | LHG | C4-O6-P-O3 |
| 24 | 4 | 622 | LHG | C3-O3-P-O6 |
| 24 | 5 | 623 | LHG | C4-O6-P-O3 |
| 22 | A | 835 | CLA | C3-C5-C6-C7 |
| 22 | B | 834 | CLA | C3-C5-C6-C7 |
| 22 | 8 | 613 | CLA | C3-C5-C6-C7 |
| 22 | B | 811 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 813 | CLA | CBA-CGA-O2A-C1 |
| 22 | F | 304 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | 7 | 602 | CLA | CBA-CGA-O2A-C1 |
| 24 | 4 | 622 | LHG | C24-C23-O8-C6 |
| 29 | 7 | 607 | CHL | CBA-CGA-O2A-C1 |
| 22 | B | 823 | CLA | O1D-CGD-O2D-CED |
| 22 | Z | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | 6 | 601 | CLA | C5-C6-C7-C8 |
| 22 | A | 811 | CLA | O1D-CGD-O2D-CED |
| 29 | 9 | 606 | CHL | O1D-CGD-O2D-CED |
| 22 | 6 | 612 | CLA | C4-C3-C5-C6 |
| 29 | 7 | 607 | CHL | C4-C3-C5-C6 |
| 22 | 7 | 610 | CLA | C10-C11-C12-C13 |
| 22 | 6 | 602 | CLA | C10-C11-C12-C13 |
| 22 | A | 803 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 809 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 834 | CLA | C2A-CAA-CBA-CGA |
| 22 | 4 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 6 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | 9 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 816 | CLA | C3-C5-C6-C7 |
| 22 | 3 | 613 | CLA | C3-C5-C6-C7 |
| 22 | 9 | 602 | CLA | C3-C5-C6-C7 |
| 22 | A | 811 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 825 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 612 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 832 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 1 | 611 | CLA | C5-C6-C7-C8 |
| 22 | 3 | 602 | CLA | CBD-CGD-O2D-CED |
| 25 | 7 | 623 | BCR | C19-C20-C21-C22 |
| 22 | 6 | 601 | CLA | C3-C5-C6-C7 |
| 28 | J | 3001 | LMG | C12-C13-C14-C15 |
| 28 | 9 | 620 | LMG | C11-C12-C13-C14 |
| 28 | 9 | 620 | LMG | C29-C30-C31-C32 |
| 22 | B | 810 | CLA | O1D-CGD-O2D-CED |
| 22 | Z | 603 | CLA | O1D-CGD-O2D-CED |
| 22 | 3 | 613 | CLA | C6-C7-C8-C10 |
| 22 | 2 | 611 | CLA | CBA-CGA-O2A-C1 |
| 22 | F | 303 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 827 | CLA | C8-C10-C11-C12 |
| 22 | G | 204 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 822 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 820 | CLA | CBA-CGA-O2A-C1 |
| 27 | B | 850 | DGD | C3B-C4B-C5B-C6B |
| 22 | A | 831 | CLA | C10-C11-C12-C13 |
| 22 | B | 826 | CLA | C10-C11-C12-C13 |
| 22 | 9 | 602 | CLA | C5-C6-C7-C8 |
| 22 | A | 825 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 813 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 604 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 814 | CLA | C16-C17-C18-C20 |
| 22 | 3 | 613 | CLA | C6-C7-C8-C9 |
| 22 | 7 | 602 | CLA | C16-C17-C18-C20 |
| 22 | 2 | 602 | CLA | O1D-CGD-O2D-CED |
| 22 | 3 | 607 | CLA | C4-C3-C5-C6 |
| 22 | 3 | 613 | CLA | C4-C3-C5-C6 |
| 22 | 6 | 610 | CLA | C2-C3-C5-C6 |
| 22 | A | 808 | CLA | C11-C12-C13-C14 |
| 22 | A | 809 | CLA | C14-C13-C15-C16 |
| 22 | A | 819 | CLA | C11-C10-C8-C9 |
| 22 | A | 822 | CLA | C11-C10-C8-C9 |
| 22 | B | 805 | CLA | C11-C10-C8-C9 |
| 22 | B | 809 | CLA | C11-C12-C13-C14 |
| 22 | B | 812 | CLA | C11-C10-C8-C9 |
| 22 | B | 832 | CLA | C6-C7-C8-C9 |
| 22 | 1 | 610 | CLA | C11-C10-C8-C9 |
| 22 | 3 | 607 | CLA | C6-C7-C8-C9 |
| 22 | Z | 613 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 6 | 602 | CLA | C6-C7-C8-C9 |
| 24 | Z | 620 | LHG | C23-C24-C25-C26 |
| 22 | A | 842 | CLA | C5-C6-C7-C8 |
| 22 | Z | 613 | CLA | C10-C11-C12-C13 |
| 22 | A | 830 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 613 | CLA | C2A-CAA-CBA-CGA |
| 29 | 3 | 608 | CHL | C2A-CAA-CBA-CGA |
| 22 | A | 818 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 602 | CLA | O1A-CGA-O2A-C1 |
| 24 | A | 847 | LHG | O1-C1-C2-C3 |
| 25 | B | 845 | BCR | C21-C22-C23-C24 |
| 25 | 8 | 619 | BCR | C17-C18-C19-C20 |
| 22 | A | 807 | CLA | C5-C6-C7-C8 |
| 22 | A | 841 | CLA | C8-C10-C11-C12 |
| 24 | 5 | 623 | LHG | C23-C24-C25-C26 |
| 27 | B | 850 | DGD | C3A-C4A-C5A-C6A |
| 27 | B | 850 | DGD | C7B-C8B-C9B-CAB |
| 29 | 6 | 606 | CHL | C6-C7-C8-C9 |
| 29 | 6 | 606 | CHL | C6-C7-C8-C10 |
| 28 | 9 | 620 | LMG | O6-C1-O1-C7 |
| 22 | B | 806 | CLA | C8-C10-C11-C12 |
| 22 | B | 812 | CLA | C15-C16-C17-C18 |
| 24 | 7 | 625 | LHG | C25-C26-C27-C28 |
| 28 | 9 | 620 | LMG | C30-C31-C32-C33 |
| 22 | Z | 616 | CLA | CBA-CGA-O2A-C1 |
| 22 | 7 | 606 | CLA | O1D-CGD-O2D-CED |
| 24 | 7 | 625 | LHG | C10-C11-C12-C13 |
| 24 | 1 | 620 | LHG | C23-C24-C25-C26 |
| 22 | B | 810 | CLA | C3-C5-C6-C7 |
| 22 | A | 819 | CLA | CBA-CGA-O2A-C1 |
| 29 | 4 | 618 | CHL | O1D-CGD-O2D-CED |
| 22 | A | 803 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 804 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 807 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 834 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 837 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 824 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 826 | CLA | C3A-C2A-CAA-CBA |
| 22 | 1 | 612 | CLA | C3A-C2A-CAA-CBA |
| 22 | 3 | 617 | CLA | C3A-C2A-CAA-CBA |
| 22 | Z | 612 | CLA | C3A-C2A-CAA-CBA |
| 22 | 5 | 601 | CLA | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 29 | Z | 601 | CHL | C3A-C2A-CAA-CBA |
| 22 | A | 820 | CLA | C13-C15-C16-C17 |
| 22 | A | 837 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 811 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 811 | CLA | O1A-CGA-O2A-C1 |
| 24 | 4 | 622 | LHG | O10-C23-O8-C6 |
| 29 | 7 | 607 | CHL | O1A-CGA-O2A-C1 |
| 29 | 3 | 608 | CHL | C16-C17-C18-C19 |
| 29 | 3 | 608 | CHL | C16-C17-C18-C20 |
| 24 | 4 | 623 | LHG | C9-C10-C11-C12 |
| 22 | A | 834 | CLA | C3-C5-C6-C7 |
| 22 | F | 304 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 603 | CLA | C10-C11-C12-C13 |
| 22 | 8 | 601 | CLA | C8-C10-C11-C12 |
| 22 | 6 | 602 | CLA | C8-C10-C11-C12 |
| 22 | B | 806 | CLA | C4-C3-C5-C6 |
| 22 | B | 816 | CLA | C4-C3-C5-C6 |
| 29 | 6 | 607 | CHL | C4-C3-C5-C6 |
| 22 | A | 822 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 828 | CLA | CBA-CGA-O2A-C1 |
| 22 | 1 | 614 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 806 | CLA | C2-C3-C5-C6 |
| 22 | B | 819 | CLA | C2-C3-C5-C6 |
| 22 | 3 | 610 | CLA | C2-C3-C5-C6 |
| 22 | 3 | 613 | CLA | C2-C3-C5-C6 |
| 22 | 4 | 613 | CLA | C2-C3-C5-C6 |
| 22 | 4 | 603 | CLA | CBA-CGA-O2A-C1 |
| 24 | A | 847 | LHG | C15-C16-C17-C18 |
| 22 | B | 820 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 602 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 602 | CLA | C16-C17-C18-C19 |
| 22 | A | 816 | CLA | C5-C6-C7-C8 |
| 22 | B | 802 | CLA | C15-C16-C17-C18 |
| 22 | A | 814 | CLA | C3-C5-C6-C7 |
| 22 | B | 817 | CLA | C3-C5-C6-C7 |
| 22 | 2 | 609 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 829 | CLA | C2-C1-O2A-CGA |
| 22 | B | 834 | CLA | C2-C1-O2A-CGA |
| 22 | 1 | 608 | CLA | C2-C1-O2A-CGA |
| 22 | 1 | 614 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 614 | CLA | C2-C1-O2A-CGA |
| 28 | J | 3001 | LMG | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 3 | 604 | CLA | C13-C15-C16-C17 |
| 24 | A | 846 | LHG | C23-C24-C25-C26 |
| 22 | B | 805 | CLA | C3-C5-C6-C7 |
| 25 | A | 848 | BCR | C5-C6-C7-C8 |
| 25 | A | 850 | BCR | C5-C6-C7-C8 |
| 25 | A | 850 | BCR | C23-C24-C25-C26 |
| 25 | A | 856 | BCR | C1-C6-C7-C8 |
| 25 | A | 856 | BCR | C5-C6-C7-C8 |
| 25 | A | 856 | BCR | C23-C24-C25-C26 |
| 25 | A | 856 | BCR | C23-C24-C25-C30 |
| 25 | B | 844 | BCR | C5-C6-C7-C8 |
| 25 | B | 846 | BCR | C5-C6-C7-C8 |
| 25 | B | 846 | BCR | C23-C24-C25-C26 |
| 25 | B | 848 | BCR | C1-C6-C7-C8 |
| 25 | B | 848 | BCR | C5-C6-C7-C8 |
| 25 | G | 205 | BCR | C5-C6-C7-C8 |
| 25 | I | 172 | BCR | C5-C6-C7-C8 |
| 25 | J | 3003 | BCR | C23-C24-C25-C26 |
| 25 | J | 3003 | BCR | C23-C24-C25-C30 |
| 25 | K | 4004 | BCR | C5-C6-C7-C8 |
| 25 | K | 4004 | BCR | C23-C24-C25-C26 |
| 25 | L | 201 | BCR | C1-C6-C7-C8 |
| 25 | L | 201 | BCR | C5-C6-C7-C8 |
| 25 | L | 201 | BCR | C23-C24-C25-C26 |
| 25 | L | 201 | BCR | C23-C24-C25-C30 |
| 25 | L | 205 | BCR | C23-C24-C25-C26 |
| 25 | L | 205 | BCR | C23-C24-C25-C30 |
| 25 | 3 | 717 | BCR | C5-C6-C7-C8 |
| 25 | 3 | 717 | BCR | C23-C24-C25-C26 |
| 25 | 3 | 717 | BCR | C23-C24-C25-C30 |
| 25 | 3 | 719 | BCR | C5-C6-C7-C8 |
| 25 | 7 | 623 | BCR | C5-C6-C7-C8 |
| 25 | 7 | 623 | BCR | C23-C24-C25-C30 |
| 25 | 7 | 624 | BCR | C5-C6-C7-C8 |
| 25 | 7 | 624 | BCR | C23-C24-C25-C26 |
| 25 | 8 | 619 | BCR | C5-C6-C7-C8 |
| 25 | 8 | 619 | BCR | C23-C24-C25-C26 |
| 25 | 8 | 619 | BCR | C23-C24-C25-C30 |
| 25 | 5 | 622 | BCR | C1-C6-C7-C8 |
| 25 | 5 | 622 | BCR | C5-C6-C7-C8 |
| 25 | 5 | 622 | BCR | C23-C24-C25-C26 |
| 25 | 5 | 622 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 25 | 5 | 625 | BCR | C5-C6-C7-C8 |
| 25 | 5 | 625 | BCR | C23-C24-C25-C26 |
| 25 | 5 | 625 | BCR | C23-C24-C25-C30 |
| 25 | 6 | 623 | BCR | C1-C6-C7-C8 |
| 25 | 6 | 623 | BCR | C23-C24-C25-C26 |
| 25 | 6 | 623 | BCR | C23-C24-C25-C30 |
| 25 | 6 | 625 | BCR | C1-C6-C7-C8 |
| 25 | 6 | 625 | BCR | C5-C6-C7-C8 |
| 30 | 1 | 617 | LUT | C1-C6-C7-C8 |
| 30 | 1 | 617 | LUT | C5-C6-C7-C8 |
| 30 | 1 | 619 | LUT | C5-C6-C7-C8 |
| 30 | 3 | 622 | LUT | C1-C6-C7-C8 |
| 30 | 3 | 622 | LUT | C5-C6-C7-C8 |
| 30 | 8 | 617 | LUT | C5-C6-C7-C8 |
| 30 | Z | 617 | LUT | C5-C6-C7-C8 |
| 30 | Z | 619 | LUT | C1-C6-C7-C8 |
| 30 | Z | 619 | LUT | C5-C6-C7-C8 |
| 30 | 4 | 620 | LUT | C5-C6-C7-C8 |
| 30 | 6 | 621 | LUT | C1-C6-C7-C8 |
| 30 | 6 | 621 | LUT | C5-C6-C7-C8 |
| 30 | 9 | 616 | LUT | C5-C6-C7-C8 |
| 30 | 9 | 617 | LUT | C1-C6-C7-C8 |
| 30 | 9 | 617 | LUT | C5-C6-C7-C8 |
| 28 | J | 3001 | LMG | O6-C5-C6-O5 |
| 24 | 4 | 622 | LHG | C15-C16-C17-C18 |
| 22 | A | 832 | CLA | CBA-CGA-O2A-C1 |
| 22 | 5 | 610 | CLA | CBA-CGA-O2A-C1 |
| 29 | 8 | 607 | CHL | CBA-CGA-O2A-C1 |
| 22 | A | 833 | CLA | C10-C11-C12-C13 |
| 22 | B | 813 | CLA | C10-C11-C12-C13 |
| 29 | 6 | 606 | CHL | C5-C6-C7-C8 |
| 22 | 8 | 604 | CLA | O1D-CGD-O2D-CED |
| 22 | 2 | 611 | CLA | O1A-CGA-O2A-C1 |
| 28 | 9 | 620 | LMG | O6-C5-C6-O5 |
| 22 | B | 823 | CLA | C10-C11-C12-C13 |
| 22 | B | 812 | CLA | C4-C3-C5-C6 |
| 22 | 4 | 613 | CLA | C4-C3-C5-C6 |
| 29 | 5 | 618 | CHL | O1D-CGD-O2D-CED |
| 22 | A | 806 | CLA | C11-C12-C13-C15 |
| 22 | A | 808 | CLA | C11-C12-C13-C15 |
| 22 | A | 808 | CLA | C12-C13-C15-C16 |
| 22 | A | 829 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 841 | CLA | C11-C10-C8-C7 |
| 22 | B | 806 | CLA | C11-C12-C13-C15 |
| 22 | B | 809 | CLA | C11-C12-C13-C15 |
| 22 | B | 812 | CLA | C2-C3-C5-C6 |
| 22 | B | 812 | CLA | C11-C10-C8-C7 |
| 22 | B | 813 | CLA | C11-C10-C8-C7 |
| 22 | B | 815 | CLA | C11-C10-C8-C7 |
| 22 | B | 816 | CLA | C2-C3-C5-C6 |
| 22 | B | 839 | CLA | C6-C7-C8-C10 |
| 22 | 1 | 608 | CLA | C2-C3-C5-C6 |
| 22 | Z | 610 | CLA | C11-C10-C8-C7 |
| 22 | Z | 613 | CLA | C6-C7-C8-C10 |
| 22 | 6 | 602 | CLA | C6-C7-C8-C10 |
| 23 | A | 844 | PQN | C22-C23-C25-C26 |
| 29 | 3 | 608 | CHL | C11-C10-C8-C7 |
| 22 | 8 | 601 | CLA | C3-C5-C6-C7 |
| 22 | A | 819 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 828 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 614 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 620 | CLA | C10-C11-C12-C13 |
| 25 | B | 801 | BCR | C15-C16-C17-C18 |
| 27 | B | 850 | DGD | C1B-C2B-C3B-C4B |
| 22 | A | 817 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 819 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 827 | CLA | CBA-CGA-O2A-C1 |
| 22 | L | 203 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 614 | CLA | CBA-CGA-O2A-C1 |
| 22 | 4 | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | 6 | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | 6 | 610 | CLA | CBA-CGA-O2A-C1 |
| 29 | 1 | 601 | CHL | CBA-CGA-O2A-C1 |
| 29 | 5 | 607 | CHL | CBA-CGA-O2A-C1 |
| 22 | F | 303 | CLA | C2A-CAA-CBA-CGA |
| 22 | 7 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 8 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 4 | 609 | CLA | C2A-CAA-CBA-CGA |
| 22 | 5 | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | 9 | 604 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 818 | CLA | C10-C11-C12-C13 |
| 22 | 7 | 601 | CLA | C5-C6-C7-C8 |
| 22 | 7 | 601 | CLA | C15-C16-C17-C18 |
| 29 | 3 | 608 | CHL | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 822 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 818 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 840 | CLA | C10-C11-C12-C13 |
| 22 | A | 841 | CLA | C15-C16-C17-C18 |
| 22 | B | 809 | CLA | C15-C16-C17-C18 |
| 22 | B | 840 | CLA | C3-C5-C6-C7 |
| 22 | A | 819 | CLA | CBD-CGD-O2D-CED |
| 22 | 4 | 609 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 805 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 812 | CLA | CBA-CGA-O2A-C1 |
| 22 | 4 | 612 | CLA | CBA-CGA-O2A-C1 |
| 24 | 7 | 625 | LHG | C11-C10-C9-C8 |
| 24 | A | 847 | LHG | C8-C7-O7-C5 |
| 24 | 8 | 620 | LHG | C8-C7-O7-C5 |
| 27 | B | 850 | DGD | C2B-C1B-O2G-C2G |
| 22 | A | 806 | CLA | C8-C10-C11-C12 |
| 22 | 8 | 613 | CLA | C10-C11-C12-C13 |
| 28 | 9 | 620 | LMG | C2-C1-O1-C7 |
| 22 | 4 | 610 | CLA | C5-C6-C7-C8 |
| 24 | A | 846 | LHG | O7-C5-C6-O8 |
| 22 | 2 | 609 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 843 | CLA | C13-C15-C16-C17 |
| 22 | A | 829 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 608 | CLA | C4-C3-C5-C6 |
| 22 | A | 822 | CLA | C2-C3-C5-C6 |
| 22 | 3 | 607 | CLA | C2-C3-C5-C6 |
| 29 | 7 | 607 | CHL | C2-C3-C5-C6 |
| 29 | 6 | 607 | CHL | C2-C3-C5-C6 |
| 22 | A | 808 | CLA | C14-C13-C15-C16 |
| 22 | A | 812 | CLA | C14-C13-C15-C16 |
| 22 | A | 818 | CLA | C6-C7-C8-C9 |
| 22 | A | 841 | CLA | C11-C10-C8-C9 |
| 22 | B | 806 | CLA | C11-C12-C13-C14 |
| 22 | B | 813 | CLA | C11-C10-C8-C9 |
| 22 | B | 815 | CLA | C11-C10-C8-C9 |
| 22 | 7 | 602 | CLA | C11-C10-C8-C9 |
| 22 | Z | 610 | CLA | C11-C10-C8-C9 |
| 22 | 6 | 604 | CLA | C6-C7-C8-C9 |
| 29 | 3 | 608 | CHL | C11-C10-C8-C9 |
| 22 | B | 828 | CLA | C3-C5-C6-C7 |
| 22 | 6 | 611 | CLA | C3-C5-C6-C7 |
| 29 | 6 | 606 | CHL | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | G | 204 | CLA | O1D-CGD-O2D-CED |
| 22 | 5 | 602 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 819 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 828 | CLA | C2A-CAA-CBA-CGA |
| 22 | 3 | 602 | CLA | C2A-CAA-CBA-CGA |
| 22 | 6 | 610 | CLA | C2A-CAA-CBA-CGA |
| 30 | 3 | 621 | LUT | C27-C28-C29-C39 |
| 22 | 1 | 602 | CLA | C5-C6-C7-C8 |
| 22 | 1 | 608 | CLA | C13-C15-C16-C17 |
| 25 | 3 | 719 | BCR | C7-C8-C9-C10 |
| 22 | A | 832 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 812 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 819 | CLA | O1A-CGA-O2A-C1 |
| 22 | Z | 614 | CLA | O1A-CGA-O2A-C1 |
| 22 | 6 | 604 | CLA | O1A-CGA-O2A-C1 |
| 29 | 1 | 601 | CHL | O1A-CGA-O2A-C1 |
| 29 | 5 | 607 | CHL | O1A-CGA-O2A-C1 |
| 22 | A | 804 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 807 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 809 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 810 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 811 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 821 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 824 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 825 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 829 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 834 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 811 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 815 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 819 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 821 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 822 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 823 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 832 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 835 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 852 | CLA | C1A-C2A-CAA-CBA |
| 22 | F | 304 | CLA | C1A-C2A-CAA-CBA |
| 22 | 1 | 602 | CLA | C1A-C2A-CAA-CBA |
| 22 | 1 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 1 | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | 1 | 612 | CLA | C1A-C2A-CAA-CBA |
| 22 | 1 | 614 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 3 | 602 | CLA | C1A-C2A-CAA-CBA |
| 22 | 3 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 3 | 617 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 602 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 614 | CLA | C1A-C2A-CAA-CBA |
| 22 | 8 | 604 | CLA | C1A-C2A-CAA-CBA |
| 22 | 8 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 8 | 614 | CLA | C1A-C2A-CAA-CBA |
| 22 | Z | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | Z | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | Z | 612 | CLA | C1A-C2A-CAA-CBA |
| 22 | 4 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 4 | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | 5 | 601 | CLA | C1A-C2A-CAA-CBA |
| 22 | 5 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 5 | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | 5 | 616 | CLA | C1A-C2A-CAA-CBA |
| 22 | 6 | 602 | CLA | C1A-C2A-CAA-CBA |
| 22 | 6 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 6 | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | 6 | 614 | CLA | C1A-C2A-CAA-CBA |
| 22 | 2 | 610 | CLA | C1A-C2A-CAA-CBA |
| 22 | 2 | 611 | CLA | C1A-C2A-CAA-CBA |
| 22 | 9 | 610 | CLA | C1A-C2A-CAA-CBA |
| 27 | B | 850 | DGD | O6E-C5E-C6E-O5E |
| 29 | 7 | 607 | CHL | C1A-C2A-CAA-CBA |
| 29 | Z | 607 | CHL | C1A-C2A-CAA-CBA |
| 22 | A | 814 | CLA | C16-C17-C18-C19 |
| 27 | B | 850 | DGD | O1B-C1B-O2G-C2G |
| 24 | 4 | 623 | LHG | C8-C7-O7-C5 |
| 22 | B | 821 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 830 | CLA | C5-C6-C7-C8 |
| 22 | A | 833 | CLA | C8-C10-C11-C12 |
| 22 | 7 | 613 | CLA | C15-C16-C17-C18 |
| 24 | A | 847 | LHG | C4-O6-P-O3 |
| 24 | 4 | 622 | LHG | C23-C24-C25-C26 |
| 22 | B | 829 | CLA | CBD-CGD-O2D-CED |
| 22 | 5 | 613 | CLA | CBD-CGD-O2D-CED |
| 29 | 8 | 607 | CHL | O1A-CGA-O2A-C1 |
| 22 | 2 | 610 | CLA | C8-C10-C11-C12 |
| 22 | 9 | 610 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 23 | A | 844 | PQN | C15-C16-C17-C18 |
| 22 | 1 | 608 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 603 | CLA | C5-C6-C7-C8 |
| 24 | 8 | 620 | LHG | O9-C7-O7-C5 |
| 22 | A | 822 | CLA | C4-C3-C5-C6 |
| 21 | A | 801 | CL0 | C15-C16-C17-C18 |
| 22 | A | 802 | CLA | C15-C16-C17-C18 |
| 22 | B | 832 | CLA | C10-C11-C12-C13 |
| 22 | L | 203 | CLA | O1A-CGA-O2A-C1 |
| 22 | 4 | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | 5 | 610 | CLA | O1A-CGA-O2A-C1 |
| 22 | 9 | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 809 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 814 | CLA | C3-C5-C6-C7 |
| 22 | B | 817 | CLA | C11-C12-C13-C14 |
| 24 | 5 | 623 | LHG | C4-C5-C6-O8 |
| 27 | B | 850 | DGD | C2B-C3B-C4B-C5B |
| 28 | J | 3001 | LMG | O1-C7-C8-C9 |
| 28 | J | 3001 | LMG | C7-C8-C9-O8 |
| 28 | 9 | 620 | LMG | C31-C32-C33-C34 |
| 22 | A | 809 | CLA | C13-C15-C16-C17 |
| 29 | 3 | 608 | CHL | C15-C16-C17-C18 |
| 22 | A | 817 | CLA | O1A-CGA-O2A-C1 |
| 22 | 6 | 610 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 610 | CLA | C10-C11-C12-C13 |
| 22 | Z | 610 | CLA | C5-C6-C7-C8 |
| 22 | B | 805 | CLA | O1A-CGA-O2A-C1 |
| 22 | K | 4003 | CLA | CBA-CGA-O2A-C1 |
| 27 | B | 850 | DGD | C7A-C8A-C9A-CAA |
| 24 | 6 | 619 | LHG | C24-C23-O8-C6 |
| 22 | 8 | 610 | CLA | C8-C10-C11-C12 |
| 22 | 1 | 608 | CLA | O1A-CGA-O2A-C1 |
| 22 | 4 | 604 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 843 | CLA | C15-C16-C17-C18 |
| 22 | B | 813 | CLA | C8-C10-C11-C12 |
| 22 | A | 826 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 614 | CLA | C4-C3-C5-C6 |
| 22 | 8 | 601 | CLA | C4-C3-C5-C6 |
| 22 | Z | 611 | CLA | C4-C3-C5-C6 |
| 22 | 6 | 613 | CLA | C4-C3-C5-C6 |
| 24 | 8 | 620 | LHG | C12-C13-C14-C15 |
| 22 | 6 | 612 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 9 | 612 | CLA | CBA-CGA-O2A-C1 |
| 24 | 4 | 623 | LHG | C13-C14-C15-C16 |
| 22 | 8 | 611 | CLA | CBD-CGD-O2D-CED |
| 29 | Z | 601 | CHL | CBD-CGD-O2D-CED |
| 22 | 3 | 613 | CLA | C5-C6-C7-C8 |
| 22 | Z | 608 | CLA | C13-C15-C16-C17 |
| 23 | A | 844 | PQN | C23-C25-C26-C27 |
| 22 | A | 810 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 817 | CLA | C2A-CAA-CBA-CGA |
| 22 | F | 304 | CLA | C2A-CAA-CBA-CGA |
| 22 | 7 | 609 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 841 | CLA | C15-C16-C17-C18 |
| 22 | A | 840 | CLA | C2-C1-O2A-CGA |
| 22 | A | 845 | CLA | C2-C1-O2A-CGA |
| 22 | B | 831 | CLA | C2-C1-O2A-CGA |
| 22 | B | 836 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 608 | CLA | C2-C1-O2A-CGA |
| 22 | 5 | 601 | CLA | C2-C1-O2A-CGA |
| 22 | 2 | 610 | CLA | C2-C1-O2A-CGA |
| 22 | B | 808 | CLA | O1D-CGD-O2D-CED |
| 22 | 4 | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | 8 | 609 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 807 | CLA | C8-C10-C11-C12 |
| 28 | 9 | 620 | LMG | C17-C18-C19-C20 |
| 22 | A | 839 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 852 | CLA | CBA-CGA-O2A-C1 |
| 22 | 8 | 601 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 832 | CLA | O1D-CGD-O2D-CED |
| 22 | Z | 612 | CLA | C3-C5-C6-C7 |
| 22 | B | 830 | CLA | CAA-CBA-CGA-O2A |
| 24 | A | 847 | LHG | O9-C7-O7-C5 |
| 22 | A | 822 | CLA | C10-C11-C12-C13 |
| 22 | 8 | 610 | CLA | C10-C11-C12-C13 |
| 22 | 9 | 612 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 845 | CLA | C4-C3-C5-C6 |
| 22 | B | 824 | CLA | C4-C3-C5-C6 |
| 22 | 5 | 613 | CLA | C4-C3-C5-C6 |
| 22 | A | 807 | CLA | C11-C12-C13-C15 |
| 22 | A | 812 | CLA | C6-C7-C8-C10 |
| 22 | A | 815 | CLA | C6-C7-C8-C10 |
| 22 | A | 818 | CLA | C6-C7-C8-C10 |
| 22 | A | 820 | CLA | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | A | 827 | CLA | C6-C7-C8-C10 |
| 22 | A | 829 | CLA | C6-C7-C8-C10 |
| 22 | A | 829 | CLA | C12-C13-C15-C16 |
| 22 | A | 831 | CLA | C11-C10-C8-C7 |
| 22 | A | 842 | CLA | C11-C10-C8-C7 |
| 22 | A | 843 | CLA | C6-C7-C8-C10 |
| 22 | B | 826 | CLA | C11-C10-C8-C7 |
| 22 | B | 832 | CLA | C6-C7-C8-C10 |
| 22 | B | 837 | CLA | C11-C10-C8-C7 |
| 22 | 1 | 610 | CLA | C6-C7-C8-C10 |
| 22 | 1 | 614 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 614 | CLA | C12-C13-C15-C16 |
| 22 | 3 | 607 | CLA | C6-C7-C8-C10 |
| 22 | 7 | 602 | CLA | C11-C10-C8-C7 |
| 22 | 7 | 604 | CLA | C6-C7-C8-C10 |
| 22 | Z | 611 | CLA | C2-C3-C5-C6 |
| 22 | 5 | 602 | CLA | C11-C10-C8-C7 |
| 22 | 5 | 602 | CLA | C12-C13-C15-C16 |
| 22 | 5 | 613 | CLA | C2-C3-C5-C6 |
| 22 | 6 | 604 | CLA | C6-C7-C8-C10 |
| 22 | 6 | 613 | CLA | C2-C3-C5-C6 |
| 22 | A | 812 | CLA | C3-C5-C6-C7 |
| 22 | Z | 604 | CLA | C3-C5-C6-C7 |
| 24 | 1 | 620 | LHG | C24-C25-C26-C27 |
| 22 | A | 807 | CLA | C11-C12-C13-C14 |
| 22 | A | 812 | CLA | C6-C7-C8-C9 |
| 22 | A | 815 | CLA | C6-C7-C8-C9 |
| 22 | A | 820 | CLA | C11-C12-C13-C14 |
| 22 | A | 829 | CLA | C6-C7-C8-C9 |
| 22 | A | 829 | CLA | C14-C13-C15-C16 |
| 22 | A | 842 | CLA | C6-C7-C8-C9 |
| 22 | B | 826 | CLA | C11-C10-C8-C9 |
| 22 | B | 826 | CLA | C11-C12-C13-C14 |
| 22 | B | 834 | CLA | C11-C10-C8-C9 |
| 22 | B | 839 | CLA | C6-C7-C8-C9 |
| 22 | 3 | 610 | CLA | C14-C13-C15-C16 |
| 22 | 7 | 604 | CLA | C6-C7-C8-C9 |
| 22 | Z | 608 | CLA | C11-C10-C8-C9 |
| 22 | 5 | 601 | CLA | C11-C10-C8-C9 |
| 22 | 5 | 602 | CLA | C11-C10-C8-C9 |
| 22 | 6 | 601 | CLA | C11-C10-C8-C9 |
| 22 | 6 | 602 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 23 | A | 844 | PQN | C19-C18-C20-C21 |
| 22 | 8 | 614 | CLA | CBA-CGA-O2A-C1 |
| 22 | 5 | 604 | CLA | CBA-CGA-O2A-C1 |
| 22 | 7 | 610 | CLA | C5-C6-C7-C8 |
| 22 | B | 833 | CLA | O1D-CGD-O2D-CED |
| 22 | 7 | 616 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 614 | CLA | C2A-CAA-CBA-CGA |
| 22 | 6 | 610 | CLA | O1D-CGD-O2D-CED |
| 25 | B | 847 | BCR | C7-C8-C9-C34 |
| 25 | J | 3003 | BCR | C7-C8-C9-C10 |
| 22 | 5 | 604 | CLA | O1D-CGD-O2D-CED |
| 24 | 4 | 623 | LHG | O9-C7-O7-C5 |
| 22 | A | 826 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 833 | CLA | CBA-CGA-O2A-C1 |
| 22 | 7 | 601 | CLA | CBA-CGA-O2A-C1 |
| 22 | 8 | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 806 | CLA | C10-C11-C12-C13 |
| 22 | B | 816 | CLA | C5-C6-C7-C8 |
| 22 | 7 | 602 | CLA | C8-C10-C11-C12 |
| 22 | 7 | 602 | CLA | C15-C16-C17-C18 |
| 22 | Z | 610 | CLA | C8-C10-C11-C12 |
| 22 | 3 | 609 | CLA | O1D-CGD-O2D-CED |
| 27 | B | 850 | DGD | C9B-CAB-CBB-CCB |
| 22 | G | 204 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 809 | CLA | C5-C6-C7-C8 |
| 24 | B | 851 | LHG | O6-C4-C5-C6 |
| 21 | A | 801 | CL0 | C3-C5-C6-C7 |
| 22 | 1 | 614 | CLA | C3-C5-C6-C7 |
| 22 | 7 | 601 | CLA | CBD-CGD-O2D-CED |
| 22 | B | 806 | CLA | C10-C11-C12-C13 |
| 22 | B | 818 | CLA | C5-C6-C7-C8 |
| 22 | A | 810 | CLA | C4-C3-C5-C6 |
| 22 | 8 | 602 | CLA | C4-C3-C5-C6 |
| 22 | Z | 614 | CLA | C4-C3-C5-C6 |
| 22 | A | 826 | CLA | C2-C3-C5-C6 |
| 22 | A | 845 | CLA | C2-C3-C5-C6 |
| 22 | B | 824 | CLA | C2-C3-C5-C6 |
| 22 | 4 | 610 | CLA | C8-C10-C11-C12 |
| 22 | 9 | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | 4 | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 823 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 807 | CLA | CBA-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | B | 822 | CLA | C10-C11-C12-C13 |
| 22 | A | 824 | CLA | C3A-C2A-CAA-CBA |
| 22 | A | 829 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 804 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 810 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 835 | CLA | C3A-C2A-CAA-CBA |
| 22 | 3 | 604 | CLA | C3A-C2A-CAA-CBA |
| 22 | 6 | 609 | CLA | C3A-C2A-CAA-CBA |
| 29 | 6 | 608 | CHL | C3A-C2A-CAA-CBA |
| 30 | Z | 618 | LUT | C29-C30-C31-C32 |
| 22 | 6 | 604 | CLA | C3-C5-C6-C7 |
| 22 | A | 830 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 807 | CLA | C13-C15-C16-C17 |
| 22 | B | 818 | CLA | C10-C11-C12-C13 |
| 24 | A | 846 | LHG | C4-C5-C6-O8 |
| 27 | B | 850 | DGD | C1G-C2G-C3G-O3G |
| 28 | 9 | 620 | LMG | O1-C7-C8-C9 |
| 22 | B | 814 | CLA | CBD-CGD-O2D-CED |
| 28 | J | 3001 | LMG | C31-C32-C33-C34 |
| 22 | Z | 610 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 829 | CLA | C5-C6-C7-C8 |
| 22 | A | 838 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 827 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 603 | CLA | C5-C6-C7-C8 |
| 22 | 7 | 612 | CLA | C4-C3-C5-C6 |
| 22 | A | 810 | CLA | C2-C3-C5-C6 |
| 22 | Z | 614 | CLA | C2-C3-C5-C6 |
| 27 | B | 850 | DGD | C4B-C5B-C6B-C7B |
| 22 | 7 | 616 | CLA | CBA-CGA-O2A-C1 |
| 24 | A | 855 | LHG | C3-O3-P-O6 |
| 29 | 4 | 606 | CHL | C3C-C2C-CMC-OMC |
| 29 | 6 | 618 | CHL | C3C-C2C-CMC-OMC |
| 29 | 9 | 606 | CHL | C3C-C2C-CMC-OMC |
| 24 | 8 | 620 | LHG | C23-C24-C25-C26 |
| 24 | 6 | 619 | LHG | O10-C23-O8-C6 |
| 22 | B | 840 | CLA | C2A-CAA-CBA-CGA |
| 22 | 1 | 604 | CLA | C2A-CAA-CBA-CGA |
| 29 | 4 | 607 | CHL | C2A-CAA-CBA-CGA |
| 24 | A | 847 | LHG | O1-C1-C2-O2 |
| 22 | 8 | 614 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 802 | CLA | C5-C6-C7-C8 |
| 22 | B | 817 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 24 | 7 | 625 | LHG | C26-C27-C28-C29 |
| 22 | B | 852 | CLA | O1A-CGA-O2A-C1 |
| 22 | 8 | 601 | CLA | O1A-CGA-O2A-C1 |
| 22 | 5 | 604 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 613 | CLA | C3-C5-C6-C7 |
| 24 | 4 | 622 | LHG | O7-C5-C6-O8 |
| 28 | J | 3001 | LMG | O7-C8-C9-O8 |
| 22 | 3 | 610 | CLA | C8-C10-C11-C12 |
| 22 | A | 810 | CLA | C2-C1-O2A-CGA |
| 22 | A | 833 | CLA | C2-C1-O2A-CGA |
| 22 | B | 802 | CLA | C2-C1-O2A-CGA |
| 22 | B | 817 | CLA | C2-C1-O2A-CGA |
| 22 | 3 | 609 | CLA | C2-C1-O2A-CGA |
| 22 | 3 | 613 | CLA | C2-C1-O2A-CGA |
| 22 | 8 | 613 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 602 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 612 | CLA | C2-C1-O2A-CGA |
| 22 | 4 | 613 | CLA | C2-C1-O2A-CGA |
| 22 | 5 | 613 | CLA | C2-C1-O2A-CGA |
| 22 | 1 | 614 | CLA | O1D-CGD-O2D-CED |
| 22 | 6 | 604 | CLA | O1D-CGD-O2D-CED |
| 22 | 2 | 601 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 816 | CLA | C14-C13-C15-C16 |
| 22 | A | 843 | CLA | C14-C13-C15-C16 |
| 22 | B | 817 | CLA | C11-C10-C8-C9 |
| 22 | B | 825 | CLA | C6-C7-C8-C9 |
| 22 | B | 837 | CLA | C11-C10-C8-C9 |
| 22 | B | 839 | CLA | C14-C13-C15-C16 |
| 22 | B | 840 | CLA | C14-C13-C15-C16 |
| 22 | 4 | 602 | CLA | C11-C10-C8-C9 |
| 22 | 5 | 602 | CLA | C14-C13-C15-C16 |
| 22 | 1 | 603 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 836 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 816 | CLA | C13-C15-C16-C17 |
| 22 | B | 808 | CLA | C13-C15-C16-C17 |
| 22 | 3 | 607 | CLA | C8-C10-C11-C12 |
| 22 | A | 826 | CLA | O1A-CGA-O2A-C1 |
| 22 | 7 | 601 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 620 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 843 | CLA | C16-C17-C18-C20 |
| 25 | A | 848 | BCR | C23-C24-C25-C26 |
| 25 | A | 848 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 25 | A | 851 | BCR | C1-C6-C7-C8 |
| 25 | A | 851 | BCR | C5-C6-C7-C8 |
| 25 | A | 851 | BCR | C23-C24-C25-C30 |
| 25 | B | 801 | BCR | C1-C6-C7-C8 |
| 25 | B | 801 | BCR | C5-C6-C7-C8 |
| 25 | B | 843 | BCR | C23-C24-C25-C26 |
| 25 | B | 843 | BCR | C23-C24-C25-C30 |
| 25 | B | 845 | BCR | C23-C24-C25-C26 |
| 25 | B | 845 | BCR | C23-C24-C25-C30 |
| 25 | B | 847 | BCR | C5-C6-C7-C8 |
| 25 | B | 847 | BCR | C23-C24-C25-C26 |
| 25 | B | 847 | BCR | C23-C24-C25-C30 |
| 25 | J | 3003 | BCR | C5-C6-C7-C8 |
| 25 | L | 205 | BCR | C1-C6-C7-C8 |
| 25 | L | 205 | BCR | C5-C6-C7-C8 |
| 25 | 3 | 718 | BCR | C23-C24-C25-C26 |
| 25 | 3 | 718 | BCR | C23-C24-C25-C30 |
| 25 | 6 | 625 | BCR | C23-C24-C25-C26 |
| 25 | 6 | 625 | BCR | C23-C24-C25-C30 |
| 30 | 3 | 621 | LUT | C1-C6-C7-C8 |
| 30 | 3 | 621 | LUT | C5-C6-C7-C8 |
| 30 | 7 | 621 | LUT | C1-C6-C7-C8 |
| 30 | 7 | 621 | LUT | C5-C6-C7-C8 |
| 30 | 8 | 618 | LUT | C5-C6-C7-C8 |
| 30 | Z | 617 | LUT | C1-C6-C7-C8 |
| 30 | 4 | 619 | LUT | C1-C6-C7-C8 |
| 30 | 4 | 619 | LUT | C5-C6-C7-C8 |
| 30 | 5 | 624 | LUT | C1-C6-C7-C8 |
| 30 | 5 | 624 | LUT | C5-C6-C7-C8 |
| 30 | 6 | 624 | LUT | C1-C6-C7-C8 |
| 30 | 6 | 624 | LUT | C5-C6-C7-C8 |
| 30 | 2 | 617 | LUT | C1-C6-C7-C8 |
| 22 | 1 | 614 | CLA | C8-C10-C11-C12 |
| 22 | Z | 611 | CLA | C15-C16-C17-C18 |
| 22 | 9 | 614 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 802 | CLA | C13-C15-C16-C17 |
| 22 | 1 | 608 | CLA | C15-C16-C17-C18 |
| 22 | 1 | 613 | CLA | C10-C11-C12-C13 |
| 22 | A | 845 | CLA | O1D-CGD-O2D-CED |
| 24 | A | 855 | LHG | C8-C7-O7-C5 |
| 24 | A | 846 | LHG | C24-C25-C26-C27 |
| 22 | 9 | 611 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 4 | 609 | CLA | O1D-CGD-O2D-CED |
| 22 | 8 | 614 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 814 | CLA | C11-C12-C13-C15 |
| 22 | A | 818 | CLA | C11-C12-C13-C15 |
| 22 | B | 817 | CLA | C11-C10-C8-C7 |
| 22 | B | 825 | CLA | C6-C7-C8-C10 |
| 22 | B | 826 | CLA | C11-C12-C13-C15 |
| 22 | B | 834 | CLA | C11-C10-C8-C7 |
| 22 | B | 839 | CLA | C12-C13-C15-C16 |
| 22 | B | 840 | CLA | C12-C13-C15-C16 |
| 22 | L | 203 | CLA | C11-C12-C13-C15 |
| 22 | 1 | 609 | CLA | C11-C10-C8-C7 |
| 22 | 1 | 610 | CLA | C11-C10-C8-C7 |
| 22 | 8 | 601 | CLA | C11-C12-C13-C15 |
| 22 | Z | 608 | CLA | C2-C3-C5-C6 |
| 22 | Z | 608 | CLA | C11-C10-C8-C7 |
| 22 | 4 | 602 | CLA | C11-C10-C8-C7 |
| 22 | 6 | 601 | CLA | C11-C10-C8-C7 |
| 22 | 6 | 602 | CLA | C11-C10-C8-C7 |
| 23 | A | 844 | PQN | C17-C18-C20-C21 |
| 29 | 3 | 608 | CHL | C12-C13-C15-C16 |
| 27 | B | 850 | DGD | CDB-CEB-CFB-CGB |
| 25 | B | 801 | BCR | C19-C20-C21-C22 |
| 25 | B | 843 | BCR | C15-C16-C17-C18 |
| 25 | K | 4001 | BCR | C13-C14-C15-C16 |
| 30 | 1 | 618 | LUT | C29-C30-C31-C32 |
| 22 | A | 842 | CLA | C3-C5-C6-C7 |
| 22 | B | 832 | CLA | C3-C5-C6-C7 |
| 22 | 2 | 603 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 815 | CLA | C10-C11-C12-C13 |
| 22 | B | 805 | CLA | C10-C11-C12-C13 |
| 23 | B | 842 | PQN | C15-C16-C17-C18 |
| 22 | 3 | 613 | CLA | CBA-CGA-O2A-C1 |
| 22 | 4 | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | 2 | 607 | CLA | CBA-CGA-O2A-C1 |
| 24 | 8 | 620 | LHG | C24-C23-O8-C6 |
| 22 | A | 804 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 807 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 812 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 817 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 827 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 842 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | B | 825 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 829 | CLA | CAD-CBD-CGD-O2D |
| 22 | F | 303 | CLA | CAD-CBD-CGD-O2D |
| 22 | 1 | 610 | CLA | CAD-CBD-CGD-O2D |
| 22 | 3 | 607 | CLA | CAD-CBD-CGD-O2D |
| 22 | 8 | 608 | CLA | CAD-CBD-CGD-O2D |
| 22 | Z | 602 | CLA | CAD-CBD-CGD-O2D |
| 22 | 4 | 602 | CLA | CAD-CBD-CGD-O2D |
| 22 | 4 | 610 | CLA | CAD-CBD-CGD-O2D |
| 22 | 4 | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | 6 | 604 | CLA | CAD-CBD-CGD-O2D |
| 22 | 6 | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | 2 | 602 | CLA | CAD-CBD-CGD-O2D |
| 22 | 2 | 603 | CLA | CAD-CBD-CGD-O2D |
| 22 | 2 | 606 | CLA | CAD-CBD-CGD-O2D |
| 22 | 2 | 612 | CLA | CAD-CBD-CGD-O2D |
| 22 | 9 | 602 | CLA | CAD-CBD-CGD-O2D |
| 29 | 4 | 608 | CHL | CAD-CBD-CGD-O2D |
| 22 | A | 806 | CLA | C15-C16-C17-C18 |
| 22 | 8 | 610 | CLA | C5-C6-C7-C8 |
| 22 | A | 805 | CLA | C4-C3-C5-C6 |
| 22 | Z | 608 | CLA | C4-C3-C5-C6 |
| 23 | B | 842 | PQN | C14-C13-C15-C16 |
| 21 | A | 801 | CL0 | C16-C17-C18-C20 |
| 22 | A | 842 | CLA | C16-C17-C18-C19 |
| 22 | B | 834 | CLA | C8-C10-C11-C12 |
| 22 | A | 805 | CLA | C2-C3-C5-C6 |
| 28 | 9 | 620 | LMG | C7-C8-C9-O8 |
| 24 | B | 851 | LHG | O6-C4-C5-O7 |
| 24 | 7 | 625 | LHG | O6-C4-C5-O7 |
| 22 | B | 809 | CLA | O1D-CGD-O2D-CED |
| 24 | 6 | 619 | LHG | C16-C17-C18-C19 |
| 22 | 1 | 609 | CLA | C2A-CAA-CBA-CGA |
| 22 | 6 | 601 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 611 | CLA | C2A-CAA-CBA-CGA |
| 22 | 3 | 613 | CLA | O1A-CGA-O2A-C1 |
| 22 | 8 | 610 | CLA | C11-C12-C13-C15 |
| 24 | A | 855 | LHG | O9-C7-O7-C5 |
| 22 | A | 806 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 806 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 807 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 809 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | A | 814 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 815 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 826 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 826 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 839 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 839 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 840 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 840 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 845 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 845 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 854 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 854 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 815 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 823 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 837 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 837 | CLA | CHA-CBD-CGD-O2D |
| 22 | F | 301 | CLA | CHA-CBD-CGD-O2D |
| 22 | J | 3002 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 601 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 601 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 611 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 611 | CLA | CHA-CBD-CGD-O2D |
| 22 | 8 | 601 | CLA | CHA-CBD-CGD-O1D |
| 22 | 8 | 601 | CLA | CHA-CBD-CGD-O2D |
| 22 | 8 | 602 | CLA | CHA-CBD-CGD-O1D |
| 22 | 8 | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | 8 | 611 | CLA | CHA-CBD-CGD-O1D |
| 22 | 8 | 611 | CLA | CHA-CBD-CGD-O2D |
| 22 | 4 | 601 | CLA | CHA-CBD-CGD-O1D |
| 22 | 4 | 601 | CLA | CHA-CBD-CGD-O2D |
| 22 | 5 | 611 | CLA | CHA-CBD-CGD-O1D |
| 22 | 5 | 611 | CLA | CHA-CBD-CGD-O2D |
| 22 | 5 | 621 | CLA | CHA-CBD-CGD-O2D |
| 22 | 6 | 601 | CLA | CHA-CBD-CGD-O1D |
| 22 | 6 | 601 | CLA | CHA-CBD-CGD-O2D |
| 22 | 2 | 601 | CLA | CHA-CBD-CGD-O1D |
| 22 | 9 | 601 | CLA | CHA-CBD-CGD-O1D |
| 22 | 9 | 601 | CLA | CHA-CBD-CGD-O2D |
| 22 | 9 | 604 | CLA | CHA-CBD-CGD-O1D |
| 22 | 9 | 604 | CLA | CHA-CBD-CGD-O2D |
| 22 | 4 | 603 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | Z | 603 | CLA | C3-C5-C6-C7 |
| 22 | A | 830 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 833 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 819 | CLA | O1D-CGD-O2D-CED |
| 24 | 5 | 623 | LHG | O7-C5-C6-O8 |
| 28 | 9 | 620 | LMG | O7-C8-C9-O8 |
| 22 | A | 823 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 842 | CLA | C16-C17-C18-C20 |
| 22 | B | 829 | CLA | O1D-CGD-O2D-CED |
| 24 | 1 | 620 | LHG | C25-C26-C27-C28 |
| 22 | B | 807 | CLA | C4-C3-C5-C6 |
| 22 | 3 | 604 | CLA | C4-C3-C5-C6 |
| 22 | B | 807 | CLA | O1A-CGA-O2A-C1 |
| 22 | 1 | 603 | CLA | O1A-CGA-O2A-C1 |
| 22 | 3 | 604 | CLA | C2-C3-C5-C6 |
| 23 | B | 842 | PQN | C12-C13-C15-C16 |
| 22 | 8 | 602 | CLA | O1D-CGD-O2D-CED |
| 22 | Z | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 829 | CLA | C5-C6-C7-C8 |
| 22 | A | 814 | CLA | C11-C12-C13-C14 |
| 22 | A | 818 | CLA | C11-C12-C13-C14 |
| 22 | A | 854 | CLA | C14-C13-C15-C16 |
| 22 | B | 812 | CLA | C11-C12-C13-C14 |
| 22 | B | 841 | CLA | C6-C7-C8-C9 |
| 22 | 2 | 610 | CLA | C11-C10-C8-C9 |
| 29 | Z | 601 | CHL | O1D-CGD-O2D-CED |
| 22 | A | 819 | CLA | CAA-CBA-CGA-O2A |
| 24 | A | 846 | LHG | C10-C11-C12-C13 |
| 22 | A | 839 | CLA | O1A-CGA-O2A-C1 |
| 22 | L | 204 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 803 | CLA | C8-C10-C11-C12 |
| 22 | Z | 616 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 803 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 816 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 845 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 826 | CLA | C1A-C2A-CAA-CBA |
| 22 | K | 4002 | CLA | C1A-C2A-CAA-CBA |
| 22 | L | 203 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 604 | CLA | C1A-C2A-CAA-CBA |
| 22 | Z | 614 | CLA | C1A-C2A-CAA-CBA |
| 22 | 4 | 614 | CLA | C1A-C2A-CAA-CBA |
| 22 | 6 | 604 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 2 | 607 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 612 | CLA | C2-C1-O2A-CGA |
| 22 | 7 | 601 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 808 | CLA | C13-C15-C16-C17 |
| 22 | 7 | 613 | CLA | C10-C11-C12-C13 |
| 24 | A | 846 | LHG | C3-O3-P-O6 |
| 24 | 4 | 622 | LHG | C4-O6-P-O3 |
| 24 | 6 | 619 | LHG | C4-O6-P-O3 |
| 24 | 6 | 619 | LHG | C11-C10-C9-C8 |
| 22 | B | 828 | CLA | C4-C3-C5-C6 |
| 22 | B | 832 | CLA | CAA-CBA-CGA-O2A |
| 22 | L | 203 | CLA | C3-C5-C6-C7 |
| 22 | 1 | 609 | CLA | C3-C5-C6-C7 |
| 22 | 8 | 602 | CLA | C2-C3-C5-C6 |
| 22 | 2 | 607 | CLA | O1A-CGA-O2A-C1 |
| 24 | A | 847 | LHG | C4-O6-P-O5 |
| 24 | B | 851 | LHG | C3-O3-P-O4 |
| 24 | 7 | 625 | LHG | C4-O6-P-O4 |
| 24 | 8 | 620 | LHG | C3-O3-P-O5 |
| 24 | 8 | 620 | LHG | C4-O6-P-O5 |
| 24 | 5 | 623 | LHG | C4-O6-P-O4 |
| 24 | 6 | 619 | LHG | C3-O3-P-O4 |
| 22 | B | 809 | CLA | C16-C17-C18-C20 |
| 22 | L | 203 | CLA | C16-C17-C18-C20 |
| 22 | 7 | 601 | CLA | C10-C11-C12-C13 |
| 22 | A | 834 | CLA | CBA-CGA-O2A-C1 |
| 24 | 7 | 625 | LHG | O6-C4-C5-C6 |
| 22 | 8 | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | 1 | 612 | CLA | C3-C5-C6-C7 |
| 22 | B | 816 | CLA | C6-C7-C8-C10 |
| 22 | A | 806 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 814 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 815 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 816 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 826 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 839 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 845 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 854 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 837 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 841 | CLA | CAD-CBD-CGD-O1D |
| 22 | J | 3002 | CLA | CAD-CBD-CGD-O1D |
| 22 | 7 | 601 | CLA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 7 | 606 | CLA | CAD-CBD-CGD-O1D |
| 22 | 7 | 620 | CLA | CAD-CBD-CGD-O1D |
| 22 | 8 | 601 | CLA | CAD-CBD-CGD-O1D |
| 22 | 4 | 601 | CLA | CAD-CBD-CGD-O1D |
| 22 | 6 | 601 | CLA | CAD-CBD-CGD-O1D |
| 22 | 2 | 601 | CLA | CAD-CBD-CGD-O1D |
| 22 | 9 | 601 | CLA | CAD-CBD-CGD-O1D |
| 22 | 9 | 604 | CLA | CAD-CBD-CGD-O1D |
| 29 | Z | 601 | CHL | CAD-CBD-CGD-O1D |
| 24 | A | 846 | LHG | C9-C10-C11-C12 |
| 22 | A | 804 | CLA | C13-C15-C16-C17 |
| 22 | A | 854 | CLA | C13-C15-C16-C17 |
| 22 | 7 | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 807 | CLA | C12-C13-C15-C16 |
| 22 | A | 816 | CLA | C12-C13-C15-C16 |
| 22 | A | 819 | CLA | C6-C7-C8-C10 |
| 22 | A | 833 | CLA | C11-C10-C8-C7 |
| 22 | A | 839 | CLA | C12-C13-C15-C16 |
| 22 | A | 854 | CLA | C12-C13-C15-C16 |
| 22 | B | 819 | CLA | C12-C13-C15-C16 |
| 22 | B | 827 | CLA | C6-C7-C8-C10 |
| 22 | 2 | 610 | CLA | C11-C10-C8-C7 |
| 23 | A | 844 | PQN | C21-C22-C23-C25 |
| 29 | 5 | 607 | CHL | C3A-C2A-CAA-CBA |
| 25 | L | 205 | BCR | C13-C14-C15-C16 |
| 22 | A | 804 | CLA | C8-C10-C11-C12 |
| 24 | 4 | 622 | LHG | C13-C14-C15-C16 |
| 22 | A | 834 | CLA | O1A-CGA-O2A-C1 |
| 22 | L | 204 | CLA | O1A-CGA-O2A-C1 |
| 22 | 8 | 610 | CLA | O1A-CGA-O2A-C1 |
| 22 | 5 | 616 | CLA | C2A-CAA-CBA-CGA |
| 24 | 7 | 625 | LHG | C23-C24-C25-C26 |
| 29 | 1 | 607 | CHL | C1C-C2C-CMC-OMC |
| 29 | 3 | 608 | CHL | C1C-C2C-CMC-OMC |
| 29 | 4 | 606 | CHL | C1C-C2C-CMC-OMC |
| 29 | 4 | 618 | CHL | C1C-C2C-CMC-OMC |
| 29 | 5 | 618 | CHL | C1C-C2C-CMC-OMC |
| 29 | 6 | 618 | CHL | C1C-C2C-CMC-OMC |
| 29 | 9 | 606 | CHL | C1C-C2C-CMC-OMC |
| 29 | 9 | 607 | CHL | C1C-C2C-CMC-OMC |
| 24 | A | 855 | LHG | O7-C5-C6-O8 |
| 22 | 4 | 601 | CLA | C8-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | 4 | 607 | CHL | CAA-CBA-CGA-O2A |
| 22 | 9 | 611 | CLA | C6-C7-C8-C10 |
| 22 | Z | 614 | CLA | C3-C5-C6-C7 |
| 22 | A | 836 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 820 | CLA | C4-C3-C5-C6 |
| 22 | B | 827 | CLA | C4-C3-C5-C6 |
| 22 | 8 | 601 | CLA | C2-C3-C5-C6 |
| 22 | A | 819 | CLA | C6-C7-C8-C9 |
| 22 | A | 831 | CLA | C11-C10-C8-C9 |
| 22 | B | 827 | CLA | C11-C10-C8-C9 |
| 22 | L | 203 | CLA | C11-C12-C13-C14 |
| 22 | 1 | 602 | CLA | C6-C7-C8-C9 |
| 22 | 1 | 609 | CLA | C11-C10-C8-C9 |
| 22 | 8 | 613 | CLA | C6-C7-C8-C9 |
| 22 | A | 831 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 827 | CLA | C3-C5-C6-C7 |
| 24 | 4 | 622 | LHG | C27-C28-C29-C30 |
| 22 | 4 | 601 | CLA | O1A-CGA-O2A-C1 |
| 24 | 8 | 620 | LHG | O10-C23-O8-C6 |
| 22 | Z | 614 | CLA | C2A-CAA-CBA-CGA |
| 25 | B | 801 | BCR | C13-C14-C15-C16 |
| 22 | A | 828 | CLA | C10-C11-C12-C13 |
| 22 | 3 | 602 | CLA | O1D-CGD-O2D-CED |
| 25 | L | 205 | BCR | C7-C8-C9-C10 |
| 30 | 3 | 621 | LUT | C27-C28-C29-C30 |
| 27 | B | 850 | DGD | CAB-CBB-CCB-CDB |
| 22 | B | 807 | CLA | C2-C3-C5-C6 |
| 22 | F | 304 | CLA | C15-C16-C17-C18 |
| 22 | 7 | 613 | CLA | C13-C15-C16-C17 |
| 22 | B | 816 | CLA | C6-C7-C8-C9 |
| 24 | A | 847 | LHG | C18-C19-C20-C21 |
| 24 | A | 846 | LHG | C14-C15-C16-C17 |
| 22 | A | 823 | CLA | C1-C2-C3-C4 |
| 22 | B | 831 | CLA | C1-C2-C3-C4 |
| 22 | Z | 608 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 835 | CLA | C2A-CAA-CBA-CGA |
| 29 | Z | 601 | CHL | C2A-CAA-CBA-CGA |
| 22 | 4 | 601 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 807 | CLA | C2-C1-O2A-CGA |
| 22 | A | 831 | CLA | C2-C1-O2A-CGA |
| 22 | A | 834 | CLA | C2-C1-O2A-CGA |
| 22 | A | 854 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 1 | 604 | CLA | C2-C1-O2A-CGA |
| 22 | 1 | 609 | CLA | C2-C1-O2A-CGA |
| 22 | 8 | 612 | CLA | C2-C1-O2A-CGA |
| 22 | 5 | 609 | CLA | C2-C1-O2A-CGA |
| 29 | 3 | 608 | CHL | C2-C1-O2A-CGA |
| 29 | 6 | 607 | CHL | C2-C1-O2A-CGA |
| 22 | 3 | 609 | CLA | CAA-CBA-CGA-O2A |
| 22 | Z | 609 | CLA | C3-C5-C6-C7 |
| 22 | K | 4003 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 831 | CLA | CBA-CGA-O2A-C1 |
| 24 | 8 | 620 | LHG | O6-C4-C5-O7 |
| 22 | B | 807 | CLA | C5-C6-C7-C8 |
| 25 | A | 849 | BCR | C1-C6-C7-C8 |
| 25 | A | 851 | BCR | C23-C24-C25-C26 |
| 25 | B | 847 | BCR | C1-C6-C7-C8 |
| 25 | J | 3003 | BCR | C1-C6-C7-C8 |
| 30 | Z | 618 | LUT | C5-C6-C7-C8 |
| 30 | 2 | 617 | LUT | C5-C6-C7-C8 |
| 24 | A | 847 | LHG | C10-C11-C12-C13 |
| 24 | 4 | 623 | LHG | C11-C10-C9-C8 |
| 22 | A | 805 | CLA | C6-C7-C8-C9 |
| 22 | A | 843 | CLA | C16-C17-C18-C19 |
| 22 | A | 843 | CLA | C8-C10-C11-C12 |
| 28 | J | 3001 | LMG | O1-C7-C8-O7 |
| 24 | A | 846 | LHG | C4-O6-P-O3 |
| 24 | A | 847 | LHG | C3-O3-P-O6 |
| 24 | 1 | 620 | LHG | C3-O3-P-O6 |
| 24 | 1 | 620 | LHG | C4-O6-P-O3 |
| 24 | 7 | 625 | LHG | C3-O3-P-O6 |
| 24 | Z | 620 | LHG | C3-O3-P-O6 |
| 24 | Z | 620 | LHG | C4-O6-P-O3 |
| 24 | 4 | 623 | LHG | C3-O3-P-O6 |
| 24 | 4 | 623 | LHG | C4-O6-P-O3 |
| 24 | 5 | 623 | LHG | C3-O3-P-O6 |
| 22 | A | 812 | CLA | C10-C11-C12-C13 |
| 22 | B | 808 | CLA | C4-C3-C5-C6 |
| 22 | A | 810 | CLA | C12-C13-C15-C16 |
| 22 | B | 805 | CLA | C11-C10-C8-C7 |
| 22 | B | 818 | CLA | C6-C7-C8-C10 |
| 22 | A | 807 | CLA | C14-C13-C15-C16 |
| 22 | A | 842 | CLA | C11-C10-C8-C9 |
| 22 | A | 843 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | 1 | 614 | CLA | C14-C13-C15-C16 |
| 25 | B | 846 | BCR | C19-C20-C21-C22 |
| 30 | 8 | 618 | LUT | C29-C30-C31-C32 |
| 30 | Z | 617 | LUT | C7-C8-C9-C19 |
| 30 | Z | 619 | LUT | C27-C28-C29-C39 |
| 22 | Z | 608 | CLA | CBA-CGA-O2A-C1 |
| 29 | 6 | 606 | CHL | CBA-CGA-O2A-C1 |
| 22 | 9 | 611 | CLA | C5-C6-C7-C8 |
| 24 | 4 | 622 | LHG | C12-C13-C14-C15 |
| 22 | A | 826 | CLA | C15-C16-C17-C18 |
| 22 | A | 822 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 827 | CLA | CBA-CGA-O2A-C1 |
| 24 | 4 | 622 | LHG | C11-C12-C13-C14 |
| 22 | A | 813 | CLA | C2A-CAA-CBA-CGA |
| 22 | 7 | 610 | CLA | C2A-CAA-CBA-CGA |
| 25 | 4 | 621 | BCR | C9-C10-C11-C12 |
| 25 | 5 | 622 | BCR | C13-C14-C15-C16 |
| 25 | 6 | 625 | BCR | C13-C14-C15-C16 |
| 30 | 5 | 624 | LUT | C29-C30-C31-C32 |
| 30 | 6 | 624 | LUT | C29-C30-C31-C32 |
| 24 | 8 | 620 | LHG | O6-C4-C5-C6 |
| 22 | A | 822 | CLA | O1D-CGD-O2D-CED |
| 24 | A | 846 | LHG | O6-C4-C5-O7 |
| 24 | A | 847 | LHG | O6-C4-C5-O7 |
| 22 | 4 | 610 | CLA | O1A-CGA-O2A-C1 |
| 22 | B | 837 | CLA | C5-C6-C7-C8 |
| 22 | 7 | 613 | CLA | C2-C3-C5-C6 |
| 22 | A | 828 | CLA | C5-C6-C7-C8 |
| 22 | 6 | 611 | CLA | C5-C6-C7-C8 |
| 24 | 4 | 623 | LHG | O2-C2-C3-O3 |
| 22 | A | 813 | CLA | C6-C7-C8-C9 |
| 22 | B | 834 | CLA | CBD-CGD-O2D-CED |
| 21 | A | 801 | CL0 | C2-C1-O2A-CGA |
| 22 | A | 805 | CLA | C2-C1-O2A-CGA |
| 22 | A | 822 | CLA | C2-C1-O2A-CGA |
| 22 | A | 830 | CLA | C2-C1-O2A-CGA |
| 22 | A | 842 | CLA | C2-C1-O2A-CGA |
| 22 | B | 827 | CLA | C2-C1-O2A-CGA |
| 22 | B | 833 | CLA | C2-C1-O2A-CGA |
| 22 | 1 | 612 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 604 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 611 | CLA | C2-C1-O2A-CGA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | 8 | 607 | CHL | C2-C1-O2A-CGA |
| 24 | Z | 620 | LHG | C28-C29-C30-C31 |
| 29 | 6 | 606 | CHL | O1A-CGA-O2A-C1 |
| 22 | A | 843 | CLA | C2A-CAA-CBA-CGA |
| 22 | B | 807 | CLA | C2A-CAA-CBA-CGA |
| 22 | 3 | 613 | CLA | C2A-CAA-CBA-CGA |
| 22 | Z | 604 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 603 | CLA | C2A-CAA-CBA-CGA |
| 22 | 9 | 613 | CLA | C2A-CAA-CBA-CGA |
| 24 | 6 | 619 | LHG | O7-C5-C6-O8 |
| 22 | 4 | 613 | CLA | C3A-C2A-CAA-CBA |
| 29 | 6 | 606 | CHL | C3A-C2A-CAA-CBA |
| 24 | 6 | 619 | LHG | C11-C12-C13-C14 |
| 22 | B | 827 | CLA | C2-C3-C5-C6 |
| 22 | B | 828 | CLA | C2-C3-C5-C6 |
| 22 | A | 804 | CLA | C6-C7-C8-C9 |
| 22 | A | 826 | CLA | C6-C7-C8-C9 |
| 22 | B | 808 | CLA | C14-C13-C15-C16 |
| 22 | B | 809 | CLA | C6-C7-C8-C9 |
| 22 | 8 | 610 | CLA | C11-C10-C8-C9 |
| 22 | 4 | 601 | CLA | C11-C12-C13-C14 |
| 29 | 3 | 608 | CHL | C6-C7-C8-C9 |
| 22 | A | 820 | CLA | C16-C17-C18-C19 |
| 22 | A | 843 | CLA | C10-C11-C12-C13 |
| 24 | A | 855 | LHG | C4-C5-C6-O8 |
| 25 | A | 852 | BCR | C11-C10-C9-C34 |
| 25 | A | 852 | BCR | C16-C17-C18-C36 |
| 25 | B | 845 | BCR | C11-C10-C9-C34 |
| 25 | B | 845 | BCR | C20-C21-C22-C37 |
| 25 | F | 305 | BCR | C35-C13-C14-C15 |
| 25 | L | 201 | BCR | C11-C10-C9-C34 |
| 22 | 3 | 604 | CLA | C2A-CAA-CBA-CGA |
| 22 | 2 | 609 | CLA | C2A-CAA-CBA-CGA |
| 22 | F | 301 | CLA | C8-C10-C11-C12 |
| 22 | B | 834 | CLA | O1D-CGD-O2D-CED |
| 22 | A | 826 | CLA | C16-C17-C18-C19 |
| 22 | B | 809 | CLA | C16-C17-C18-C19 |
| 22 | L | 203 | CLA | C16-C17-C18-C19 |
| 22 | A | 806 | CLA | O2A-C1-C2-C3 |
| 29 | 5 | 607 | CHL | O2A-C1-C2-C3 |
| 25 | A | 852 | BCR | C37-C22-C23-C24 |
| 25 | B | 801 | BCR | C7-C8-C9-C34 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 25 | L | 201 | BCR | C37-C22-C23-C24 |
| 24 | 4 | 622 | LHG | C10-C11-C12-C13 |
| 22 | 4 | 610 | CLA | C10-C11-C12-C13 |
| 22 | A | 840 | CLA | C4-C3-C5-C6 |
| 22 | B | 810 | CLA | C4-C3-C5-C6 |
| 22 | L | 203 | CLA | C4-C3-C5-C6 |
| 22 | A | 808 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 831 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 814 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 827 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 838 | CLA | C1A-C2A-CAA-CBA |
| 22 | L | 204 | CLA | C1A-C2A-CAA-CBA |
| 22 | 3 | 604 | CLA | C1A-C2A-CAA-CBA |
| 22 | 7 | 608 | CLA | C1A-C2A-CAA-CBA |
| 22 | 4 | 602 | CLA | C1A-C2A-CAA-CBA |
| 22 | 9 | 602 | CLA | C1A-C2A-CAA-CBA |
| 29 | Z | 601 | CHL | C1A-C2A-CAA-CBA |
| 29 | 6 | 606 | CHL | C1A-C2A-CAA-CBA |
| 22 | A | 822 | CLA | C11-C12-C13-C15 |
| 22 | A | 831 | CLA | C12-C13-C15-C16 |
| 22 | B | 841 | CLA | C6-C7-C8-C10 |
| 22 | 7 | 601 | CLA | C11-C12-C13-C15 |
| 22 | 8 | 613 | CLA | C6-C7-C8-C10 |
| 22 | Z | 610 | CLA | C6-C7-C8-C10 |
| 22 | Z | 611 | CLA | C12-C13-C15-C16 |
| 22 | A | 829 | CLA | C13-C15-C16-C17 |
| 24 | B | 851 | LHG | C4-O6-P-O3 |
| 29 | 3 | 608 | CHL | C3C-C2C-CMC-OMC |
| 24 | A | 846 | LHG | C12-C13-C14-C15 |
| 22 | B | 827 | CLA | CAA-CBA-CGA-O2A |
| 23 | A | 844 | PQN | C20-C21-C22-C23 |
| 22 | 1 | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 809 | CLA | C8-C10-C11-C12 |
| 22 | B | 830 | CLA | CAA-CBA-CGA-O1A |
| 22 | Z | 613 | CLA | C8-C10-C11-C12 |
| 29 | 7 | 607 | CHL | C5-C6-C7-C8 |
| 22 | B | 826 | CLA | C3-C5-C6-C7 |
| 22 | A | 806 | CLA | C4-C3-C5-C6 |
| 22 | A | 830 | CLA | C4-C3-C5-C6 |
| 22 | B | 820 | CLA | C4-C3-C5-C6 |
| 22 | 1 | 609 | CLA | C4-C3-C5-C6 |
| 22 | A | 827 | CLA | O1A-CGA-O2A-C1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 1 | 616 | CLA | CBD-CGD-O2D-CED |
| 25 | A | 852 | BCR | C11-C10-C9-C8 |
| 25 | A | 852 | BCR | C16-C17-C18-C19 |
| 25 | B | 845 | BCR | C11-C10-C9-C8 |
| 25 | B | 845 | BCR | C20-C21-C22-C23 |
| 25 | F | 305 | BCR | C12-C13-C14-C15 |
| 25 | L | 201 | BCR | C11-C10-C9-C8 |
| 22 | A | 826 | CLA | C8-C10-C11-C12 |
| 22 | 1 | 614 | CLA | C2A-CAA-CBA-CGA |
| 25 | A | 856 | BCR | C15-C16-C17-C18 |
| 25 | K | 4001 | BCR | C15-C16-C17-C18 |
| 22 | 7 | 616 | CLA | O1A-CGA-O2A-C1 |
| 24 | 5 | 623 | LHG | C1-C2-C3-O3 |
| 29 | 7 | 607 | CHL | O1D-CGD-O2D-CED |
| 22 | A | 813 | CLA | C4-C3-C5-C6 |
| 22 | B | 822 | CLA | C4-C3-C5-C6 |
| 22 | F | 301 | CLA | C4-C3-C5-C6 |
| 22 | 7 | 604 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 606 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 609 | CLA | C2-C1-O2A-CGA |
| 22 | 5 | 606 | CLA | C2-C1-O2A-CGA |
| 22 | 9 | 613 | CLA | C2-C1-O2A-CGA |
| 29 | 4 | 607 | CHL | C2-C1-O2A-CGA |
| 22 | B | 814 | CLA | O1D-CGD-O2D-CED |
| 22 | 2 | 603 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 810 | CLA | C2-C3-C5-C6 |
| 22 | L | 203 | CLA | C2-C3-C5-C6 |
| 22 | B | 802 | CLA | C8-C10-C11-C12 |
| 21 | A | 801 | CL0 | CAA-CBA-CGA-O2A |
| 22 | A | 807 | CLA | C11-C10-C8-C9 |
| 22 | A | 840 | CLA | C11-C12-C13-C14 |
| 22 | A | 813 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 841 | CLA | C2A-CAA-CBA-CGA |
| 22 | Z | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 805 | CLA | C6-C7-C8-C10 |
| 22 | 3 | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 610 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 849 | BCR | C5-C6-C7-C8 |
| 25 | A | 849 | BCR | C23-C24-C25-C30 |
| 25 | B | 843 | BCR | C1-C6-C7-C8 |
| 25 | B | 844 | BCR | C23-C24-C25-C30 |
| 25 | K | 4001 | BCR | C23-C24-C25-C30 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 30 | 1 | 618 | LUT | C1-C6-C7-C8 |
| 30 | 7 | 622 | LUT | C1-C6-C7-C8 |
| 30 | 8 | 618 | LUT | C1-C6-C7-C8 |
| 30 | Z | 618 | LUT | C1-C6-C7-C8 |
| 22 | A | 829 | CLA | CAA-CBA-CGA-O2A |
| 24 | B | 851 | LHG | C4-C5-C6-O8 |
| 25 | 3 | 717 | BCR | C15-C16-C17-C18 |
| 22 | B | 802 | CLA | C4-C3-C5-C6 |
| 22 | B | 814 | CLA | C4-C3-C5-C6 |
| 22 | 7 | 613 | CLA | C4-C3-C5-C6 |
| 23 | A | 844 | PQN | C14-C13-C15-C16 |
| 25 | B | 847 | BCR | C7-C8-C9-C10 |
| 22 | Z | 614 | CLA | C10-C11-C12-C13 |
| 22 | A | 806 | CLA | C2-C3-C5-C6 |
| 22 | A | 820 | CLA | C2-C3-C5-C6 |
| 22 | B | 808 | CLA | C2-C3-C5-C6 |
| 22 | 3 | 614 | CLA | CAA-CBA-CGA-O2A |
| 22 | Z | 611 | CLA | C2A-CAA-CBA-CGA |
| 23 | A | 844 | PQN | C18-C20-C21-C22 |
| 27 | B | 850 | DGD | CEA-CFA-CGA-CHA |
| 22 | 2 | 609 | CLA | CAA-CBA-CGA-O2A |
| 24 | 6 | 619 | LHG | C10-C11-C12-C13 |
| 29 | 6 | 607 | CHL | C3-C5-C6-C7 |
| 22 | 3 | 614 | CLA | CAA-CBA-CGA-O1A |
| 22 | 8 | 613 | CLA | C13-C15-C16-C17 |
| 22 | 5 | 602 | CLA | C8-C10-C11-C12 |
| 28 | J | 3001 | LMG | C10-C11-C12-C13 |
| 22 | B | 817 | CLA | C4-C3-C5-C6 |
| 22 | 8 | 613 | CLA | C4-C3-C5-C6 |
| 22 | A | 807 | CLA | C11-C10-C8-C7 |
| 22 | A | 812 | CLA | C12-C13-C15-C16 |
| 22 | A | 828 | CLA | C2-C3-C5-C6 |
| 22 | A | 828 | CLA | C12-C13-C15-C16 |
| 22 | B | 827 | CLA | C11-C10-C8-C7 |
| 22 | 4 | 613 | CLA | C6-C7-C8-C10 |
| 29 | 3 | 608 | CHL | CBA-CGA-O2A-C1 |
| 22 | B | 819 | CLA | C10-C11-C12-C13 |
| 25 | 6 | 623 | BCR | C13-C14-C15-C16 |
| 30 | 4 | 620 | LUT | C9-C10-C11-C12 |
| 22 | 1 | 616 | CLA | CAA-CBA-CGA-O2A |
| 22 | 4 | 613 | CLA | CAA-CBA-CGA-O2A |
| 24 | 1 | 620 | LHG | O7-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 24 | 4 | 622 | LHG | O7-C7-C8-C9 |
| 22 | 1 | 606 | CLA | O1A-CGA-O2A-C1 |
| 22 | A | 809 | CLA | C4-C3-C5-C6 |
| 22 | B | 809 | CLA | C4-C3-C5-C6 |
| 22 | A | 840 | CLA | C2-C3-C5-C6 |
| 22 | F | 301 | CLA | C2-C3-C5-C6 |
| 22 | 7 | 612 | CLA | C2-C3-C5-C6 |
| 22 | 7 | 613 | CLA | CBD-CGD-O2D-CED |
| 24 | A | 846 | LHG | C16-C17-C18-C19 |
| 22 | B | 807 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 824 | CLA | CAA-CBA-CGA-O2A |
| 22 | 3 | 612 | CLA | CAA-CBA-CGA-O2A |
| 22 | Z | 612 | CLA | CAA-CBA-CGA-O2A |
| 24 | 4 | 622 | LHG | C14-C15-C16-C17 |
| 22 | A | 812 | CLA | C11-C10-C8-C9 |
| 22 | A | 826 | CLA | C14-C13-C15-C16 |
| 22 | A | 828 | CLA | C11-C10-C8-C9 |
| 22 | A | 833 | CLA | C11-C10-C8-C9 |
| 22 | B | 819 | CLA | C14-C13-C15-C16 |
| 22 | B | 827 | CLA | C6-C7-C8-C9 |
| 22 | 3 | 604 | CLA | C11-C12-C13-C14 |
| 22 | 8 | 601 | CLA | C11-C12-C13-C14 |
| 22 | Z | 611 | CLA | C14-C13-C15-C16 |
| 22 | A | 854 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 827 | CLA | C3A-C2A-CAA-CBA |
| 22 | B | 834 | CLA | C3A-C2A-CAA-CBA |
| 22 | 2 | 603 | CLA | C3A-C2A-CAA-CBA |
| 22 | 2 | 613 | CLA | C3A-C2A-CAA-CBA |
| 29 | 8 | 607 | CHL | C3A-C2A-CAA-CBA |
| 24 | 5 | 623 | LHG | O2-C2-C3-O3 |
| 24 | Z | 620 | LHG | C24-C25-C26-C27 |
| 22 | K | 4002 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 821 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 838 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 803 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 805 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 814 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 820 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 824 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 830 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 836 | CLA | CAD-CBD-CGD-O2D |
| 22 | B | 838 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | K | 4002 | CLA | CAD-CBD-CGD-O2D |
| 22 | 1 | 603 | CLA | CAD-CBD-CGD-O2D |
| 22 | 1 | 604 | CLA | CAD-CBD-CGD-O2D |
| 22 | 1 | 608 | CLA | CAD-CBD-CGD-O2D |
| 22 | 3 | 609 | CLA | CAD-CBD-CGD-O2D |
| 22 | 3 | 610 | CLA | CAD-CBD-CGD-O2D |
| 22 | 7 | 612 | CLA | CAD-CBD-CGD-O2D |
| 22 | 7 | 614 | CLA | CAD-CBD-CGD-O2D |
| 22 | Z | 603 | CLA | CAD-CBD-CGD-O2D |
| 22 | Z | 604 | CLA | CAD-CBD-CGD-O2D |
| 22 | 5 | 603 | CLA | CAD-CBD-CGD-O2D |
| 22 | 5 | 610 | CLA | CAD-CBD-CGD-O2D |
| 22 | 9 | 611 | CLA | CAD-CBD-CGD-O2D |
| 22 | 9 | 612 | CLA | CAD-CBD-CGD-O2D |
| 22 | A | 804 | CLA | C2A-CAA-CBA-CGA |
| 22 | 4 | 610 | CLA | C2A-CAA-CBA-CGA |
| 22 | A | 845 | CLA | C4C-C3C-CAC-CBC |
| 22 | B | 813 | CLA | CAA-CBA-CGA-O2A |
| 22 | 7 | 616 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 801 | CL0 | O1A-CGA-O2A-C1 |
| 22 | A | 803 | CLA | C4-C3-C5-C6 |
| 22 | A | 807 | CLA | C4-C3-C5-C6 |
| 22 | A | 811 | CLA | C4-C3-C5-C6 |
| 22 | B | 836 | CLA | C3-C5-C6-C7 |
| 22 | B | 805 | CLA | C13-C15-C16-C17 |
| 22 | A | 807 | CLA | C2-C3-C5-C6 |
| 22 | A | 830 | CLA | C2-C3-C5-C6 |
| 22 | B | 814 | CLA | C2-C3-C5-C6 |
| 22 | B | 820 | CLA | C2-C3-C5-C6 |
| 22 | 1 | 609 | CLA | C2-C3-C5-C6 |
| 23 | A | 844 | PQN | C12-C13-C15-C16 |
| 22 | B | 838 | CLA | CAA-CBA-CGA-O2A |
| 22 | 1 | 612 | CLA | CAA-CBA-CGA-O2A |
| 22 | 1 | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | 6 | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | 9 | 604 | CLA | CAA-CBA-CGA-O2A |
| 29 | 3 | 608 | CHL | CAA-CBA-CGA-O2A |
| 29 | 8 | 607 | CHL | CAA-CBA-CGA-O2A |
| 22 | 2 | 610 | CLA | O1A-CGA-O2A-C1 |
| 25 | A | 852 | BCR | C7-C8-C9-C10 |
| 25 | B | 801 | BCR | C7-C8-C9-C10 |
| 25 | B | 847 | BCR | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 30 | 7 | 621 | LUT | C11-C12-C13-C14 |
| 24 | 4 | 622 | LHG | C4-C5-C6-O8 |
| 22 | 1 | 606 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 802 | CLA | CAA-CBA-CGA-O2A |
| 22 | 3 | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | 7 | 613 | CLA | CAA-CBA-CGA-O2A |
| 24 | A | 855 | LHG | O8-C23-C24-C25 |
| 24 | A | 846 | LHG | C25-C26-C27-C28 |
| 29 | 5 | 608 | CHL | O2A-C1-C2-C3 |
| 22 | A | 806 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 817 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 837 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 837 | CLA | CAA-CBA-CGA-O2A |
| 22 | 6 | 622 | CLA | CAA-CBA-CGA-O2A |
| 22 | 1 | 610 | CLA | CBD-CGD-O2D-CED |
| 22 | A | 814 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 815 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 816 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 820 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 822 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 822 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 823 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 824 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 824 | CLA | CHA-CBD-CGD-O2D |
| 22 | A | 829 | CLA | CHA-CBD-CGD-O1D |
| 22 | A | 829 | CLA | CHA-CBD-CGD-O2D |
| 22 | B | 804 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 813 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 815 | CLA | CHA-CBD-CGD-O1D |
| 22 | B | 821 | CLA | CHA-CBD-CGD-O1D |
| 22 | G | 204 | CLA | CHA-CBD-CGD-O2D |
| 22 | 1 | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | 3 | 602 | CLA | CHA-CBD-CGD-O1D |
| 22 | 3 | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 602 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 613 | CLA | CHA-CBD-CGD-O2D |
| 22 | 7 | 620 | CLA | CHA-CBD-CGD-O1D |
| 22 | 7 | 620 | CLA | CHA-CBD-CGD-O2D |
| 22 | 8 | 606 | CLA | CHA-CBD-CGD-O1D |
| 22 | 8 | 606 | CLA | CHA-CBD-CGD-O2D |
| 22 | 4 | 602 | CLA | CHA-CBD-CGD-O2D |
| 22 | 4 | 604 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | 4 | 604 | CLA | CHA-CBD-CGD-O2D |
| 22 | 5 | 616 | CLA | CHA-CBD-CGD-O1D |
| 22 | 5 | 616 | CLA | CHA-CBD-CGD-O2D |
| 22 | 6 | 603 | CLA | CHA-CBD-CGD-O2D |
| 22 | 2 | 601 | CLA | CHA-CBD-CGD-O2D |
| 22 | 3 | 620 | CLA | CAA-CBA-CGA-O2A |
| 22 | 9 | 601 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 817 | CLA | C2-C3-C5-C6 |
| 24 | 5 | 623 | LHG | O6-C4-C5-C6 |
| 22 | 8 | 603 | CLA | CAA-CBA-CGA-O2A |
| 24 | 4 | 622 | LHG | C11-C10-C9-C8 |
| 24 | 6 | 619 | LHG | C13-C14-C15-C16 |
| 22 | Z | 604 | CLA | C5-C6-C7-C8 |
| 22 | A | 843 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 809 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 812 | CLA | CAA-CBA-CGA-O2A |
| 22 | 8 | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | 4 | 601 | CLA | CAA-CBA-CGA-O2A |
| 29 | 1 | 607 | CHL | CAA-CBA-CGA-O2A |
| 28 | 9 | 620 | LMG | C23-C24-C25-C26 |
| 22 | A | 813 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 828 | CLA | CAA-CBA-CGA-O2A |
| 22 | 1 | 603 | CLA | CAA-CBA-CGA-O2A |
| 22 | 8 | 616 | CLA | CAA-CBA-CGA-O2A |
| 22 | 5 | 606 | CLA | CAA-CBA-CGA-O2A |
| 22 | 6 | 601 | CLA | CAA-CBA-CGA-O2A |
| 22 | 9 | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 823 | CLA | C2A-CAA-CBA-CGA |
| 22 | 6 | 617 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 841 | CLA | C4C-C3C-CAC-CBC |
| 22 | 2 | 610 | CLA | CBA-CGA-O2A-C1 |
| 22 | B | 806 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 811 | CLA | CAA-CBA-CGA-O2A |
| 22 | 5 | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | 3 | 610 | CLA | CBD-CGD-O2D-CED |
| 22 | K | 4002 | CLA | CAA-CBA-CGA-O1A |
| 22 | 5 | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | 5 | 601 | CLA | C13-C15-C16-C17 |
| 22 | A | 811 | CLA | C2-C3-C5-C6 |
| 22 | B | 805 | CLA | C6-C7-C8-C10 |
| 22 | B | 812 | CLA | C11-C12-C13-C15 |
| 22 | F | 304 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 22 | Z | 609 | CLA | C11-C10-C8-C7 |
| 22 | 6 | 601 | CLA | C6-C7-C8-C10 |
| 22 | 8 | 610 | CLA | C11-C12-C13-C14 |
| 22 | B | 816 | CLA | CAA-CBA-CGA-O2A |
| 22 | 8 | 609 | CLA | CAA-CBA-CGA-O2A |
| 22 | Z | 613 | CLA | CAA-CBA-CGA-O2A |
| 22 | 2 | 607 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 810 | CLA | C14-C13-C15-C16 |
| 22 | 3 | 610 | CLA | C6-C7-C8-C9 |
| 22 | B | 807 | CLA | CAA-CBA-CGA-O1A |
| 24 | 1 | 620 | LHG | O9-C7-C8-C9 |
| 25 | B | 843 | BCR | C13-C14-C15-C16 |
| 25 | 5 | 625 | BCR | C9-C10-C11-C12 |
| 30 | 7 | 622 | LUT | C29-C30-C31-C32 |
| 22 | 8 | 601 | CLA | C10-C11-C12-C13 |
| 22 | A | 813 | CLA | CBA-CGA-O2A-C1 |
| 22 | A | 823 | CLA | CAA-CBA-CGA-O2A |
| 22 | 7 | 616 | CLA | CAA-CBA-CGA-O1A |
| 29 | 6 | 607 | CHL | C2A-CAA-CBA-CGA |
| 22 | 7 | 613 | CLA | CAA-CBA-CGA-O1A |
| 22 | Z | 616 | CLA | CAA-CBA-CGA-O2A |
| 24 | 8 | 620 | LHG | O7-C7-C8-C9 |
| 22 | 4 | 613 | CLA | CAA-CBA-CGA-O1A |
| 29 | 8 | 607 | CHL | CAA-CBA-CGA-O1A |
| 22 | A | 820 | CLA | C16-C17-C18-C20 |
| 22 | 3 | 603 | CLA | C2-C3-C5-C6 |
| 22 | 8 | 613 | CLA | C2-C3-C5-C6 |
| 25 | L | 201 | BCR | C21-C22-C23-C24 |
| 30 | Z | 619 | LUT | C27-C28-C29-C30 |
| 22 | A | 828 | CLA | CBA-CGA-O2A-C1 |
| 22 | Z | 603 | CLA | CBA-CGA-O2A-C1 |
| 24 | A | 846 | LHG | C29-C30-C31-C32 |
| 22 | A | 817 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 838 | CLA | C1A-C2A-CAA-CBA |
| 22 | A | 854 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 804 | CLA | C1A-C2A-CAA-CBA |
| 22 | B | 834 | CLA | C1A-C2A-CAA-CBA |
| 22 | 5 | 604 | CLA | C1A-C2A-CAA-CBA |
| 22 | 6 | 609 | CLA | C1A-C2A-CAA-CBA |
| 22 | 2 | 603 | CLA | C1A-C2A-CAA-CBA |
| 22 | 9 | 614 | CLA | C1A-C2A-CAA-CBA |
| 29 | 4 | 606 | CHL | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | 4 | 608 | CHL | C1A-C2A-CAA-CBA |
| 22 | A | 802 | CLA | CAA-CBA-CGA-O1A |
| 22 | 3 | 612 | CLA | CAA-CBA-CGA-O1A |
| 22 | 3 | 613 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 823 | CLA | C2-C1-O2A-CGA |
| 22 | B | 814 | CLA | C2-C1-O2A-CGA |
| 22 | 1 | 602 | CLA | C2-C1-O2A-CGA |
| 22 | Z | 608 | CLA | C10-C11-C12-C13 |
| 22 | B | 813 | CLA | CAA-CBA-CGA-O1A |
| 22 | B | 824 | CLA | CAA-CBA-CGA-O1A |
| 22 | Z | 616 | CLA | CAA-CBA-CGA-O1A |
| 22 | 2 | 601 | CLA | CAA-CBA-CGA-O1A |
| 24 | 1 | 620 | LHG | C4-C5-C6-O8 |
| 22 | B | 805 | CLA | CAA-CBA-CGA-O2A |
| 24 | Z | 620 | LHG | C13-C14-C15-C16 |
| 22 | A | 842 | CLA | C2A-CAA-CBA-CGA |
| 22 | 3 | 610 | CLA | C2A-CAA-CBA-CGA |
| 29 | 5 | 607 | CHL | C2A-CAA-CBA-CGA |
| 22 | A | 845 | CLA | C2C-C3C-CAC-CBC |
| 29 | 6 | 607 | CHL | C2C-C3C-CAC-CBC |
| 22 | A | 812 | CLA | C16-C17-C18-C19 |
| 22 | 1 | 613 | CLA | CAA-CBA-CGA-O1A |
| 22 | 9 | 601 | CLA | CAA-CBA-CGA-O1A |
| 24 | 4 | 622 | LHG | O9-C7-C8-C9 |
| 22 | A | 842 | CLA | C13-C15-C16-C17 |
| 24 | 4 | 622 | LHG | C32-C33-C34-C35 |
| 22 | B | 804 | CLA | CAA-CBA-CGA-O2A |
| 22 | 8 | 603 | CLA | CAA-CBA-CGA-O1A |
| 24 | Z | 620 | LHG | O7-C7-C8-C9 |
| 22 | B | 809 | CLA | CAA-CBA-CGA-O1A |
| 22 | B | 838 | CLA | CAA-CBA-CGA-O1A |
| 22 | Z | 612 | CLA | CAA-CBA-CGA-O1A |
| 22 | Z | 613 | CLA | CAA-CBA-CGA-O1A |
| 22 | 9 | 604 | CLA | CAA-CBA-CGA-O1A |
| 22 | 9 | 613 | CLA | CAA-CBA-CGA-O1A |
| 24 | 8 | 620 | LHG | O9-C7-C8-C9 |
| 29 | 3 | 608 | CHL | O1A-CGA-O2A-C1 |
| 22 | 6 | 622 | CLA | CAA-CBA-CGA-O1A |
| 24 | A | 855 | LHG | C3-O3-P-O4 |
| 24 | Z | 620 | LHG | C3-O3-P-O5 |
| 24 | 4 | 623 | LHG | C4-O6-P-O5 |
| 24 | 1 | 620 | LHG | O7-C5-C6-O8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | A | 806 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 843 | CLA | CAA-CBA-CGA-O1A |
| 22 | 1 | 603 | CLA | CAA-CBA-CGA-O1A |
| 22 | 1 | 612 | CLA | CAA-CBA-CGA-O1A |
| 22 | 1 | 616 | CLA | CAA-CBA-CGA-O1A |
| 22 | 3 | 620 | CLA | CAA-CBA-CGA-O1A |
| 24 | A | 855 | LHG | O10-C23-C24-C25 |
| 22 | Z | 603 | CLA | O1A-CGA-O2A-C1 |
| 25 | B | 843 | BCR | C5-C6-C7-C8 |
| 25 | B | 848 | BCR | C23-C24-C25-C30 |
| 30 | 1 | 618 | LUT | C5-C6-C7-C8 |
| 30 | 7 | 622 | LUT | C5-C6-C7-C8 |
| 22 | Z | 611 | CLA | C8-C10-C11-C12 |
| 22 | 6 | 613 | CLA | CAA-CBA-CGA-O1A |
| 28 | J | 3001 | LMG | O10-C28-C29-C30 |
| 22 | 7 | 610 | CLA | O1A-CGA-O2A-C1 |
| 29 | 4 | 608 | CHL | CAA-CBA-CGA-O2A |
| 22 | F | 301 | CLA | C16-C17-C18-C20 |
| 29 | 1 | 607 | CHL | CAA-CBA-CGA-O1A |
| 22 | A | 826 | CLA | CAA-CBA-CGA-O2A |
| 22 | Z | 603 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 839 | CLA | C13-C15-C16-C17 |
| 22 | B | 806 | CLA | CAA-CBA-CGA-O1A |
| 22 | 8 | 613 | CLA | CAA-CBA-CGA-O1A |
| 29 | 3 | 608 | CHL | CAA-CBA-CGA-O1A |
| 22 | A | 838 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 813 | CLA | CAD-CBD-CGD-O1D |
| 22 | B | 826 | CLA | CAD-CBD-CGD-O1D |
| 22 | 6 | 622 | CLA | CAD-CBD-CGD-O1D |
| 22 | 2 | 614 | CLA | CAD-CBD-CGD-O1D |
| 22 | A | 828 | CLA | O1A-CGA-O2A-C1 |
| 29 | 9 | 607 | CHL | O1A-CGA-O2A-C1 |
| 22 | A | 828 | CLA | CAA-CBA-CGA-O1A |
| 22 | 4 | 601 | CLA | CAA-CBA-CGA-O1A |
| 22 | 2 | 607 | CLA | CAA-CBA-CGA-O1A |
| 22 | 5 | 610 | CLA | C5-C6-C7-C8 |
| 22 | A | 810 | CLA | C6-C7-C8-C9 |
| 22 | B | 813 | CLA | C14-C13-C15-C16 |
| 22 | F | 304 | CLA | C14-C13-C15-C16 |
| 22 | 1 | 611 | CLA | C14-C13-C15-C16 |
| 22 | Z | 608 | CLA | C14-C13-C15-C16 |
| 22 | 6 | 601 | CLA | C6-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 23 | A | 844 | PQN | C21-C22-C23-C24 |
| 22 | A | 829 | CLA | C10-C11-C12-C13 |
| 22 | A | 841 | CLA | CAA-CBA-CGA-O2A |
| 22 | B | 828 | CLA | CAA-CBA-CGA-O2A |
| 22 | 4 | 609 | CLA | CAA-CBA-CGA-O2A |
| 22 | 6 | 617 | CLA | CAA-CBA-CGA-O2A |
| 24 | A | 847 | LHG | O7-C7-C8-C9 |
| 24 | B | 851 | LHG | O7-C7-C8-C9 |
| 29 | 9 | 607 | CHL | CAA-CBA-CGA-O2A |
| 22 | A | 835 | CLA | C5-C6-C7-C8 |
| 22 | B | 816 | CLA | CAA-CBA-CGA-O1A |
| 22 | 7 | 613 | CLA | O1D-CGD-O2D-CED |
| 22 | B | 831 | CLA | CAA-CBA-CGA-O2A |
| 22 | 7 | 609 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 820 | CLA | C3-C5-C6-C7 |
| 22 | A | 828 | CLA | C4-C3-C5-C6 |
| 22 | 4 | 610 | CLA | C4-C3-C5-C6 |
| 22 | A | 809 | CLA | C6-C7-C8-C10 |
| 22 | B | 806 | CLA | C11-C10-C8-C7 |
| 22 | B | 807 | CLA | C11-C10-C8-C7 |
| 22 | B | 812 | CLA | C6-C7-C8-C10 |
| 22 | B | 814 | CLA | C6-C7-C8-C10 |
| 22 | 1 | 611 | CLA | C12-C13-C15-C16 |
| 22 | 3 | 607 | CLA | C3A-C2A-CAA-CBA |
| 22 | 3 | 607 | CLA | C11-C10-C8-C7 |
| 22 | 3 | 610 | CLA | C6-C7-C8-C10 |
| 22 | Z | 608 | CLA | C12-C13-C15-C16 |
| 29 | 6 | 607 | CHL | C3A-C2A-CAA-CBA |
| 22 | A | 813 | CLA | CAA-CBA-CGA-O1A |
| 22 | 8 | 616 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 810 | CLA | CAA-CBA-CGA-O2A |
| 22 | 3 | 617 | CLA | CAA-CBA-CGA-O2A |
| 22 | 5 | 616 | CLA | CAA-CBA-CGA-O2A |
| 22 | 9 | 611 | CLA | CAA-CBA-CGA-O2A |
| 24 | A | 846 | LHG | O8-C23-C24-C25 |
| 22 | 1 | 610 | CLA | C8-C10-C11-C12 |
| 25 | K | 4004 | BCR | C21-C22-C23-C24 |
| 30 | 3 | 621 | LUT | C11-C12-C13-C14 |
| 30 | 8 | 618 | LUT | C7-C8-C9-C10 |
| 30 | Z | 617 | LUT | C7-C8-C9-C10 |
| 30 | Z | 618 | LUT | C7-C8-C9-C10 |
| 30 | 2 | 617 | LUT | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 22 | B | 811 | CLA | CAA-CBA-CGA-O1A |
| 22 | 7 | 609 | CLA | CAA-CBA-CGA-O1A |
| 22 | 4 | 609 | CLA | CAA-CBA-CGA-O1A |
| 22 | 5 | 606 | CLA | CAA-CBA-CGA-O1A |
| 22 | 5 | 613 | CLA | CAA-CBA-CGA-O1A |
| 22 | 6 | 601 | CLA | CAA-CBA-CGA-O1A |
| 28 | J | 3001 | LMG | O8-C28-C29-C30 |
| 22 | B | 817 | CLA | C10-C11-C12-C13 |
| 22 | A | 820 | CLA | C8-C10-C11-C12 |
| 22 | 4 | 602 | CLA | C5-C6-C7-C8 |
| 22 | 5 | 601 | CLA | C10-C11-C12-C13 |
| 22 | Z | 603 | CLA | CAA-CBA-CGA-O1A |
| 24 | B | 851 | LHG | O9-C7-C8-C9 |
| 24 | Z | 620 | LHG | O9-C7-C8-C9 |
| 29 | 9 | 607 | CHL | CBA-CGA-O2A-C1 |
| 22 | B | 806 | CLA | C5-C6-C7-C8 |
| 22 | 1 | 613 | CLA | C13-C15-C16-C17 |
| 22 | A | 811 | CLA | CAA-CBA-CGA-O2A |
| 22 | K | 4003 | CLA | CAA-CBA-CGA-O2A |
| 22 | 2 | 612 | CLA | CAA-CBA-CGA-O2A |
| 22 | 9 | 603 | CLA | CAA-CBA-CGA-O2A |
| 22 | A | 823 | CLA | CAA-CBA-CGA-O1A |
| 22 | A | 854 | CLA | C8-C10-C11-C12 |
| 22 | 6 | 617 | CLA | CAA-CBA-CGA-O1A |
| 22 | 3 | 603 | CLA | C4-C3-C5-C6 |
| 22 | A | 804 | CLA | CAA-CBA-CGA-O2A |
| 22 | F | 301 | CLA | C13-C15-C16-C17 |

There are no ring outliers.

274 monomers are involved in 852 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22 | 3 | 607 | CLA | 4 | 0 |
| 25 | G | 205 | BCR | 3 | 0 |
| 22 | A | 825 | CLA | 3 | 0 |
| 22 | 3 | 609 | CLA | 1 | 0 |
| 22 | 1 | 613 | CLA | 2 | 0 |
| 22 | B | 806 | CLA | 2 | 0 |
| 22 | 7 | 610 | CLA | 2 | 0 |
| 25 | 6 | 623 | BCR | 8 | 0 |
| 25 | K | 4001 | BCR | 5 | 0 |
| 29 | 1 | 601 | CHL | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22 | 7 | 611 | CLA | 1 | 0 |
| 22 | 4 | 614 | CLA | 4 | 0 |
| 22 | 1 | 602 | CLA | 9 | 0 |
| 22 | A | 832 | CLA | 5 | 0 |
| 25 | J | 3003 | BCR | 2 | 0 |
| 24 | Z | 620 | LHG | 1 | 0 |
| 22 | 4 | 611 | CLA | 6 | 0 |
| 25 | B | 847 | BCR | 4 | 0 |
| 22 | 3 | 613 | CLA | 2 | 0 |
| 29 | 6 | 607 | CHL | 5 | 0 |
| 22 | 5 | 616 | CLA | 1 | 0 |
| 22 | A | 835 | CLA | 23 | 0 |
| 22 | Z | 604 | CLA | 1 | 0 |
| 22 | A | 809 | CLA | 4 | 0 |
| 22 | Z | 606 | CLA | 2 | 0 |
| 22 | 4 | 613 | CLA | 3 | 0 |
| 22 | 5 | 606 | CLA | 4 | 0 |
| 25 | L | 201 | BCR | 7 | 0 |
| 24 | 6 | 619 | LHG | 19 | 0 |
| 22 | A | 823 | CLA | 3 | 0 |
| 22 | 3 | 612 | CLA | 2 | 0 |
| 22 | A | 824 | CLA | 1 | 0 |
| 22 | 2 | 612 | CLA | 1 | 0 |
| 22 | B | 812 | CLA | 8 | 0 |
| 22 | 4 | 612 | CLA | 1 | 0 |
| 30 | 8 | 618 | LUT | 5 | 0 |
| 22 | 3 | 602 | CLA | 1 | 0 |
| 30 | 7 | 622 | LUT | 2 | 0 |
| 25 | 7 | 623 | BCR | 5 | 0 |
| 29 | 6 | 608 | CHL | 1 | 0 |
| 30 | 6 | 621 | LUT | 4 | 0 |
| 22 | B | 828 | CLA | 3 | 0 |
| 22 | B | 837 | CLA | 4 | 0 |
| 22 | A | 804 | CLA | 2 | 0 |
| 25 | B | 846 | BCR | 6 | 0 |
| 25 | 5 | 622 | BCR | 5 | 0 |
| 22 | 9 | 603 | CLA | 1 | 0 |
| 29 | 5 | 607 | CHL | 3 | 0 |
| 22 | J | 3002 | CLA | 1 | 0 |
| 22 | B | 808 | CLA | 1 | 0 |
| 22 | A | 842 | CLA | 10 | 0 |
| 22 | A | 821 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25 | B | 801 | BCR | 6 | 0 |
| 22 | 5 | 613 | CLA | 3 | 0 |
| 22 | B | 833 | CLA | 3 | 0 |
| 25 | B | 848 | BCR | 3 | 0 |
| 21 | A | 801 | CL0 | 3 | 0 |
| 22 | 4 | 610 | CLA | 10 | 0 |
| 25 | K | 4004 | BCR | 1 | 0 |
| 22 | 9 | 609 | CLA | 11 | 0 |
| 29 | 9 | 607 | CHL | 1 | 0 |
| 22 | A | 803 | CLA | 2 | 0 |
| 22 | B | 823 | CLA | 4 | 0 |
| 22 | 7 | 601 | CLA | 4 | 0 |
| 22 | B | 824 | CLA | 1 | 0 |
| 22 | 6 | 602 | CLA | 1 | 0 |
| 30 | 5 | 620 | LUT | 15 | 0 |
| 30 | 2 | 617 | LUT | 3 | 0 |
| 22 | 9 | 614 | CLA | 2 | 0 |
| 22 | A | 802 | CLA | 26 | 0 |
| 22 | B | 830 | CLA | 3 | 0 |
| 22 | 5 | 604 | CLA | 2 | 0 |
| 22 | 8 | 614 | CLA | 5 | 0 |
| 22 | A | 819 | CLA | 3 | 0 |
| 22 | B | 826 | CLA | 2 | 0 |
| 22 | 7 | 616 | CLA | 1 | 0 |
| 29 | 5 | 608 | CHL | 3 | 0 |
| 30 | 4 | 620 | LUT | 4 | 0 |
| 22 | 9 | 610 | CLA | 1 | 0 |
| 22 | 4 | 602 | CLA | 1 | 0 |
| 22 | 3 | 606 | CLA | 3 | 0 |
| 22 | 7 | 608 | CLA | 2 | 0 |
| 25 | 6 | 625 | BCR | 3 | 0 |
| 22 | B | 816 | CLA | 5 | 0 |
| 22 | A | 808 | CLA | 2 | 0 |
| 22 | 2 | 613 | CLA | 9 | 0 |
| 22 | 8 | 616 | CLA | 1 | 0 |
| 22 | 3 | 610 | CLA | 3 | 0 |
| 22 | B | 811 | CLA | 3 | 0 |
| 22 | A | 806 | CLA | 5 | 0 |
| 25 | A | 848 | BCR | 5 | 0 |
| 22 | A | 854 | CLA | 5 | 0 |
| 22 | 9 | 612 | CLA | 1 | 0 |
| 25 | 4 | 621 | BCR | 39 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 29 | 7 | 607 | CHL | 1 | 0 |
| 22 | 7 | 606 | CLA | 2 | 0 |
| 30 | 9 | 617 | LUT | 4 | 0 |
| 22 | F | 303 | CLA | 2 | 0 |
| 22 | A | 817 | CLA | 5 | 0 |
| 22 | A | 818 | CLA | 3 | 0 |
| 22 | 1 | 603 | CLA | 3 | 0 |
| 25 | B | 845 | BCR | 3 | 0 |
| 22 | 5 | 602 | CLA | 4 | 0 |
| 22 | 8 | 609 | CLA | 2 | 0 |
| 22 | Z | 611 | CLA | 2 | 0 |
| 22 | 5 | 621 | CLA | 1 | 0 |
| 22 | 6 | 609 | CLA | 2 | 0 |
| 29 | 4 | 618 | CHL | 7 | 0 |
| 22 | 7 | 614 | CLA | 1 | 0 |
| 22 | A | 822 | CLA | 2 | 0 |
| 22 | 2 | 610 | CLA | 2 | 0 |
| 29 | 3 | 608 | CHL | 5 | 0 |
| 24 | 1 | 620 | LHG | 2 | 0 |
| 22 | 8 | 606 | CLA | 2 | 0 |
| 30 | 3 | 621 | LUT | 4 | 0 |
| 22 | B | 840 | CLA | 4 | 0 |
| 25 | 5 | 625 | BCR | 7 | 0 |
| 22 | Z | 603 | CLA | 1 | 0 |
| 25 | A | 852 | BCR | 3 | 0 |
| 25 | 8 | 619 | BCR | 6 | 0 |
| 30 | 9 | 616 | LUT | 4 | 0 |
| 25 | A | 849 | BCR | 5 | 0 |
| 22 | A | 820 | CLA | 4 | 0 |
| 22 | 5 | 617 | CLA | 6 | 0 |
| 22 | A | 830 | CLA | 3 | 0 |
| 22 | A | 816 | CLA | 7 | 0 |
| 22 | B | 841 | CLA | 13 | 0 |
| 22 | 7 | 613 | CLA | 3 | 0 |
| 22 | A | 826 | CLA | 2 | 0 |
| 23 | B | 842 | PQN | 1 | 0 |
| 22 | A | 827 | CLA | 1 | 0 |
| 22 | 1 | 611 | CLA | 1 | 0 |
| 22 | B | 815 | CLA | 3 | 0 |
| 22 | B | 832 | CLA | 5 | 0 |
| 22 | A | 807 | CLA | 9 | 0 |
| 30 | 8 | 617 | LUT | 8 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 22 | 3 | 603 | CLA | 4 | 0 |
| 22 | B | 825 | CLA | 5 | 0 |
| 22 | Z | 609 | CLA | 1 | 0 |
| 22 | A | 836 | CLA | 2 | 0 |
| 22 | A | 811 | CLA | 4 | 0 |
| 22 | A | 833 | CLA | 4 | 0 |
| 22 | 3 | 614 | CLA | 3 | 0 |
| 22 | 8 | 610 | CLA | 6 | 0 |
| 22 | A | 831 | CLA | 8 | 0 |
| 22 | Z | 608 | CLA | 4 | 0 |
| 23 | A | 844 | PQN | 4 | 0 |
| 29 | 4 | 607 | CHL | 1 | 0 |
| 22 | B | 818 | CLA | 4 | 0 |
| 22 | 6 | 604 | CLA | 4 | 0 |
| 22 | 7 | 612 | CLA | 1 | 0 |
| 22 | 4 | 604 | CLA | 6 | 0 |
| 22 | 7 | 604 | CLA | 1 | 0 |
| 24 | A | 846 | LHG | 2 | 0 |
| 22 | 1 | 608 | CLA | 5 | 0 |
| 22 | B | 820 | CLA | 15 | 0 |
| 22 | 8 | 604 | CLA | 1 | 0 |
| 30 | 1 | 617 | LUT | 7 | 0 |
| 22 | Z | 610 | CLA | 3 | 0 |
| 22 | B | 822 | CLA | 1 | 0 |
| 22 | 5 | 603 | CLA | 1 | 0 |
| 22 | 9 | 611 | CLA | 1 | 0 |
| 25 | A | 856 | BCR | 5 | 0 |
| 22 | K | 4003 | CLA | 2 | 0 |
| 22 | 6 | 610 | CLA | 5 | 0 |
| 22 | 5 | 612 | CLA | 2 | 0 |
| 22 | Z | 612 | CLA | 1 | 0 |
| 30 | 1 | 618 | LUT | 5 | 0 |
| 22 | B | 813 | CLA | 5 | 0 |
| 22 | B | 807 | CLA | 2 | 0 |
| 28 | 9 | 620 | LMG | 1 | 0 |
| 22 | 2 | 601 | CLA | 5 | 0 |
| 22 | 4 | 601 | CLA | 6 | 0 |
| 25 | B | 843 | BCR | 5 | 0 |
| 29 | 4 | 608 | CHL | 8 | 0 |
| 25 | 7 | 624 | BCR | 1 | 0 |
| 22 | A | 845 | CLA | 1 | 0 |
| 29 | 4 | 606 | CHL | 10 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | 8 | 601 | CLA | 1 | 0 |
| 30 | Z | 617 | LUT | 4 | 0 |
| 27 | B | 850 | DGD | 1 | 0 |
| 30 | 4 | 619 | LUT | 12 | 0 |
| 22 | B | 831 | CLA | 6 | 0 |
| 24 | A | 847 | LHG | 3 | 0 |
| 22 | 6 | 614 | CLA | 2 | 0 |
| 22 | B | 803 | CLA | 4 | 0 |
| 22 | B | 838 | CLA | 3 | 0 |
| 22 | B | 827 | CLA | 4 | 0 |
| 22 | A | 814 | CLA | 2 | 0 |
| 22 | F | 301 | CLA | 4 | 0 |
| 30 | Z | 618 | LUT | 4 | 0 |
| 29 | Z | 601 | CHL | 1 | 0 |
| 22 | Z | 602 | CLA | 3 | 0 |
| 22 | A | 812 | CLA | 15 | 0 |
| 25 | 3 | 719 | BCR | 6 | 0 |
| 22 | 4 | 616 | CLA | 6 | 0 |
| 22 | 1 | 609 | CLA | 2 | 0 |
| 22 | 9 | 613 | CLA | 1 | 0 |
| 22 | 3 | 620 | CLA | 1 | 0 |
| 30 | 6 | 624 | LUT | 3 | 0 |
| 22 | 6 | 611 | CLA | 1 | 0 |
| 25 | B | 844 | BCR | 2 | 0 |
| 22 | B | 834 | CLA | 1 | 0 |
| 22 | 3 | 617 | CLA | 3 | 0 |
| 25 | A | 851 | BCR | 3 | 0 |
| 22 | A | 828 | CLA | 1 | 0 |
| 22 | A | 840 | CLA | 3 | 0 |
| 22 | A | 805 | CLA | 22 | 0 |
| 25 | I | 172 | BCR | 1 | 0 |
| 22 | B | 817 | CLA | 3 | 0 |
| 22 | A | 839 | CLA | 4 | 0 |
| 22 | 7 | 620 | CLA | 12 | 0 |
| 22 | A | 829 | CLA | 7 | 0 |
| 22 | 5 | 614 | CLA | 5 | 0 |
| 22 | 8 | 613 | CLA | 3 | 0 |
| 22 | 6 | 612 | CLA | 2 | 0 |
| 22 | Z | 614 | CLA | 2 | 0 |
| 24 | 4 | 622 | LHG | 3 | 0 |
| 22 | 8 | 612 | CLA | 1 | 0 |
| 22 | Z | 613 | CLA | 5 | 0 |

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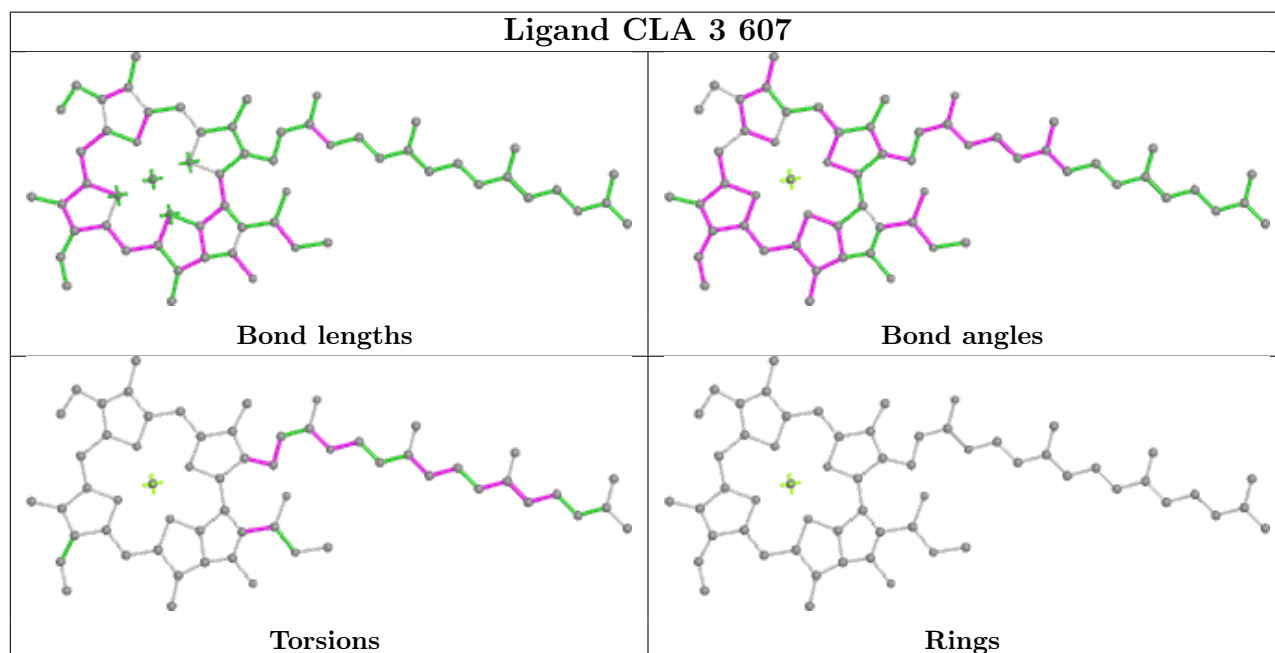
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | 1 | 616 | CLA | 1 | 0 |
| 22 | A | 813 | CLA | 2 | 0 |
| 30 | 5 | 624 | LUT | 5 | 0 |
| 22 | 3 | 604 | CLA | 3 | 0 |
| 22 | L | 203 | CLA | 1 | 0 |
| 25 | A | 850 | BCR | 5 | 0 |
| 22 | 6 | 601 | CLA | 7 | 0 |
| 22 | 7 | 602 | CLA | 2 | 0 |
| 22 | 6 | 616 | CLA | 8 | 0 |
| 22 | 2 | 602 | CLA | 2 | 0 |
| 29 | 1 | 607 | CHL | 3 | 0 |
| 29 | 6 | 606 | CHL | 4 | 0 |
| 22 | 5 | 609 | CLA | 6 | 0 |
| 22 | B | 821 | CLA | 1 | 0 |
| 22 | A | 834 | CLA | 3 | 0 |
| 22 | B | 814 | CLA | 5 | 0 |
| 22 | 1 | 610 | CLA | 5 | 0 |
| 22 | 6 | 622 | CLA | 14 | 0 |
| 22 | 5 | 610 | CLA | 1 | 0 |
| 22 | B | 805 | CLA | 5 | 0 |
| 22 | 8 | 608 | CLA | 1 | 0 |
| 25 | 3 | 718 | BCR | 5 | 0 |
| 22 | 1 | 604 | CLA | 1 | 0 |
| 22 | 1 | 606 | CLA | 3 | 0 |
| 22 | 8 | 602 | CLA | 3 | 0 |
| 25 | F | 305 | BCR | 15 | 0 |
| 22 | B | 829 | CLA | 4 | 0 |
| 22 | 2 | 611 | CLA | 1 | 0 |
| 24 | 8 | 620 | LHG | 1 | 0 |
| 22 | B | 836 | CLA | 2 | 0 |
| 22 | 1 | 614 | CLA | 3 | 0 |
| 22 | A | 841 | CLA | 11 | 0 |
| 29 | 6 | 618 | CHL | 2 | 0 |
| 30 | 7 | 621 | LUT | 6 | 0 |
| 22 | 7 | 609 | CLA | 3 | 0 |
| 22 | B | 802 | CLA | 2 | 0 |
| 25 | L | 205 | BCR | 2 | 0 |
| 30 | 3 | 622 | LUT | 3 | 0 |
| 22 | A | 838 | CLA | 1 | 0 |
| 22 | F | 304 | CLA | 2 | 0 |
| 22 | B | 835 | CLA | 2 | 0 |
| 22 | 5 | 601 | CLA | 1 | 0 |

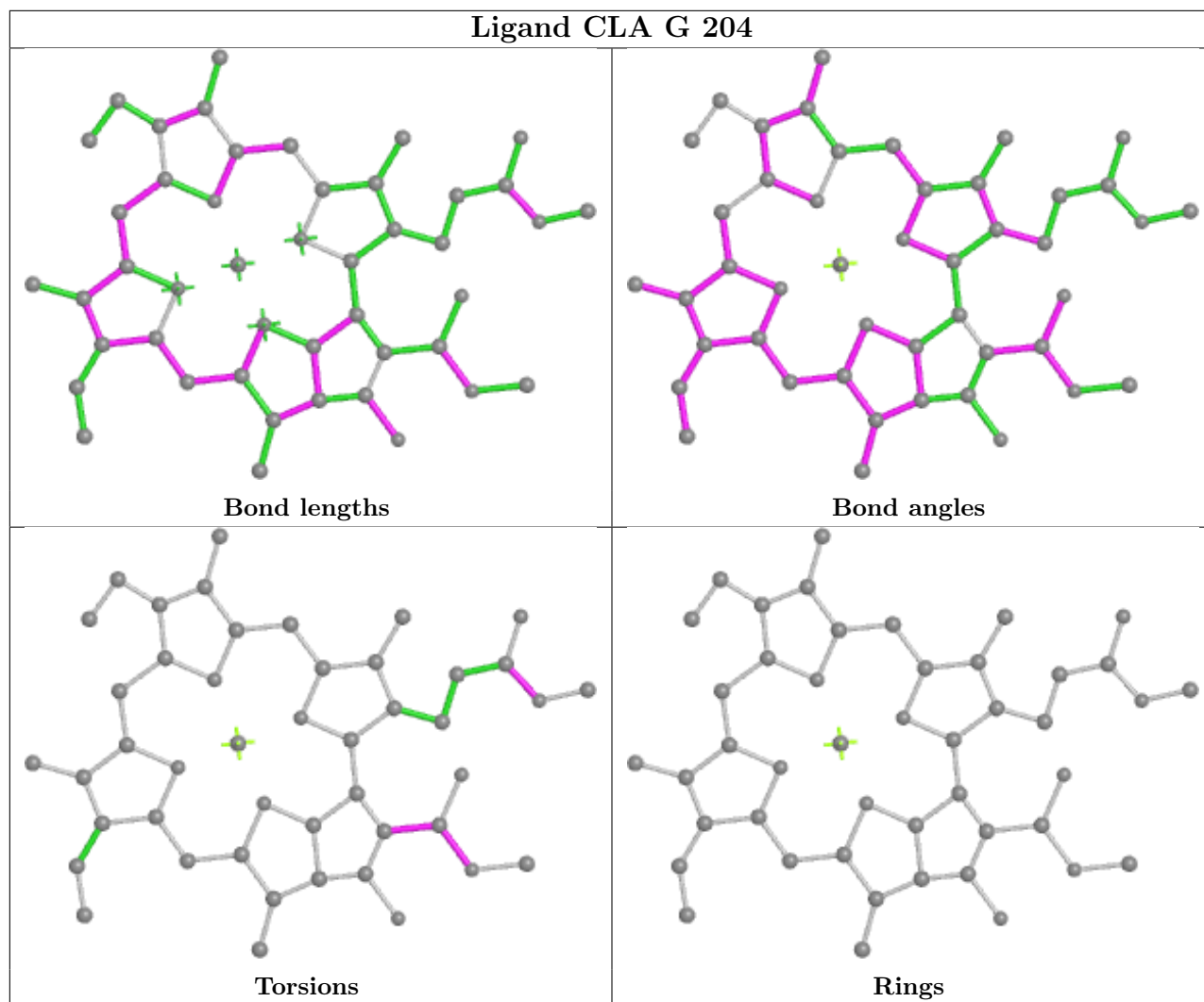
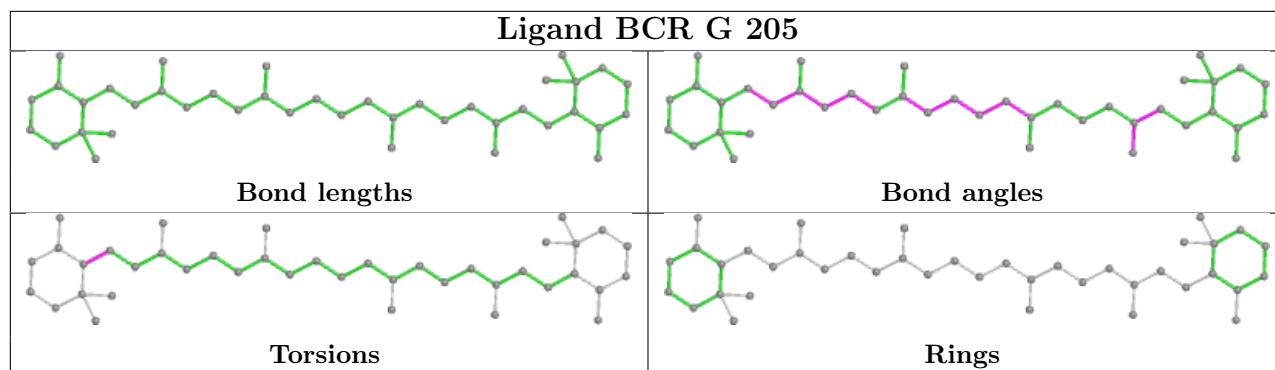
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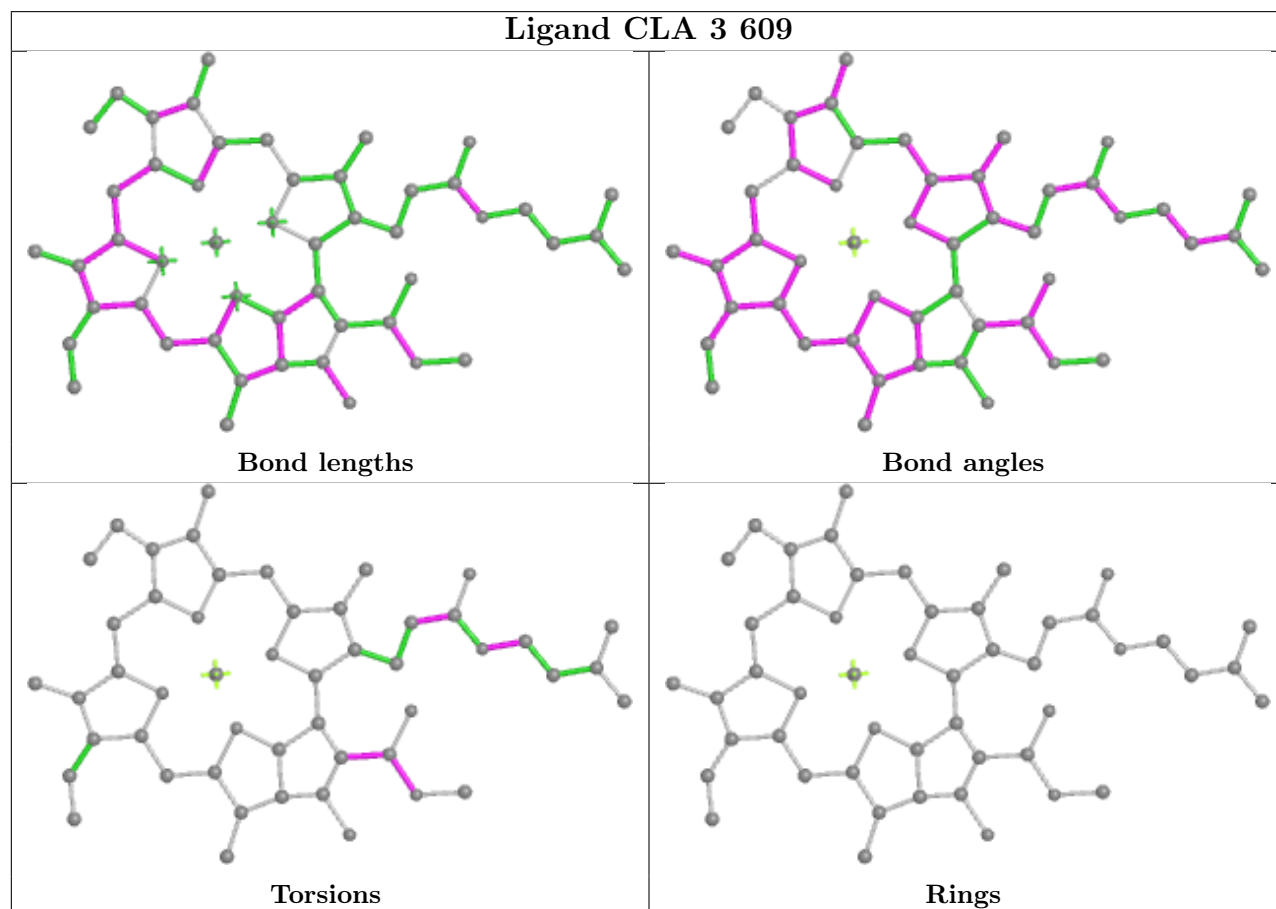
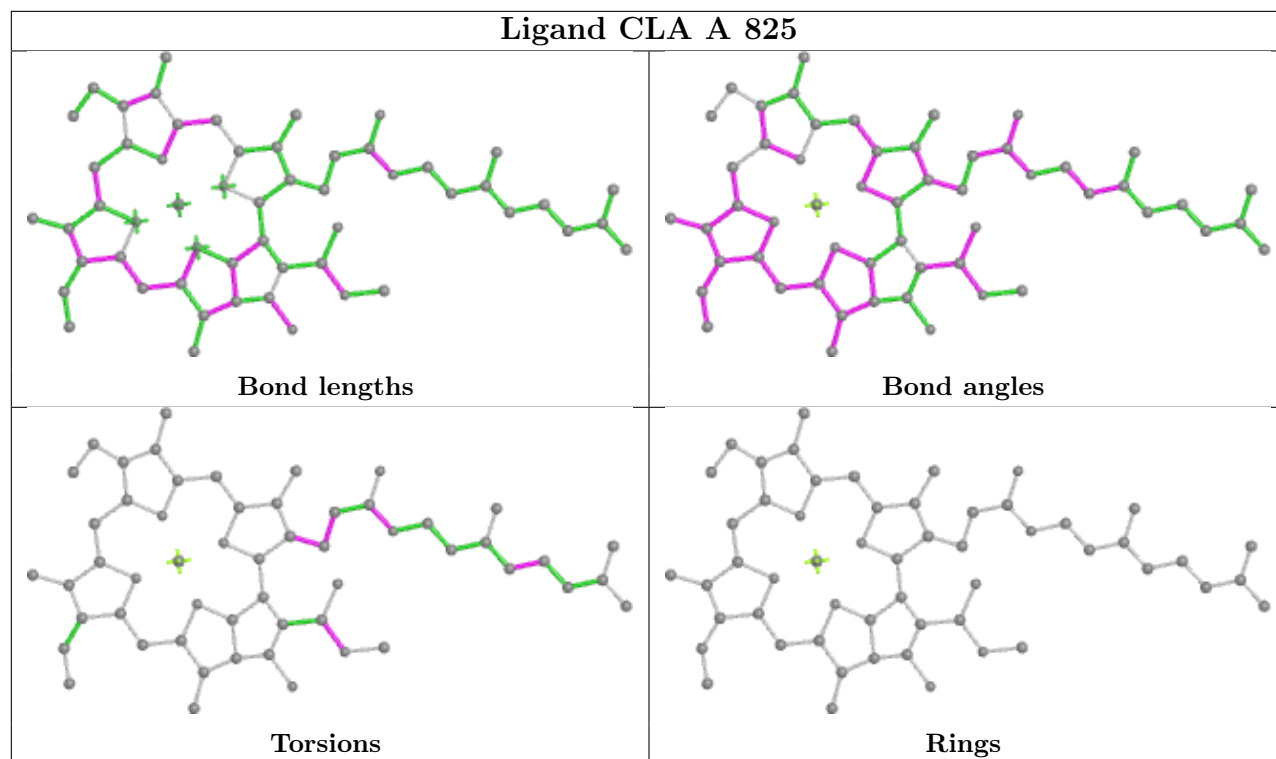
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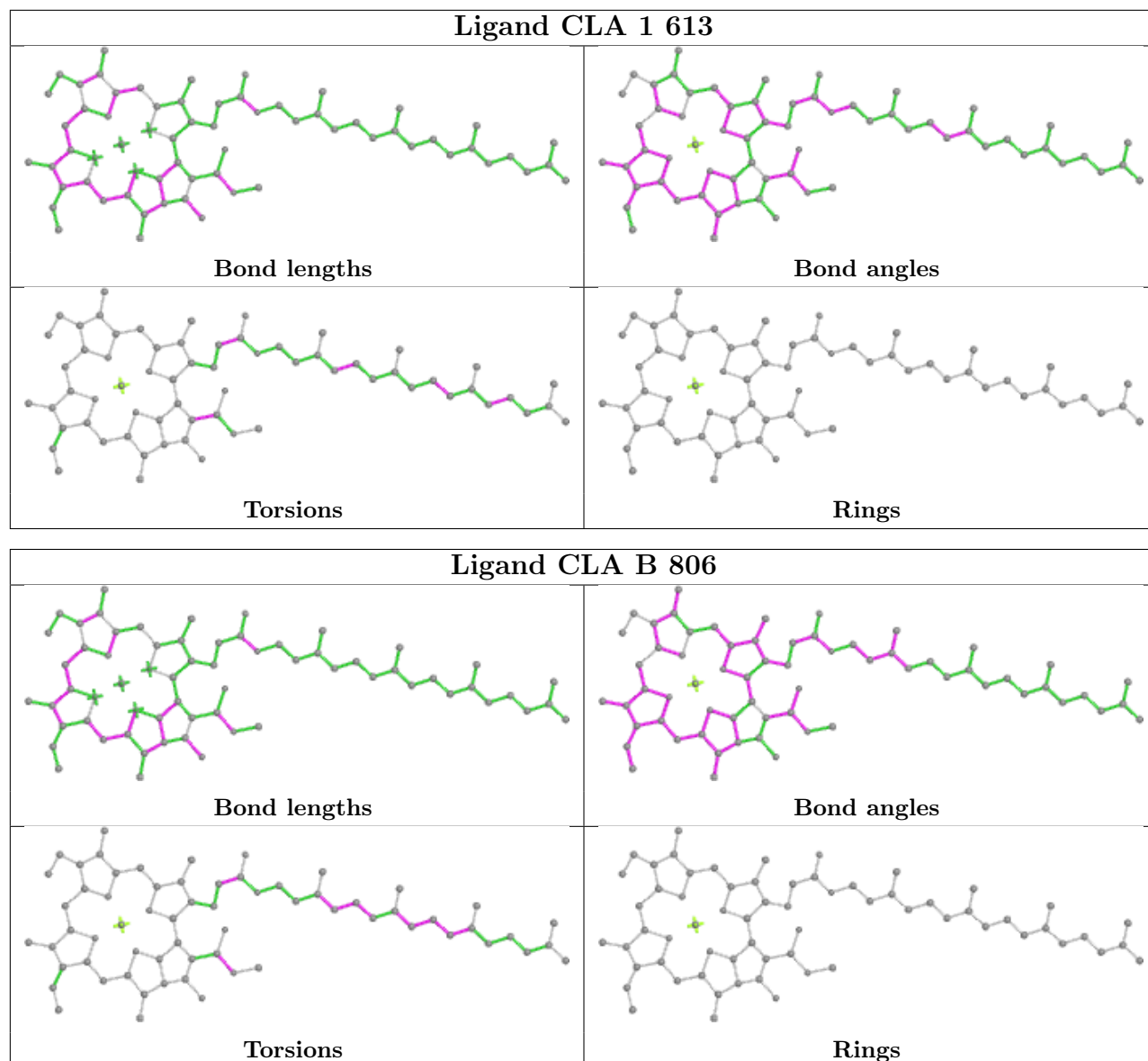
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | B | 809 | CLA | 1 | 0 |
| 22 | B | 819 | CLA | 2 | 0 |
| 22 | 9 | 602 | CLA | 3 | 0 |
| 25 | 3 | 717 | BCR | 4 | 0 |
| 22 | A | 837 | CLA | 1 | 0 |
| 30 | 2 | 616 | LUT | 3 | 0 |
| 22 | B | 839 | CLA | 4 | 0 |
| 30 | Z | 619 | LUT | 2 | 0 |
| 30 | 1 | 619 | LUT | 2 | 0 |
| 22 | A | 815 | CLA | 21 | 0 |
| 22 | A | 843 | CLA | 7 | 0 |
| 22 | 6 | 613 | CLA | 2 | 0 |

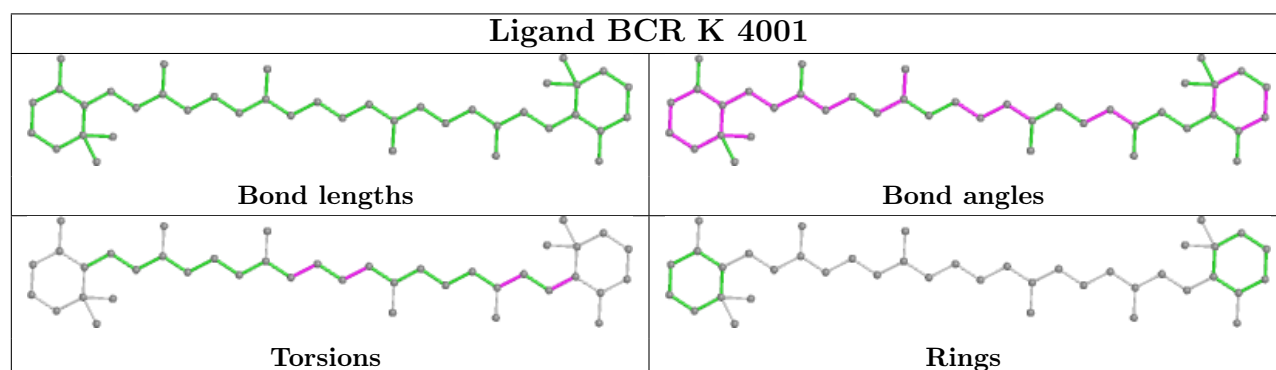
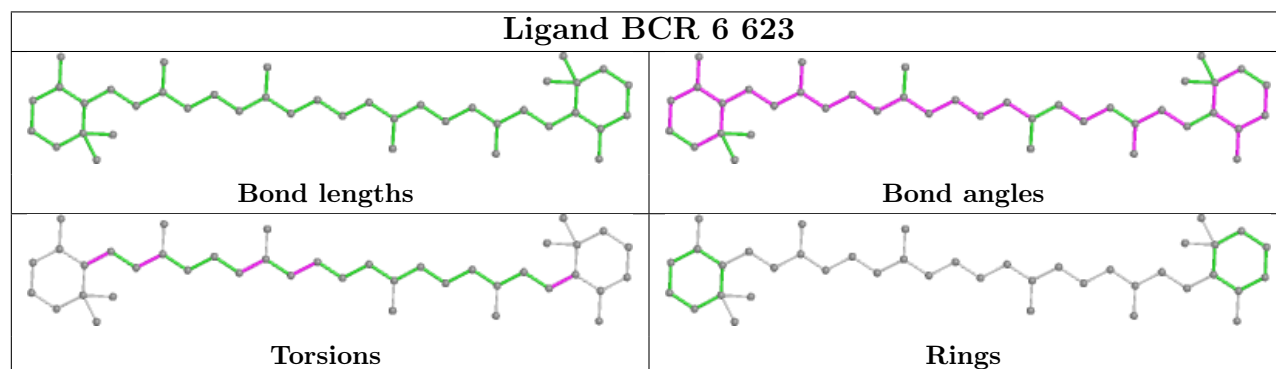
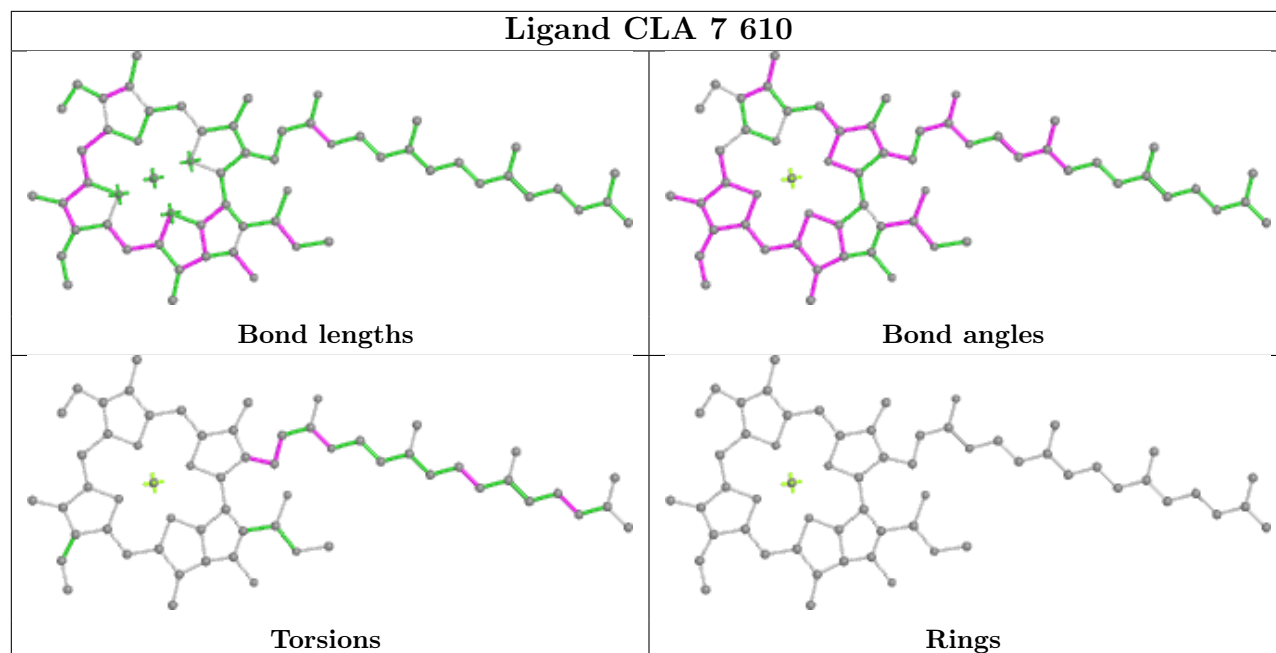
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

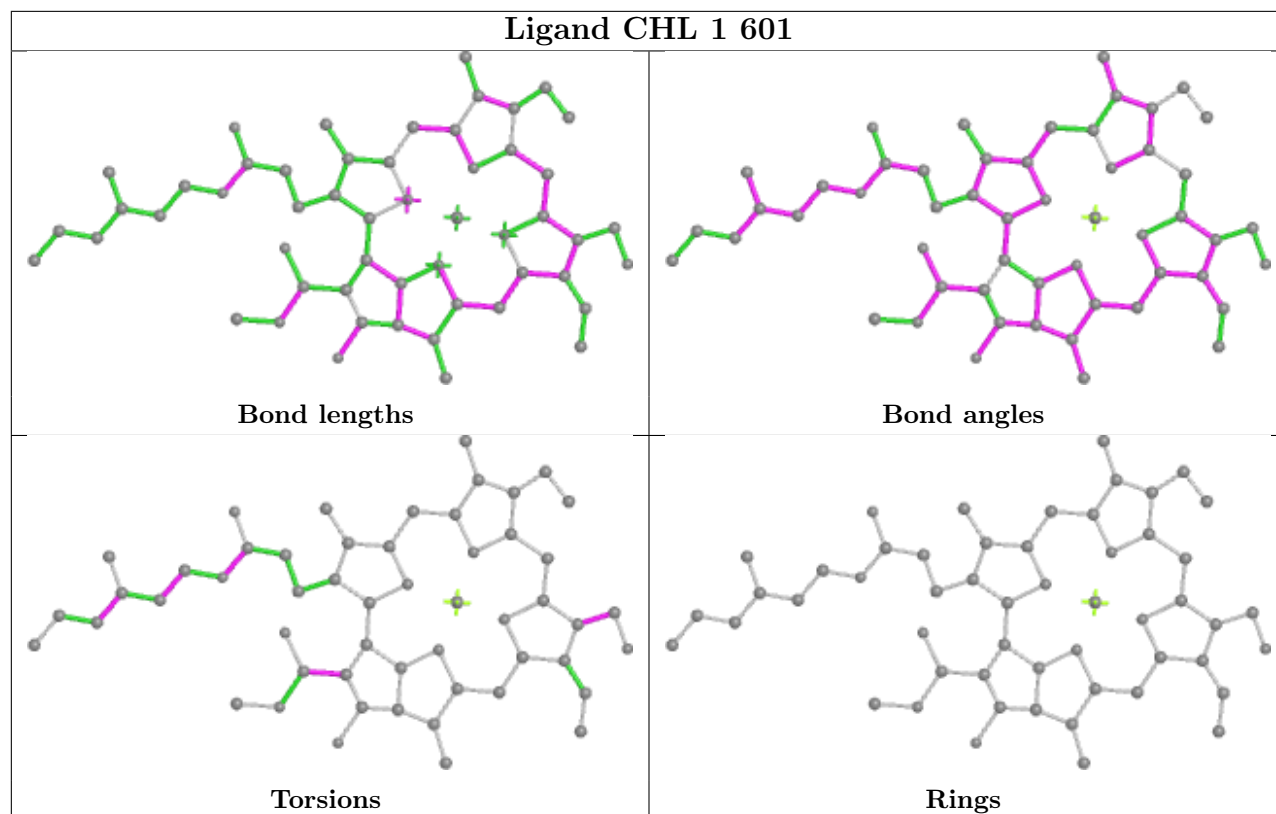


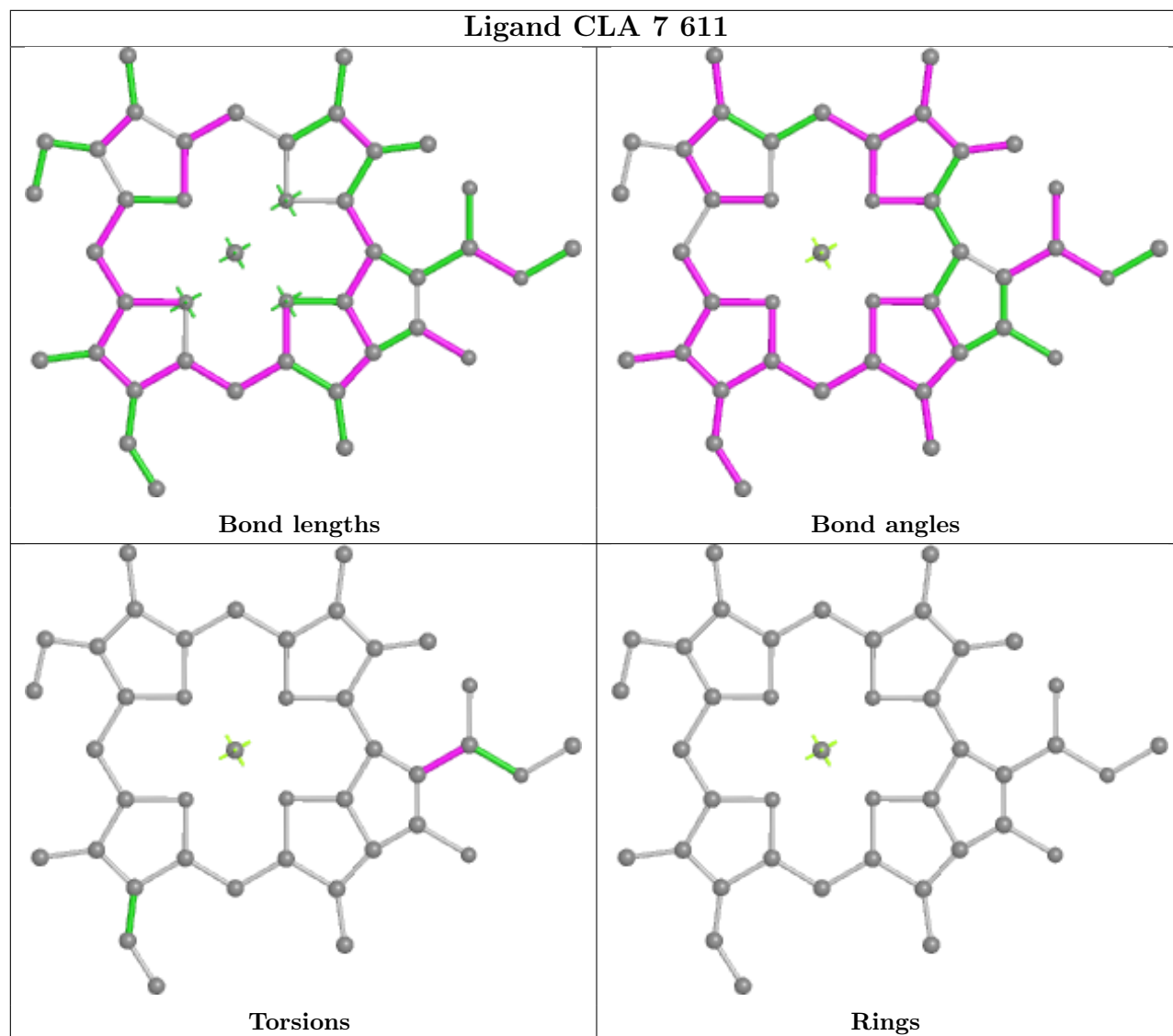


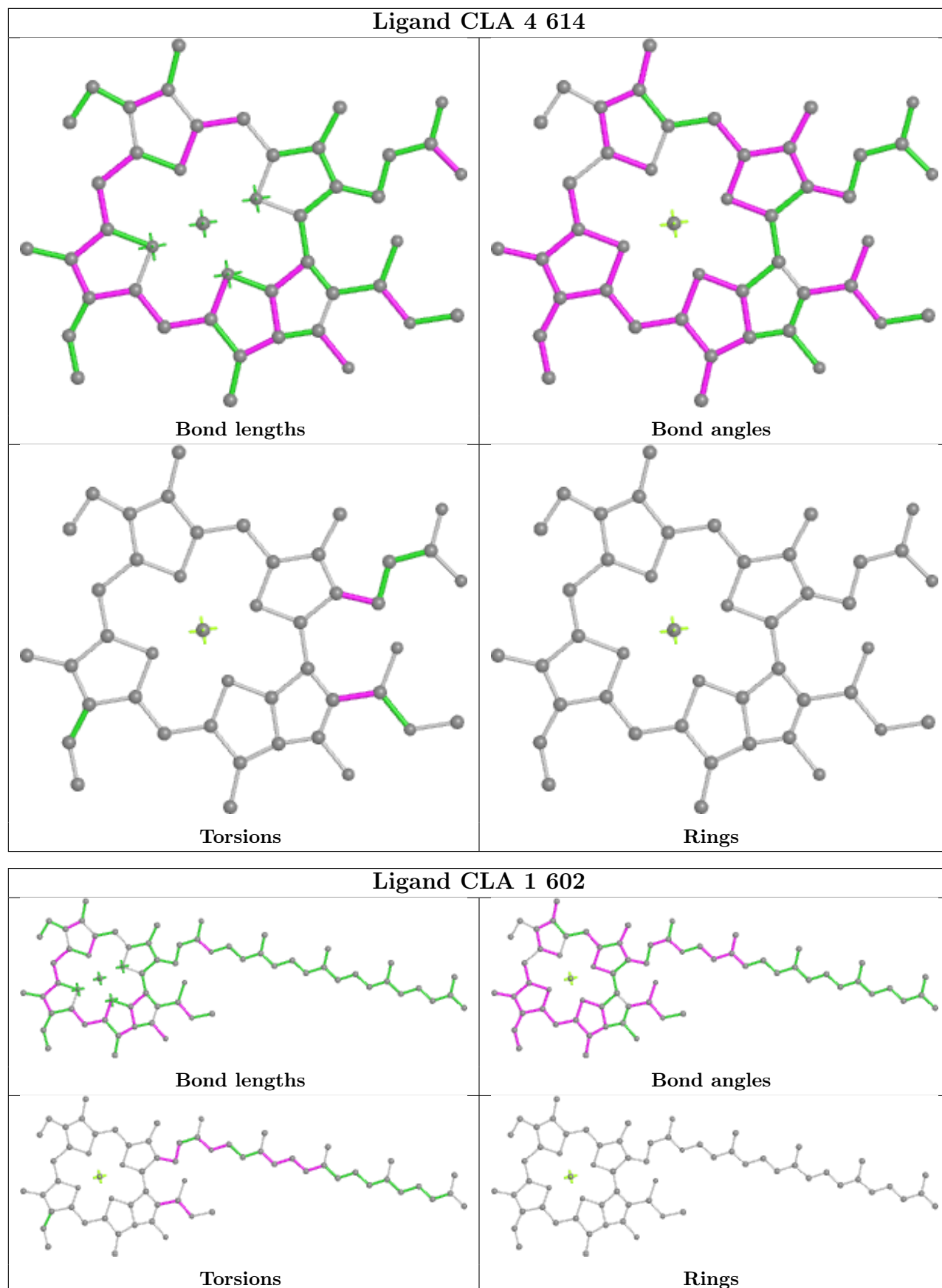


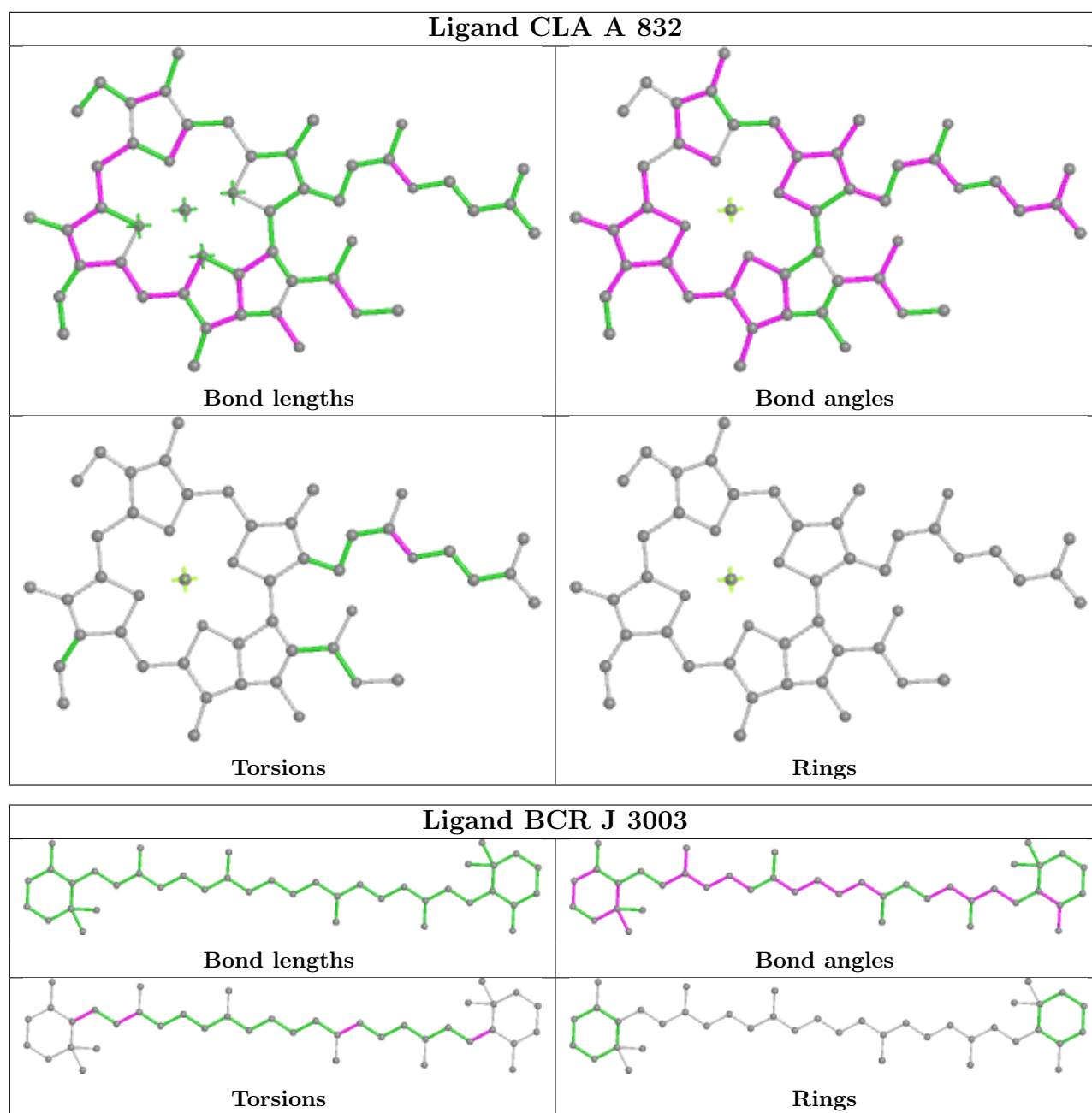


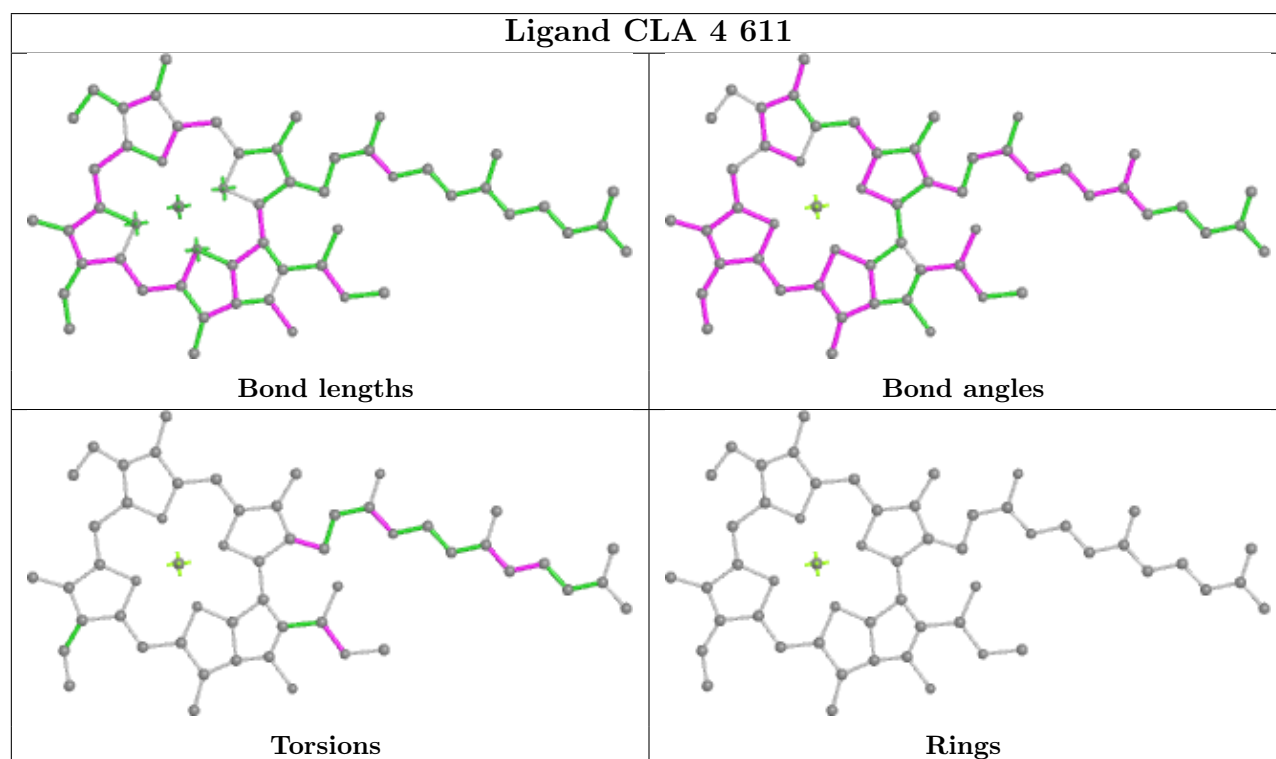
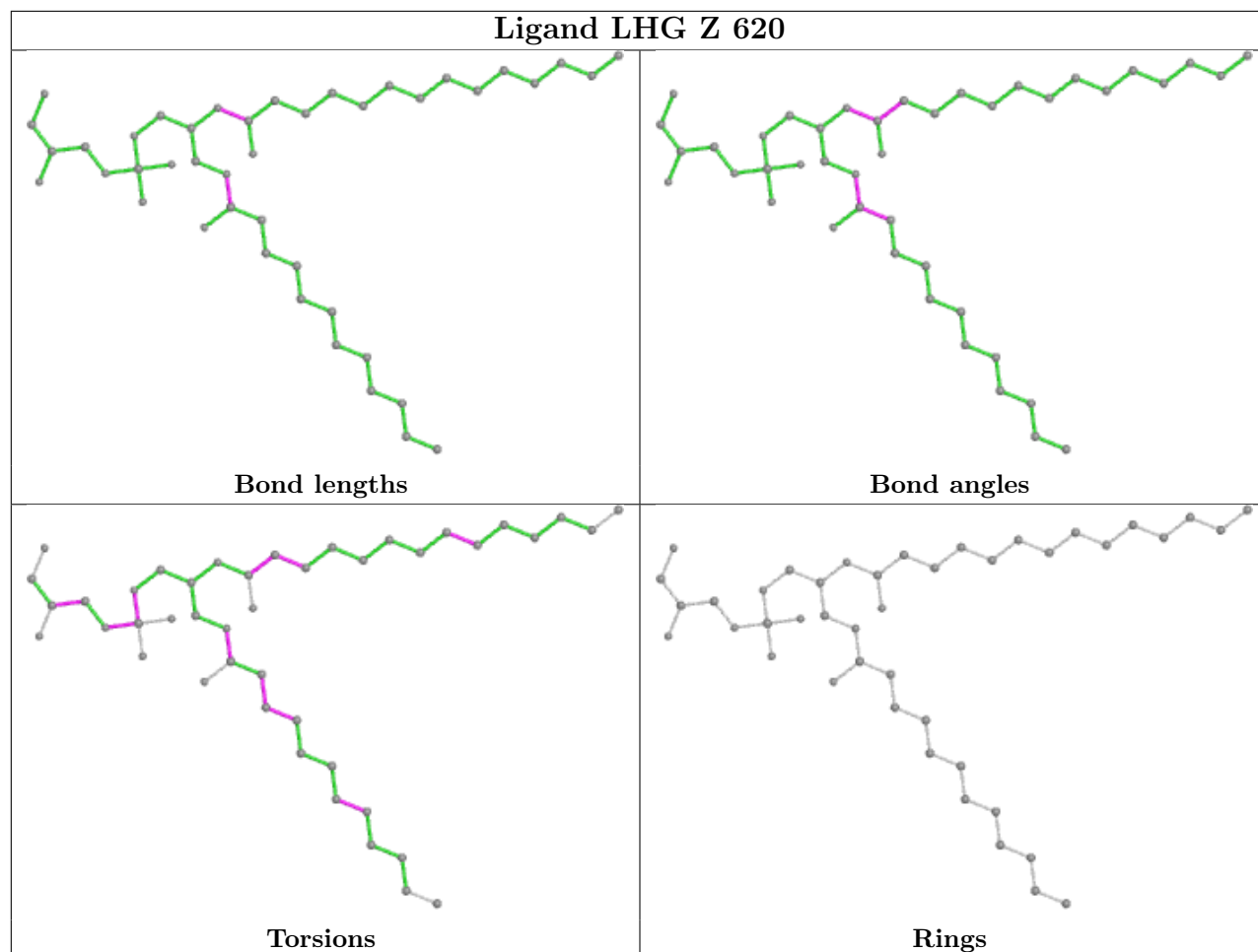


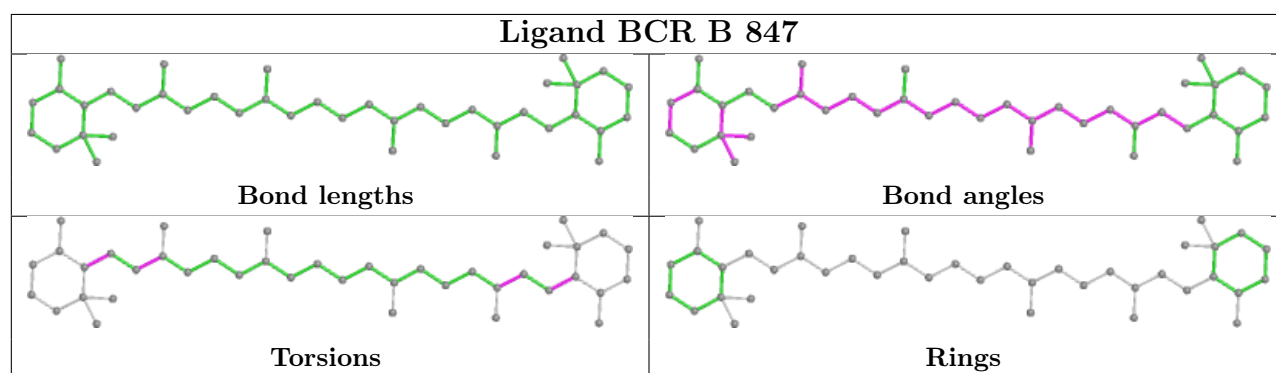
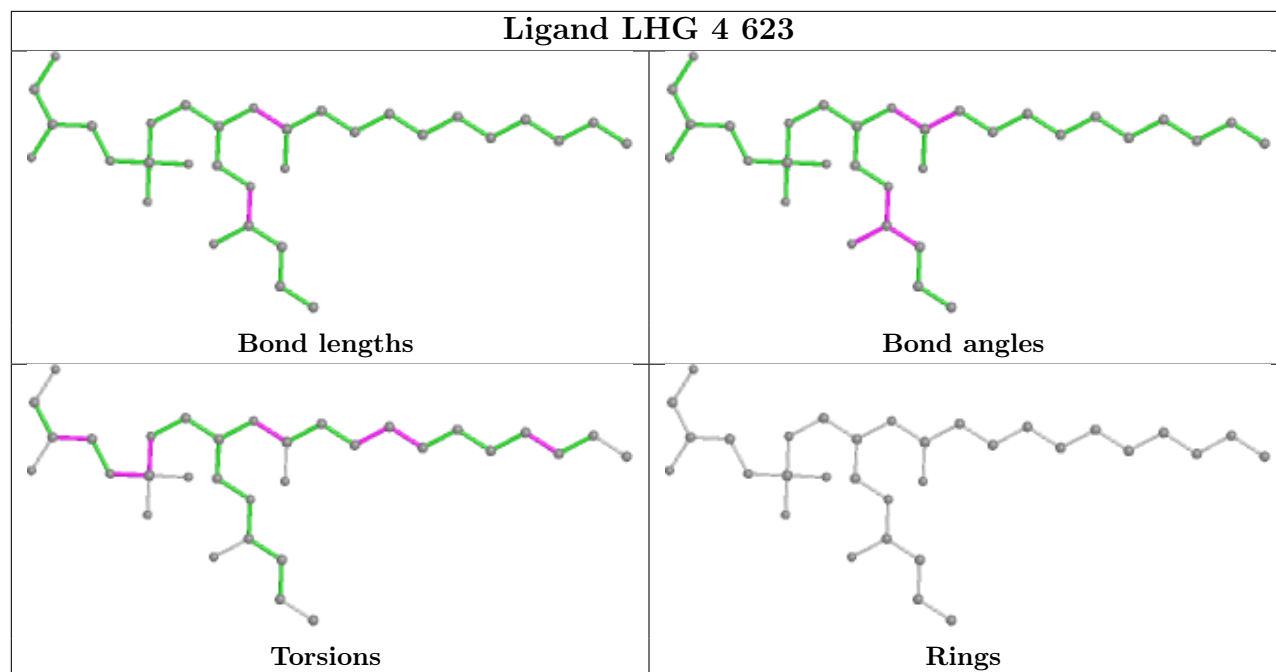


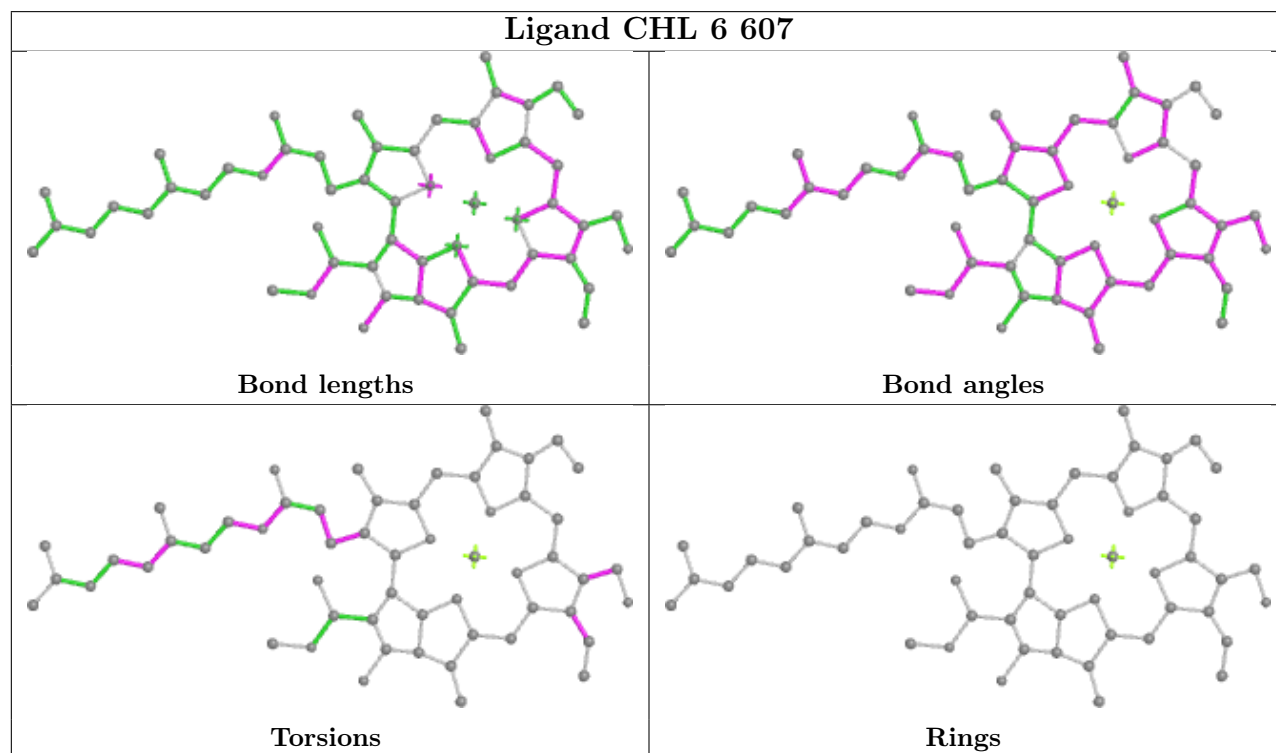
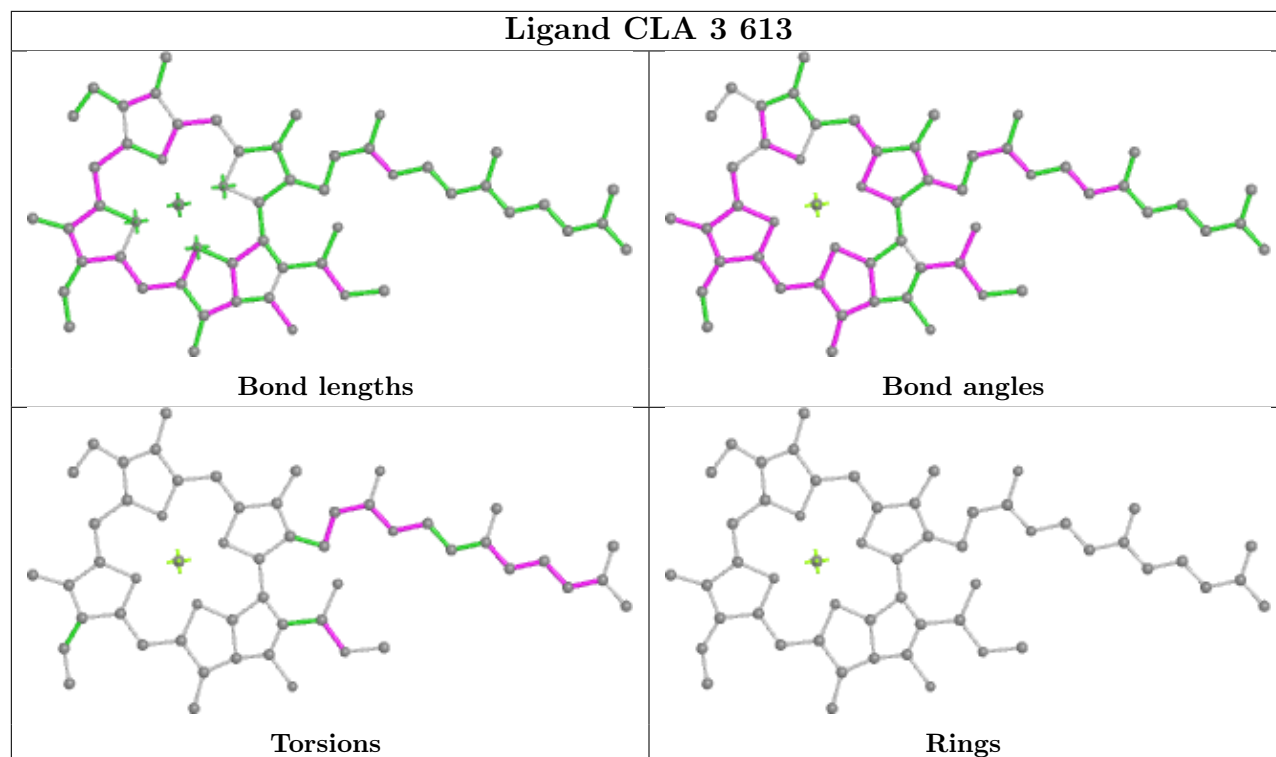


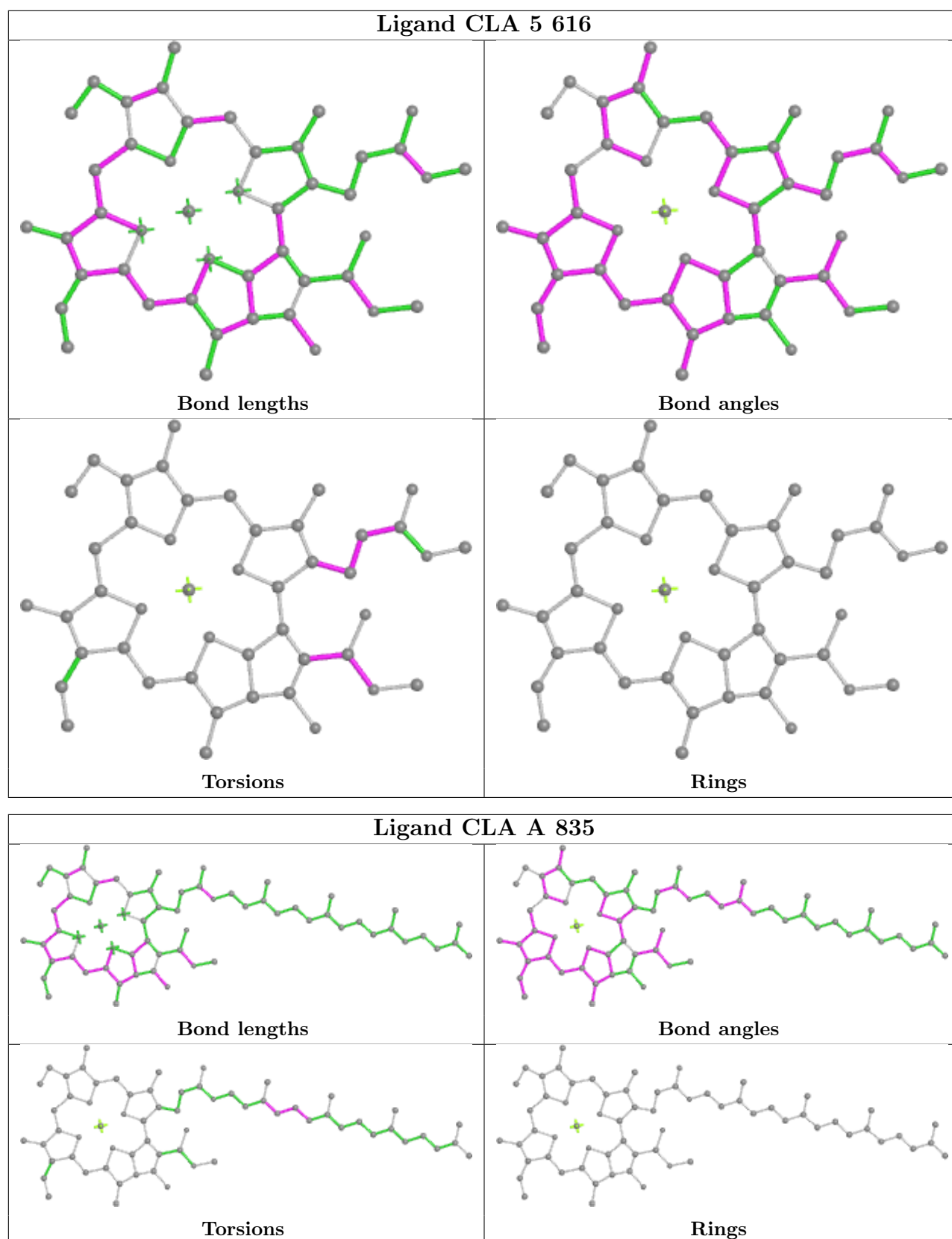


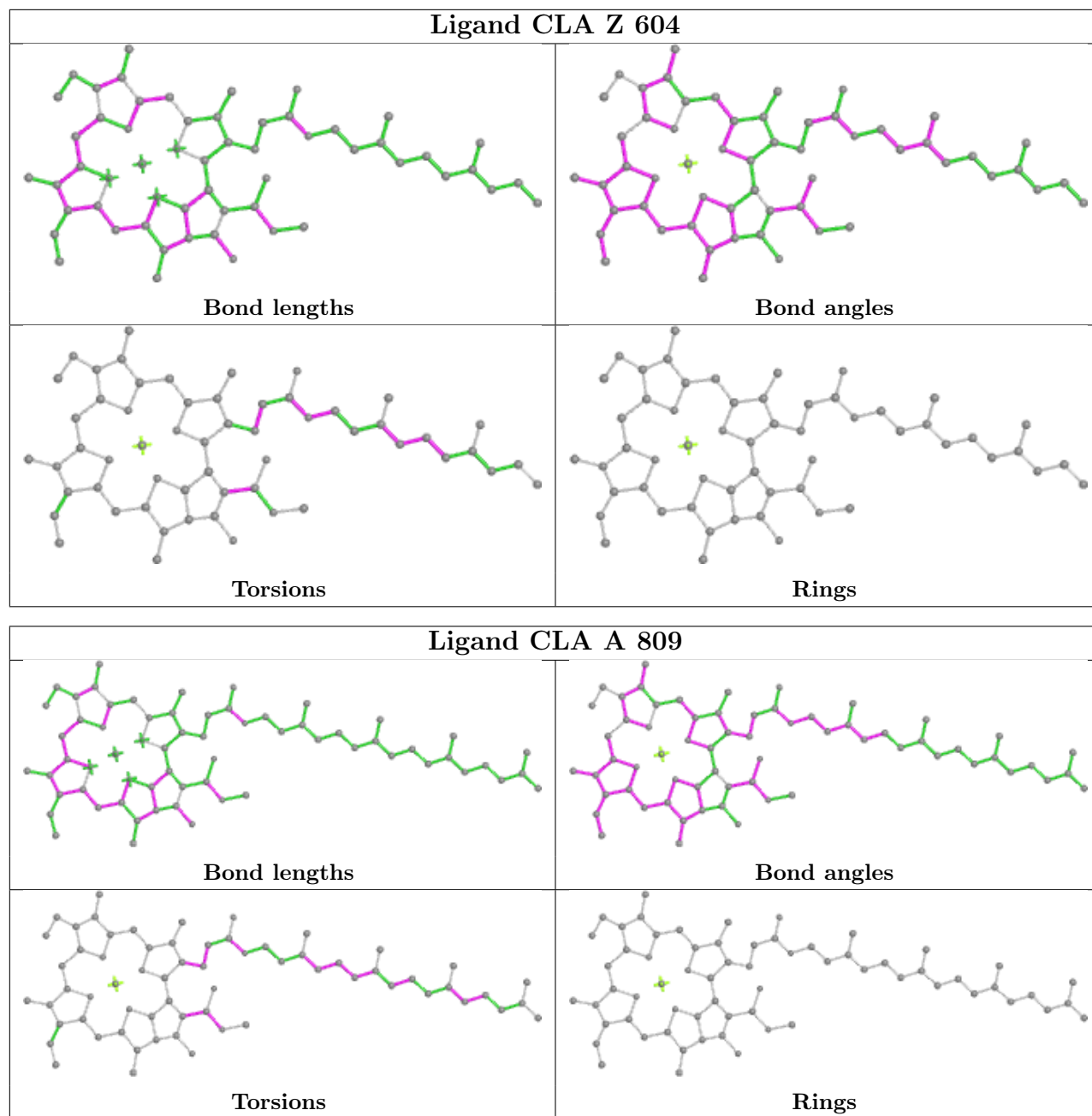


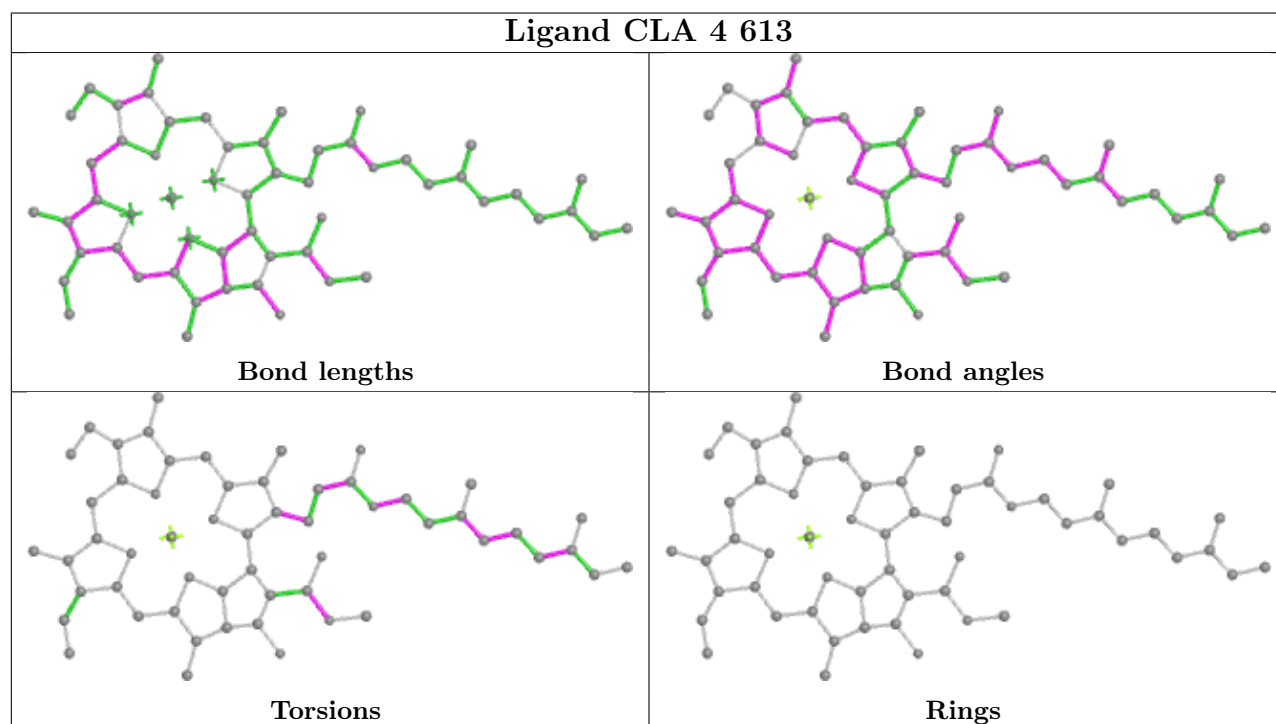
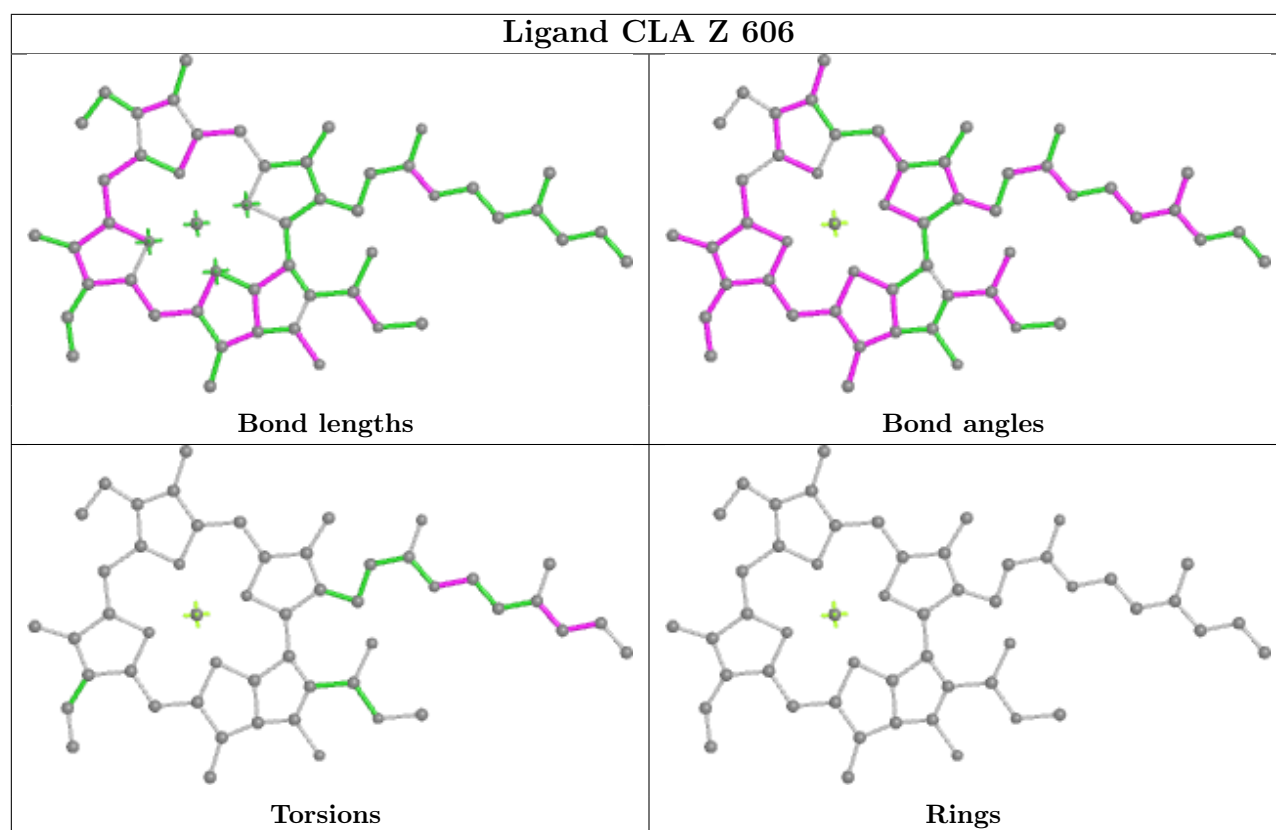


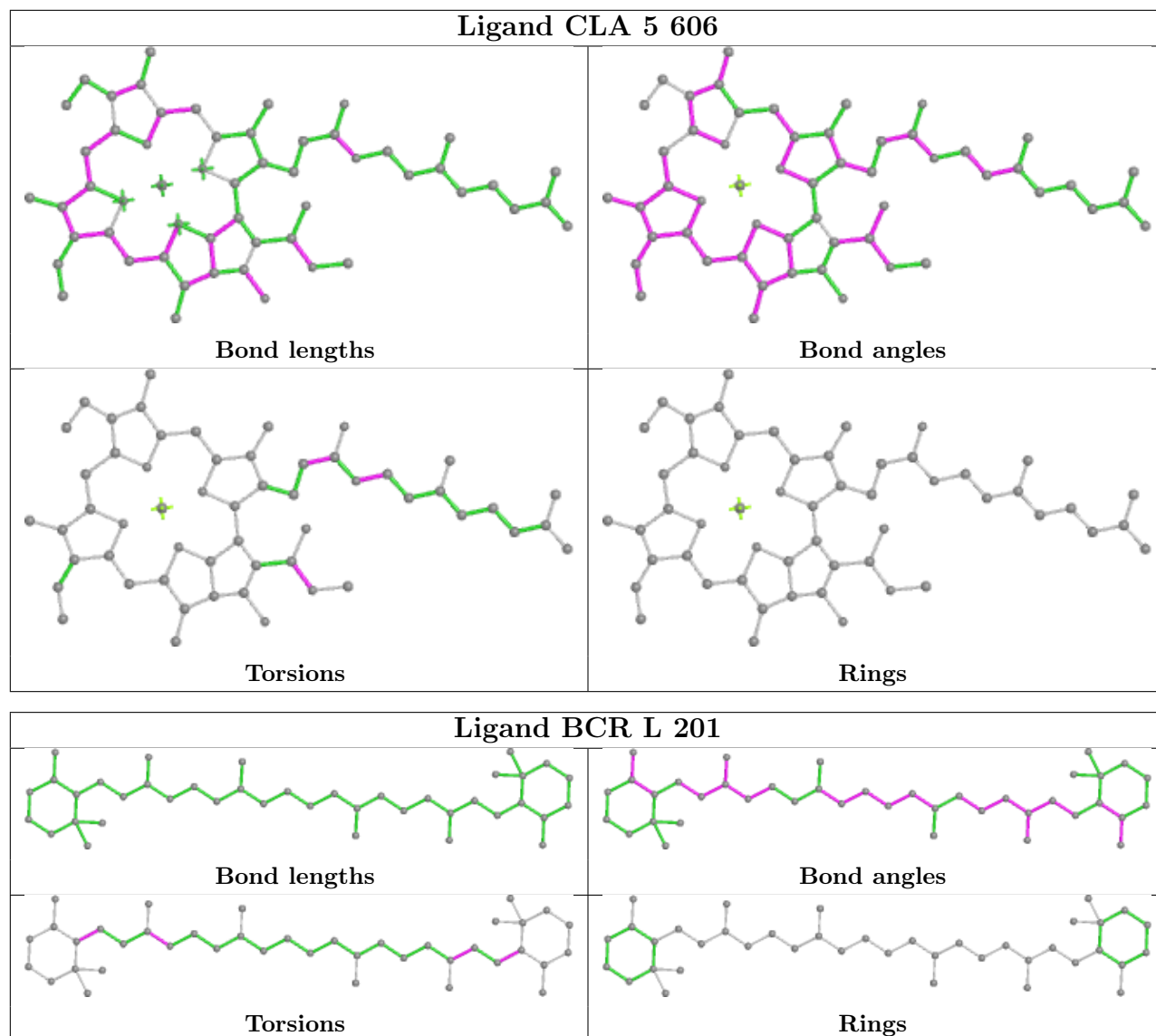


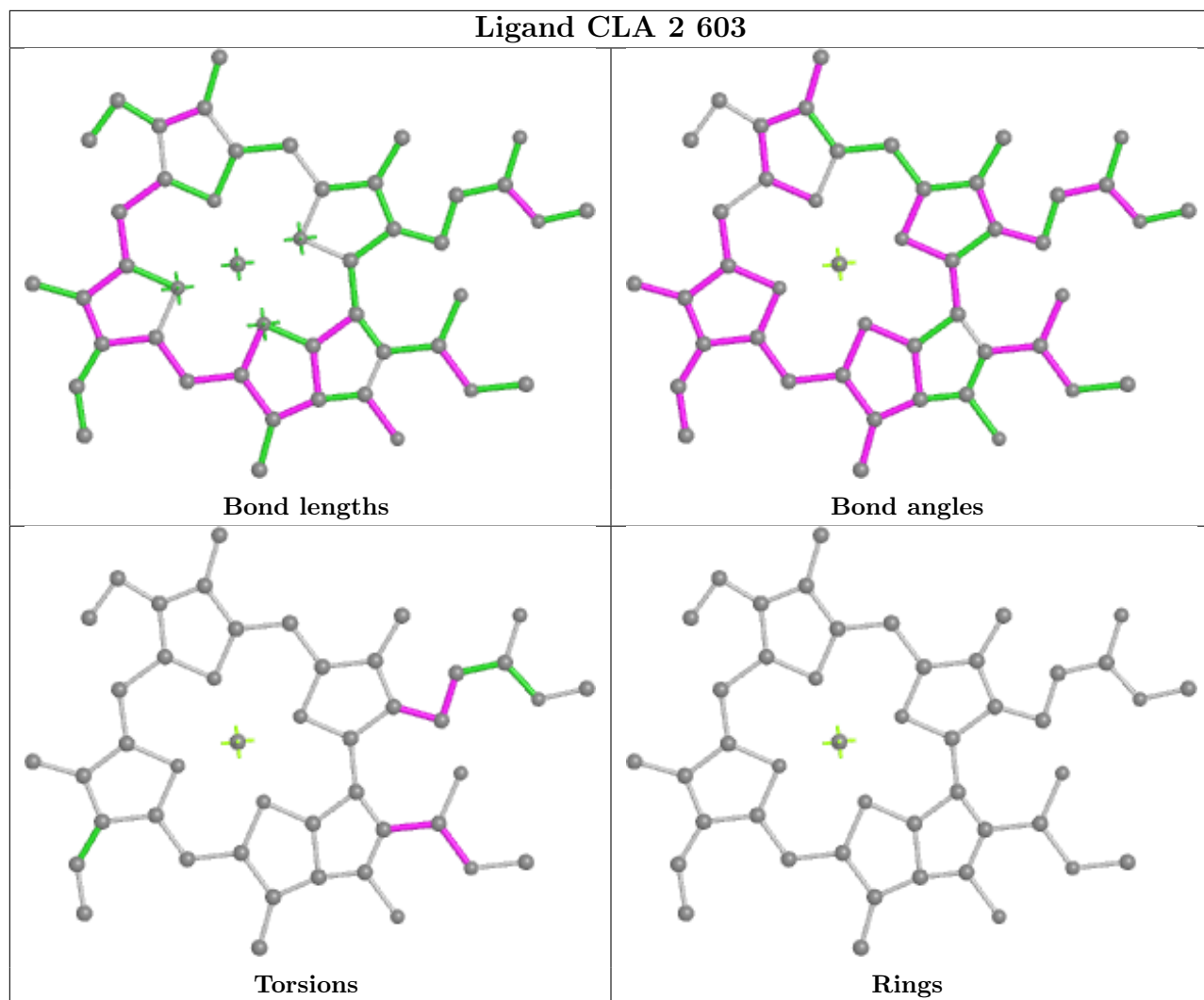


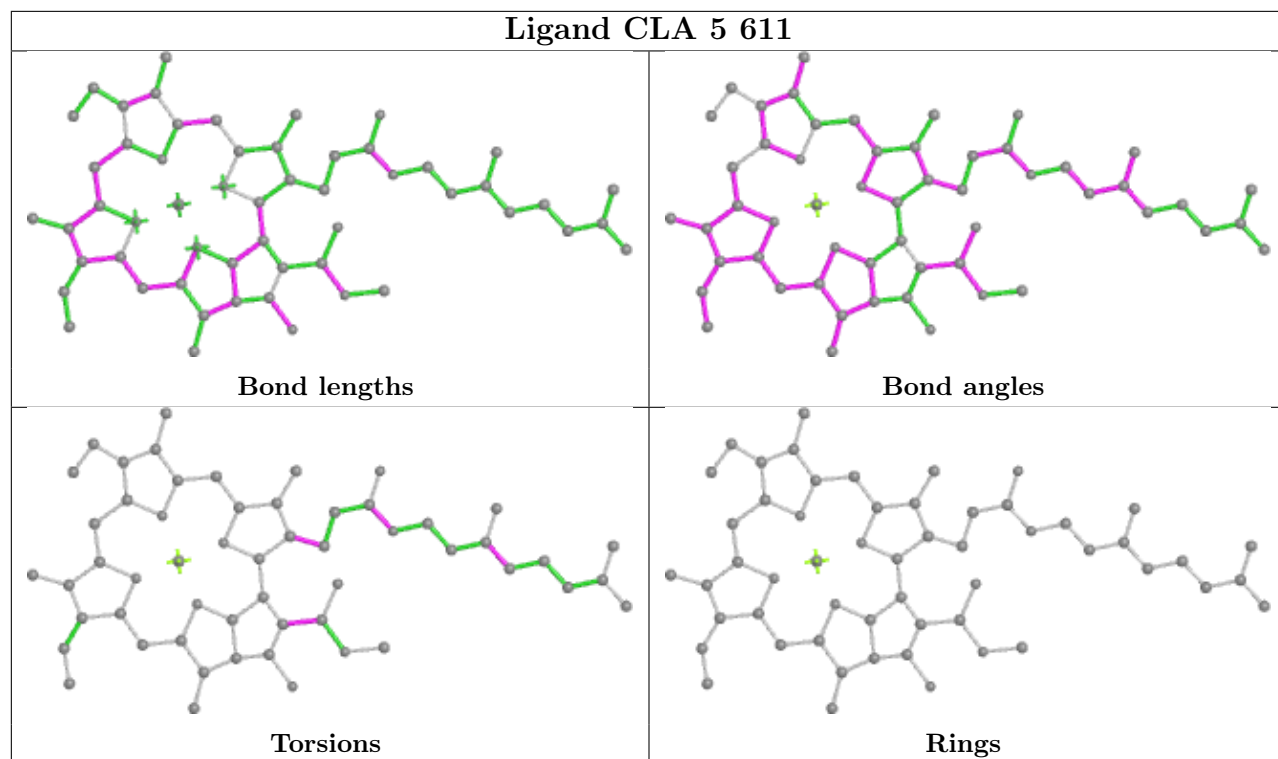


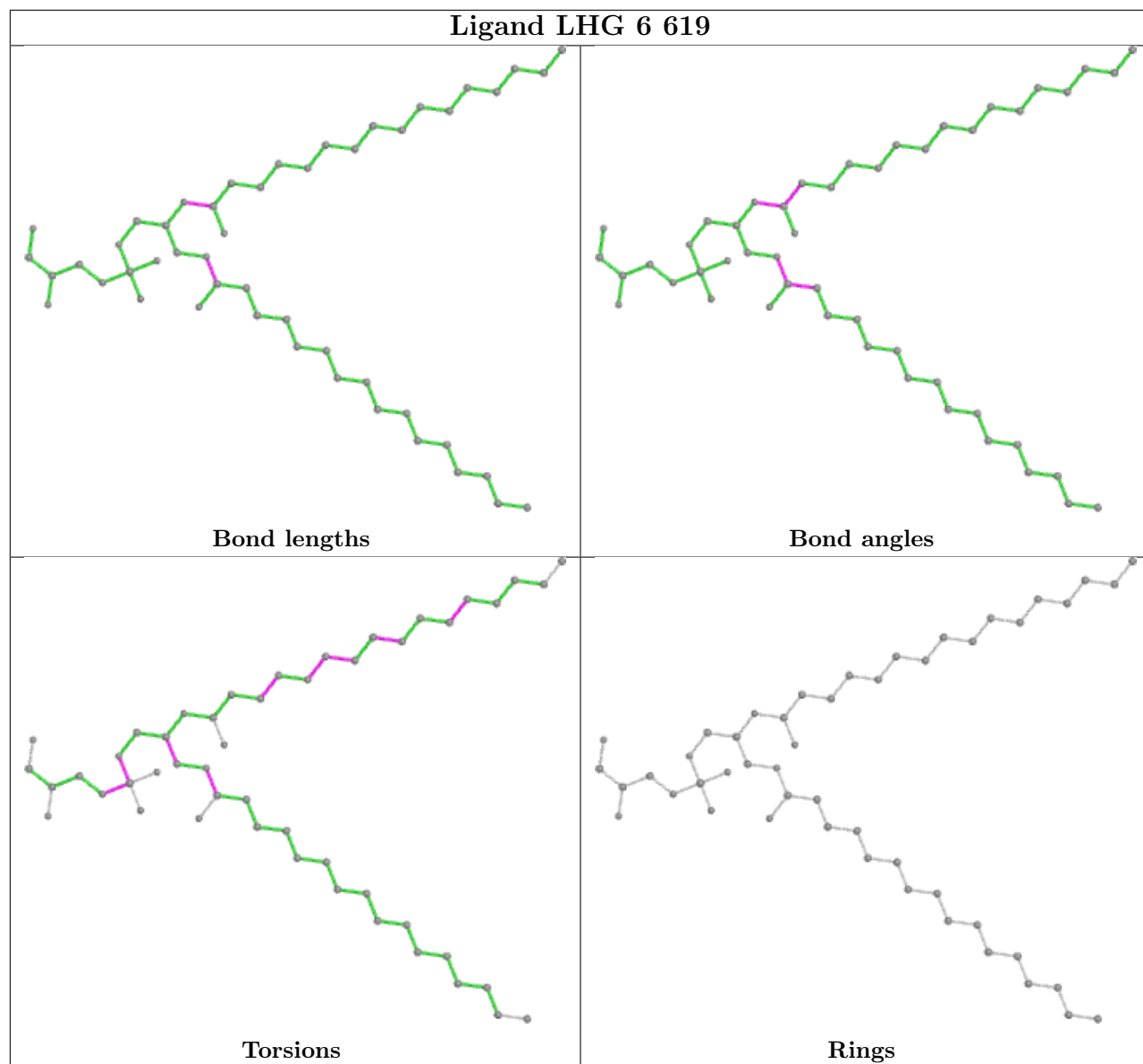


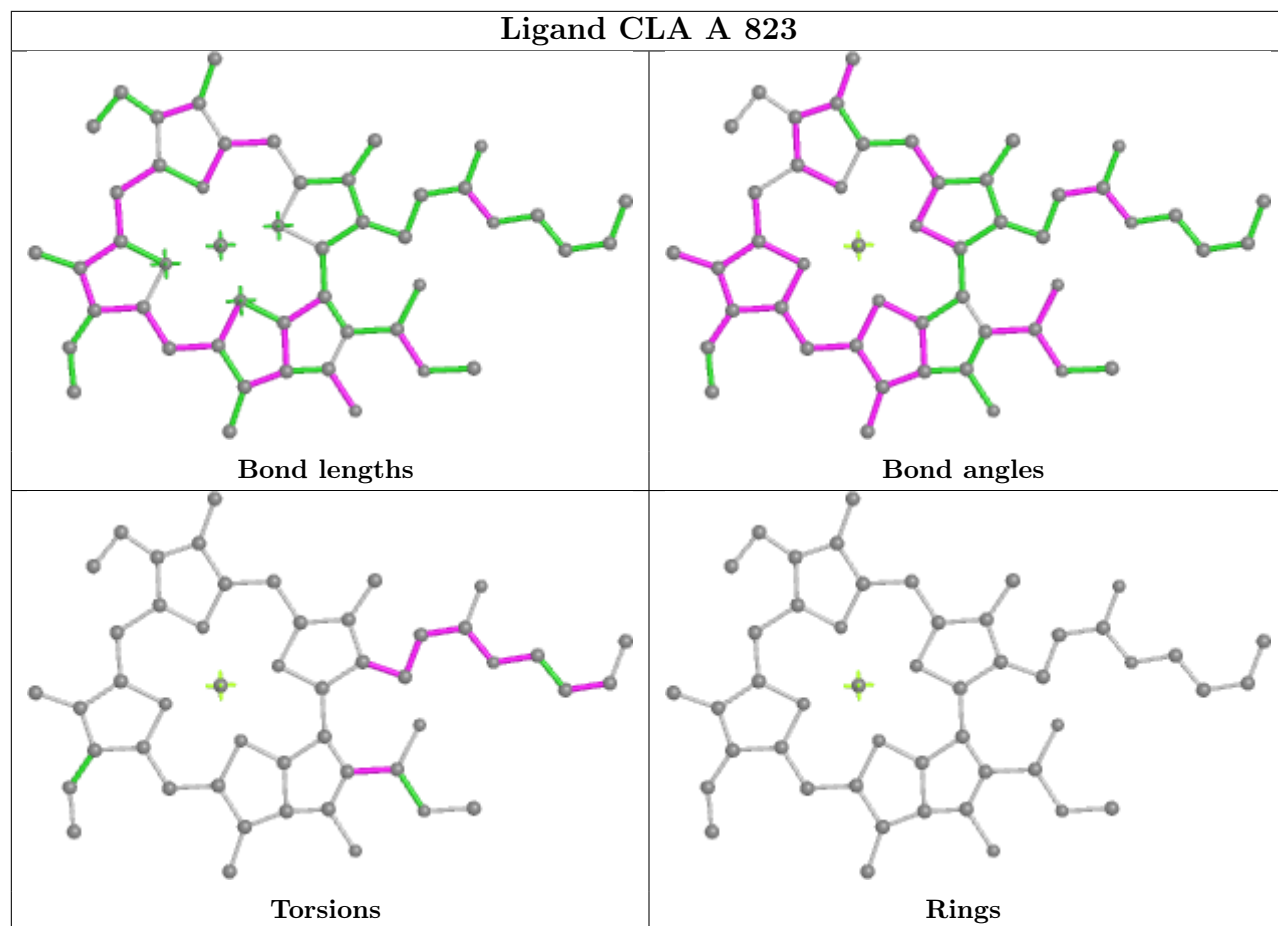


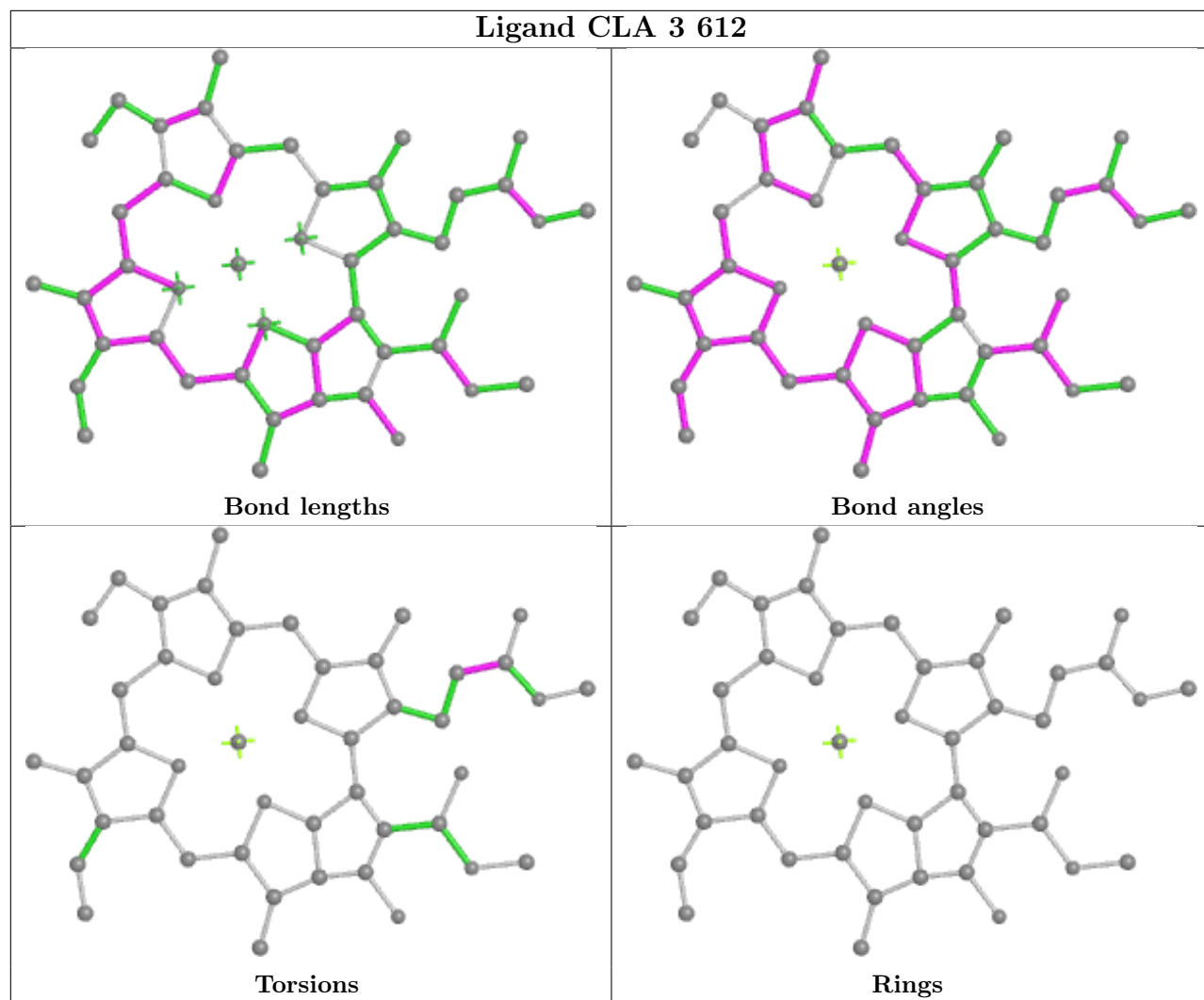


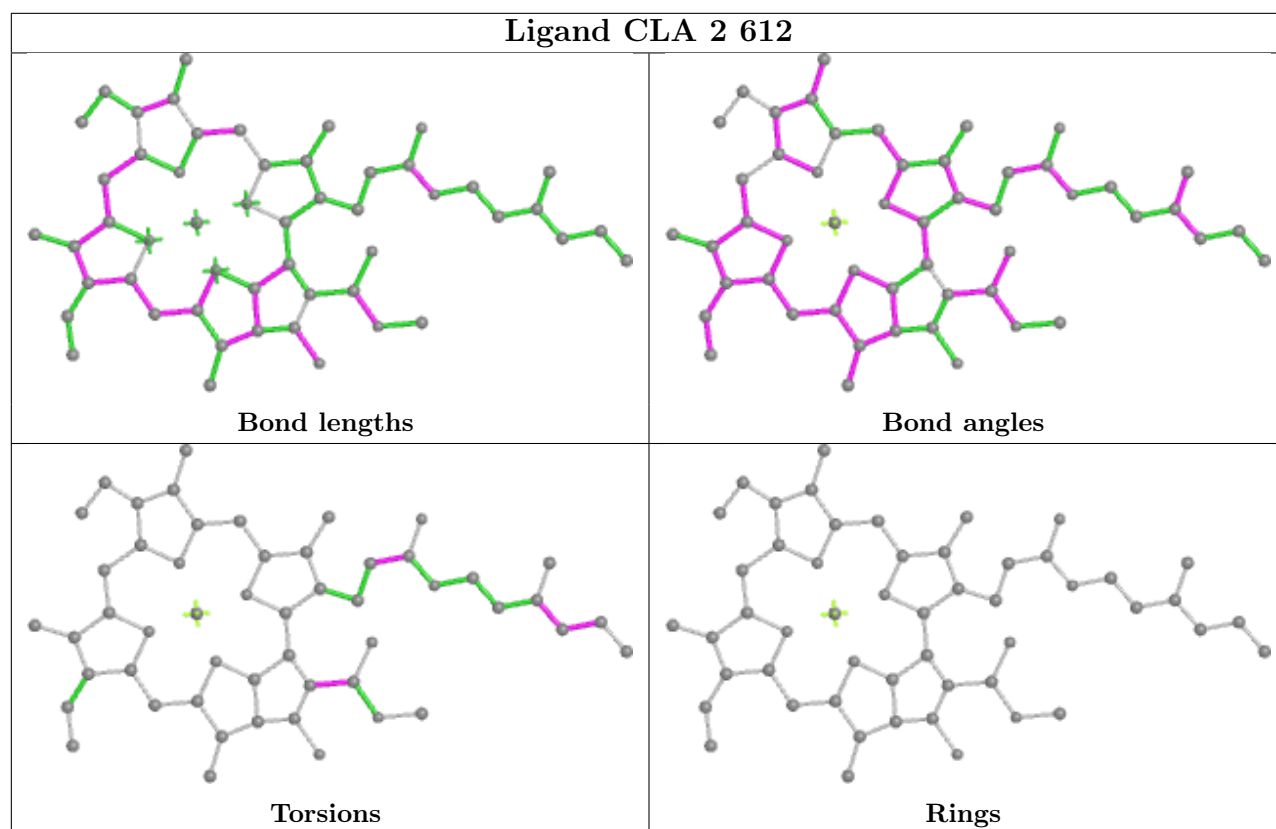
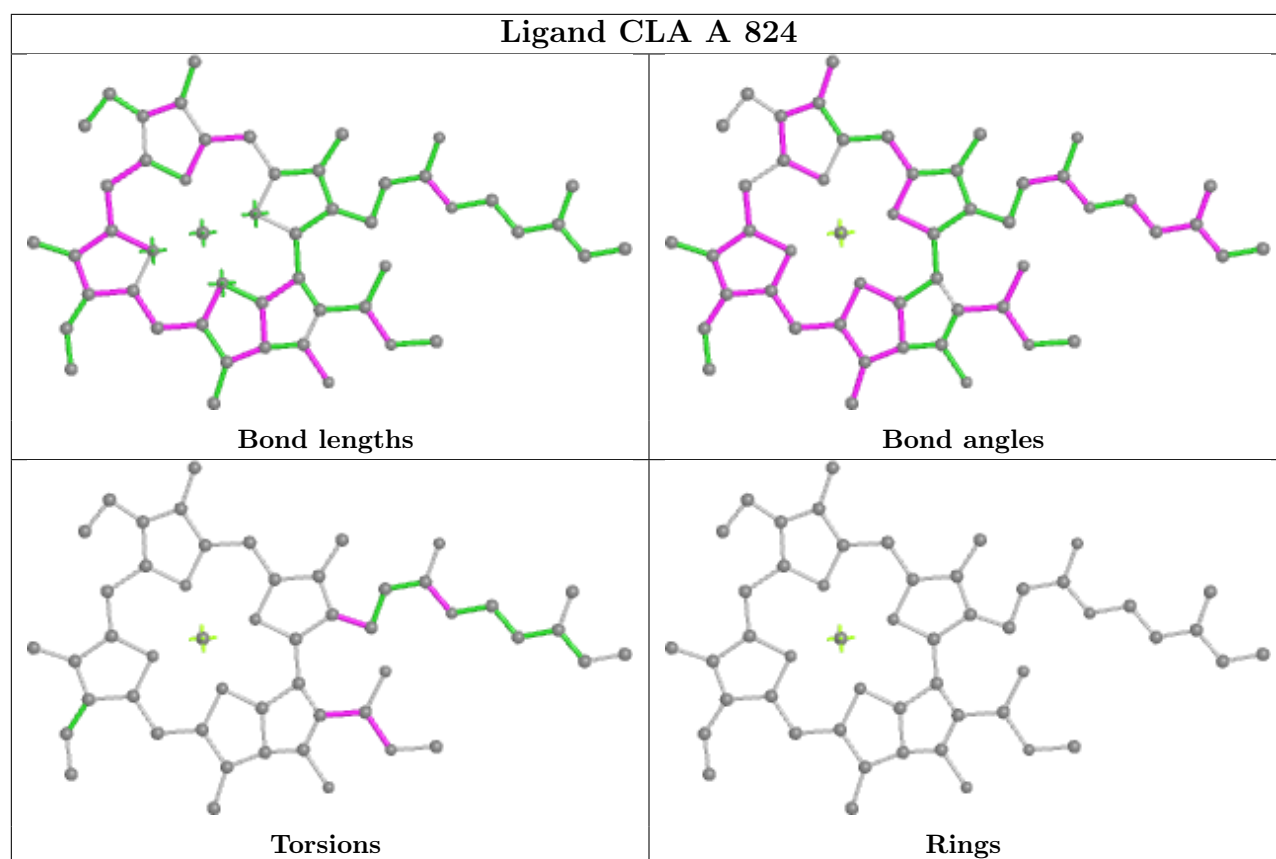


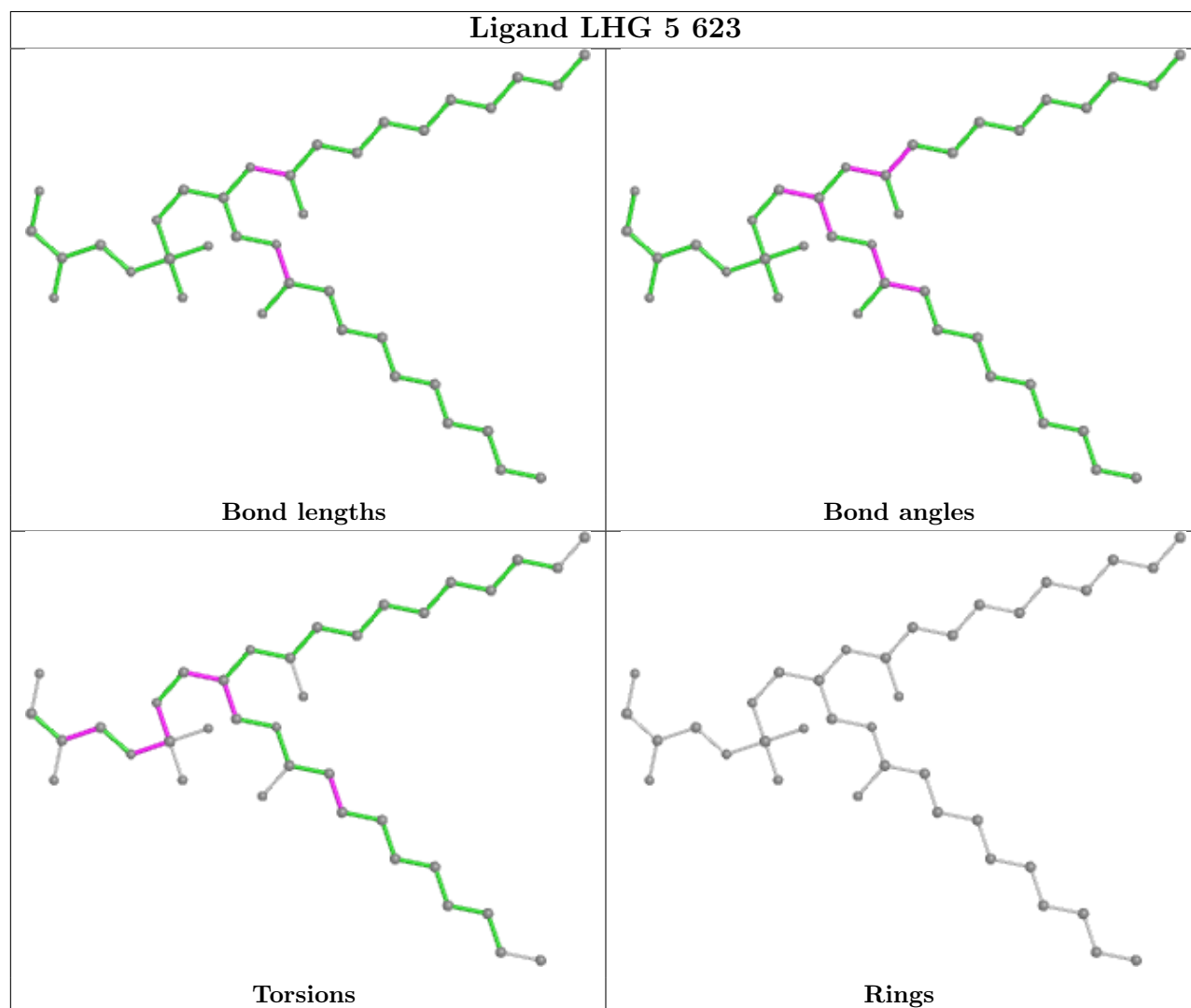
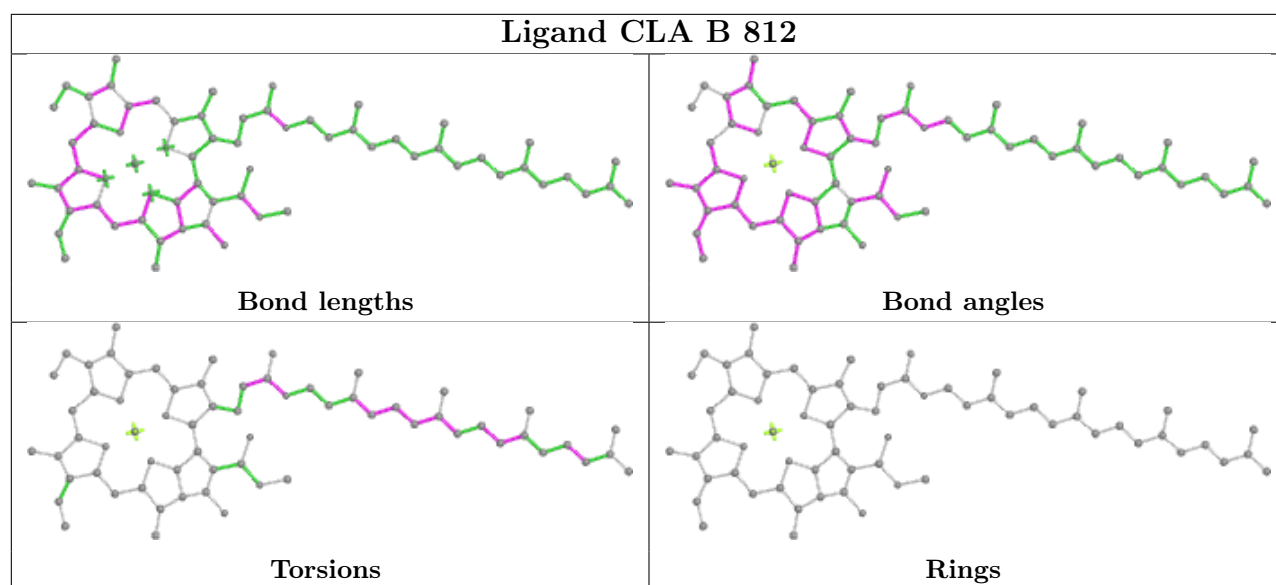


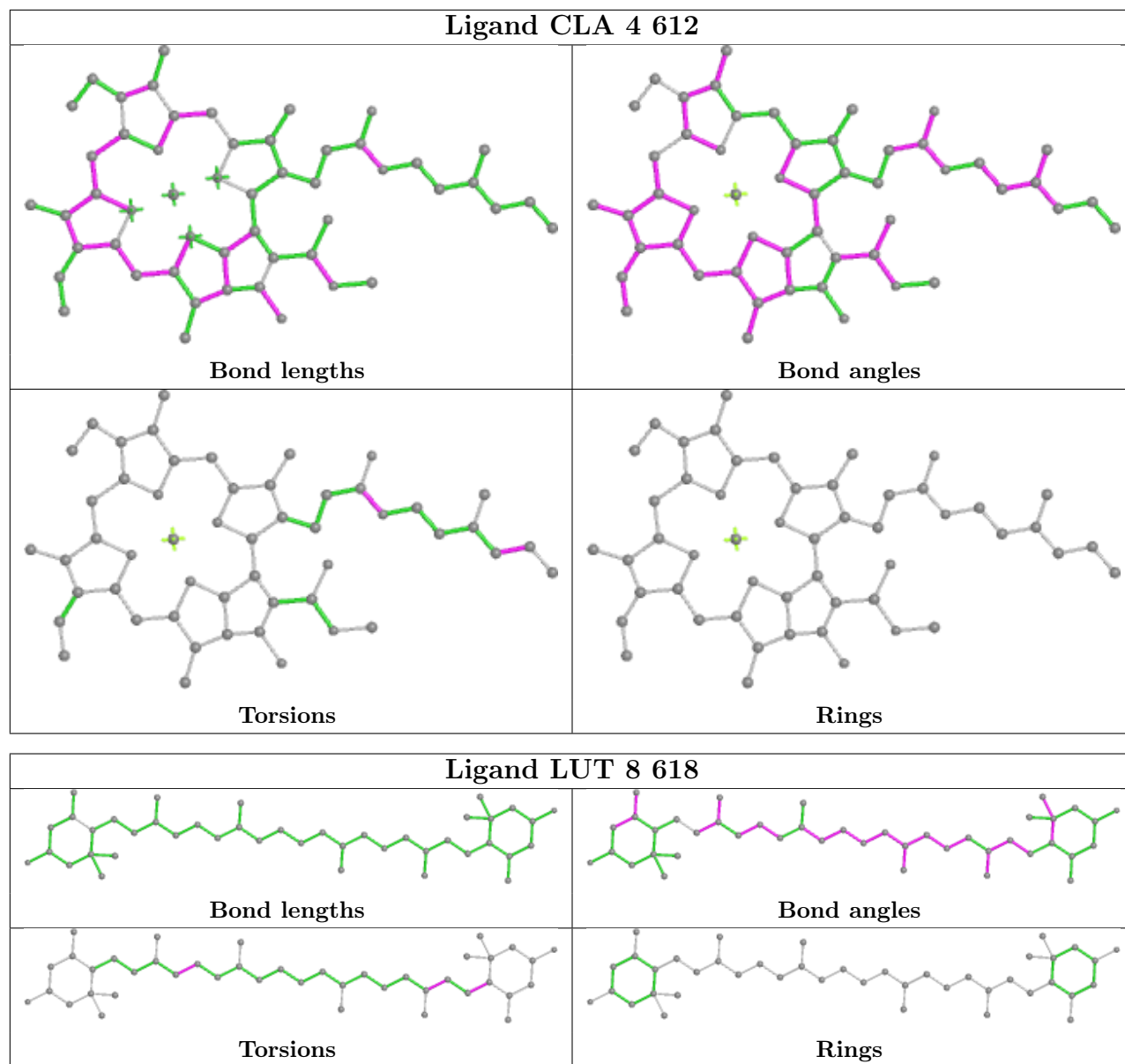


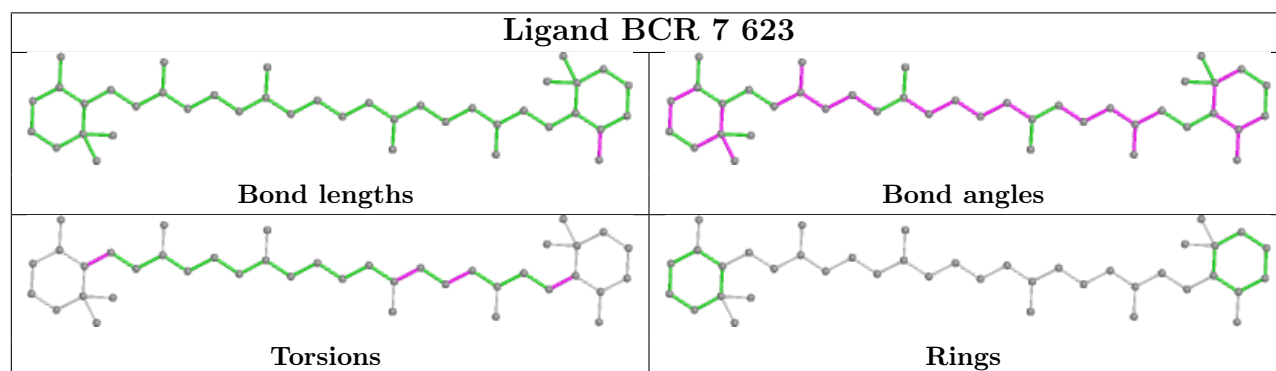
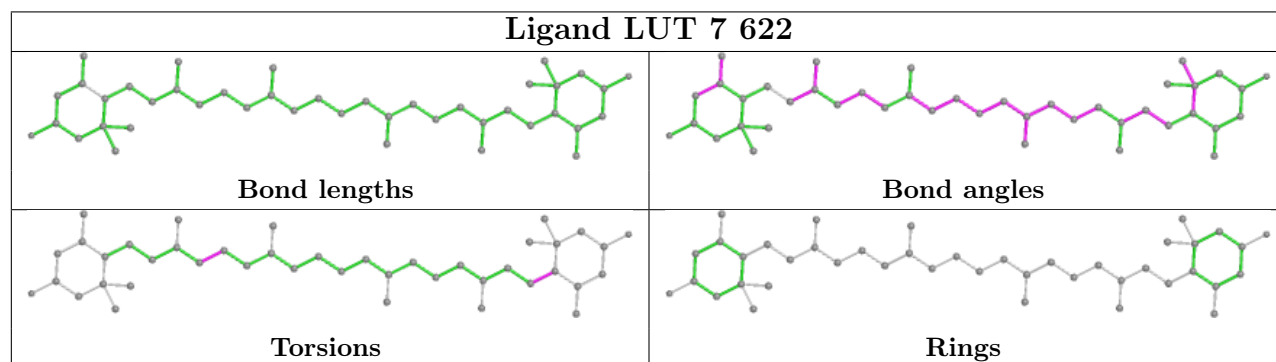
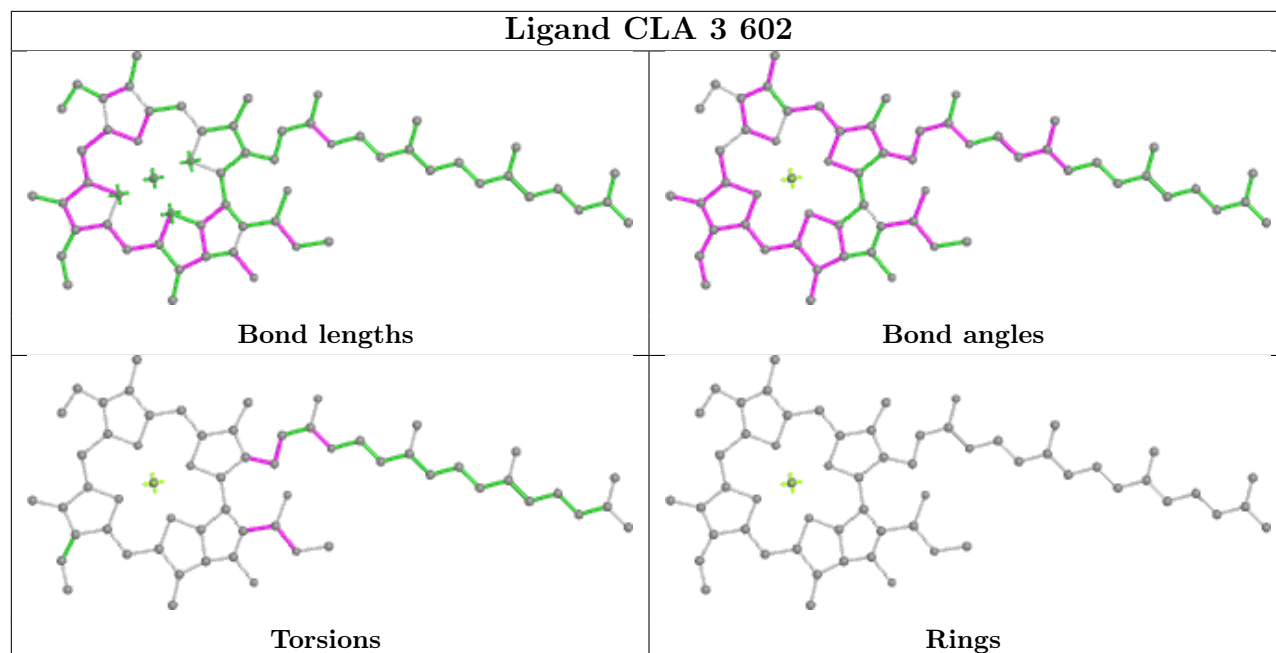


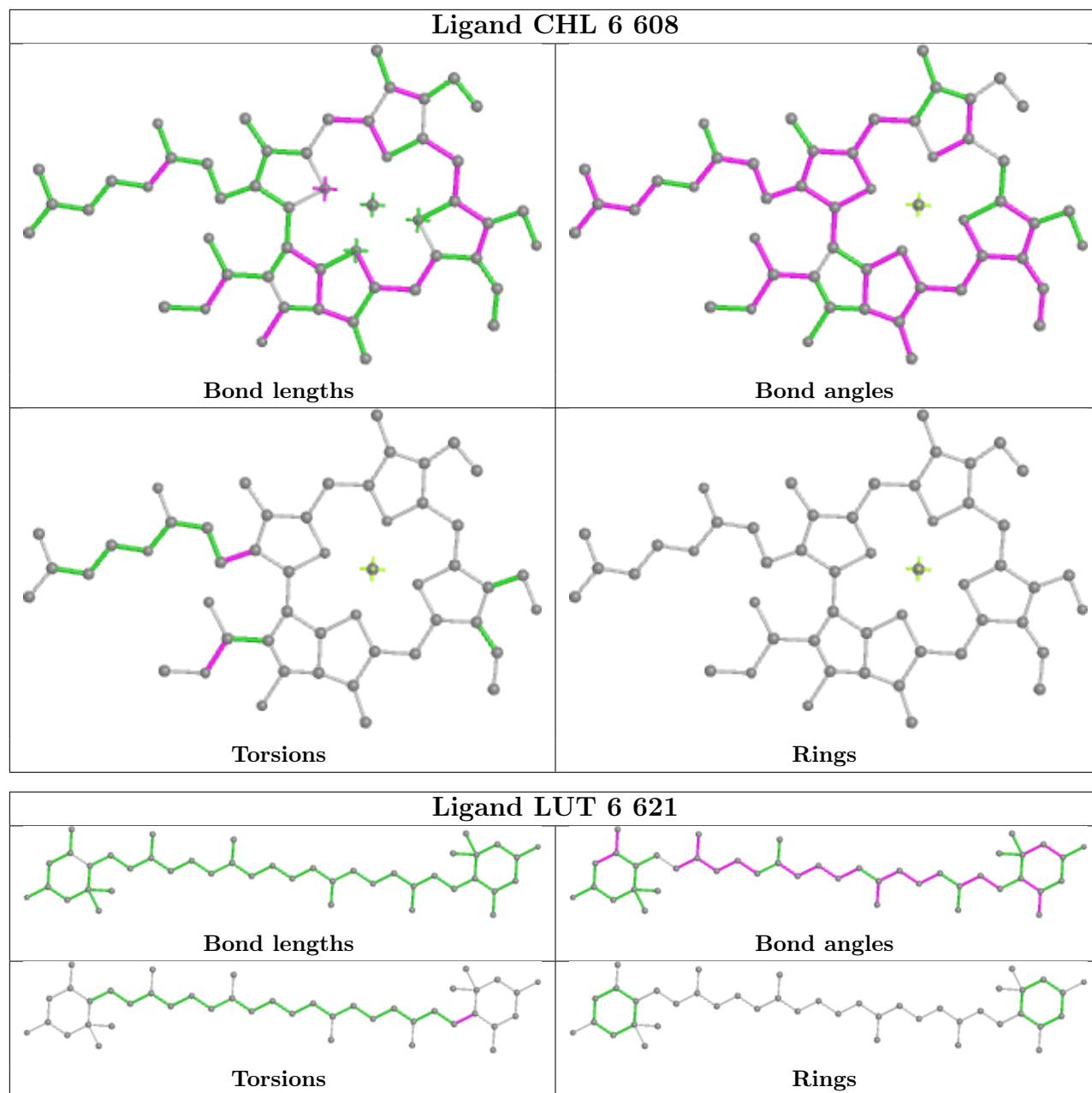


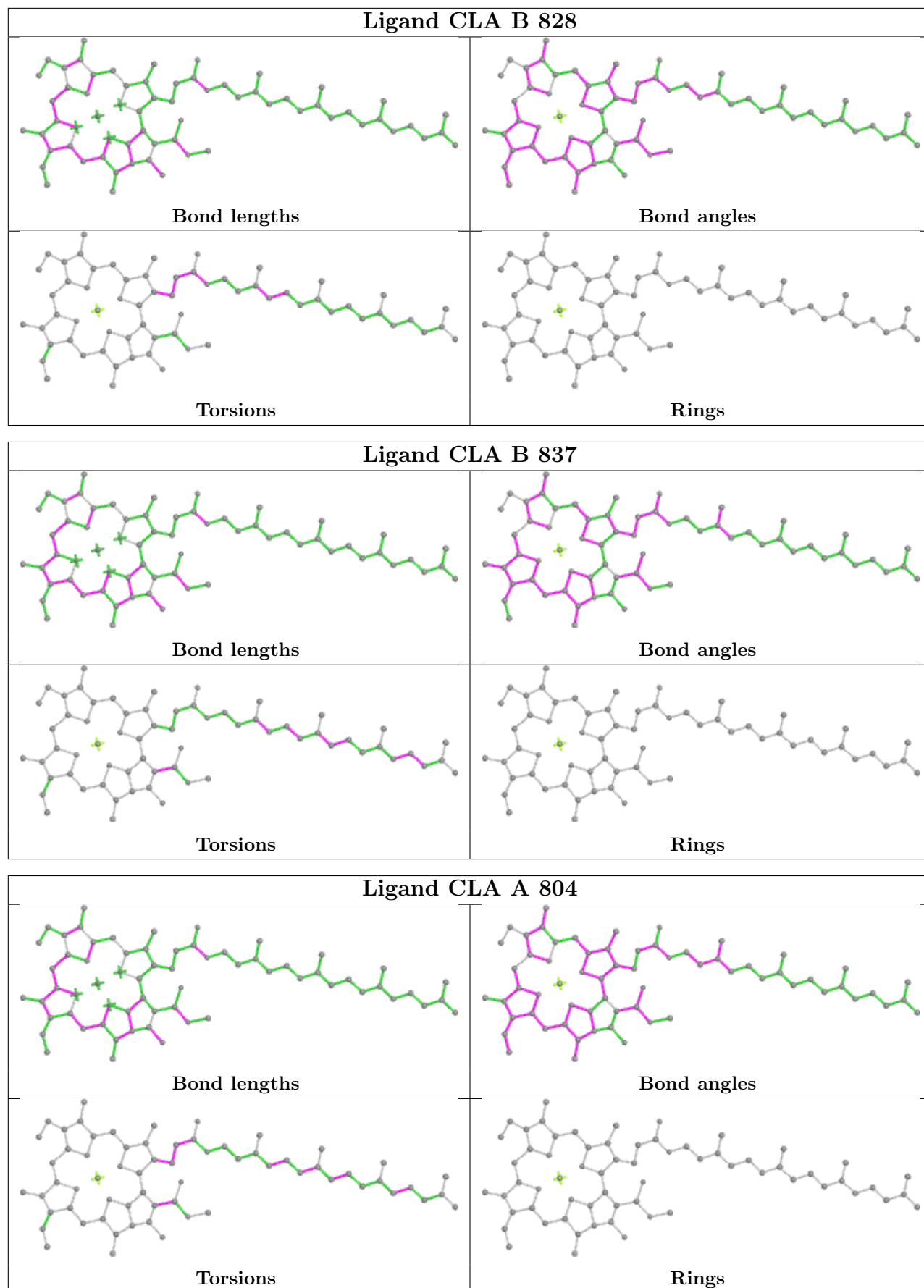


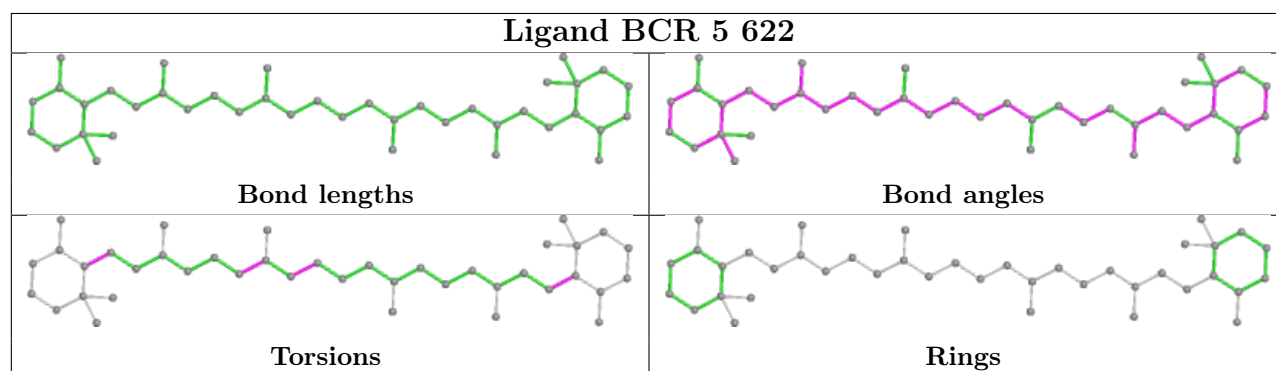
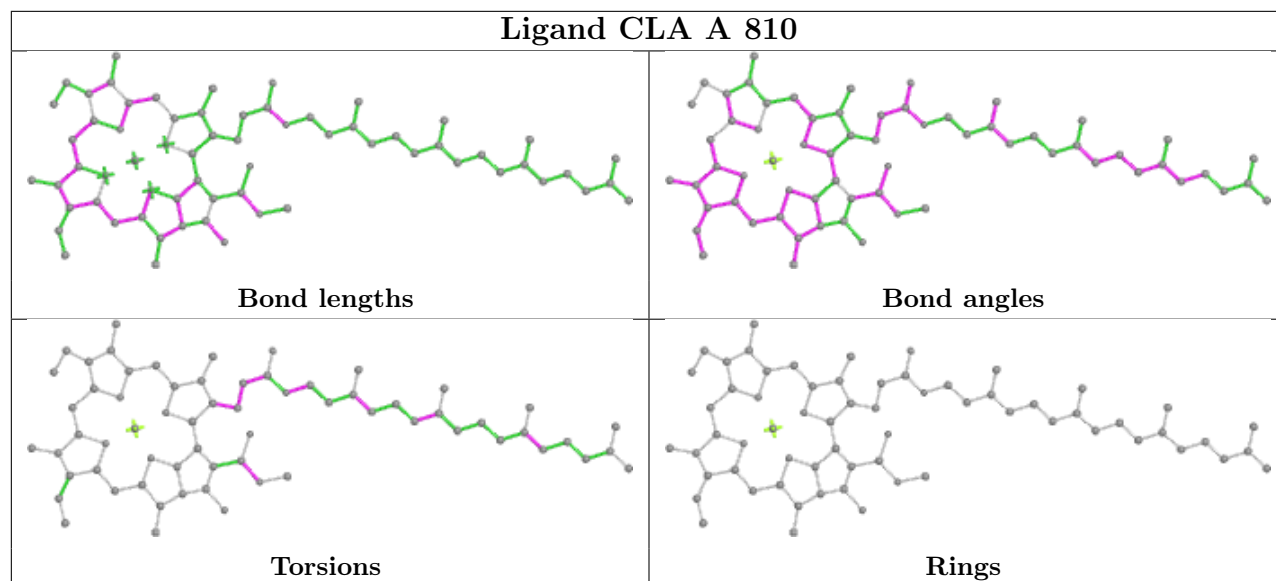
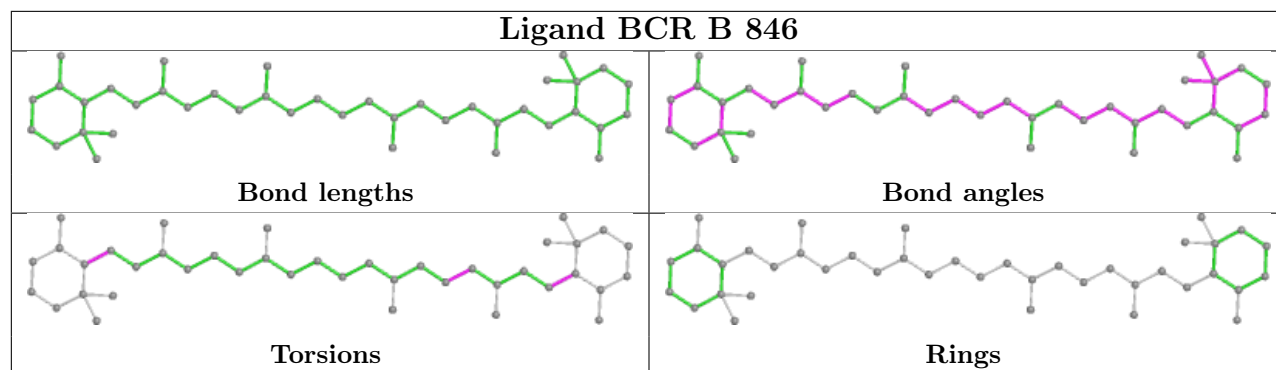


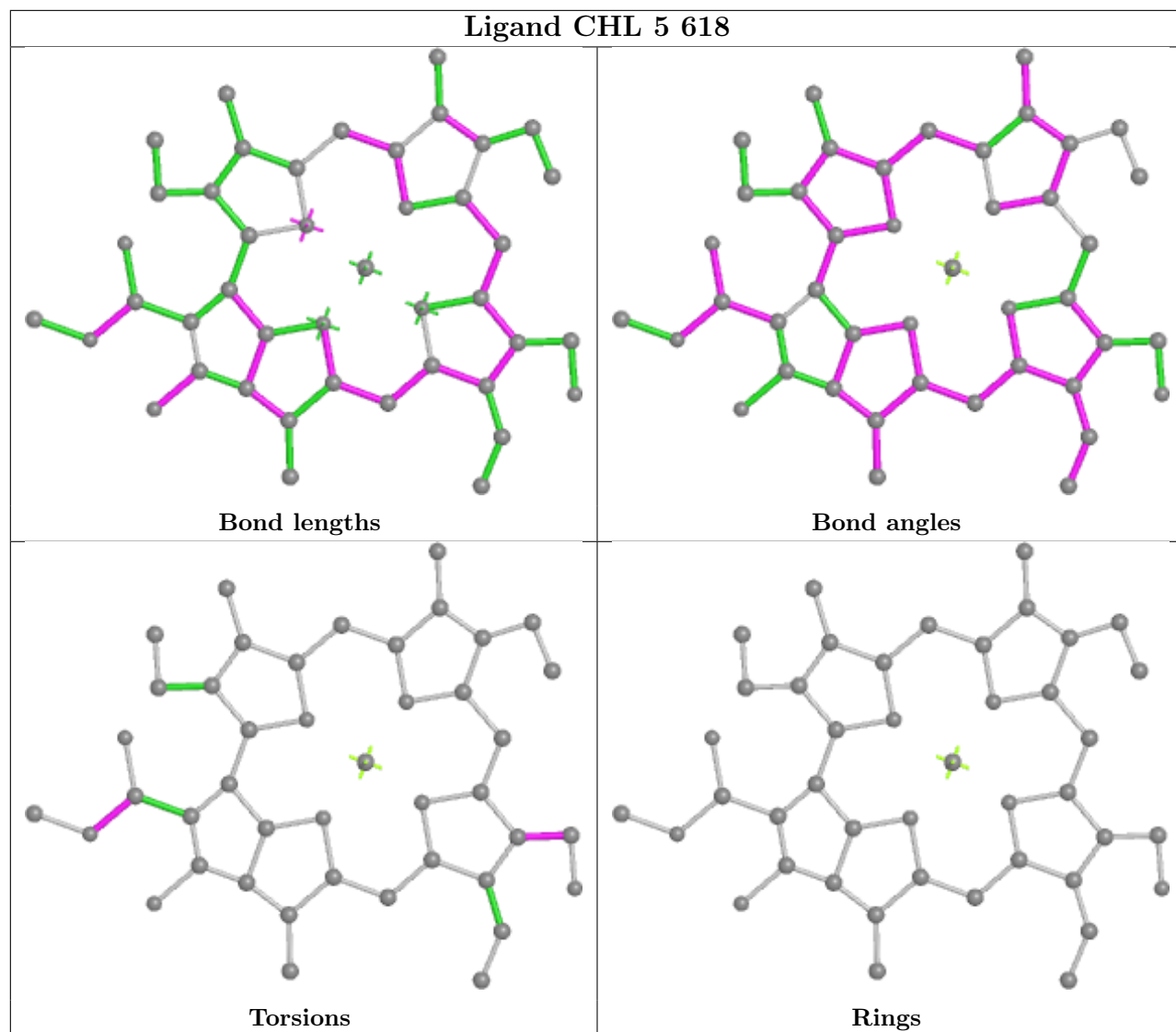


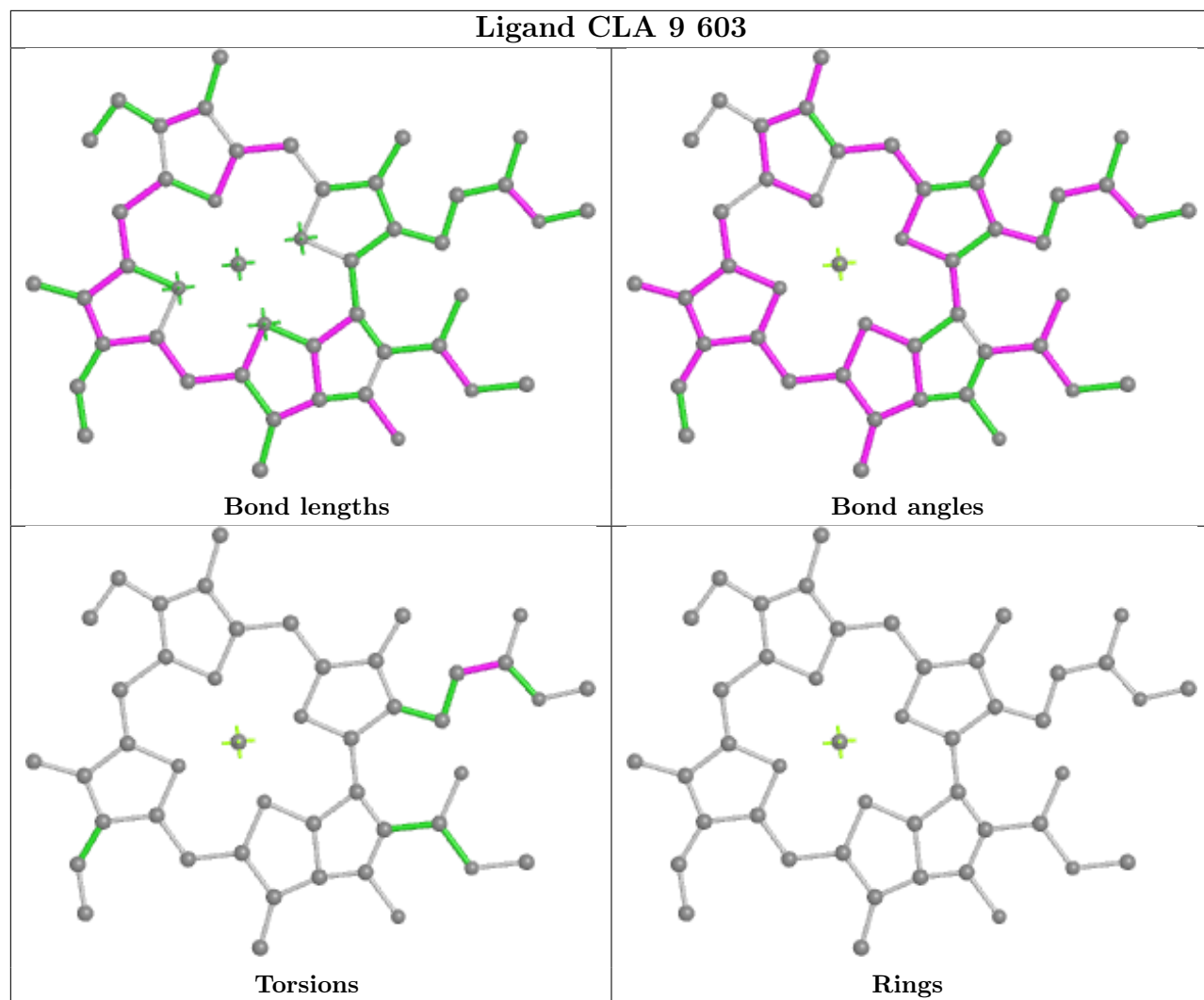


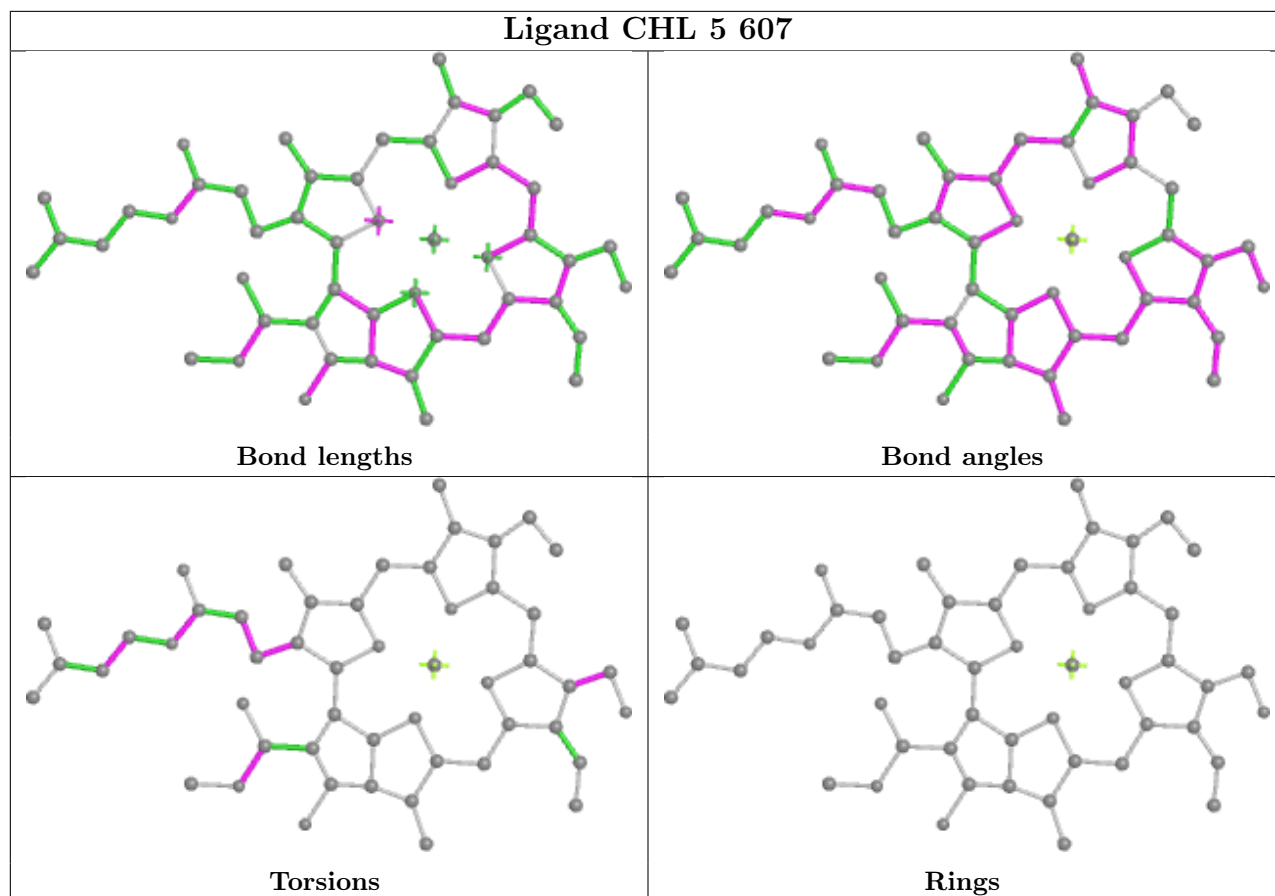


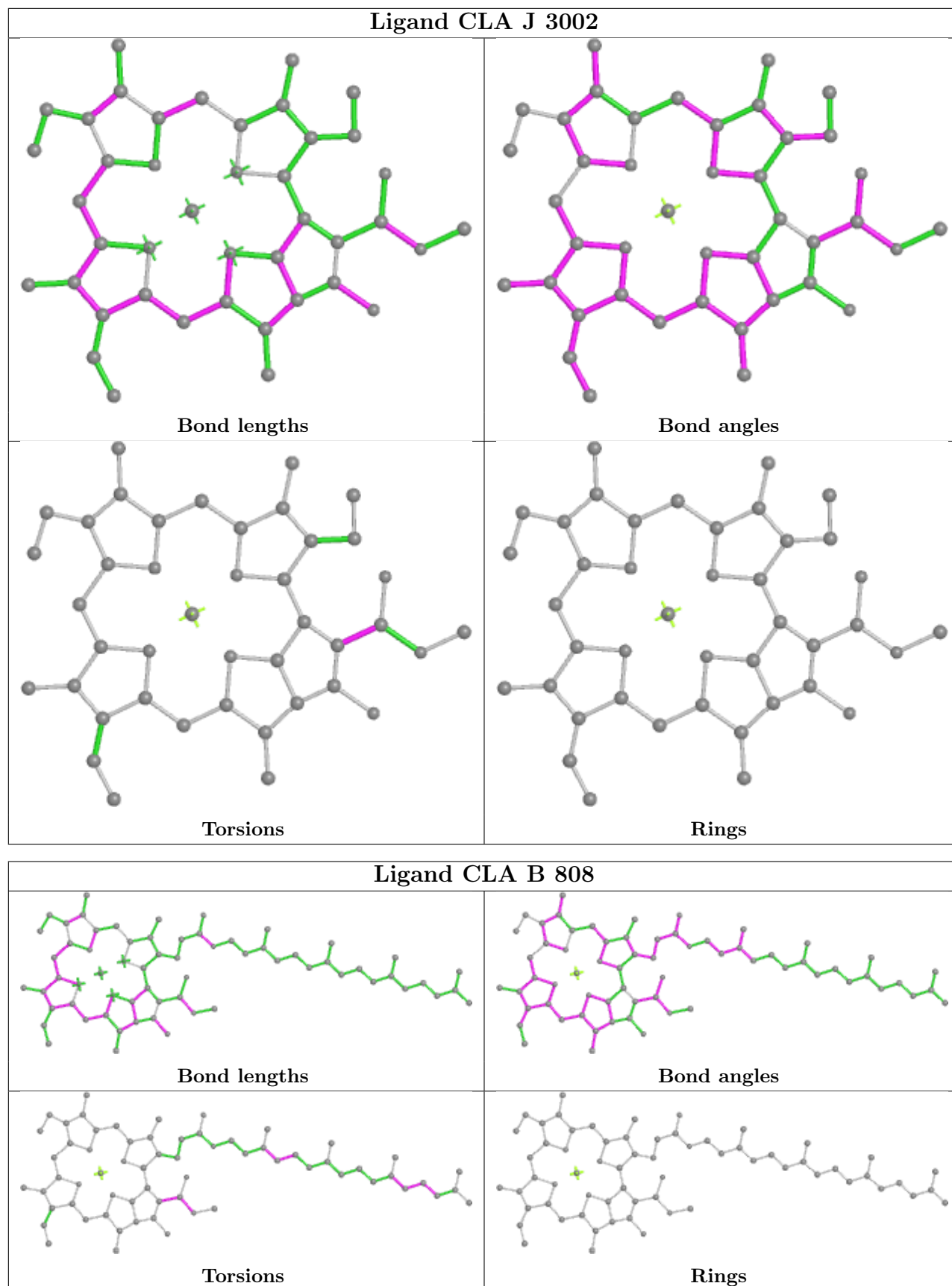


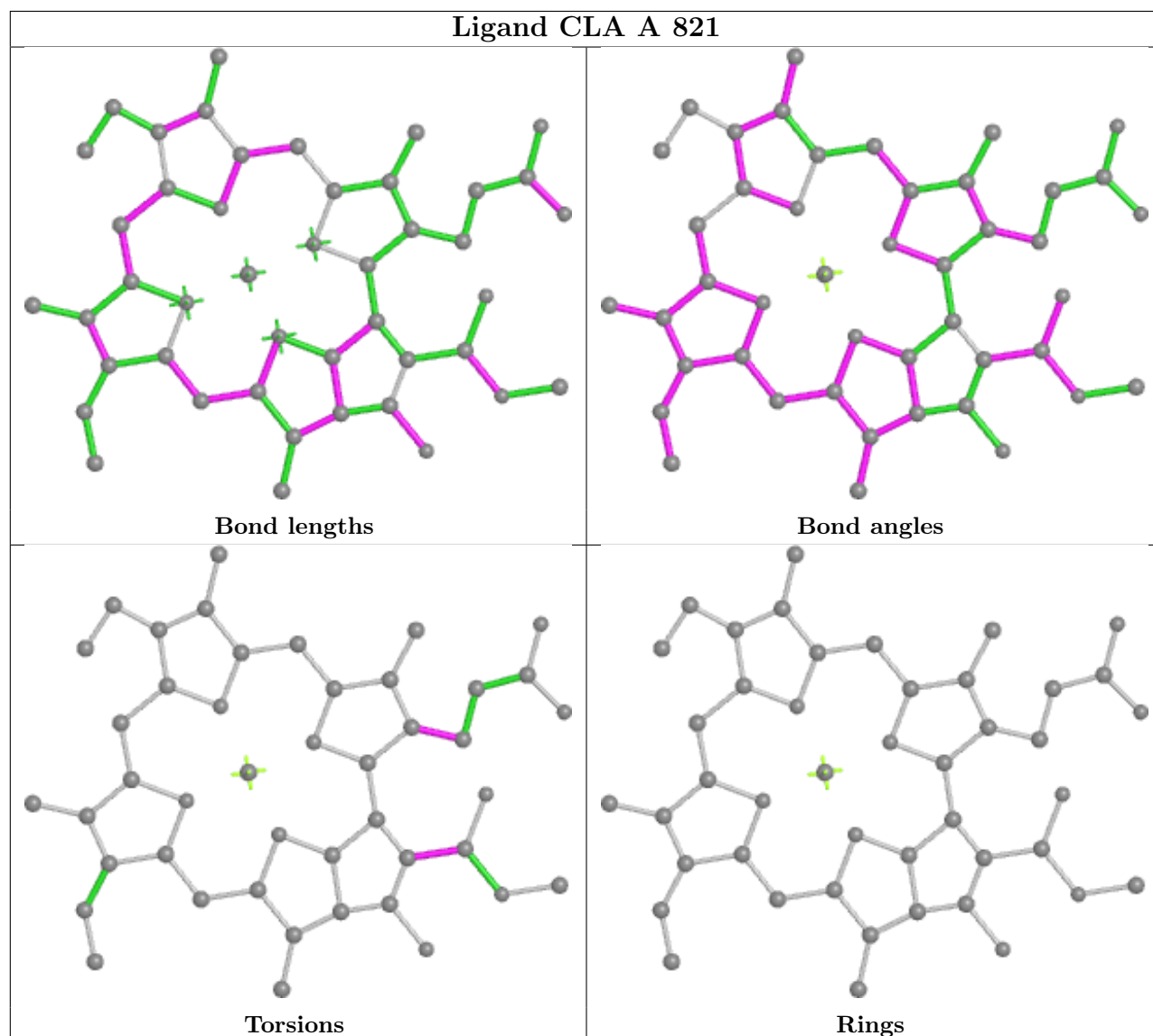
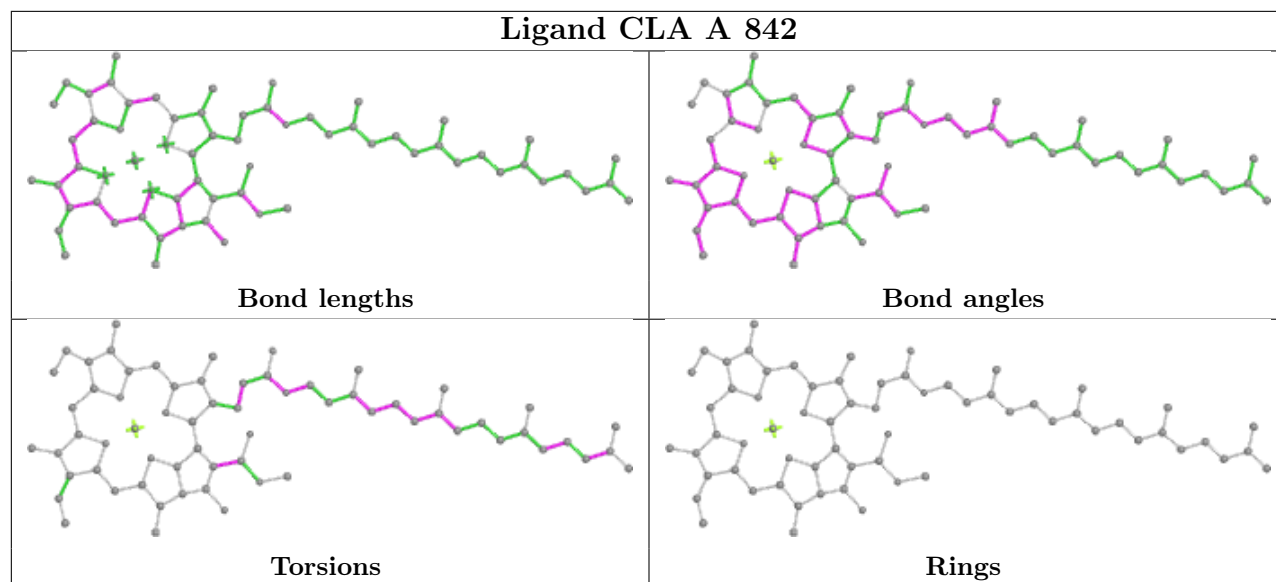


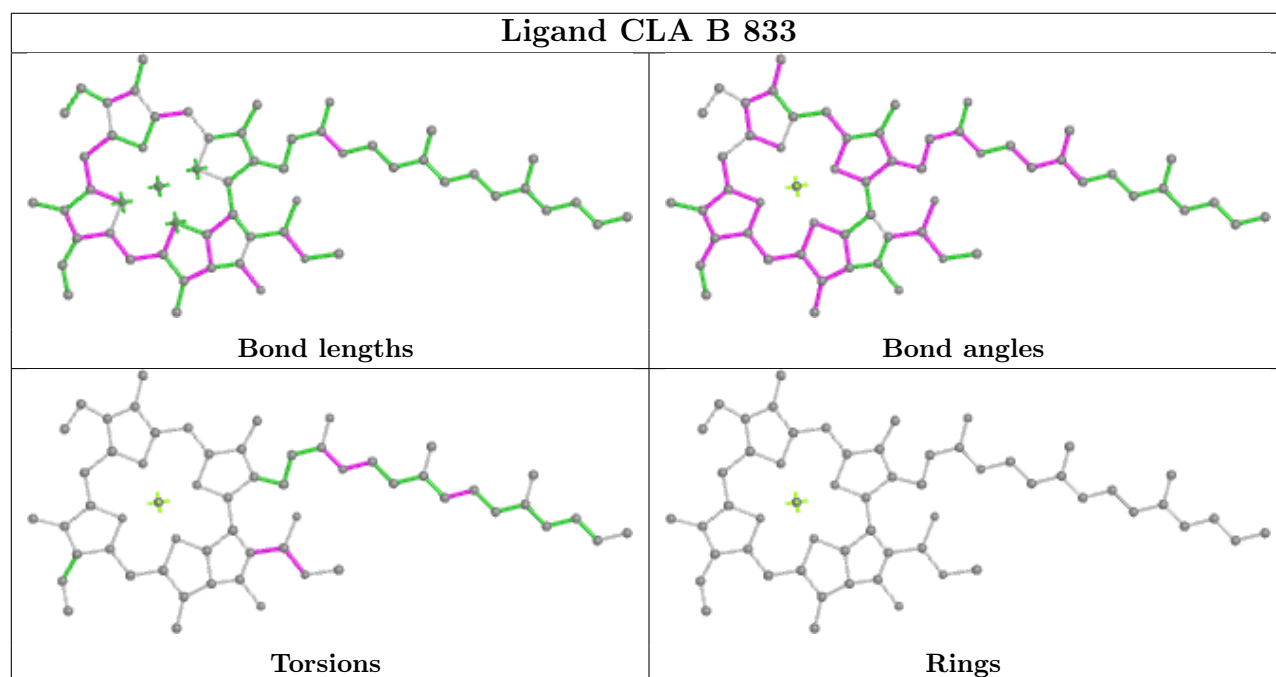
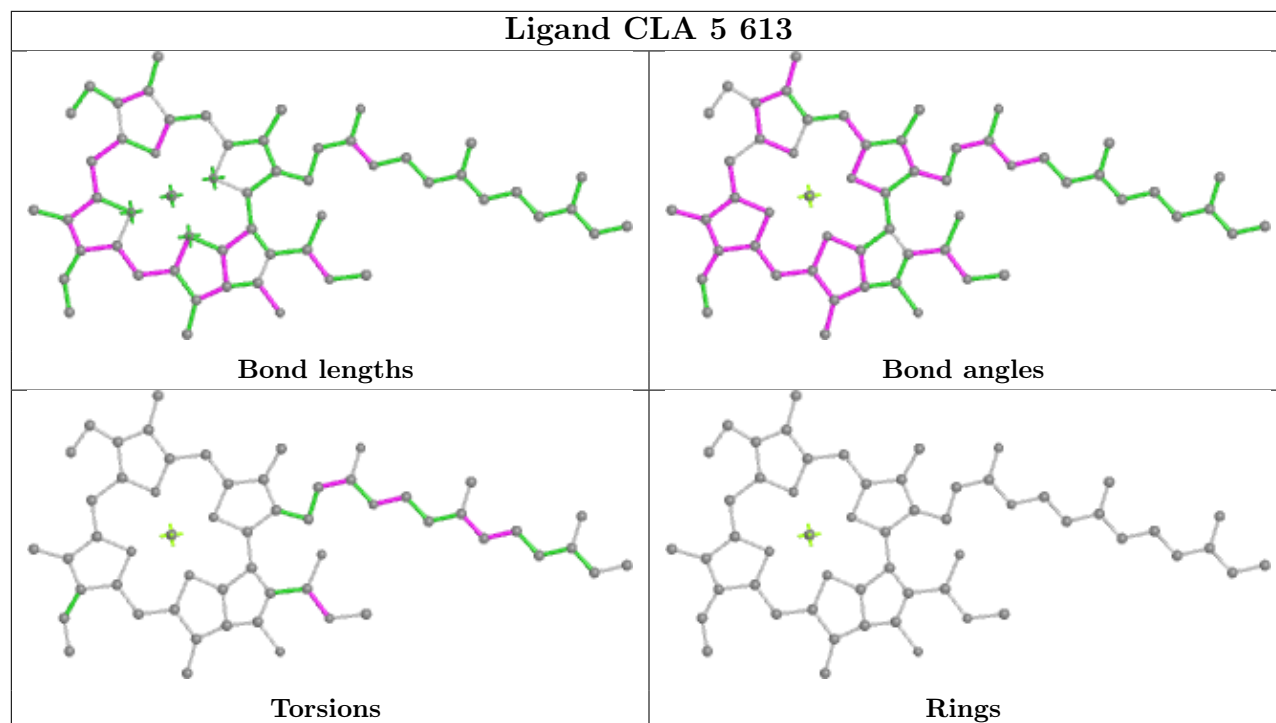
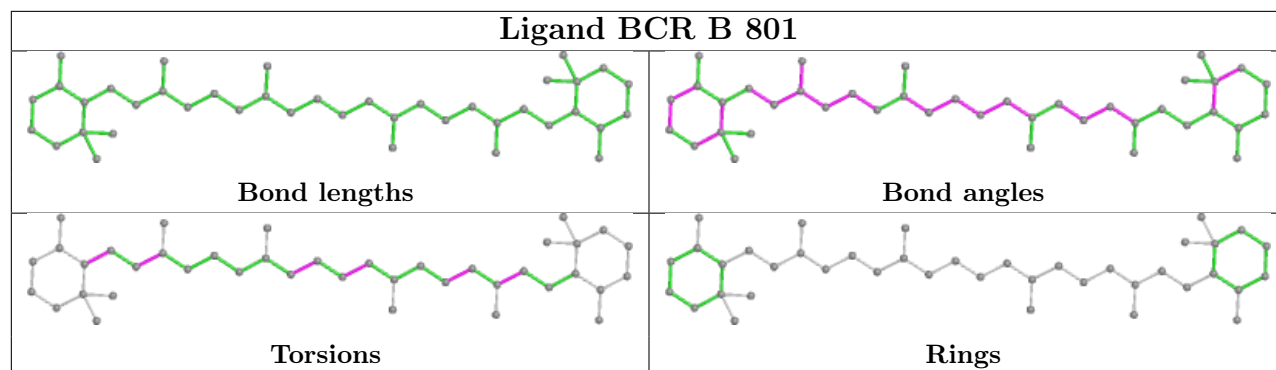


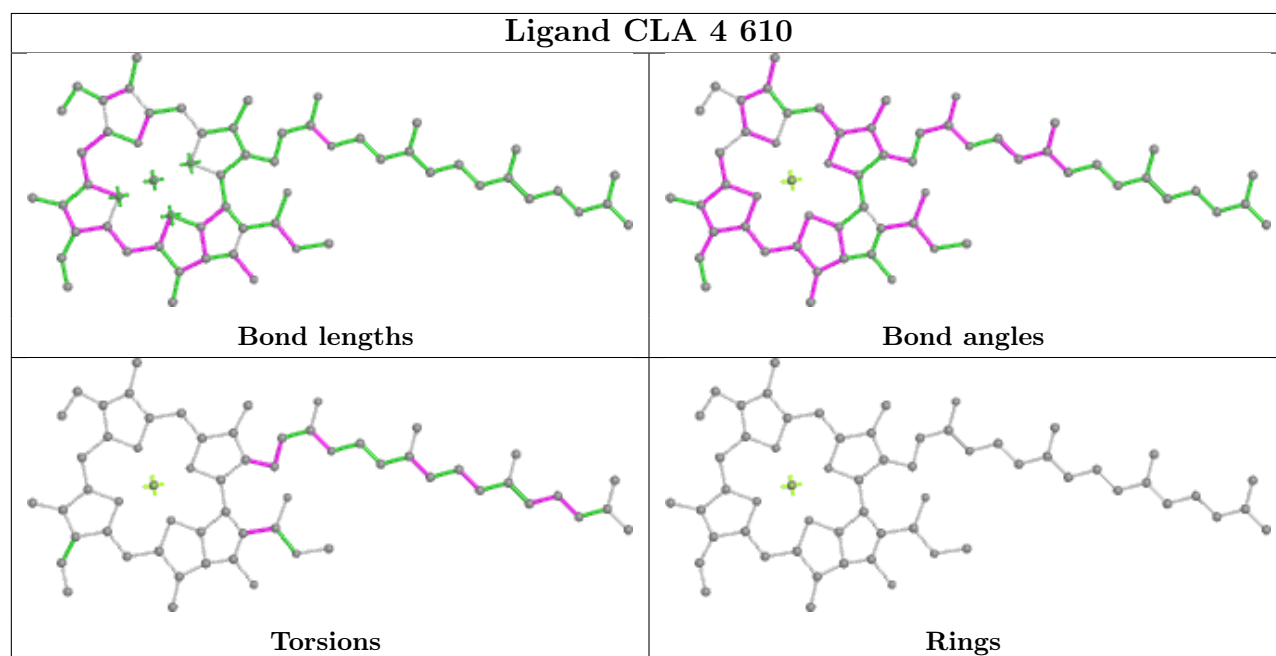
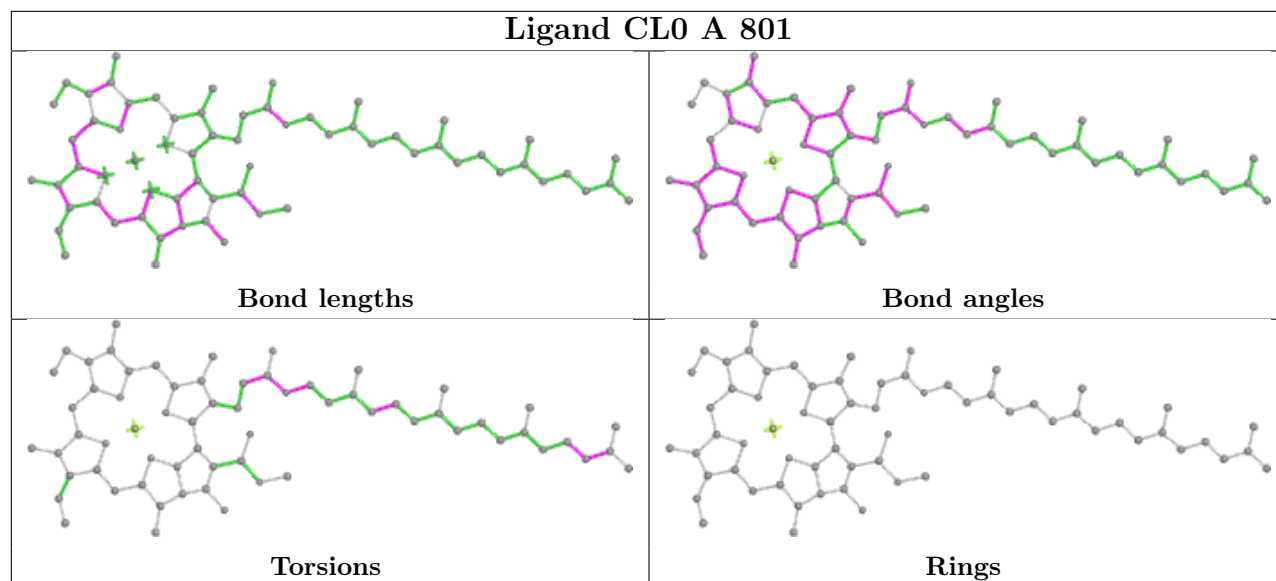
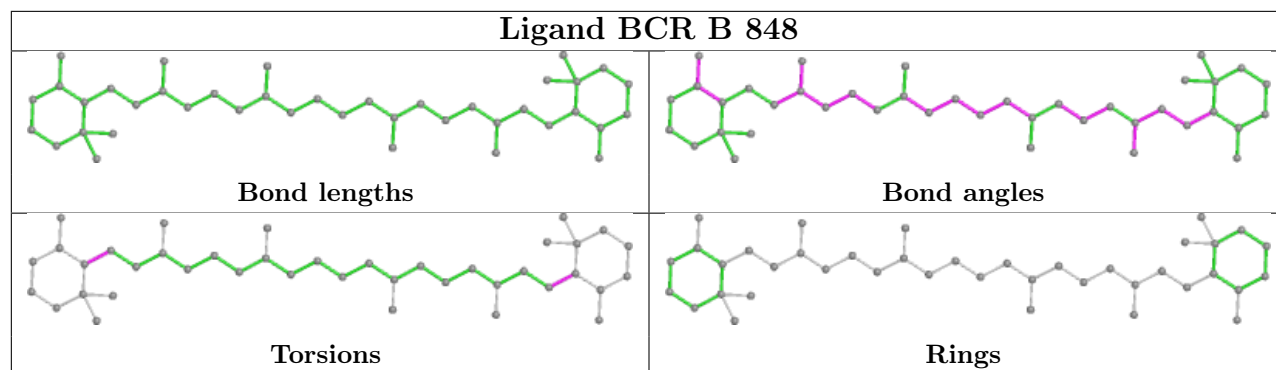


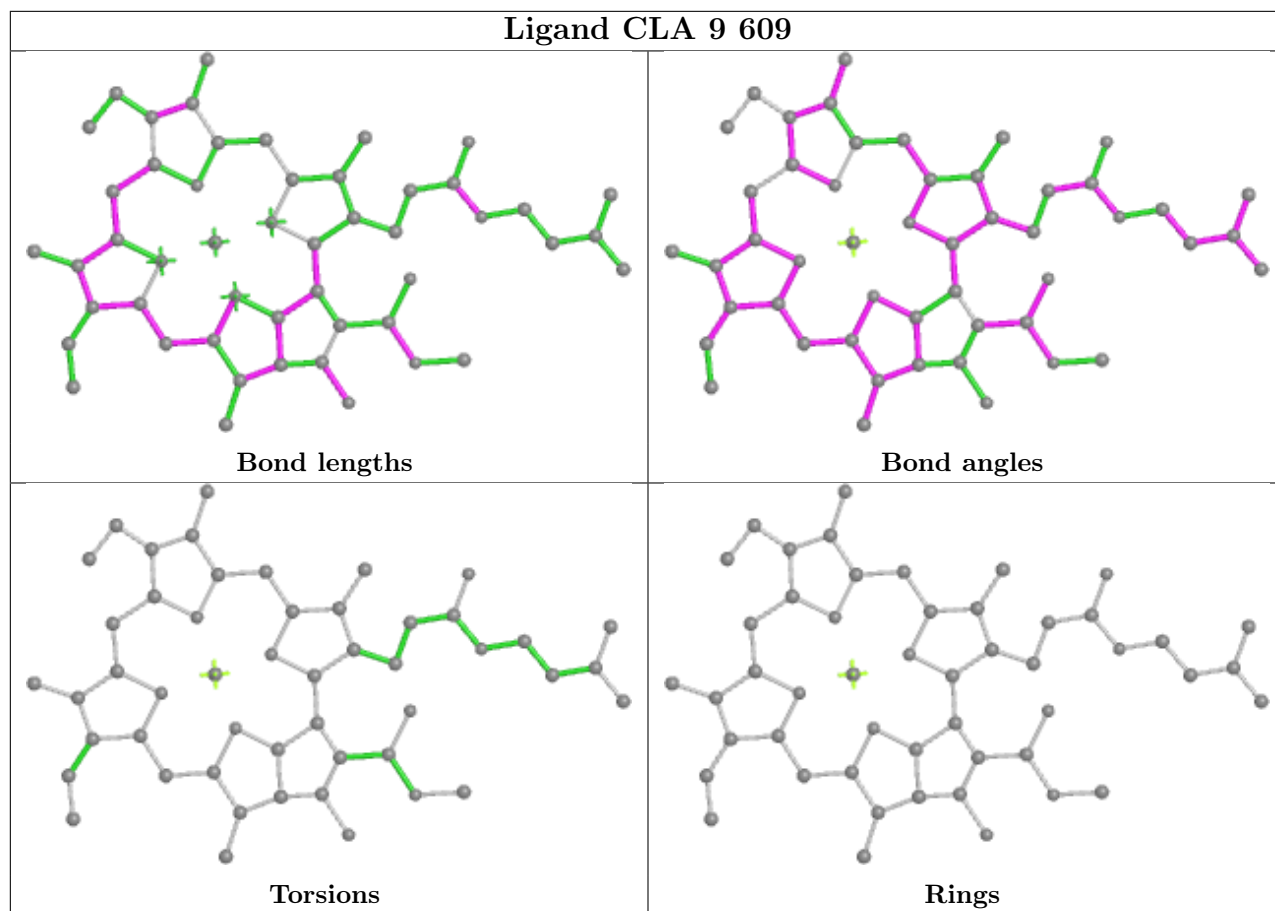
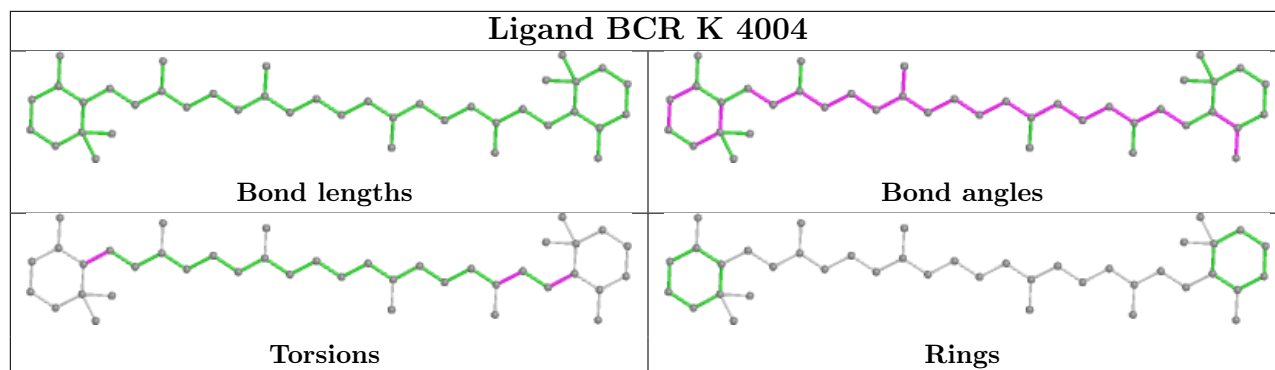


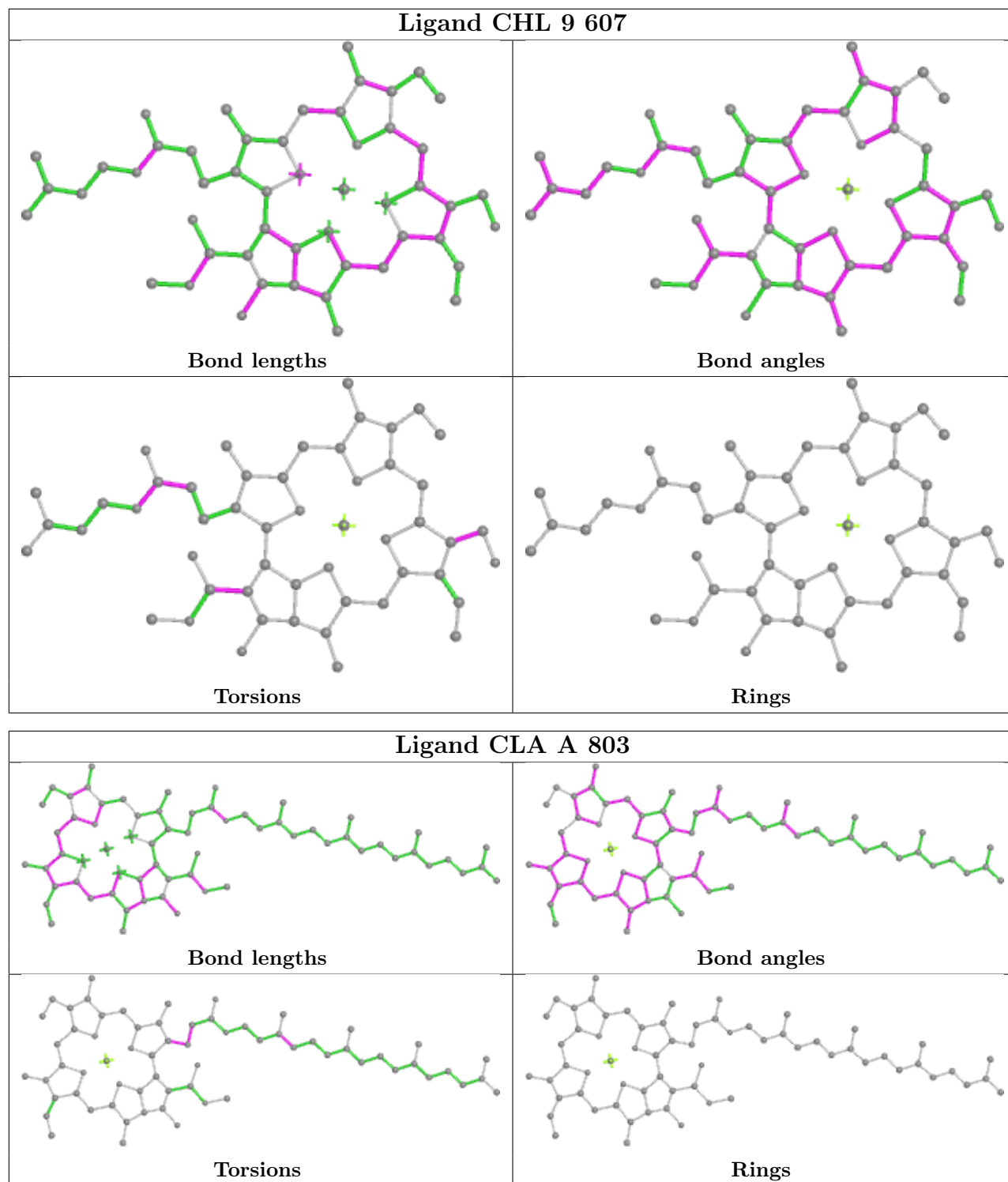


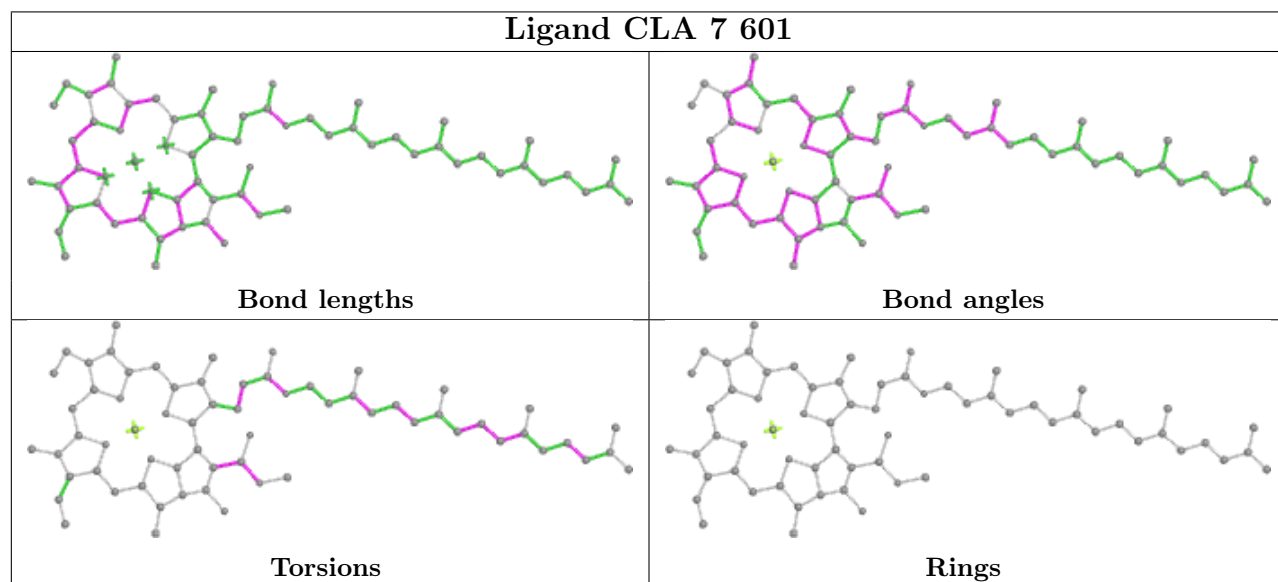
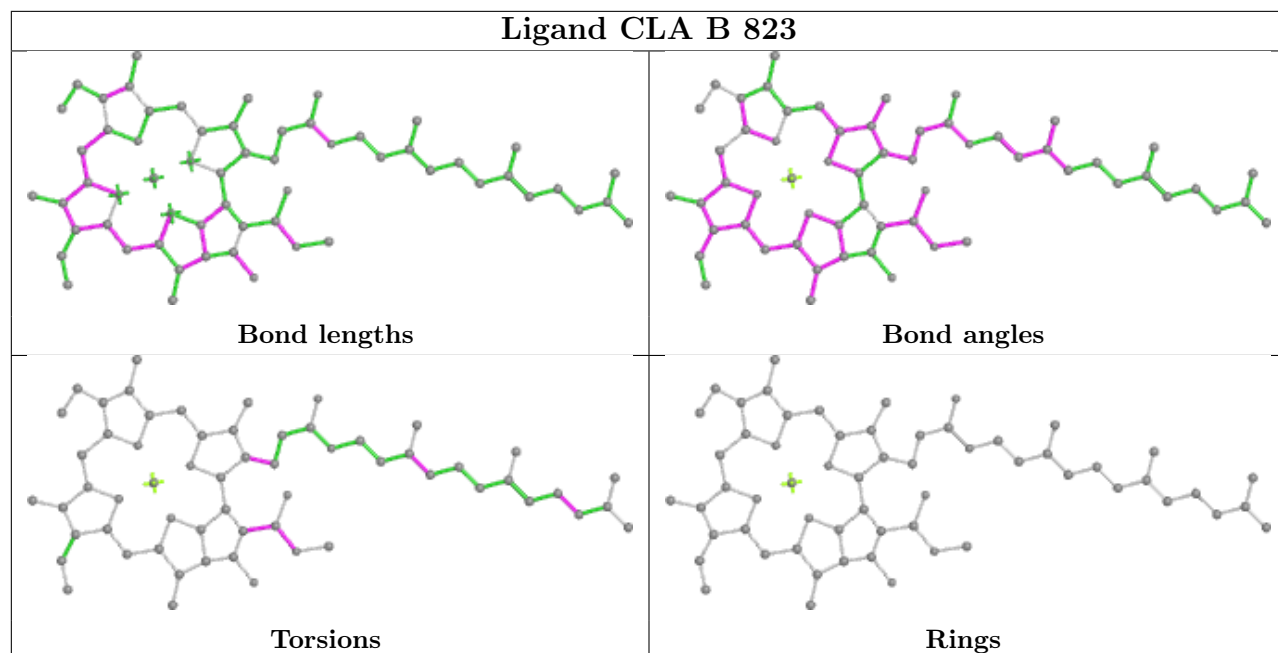


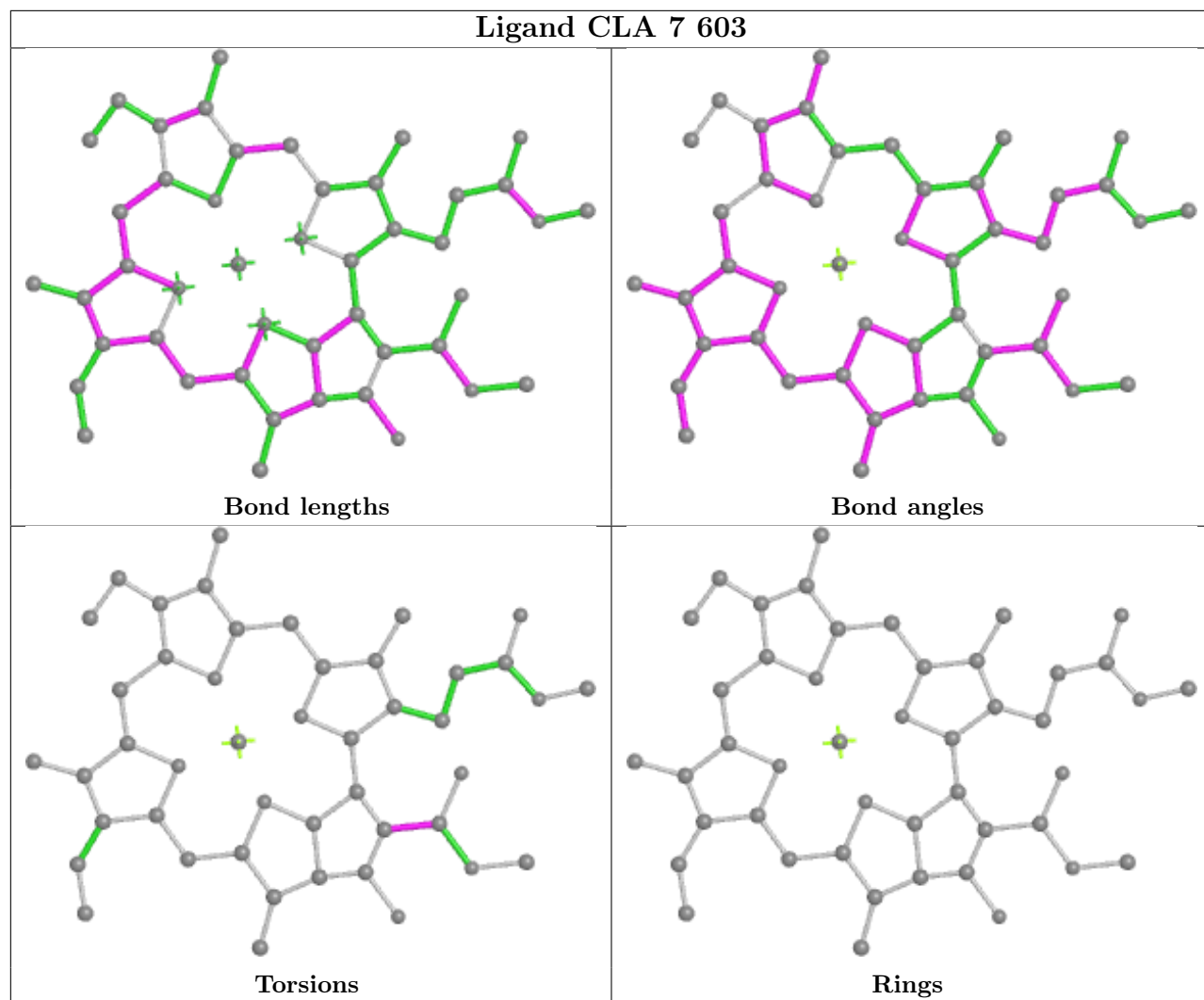


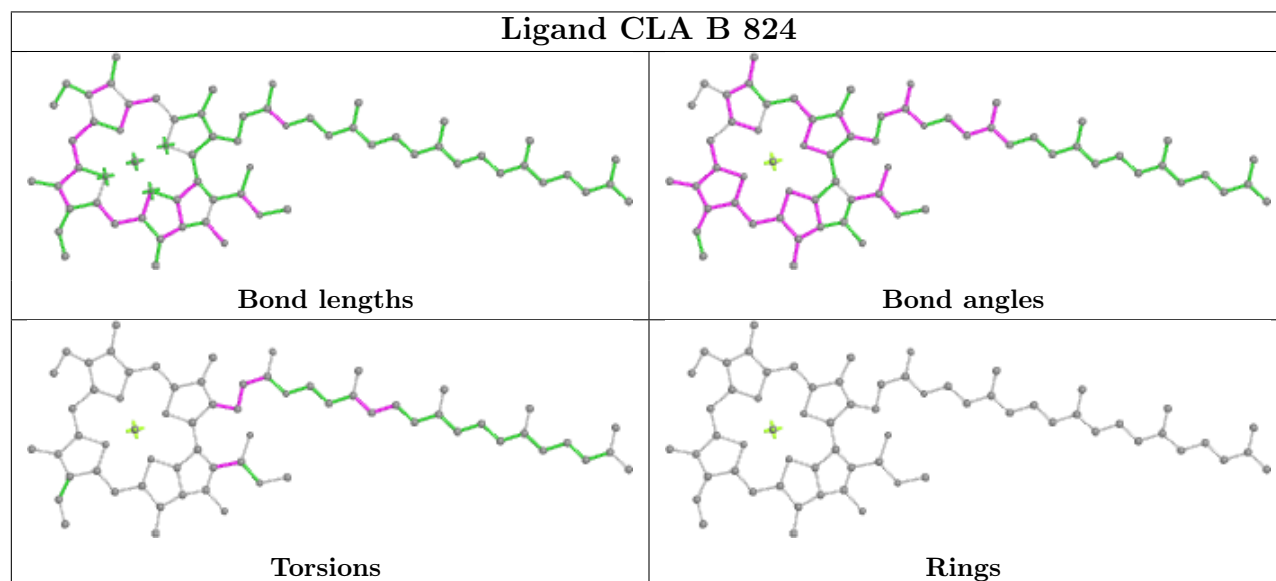
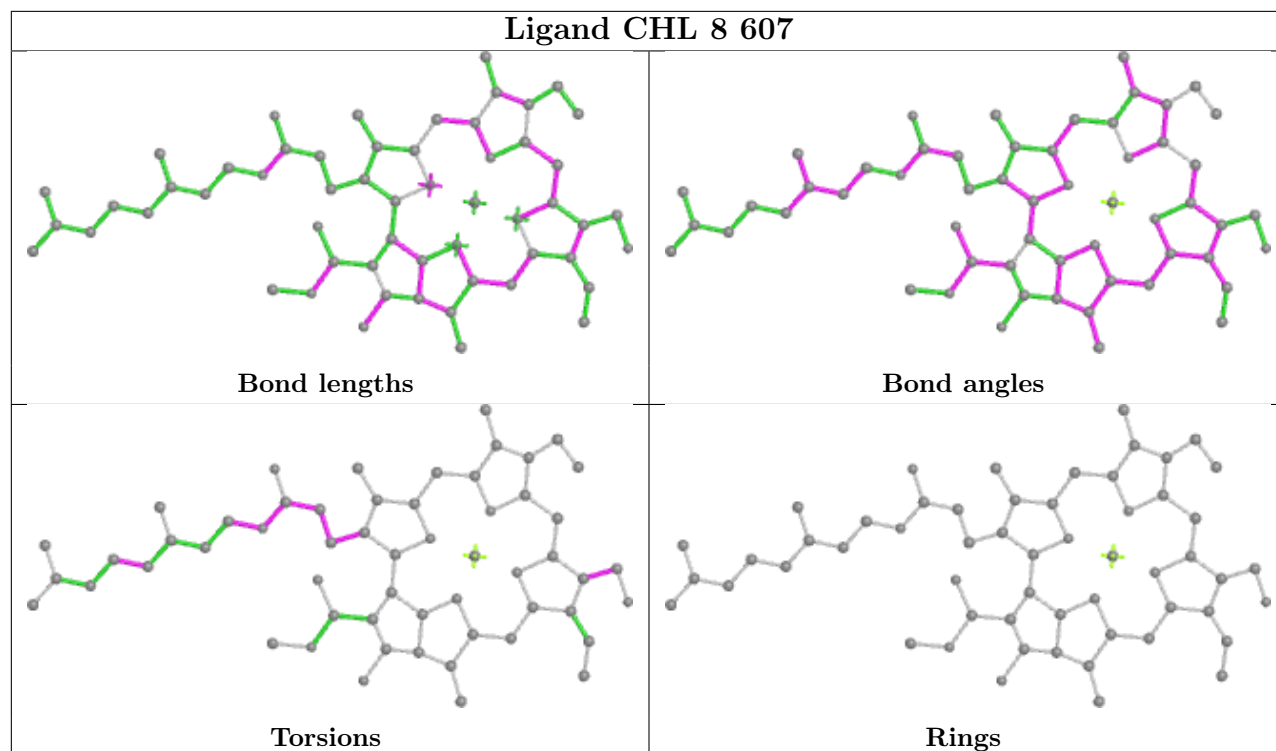


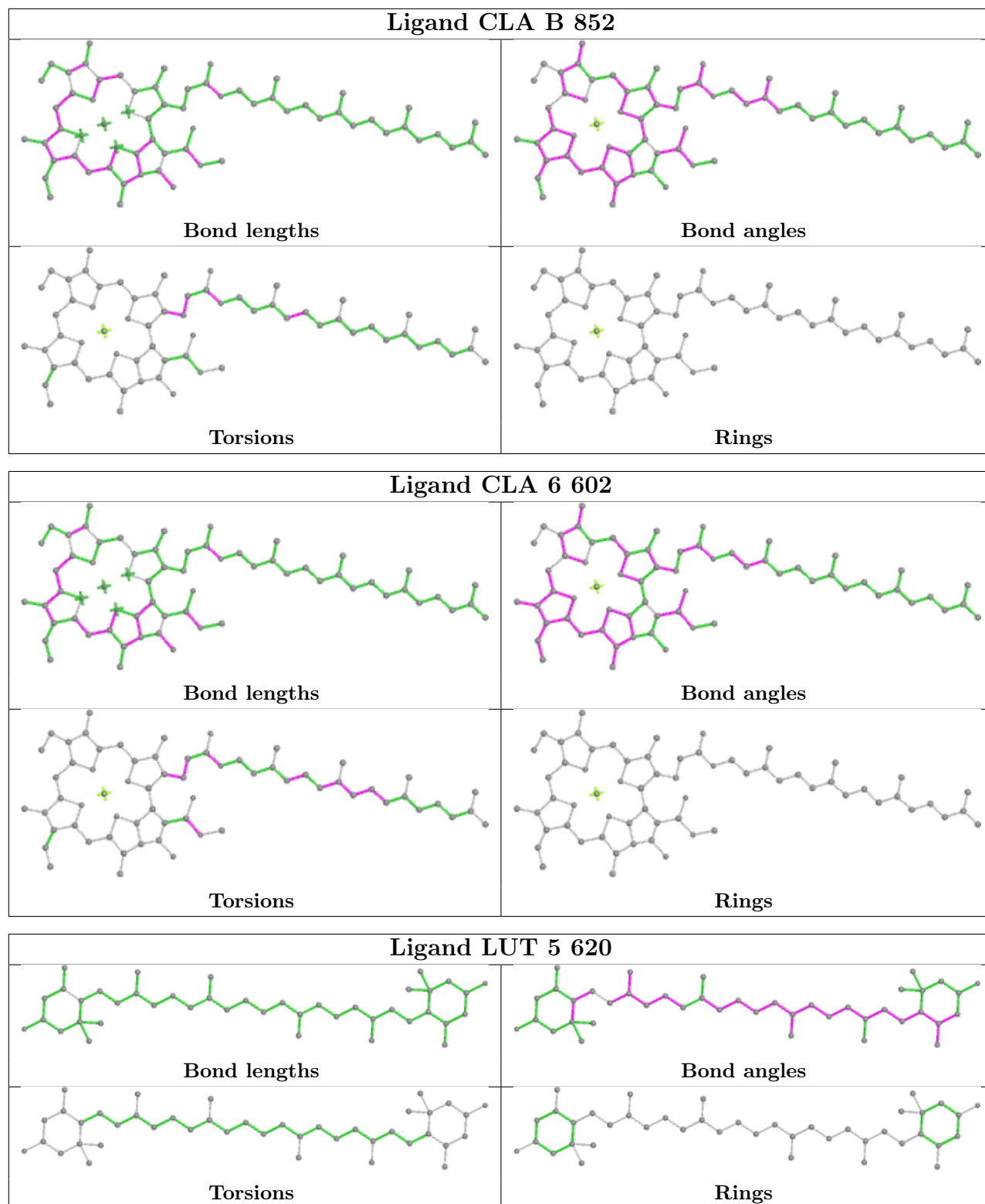


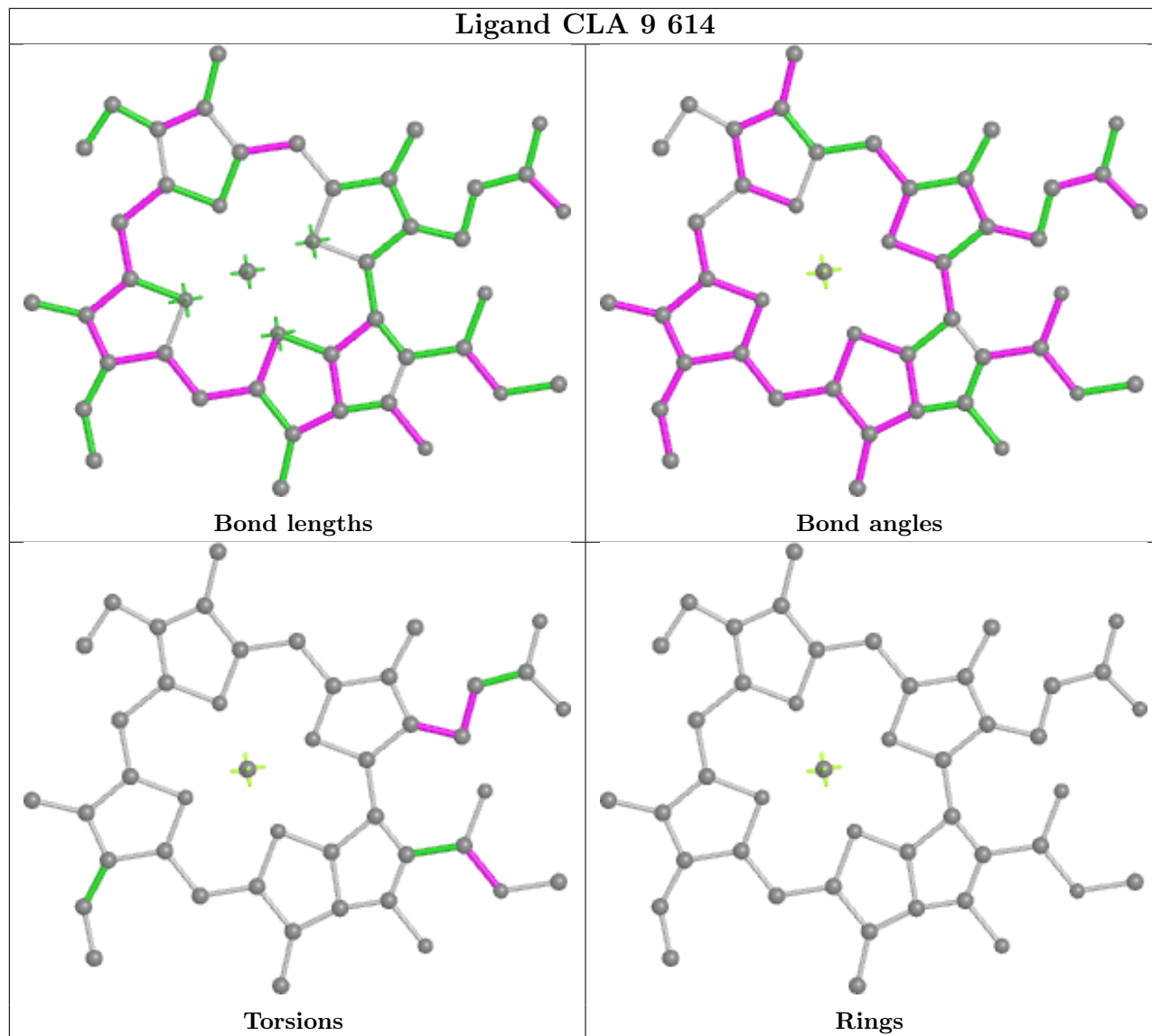
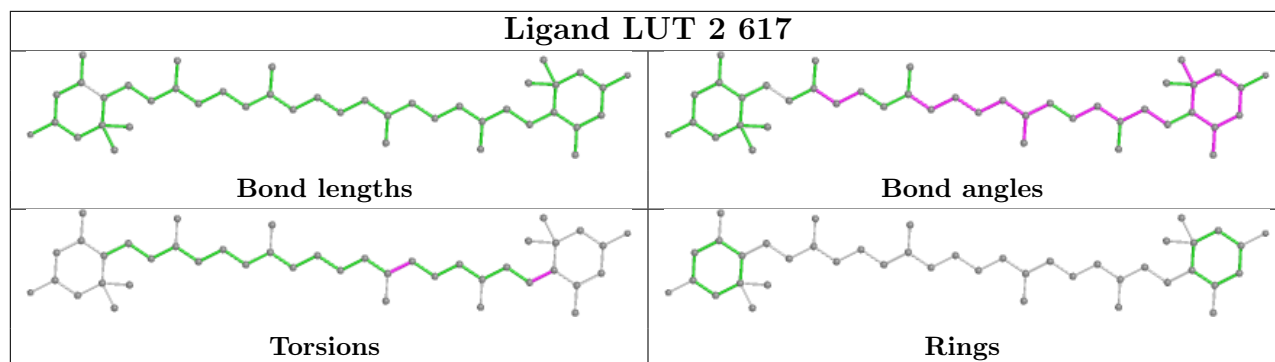


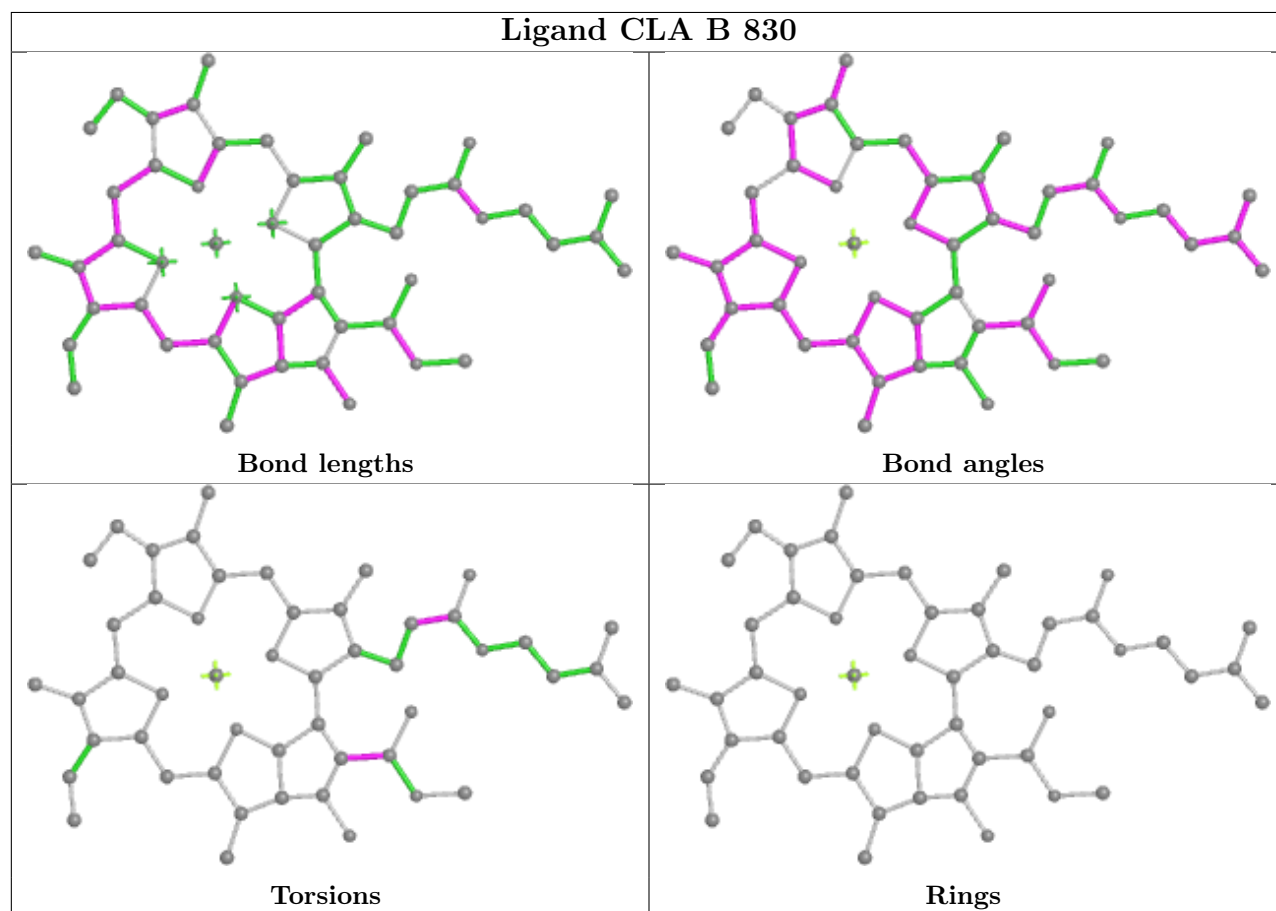
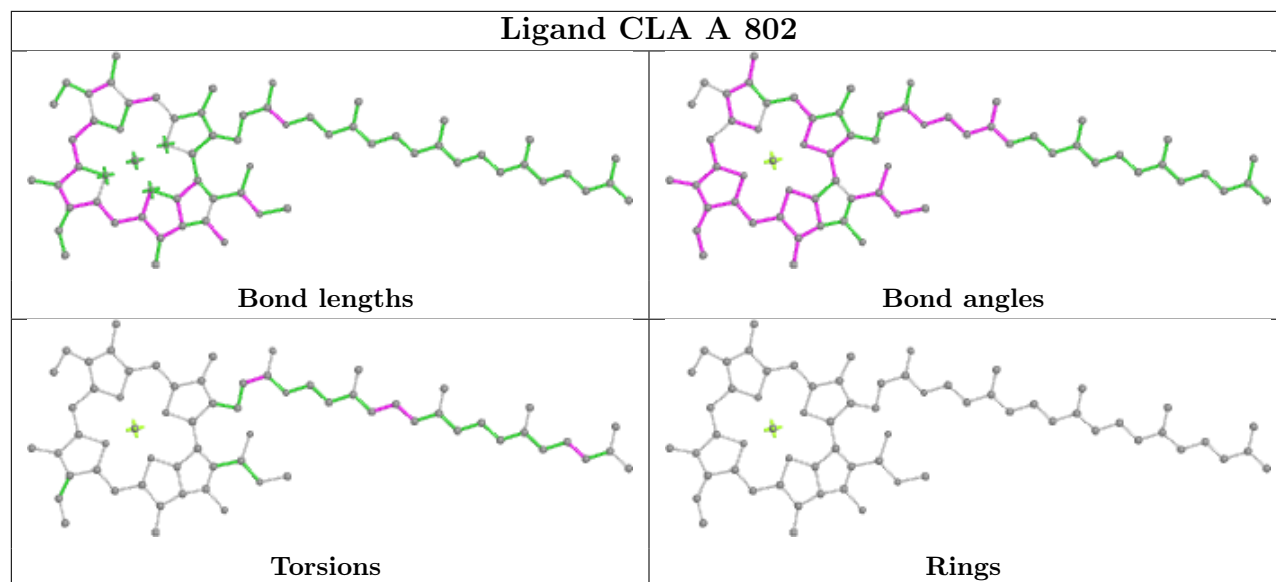


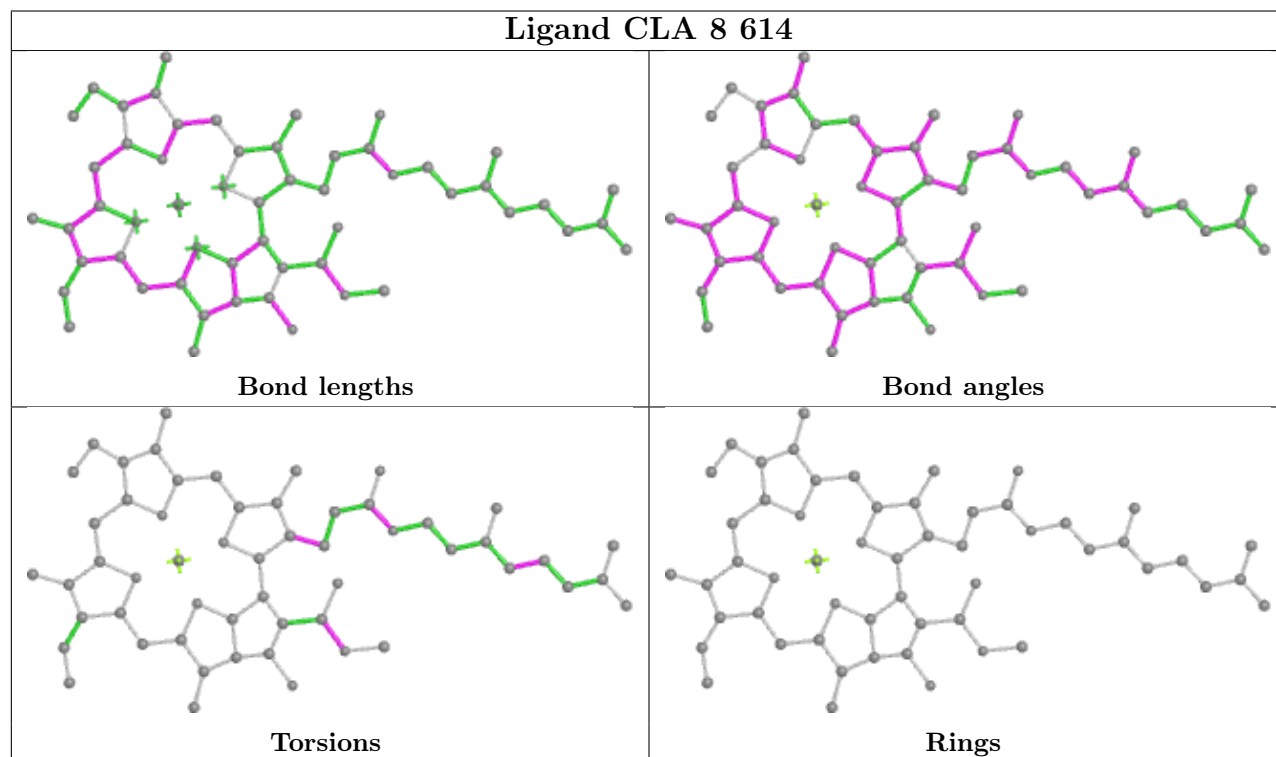
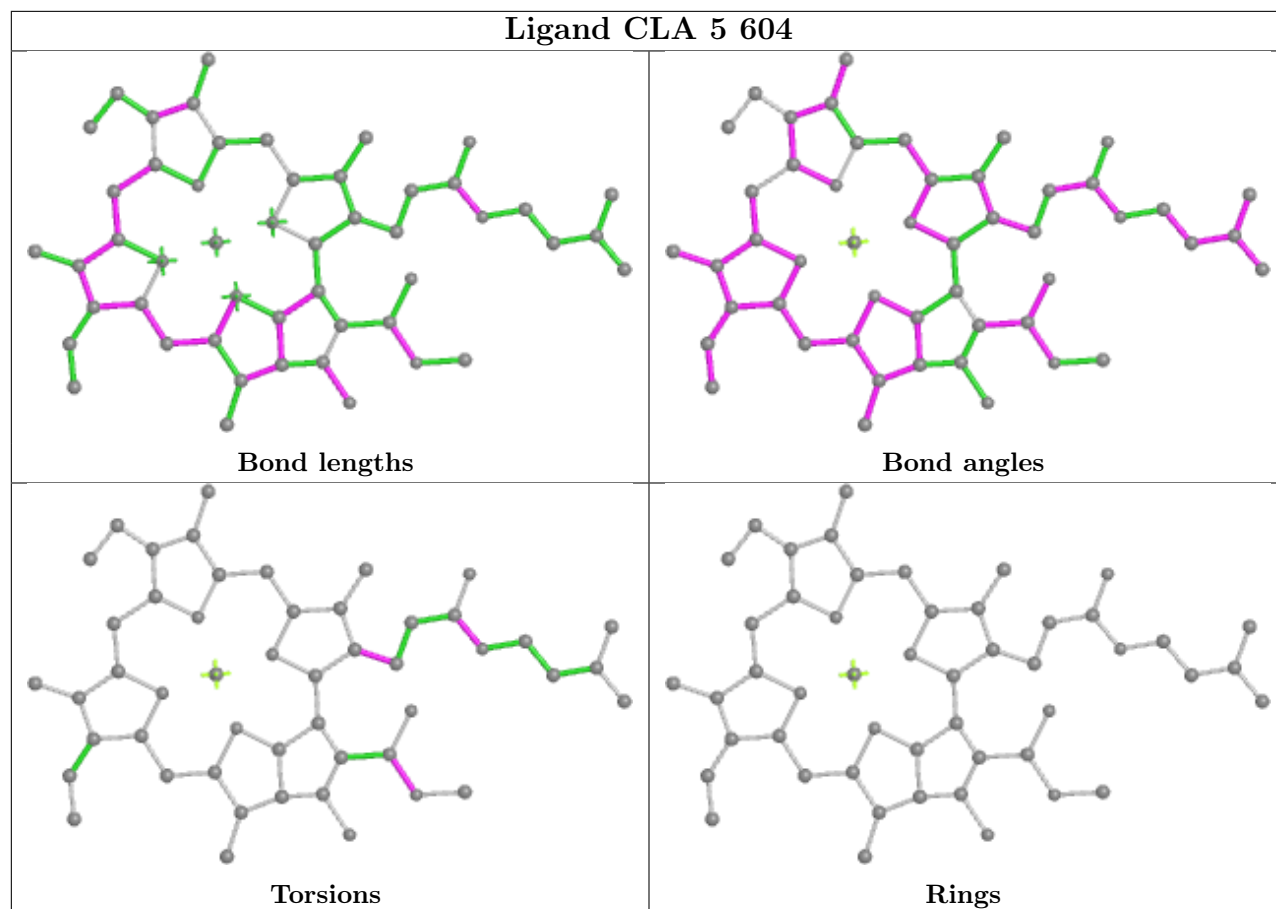


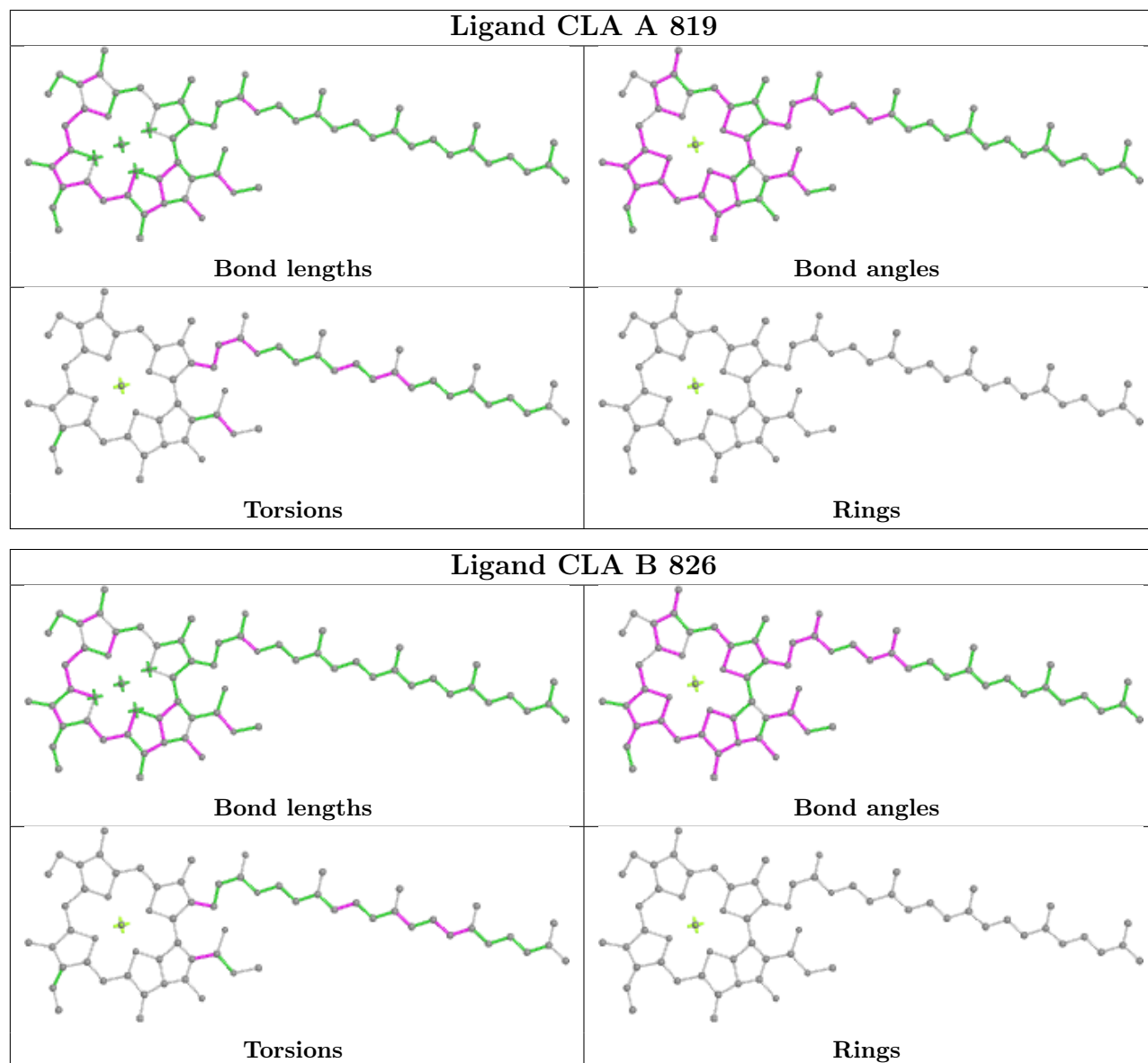


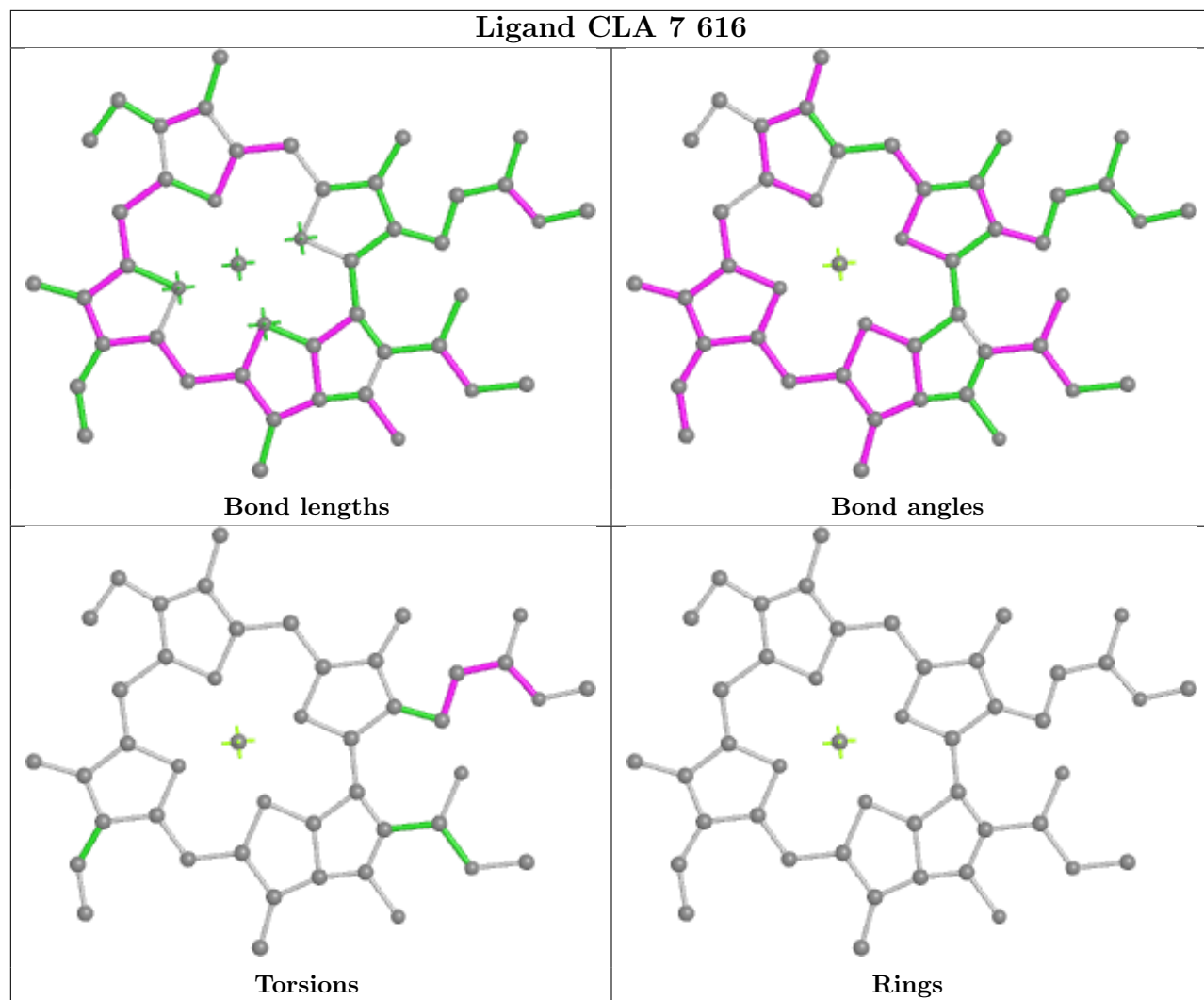


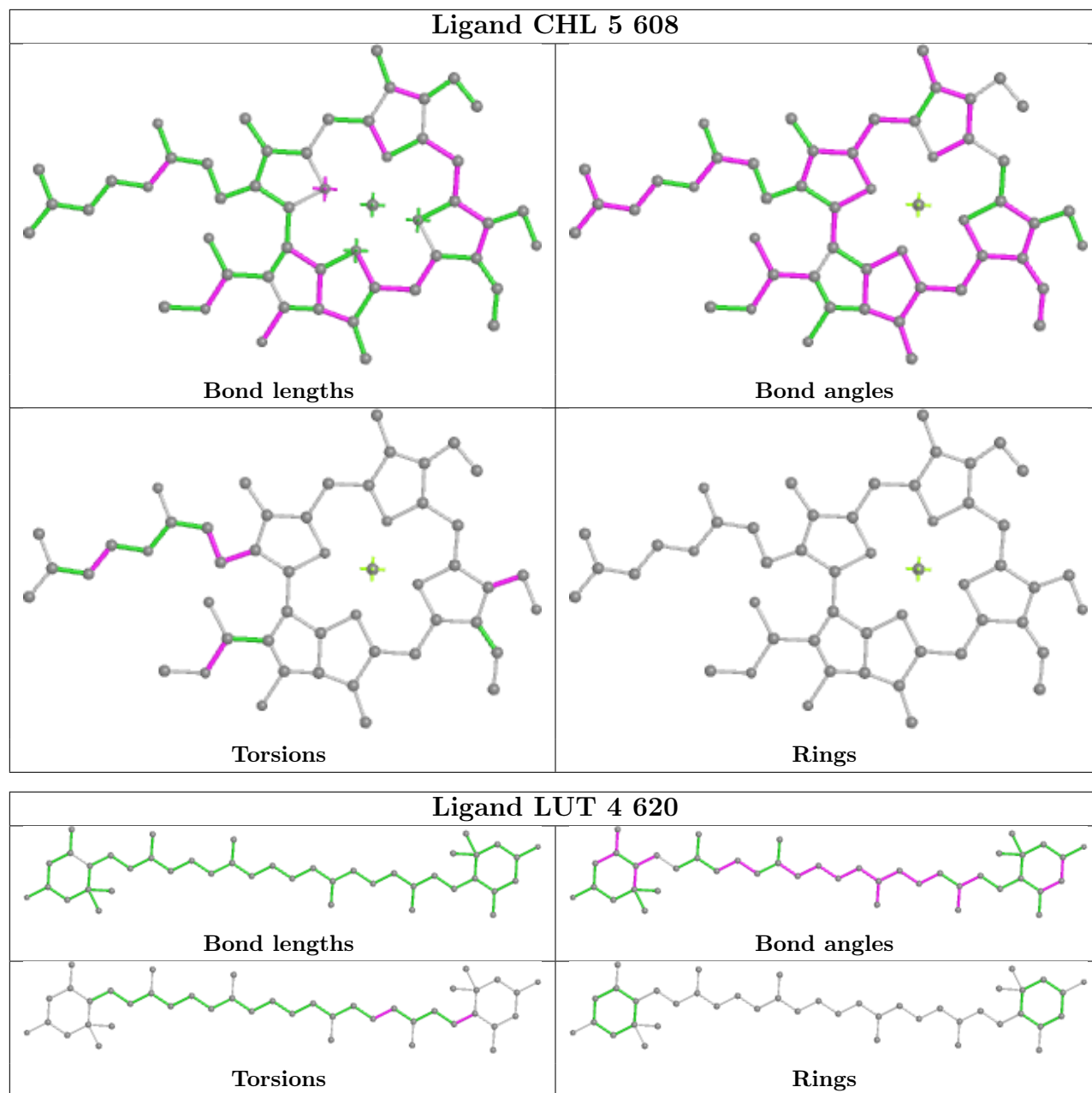


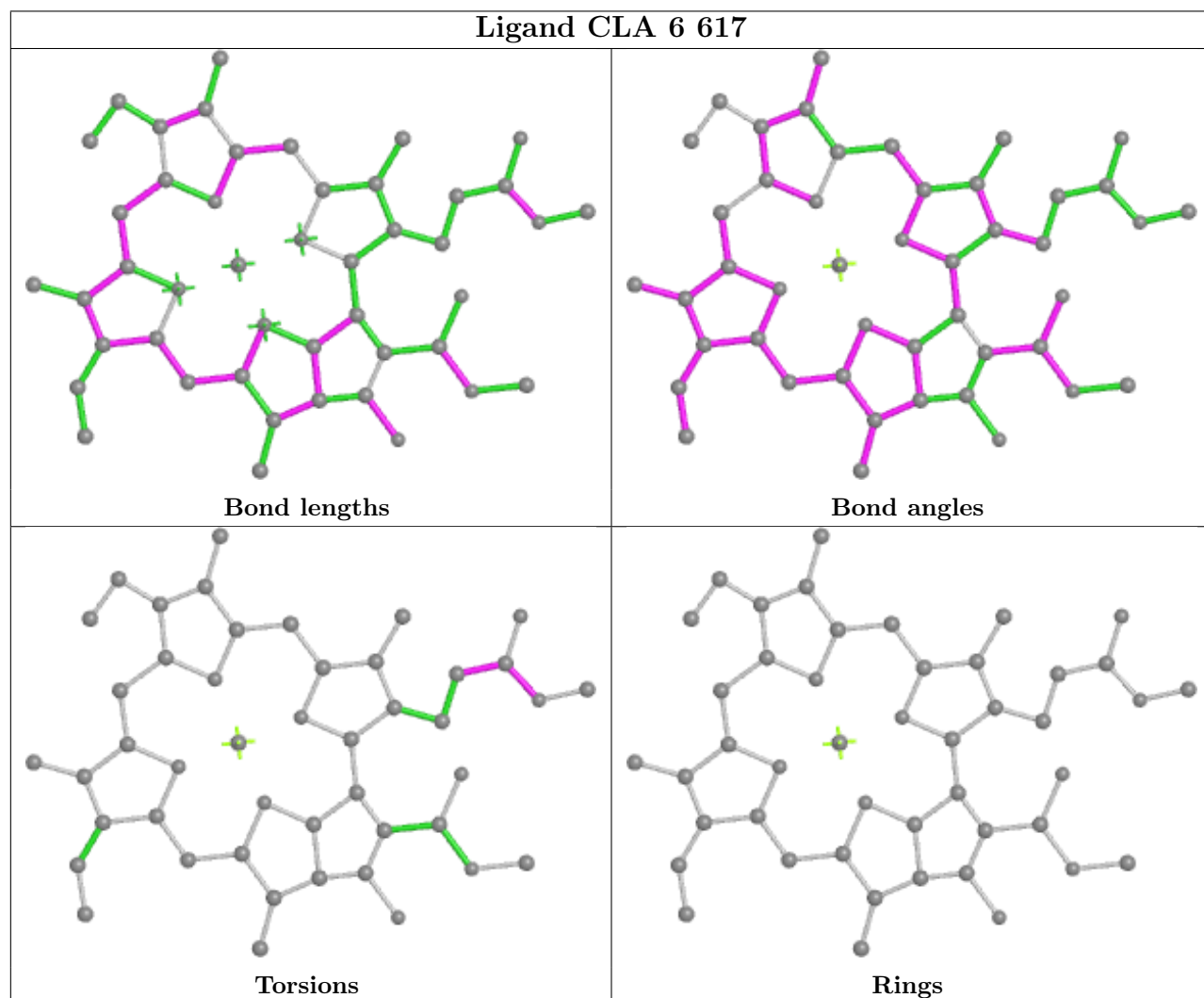
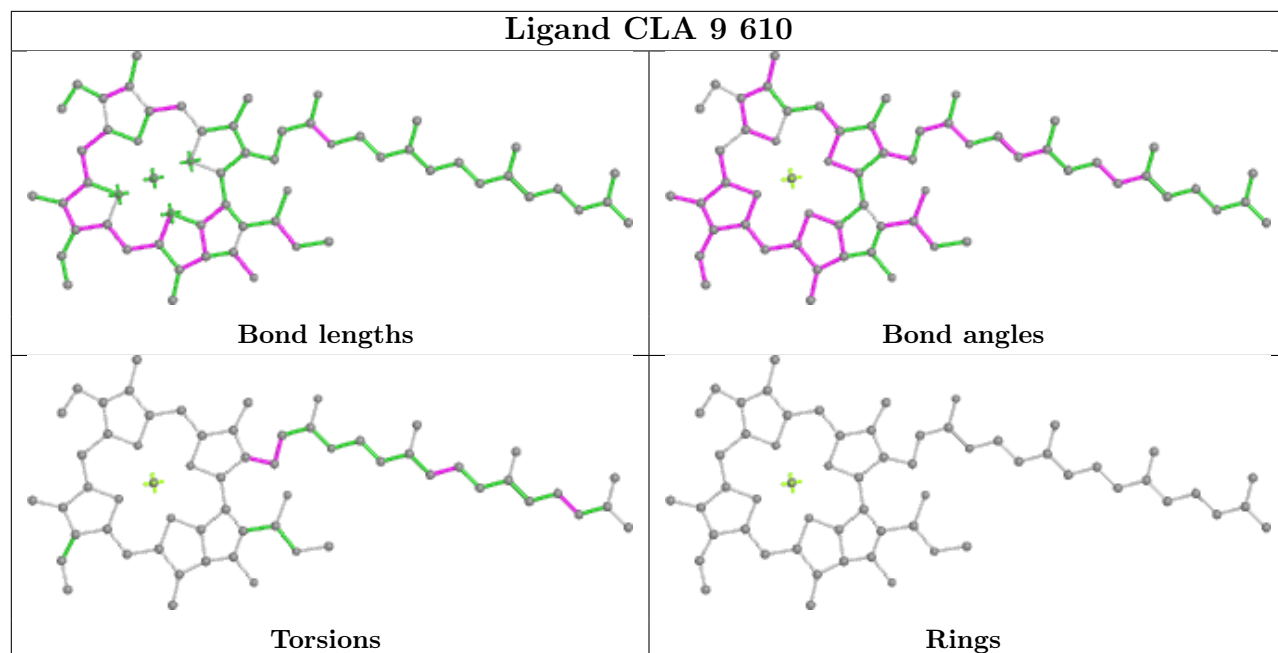


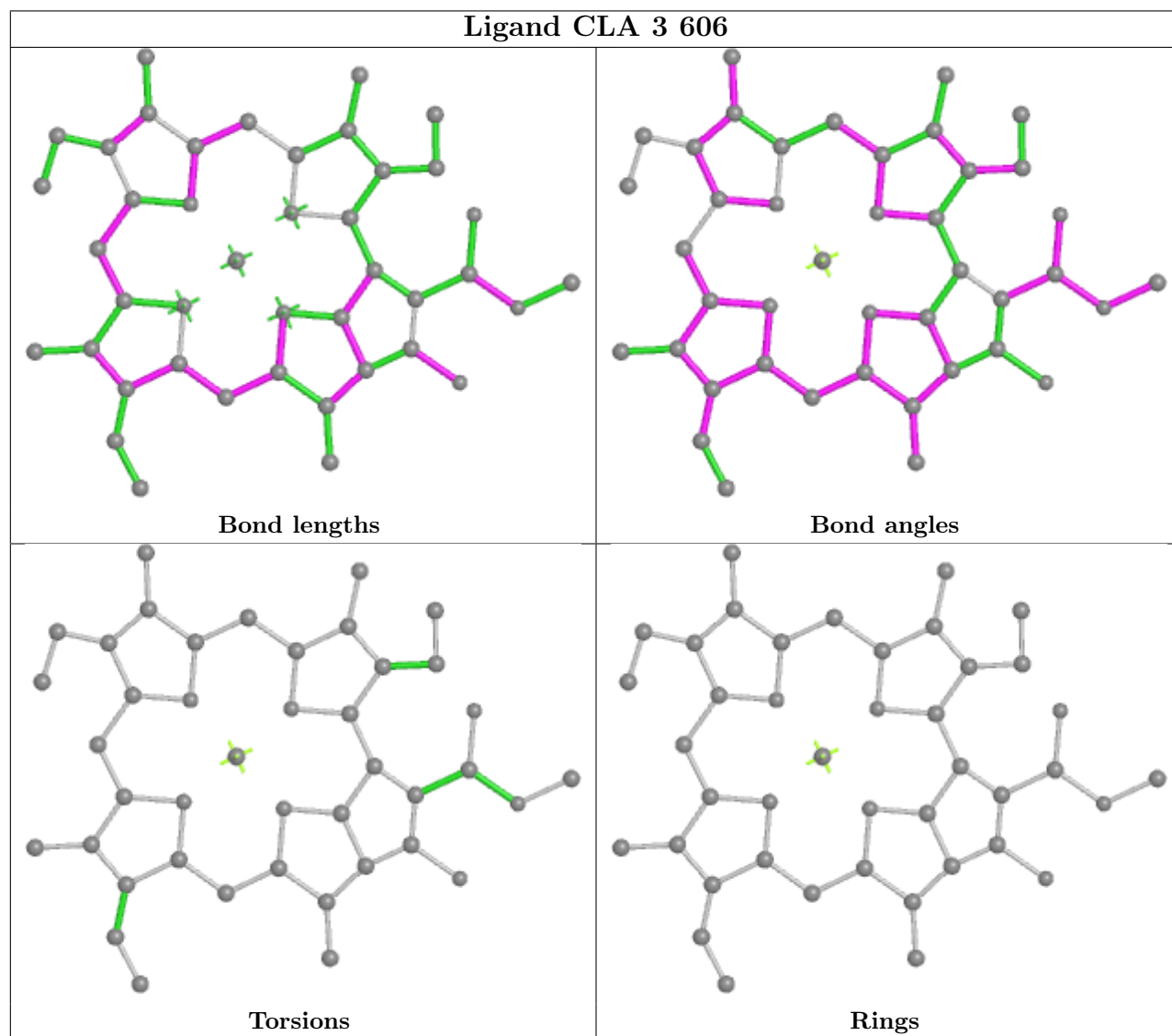
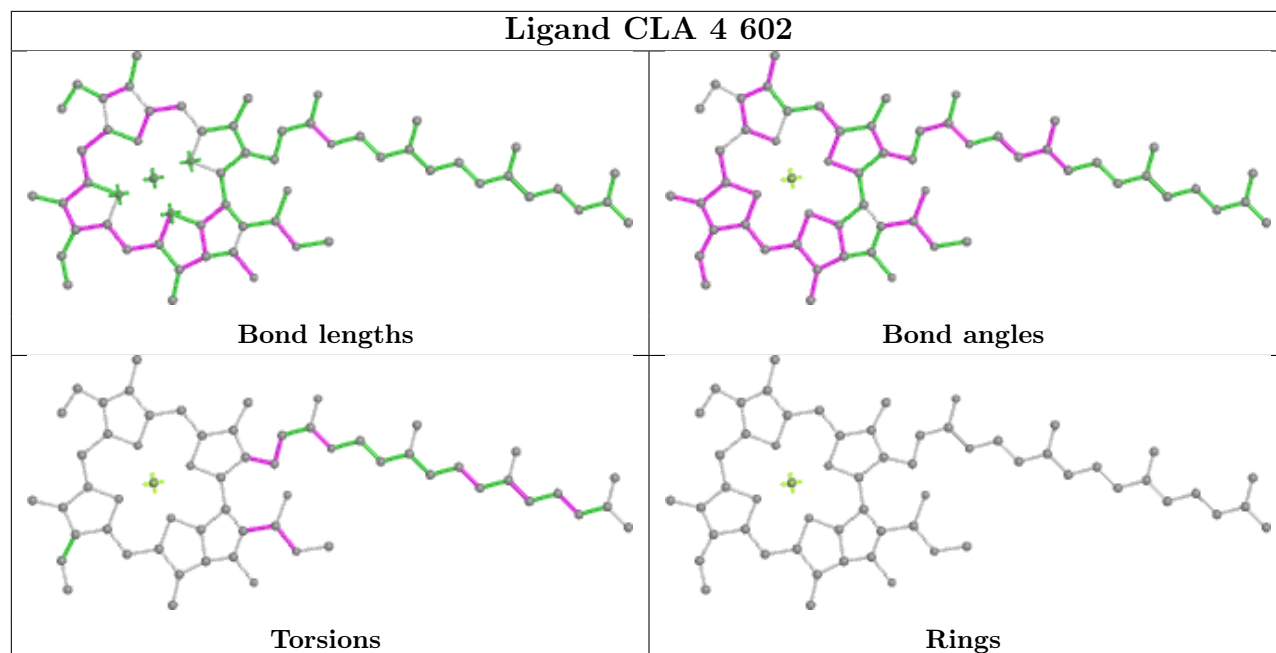


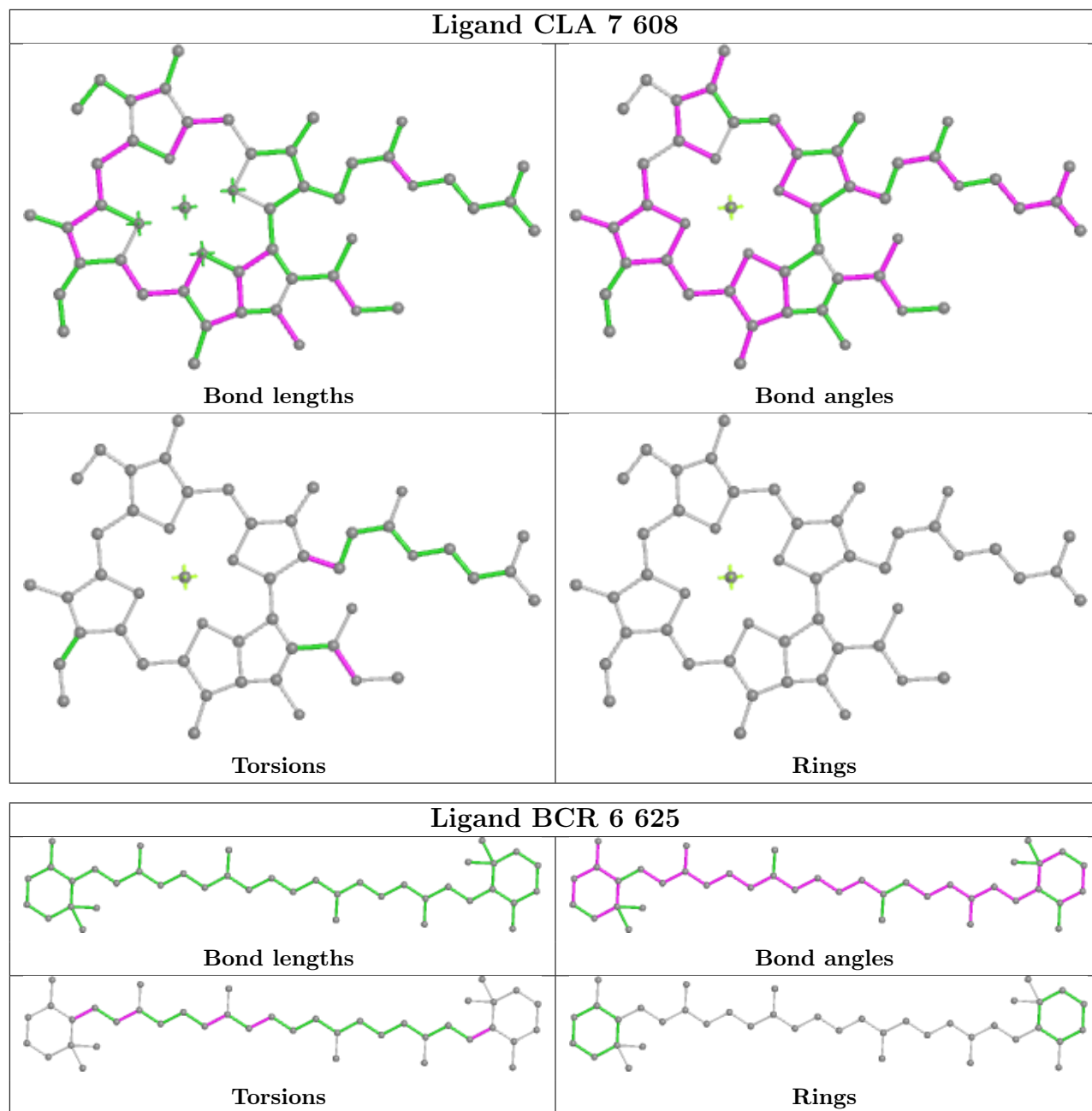


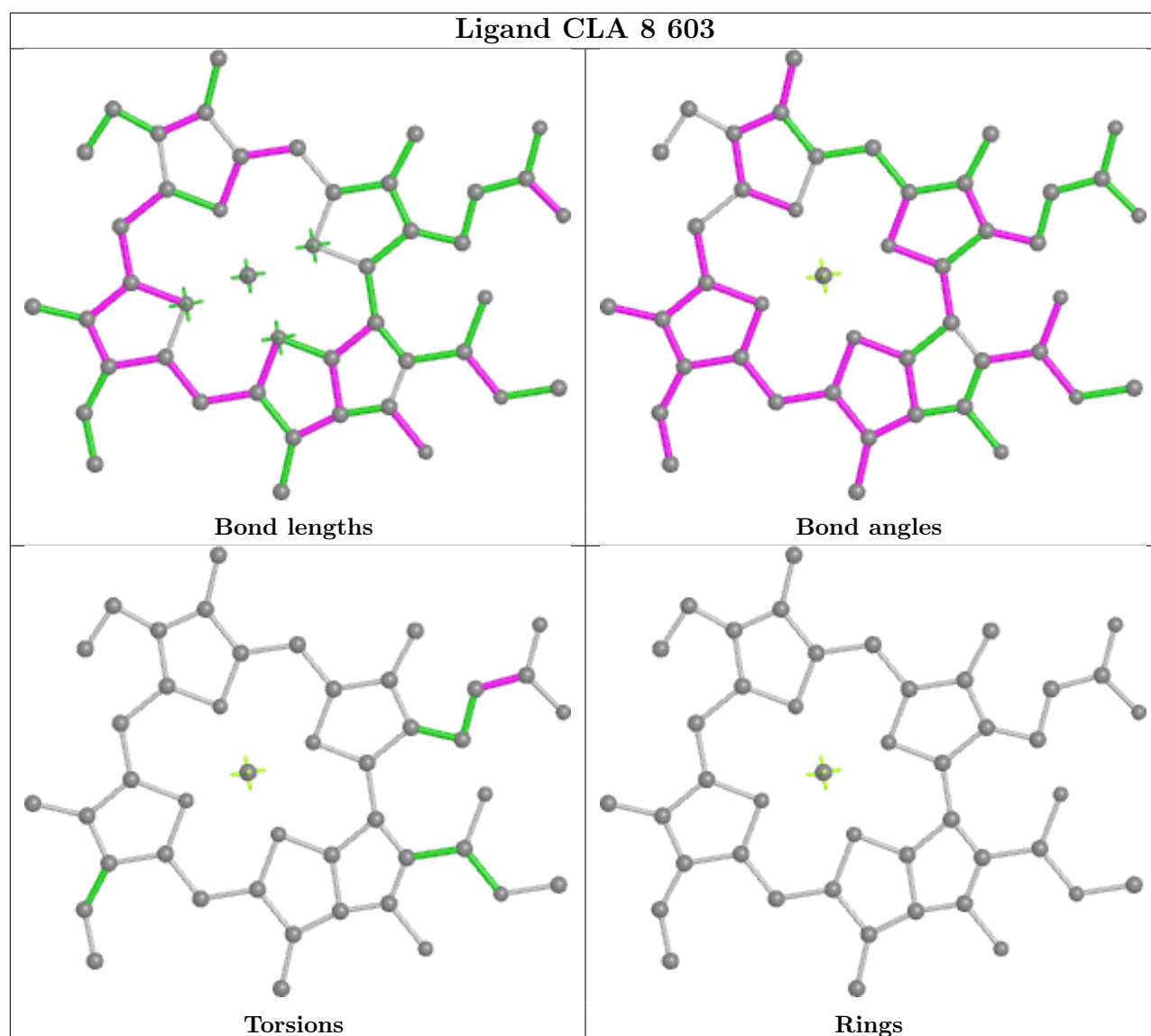


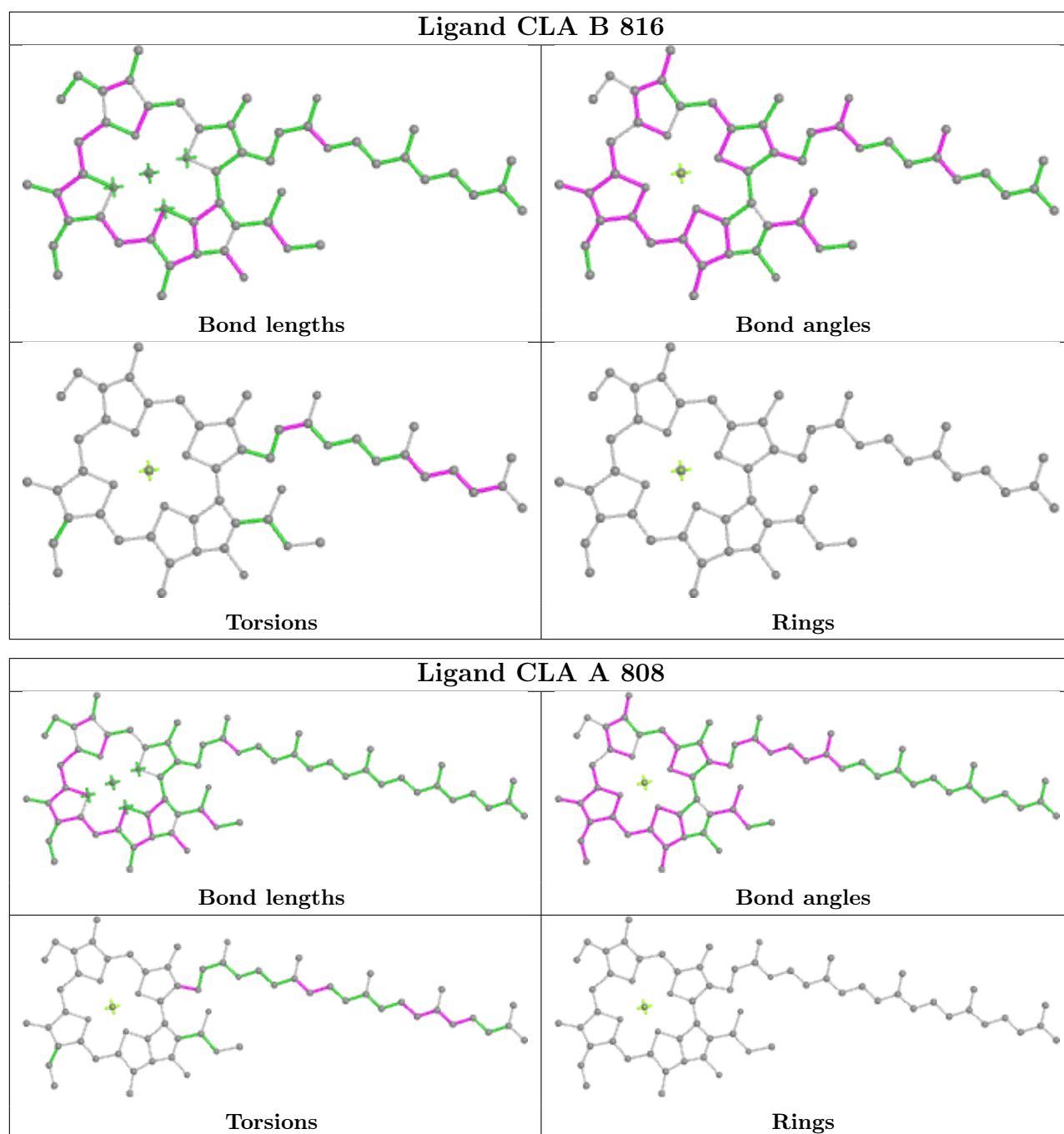


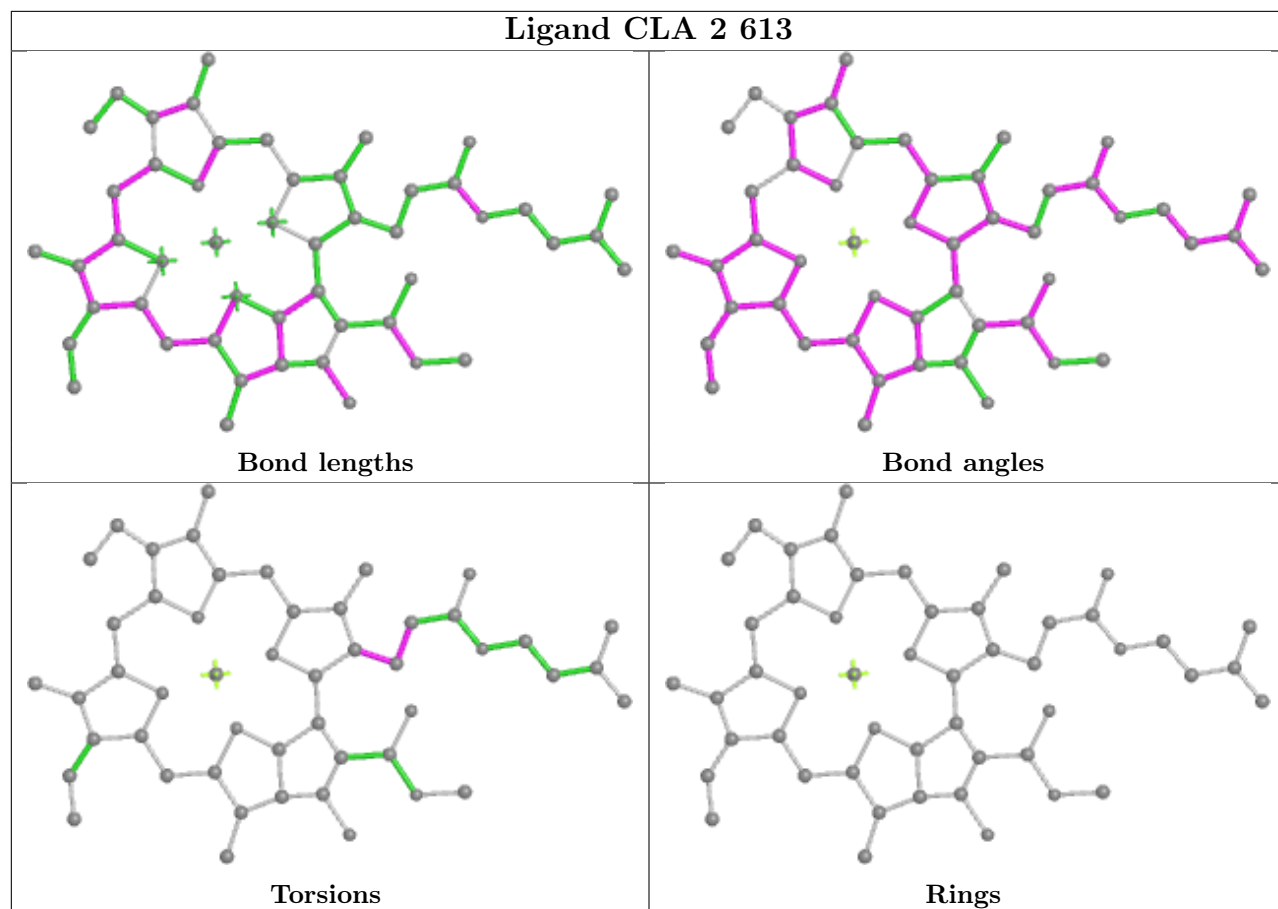


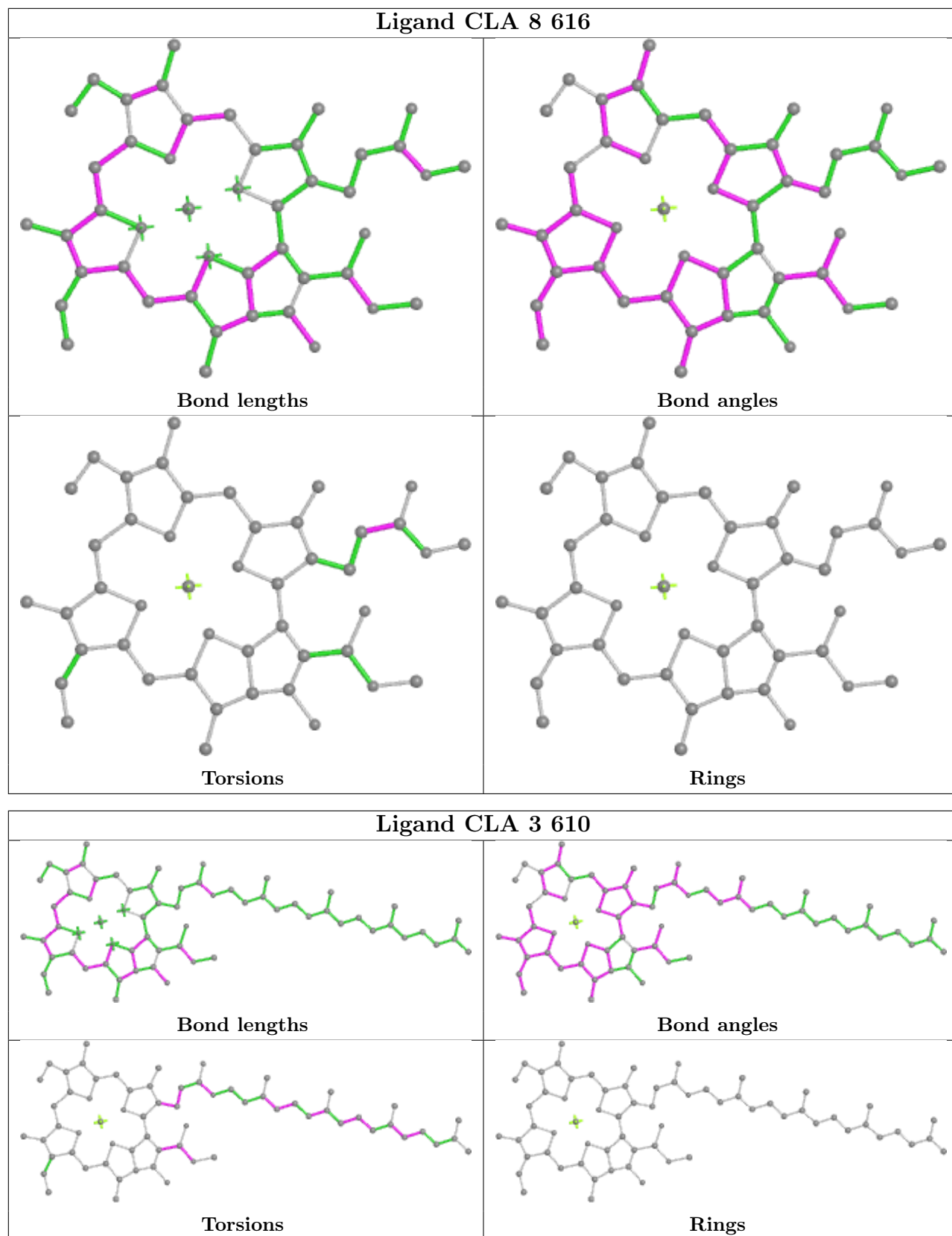


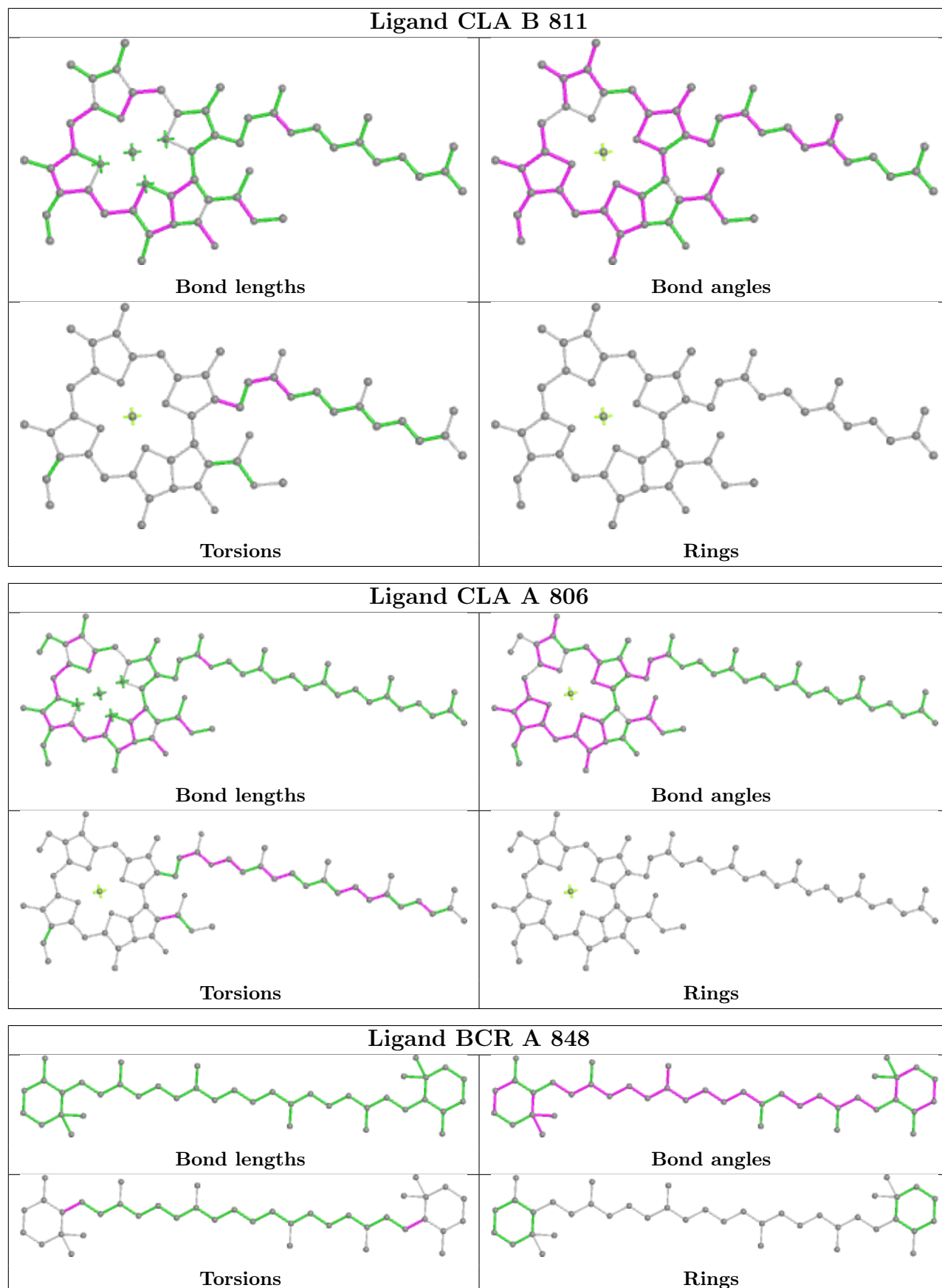


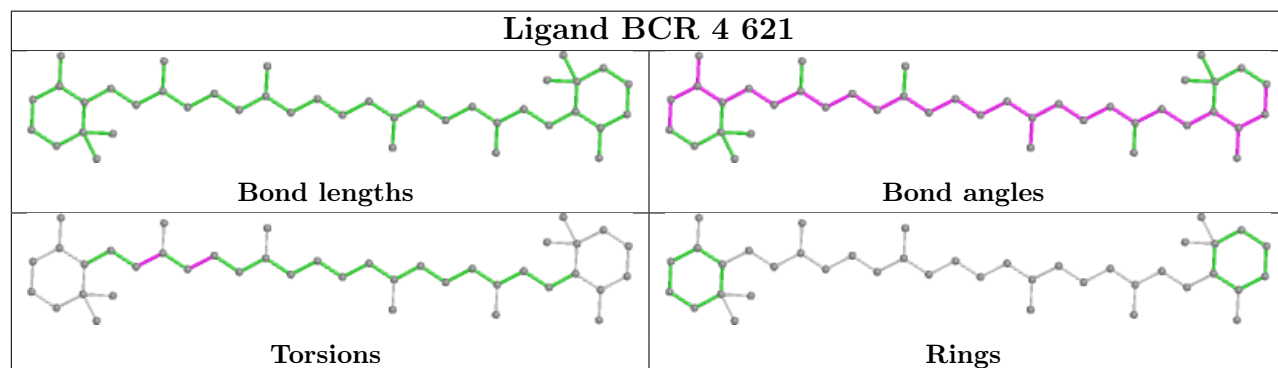
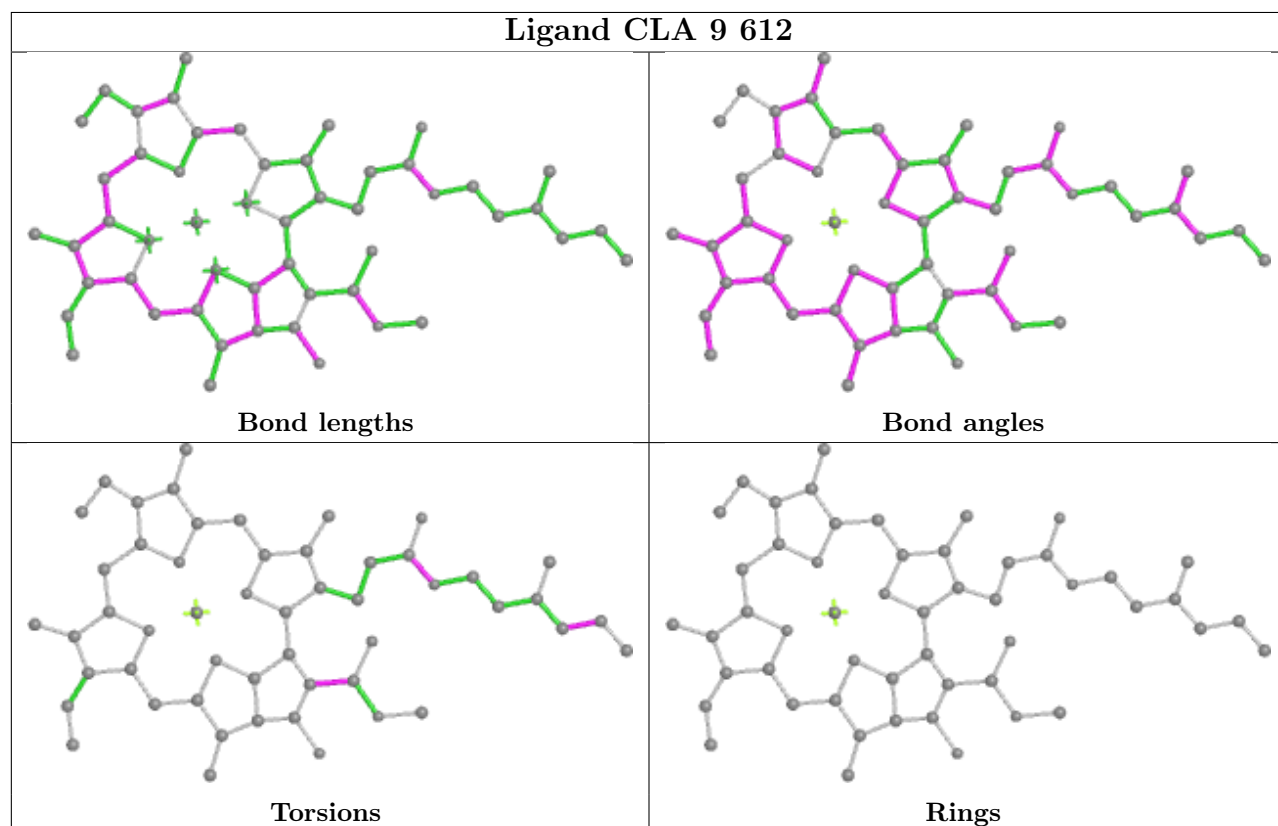
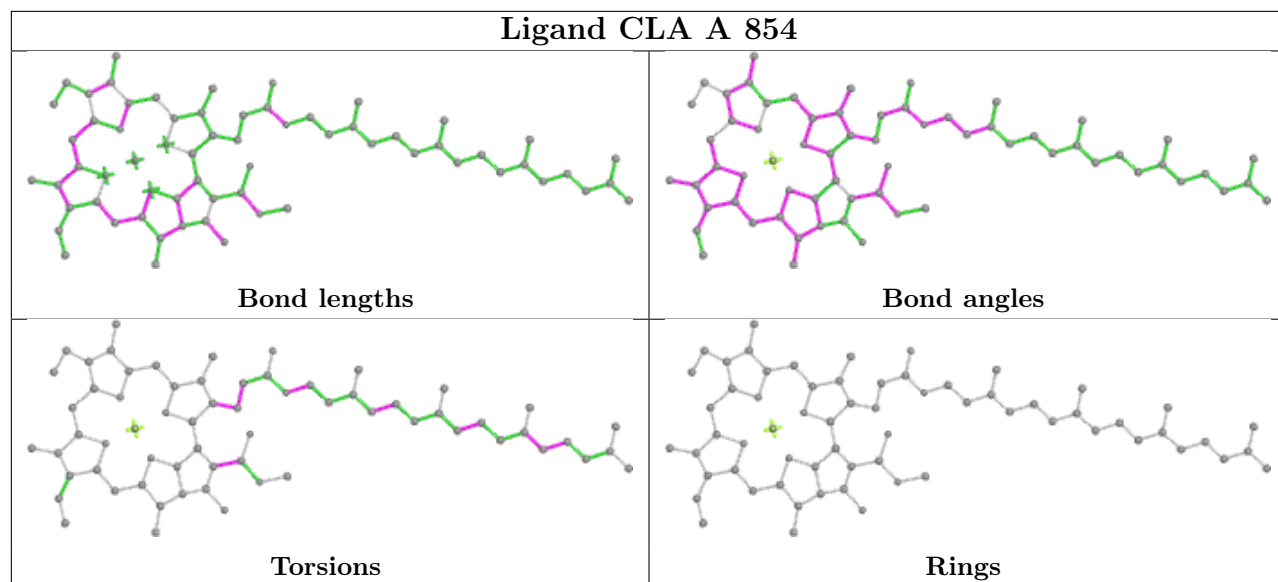


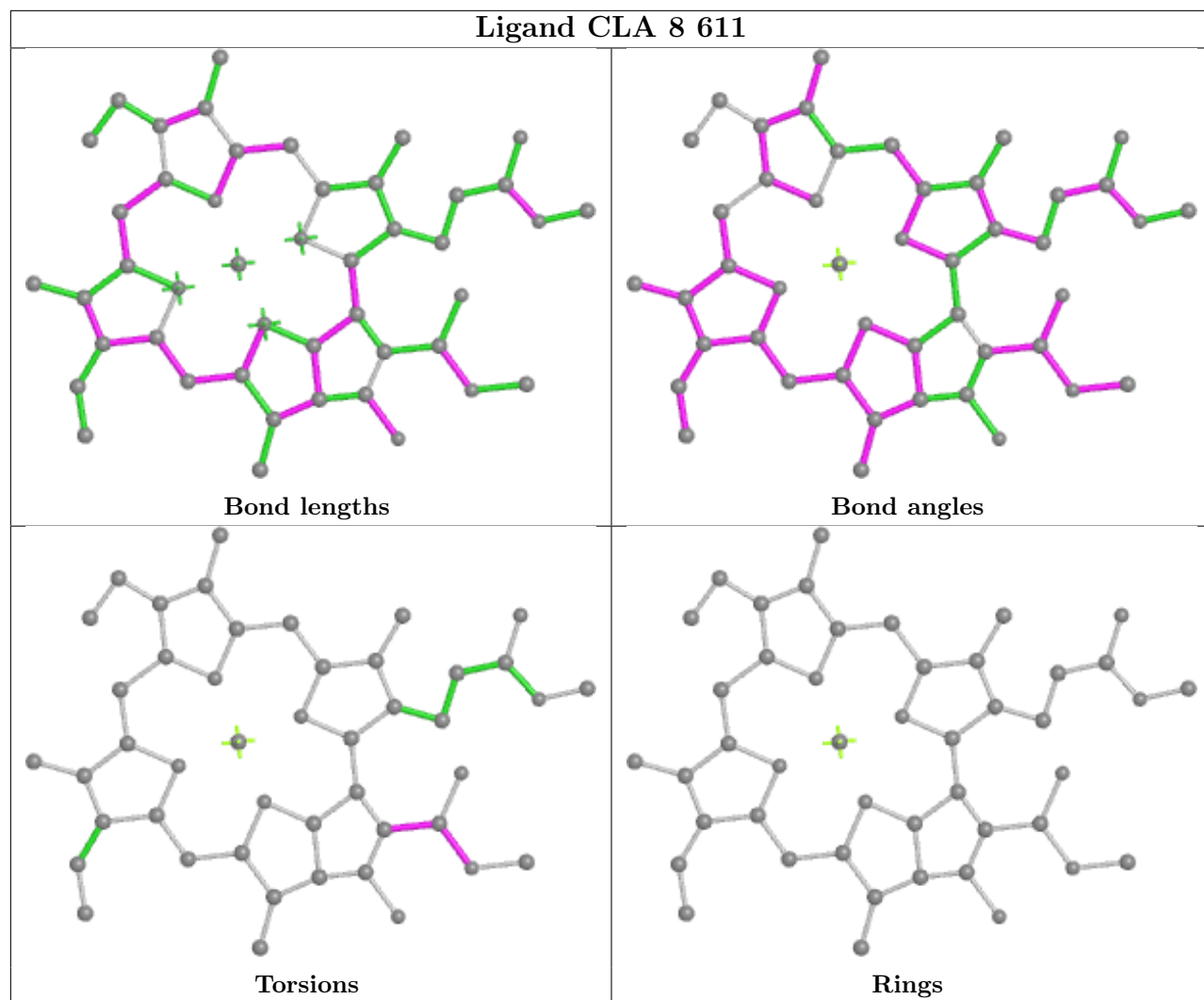


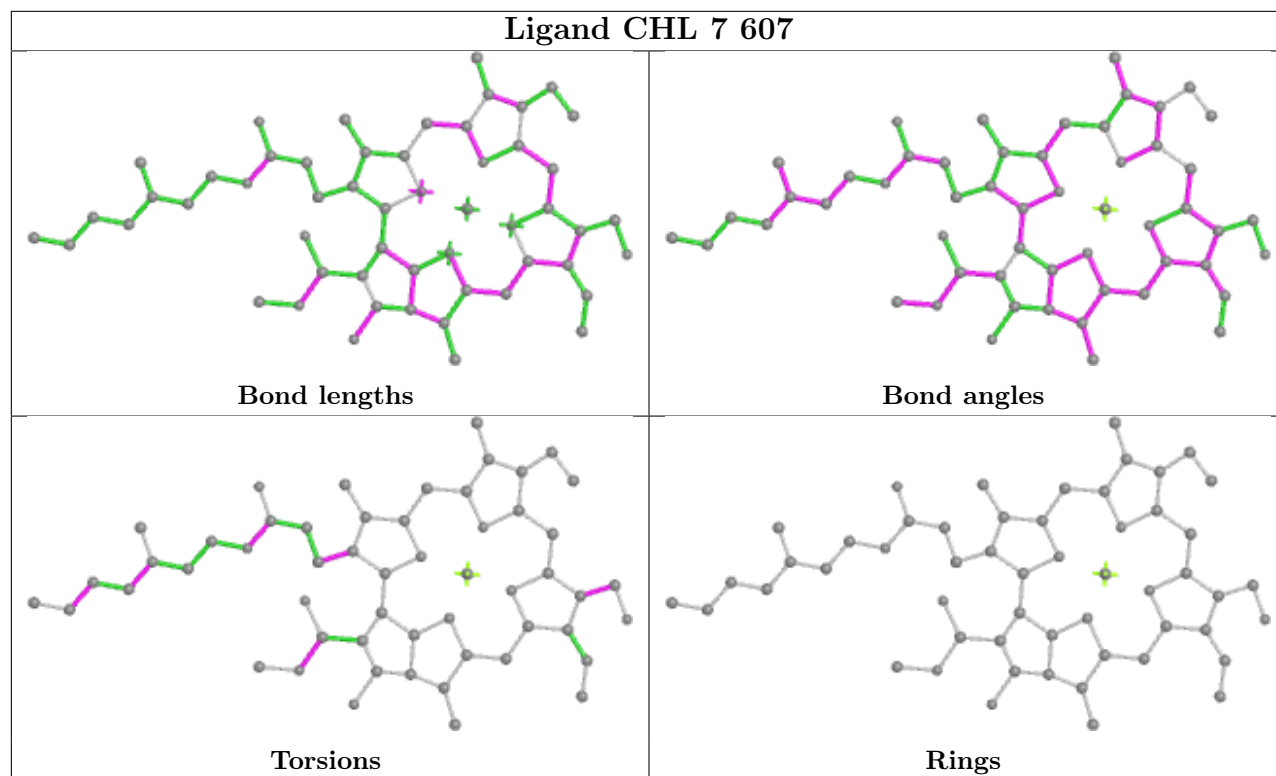


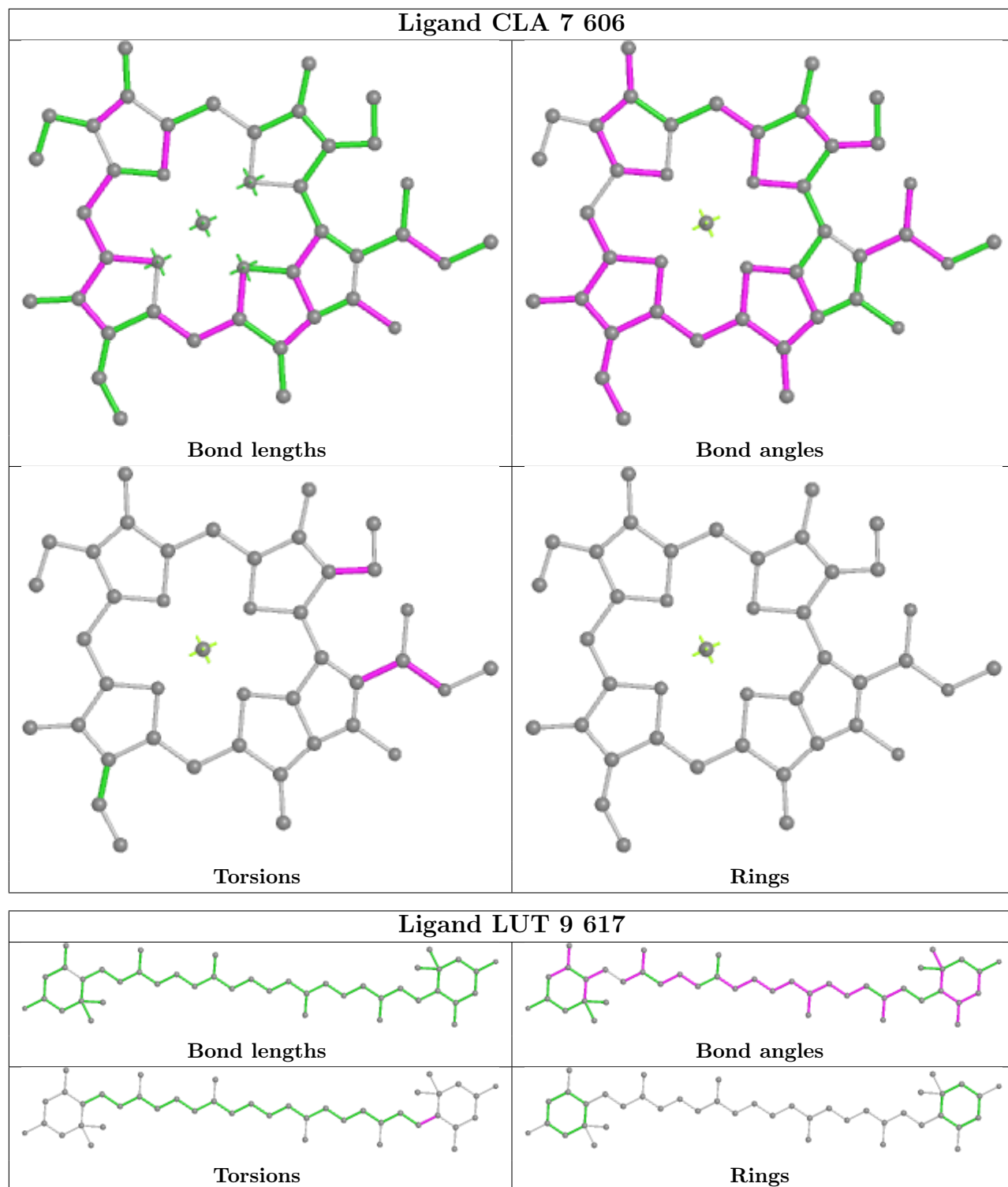


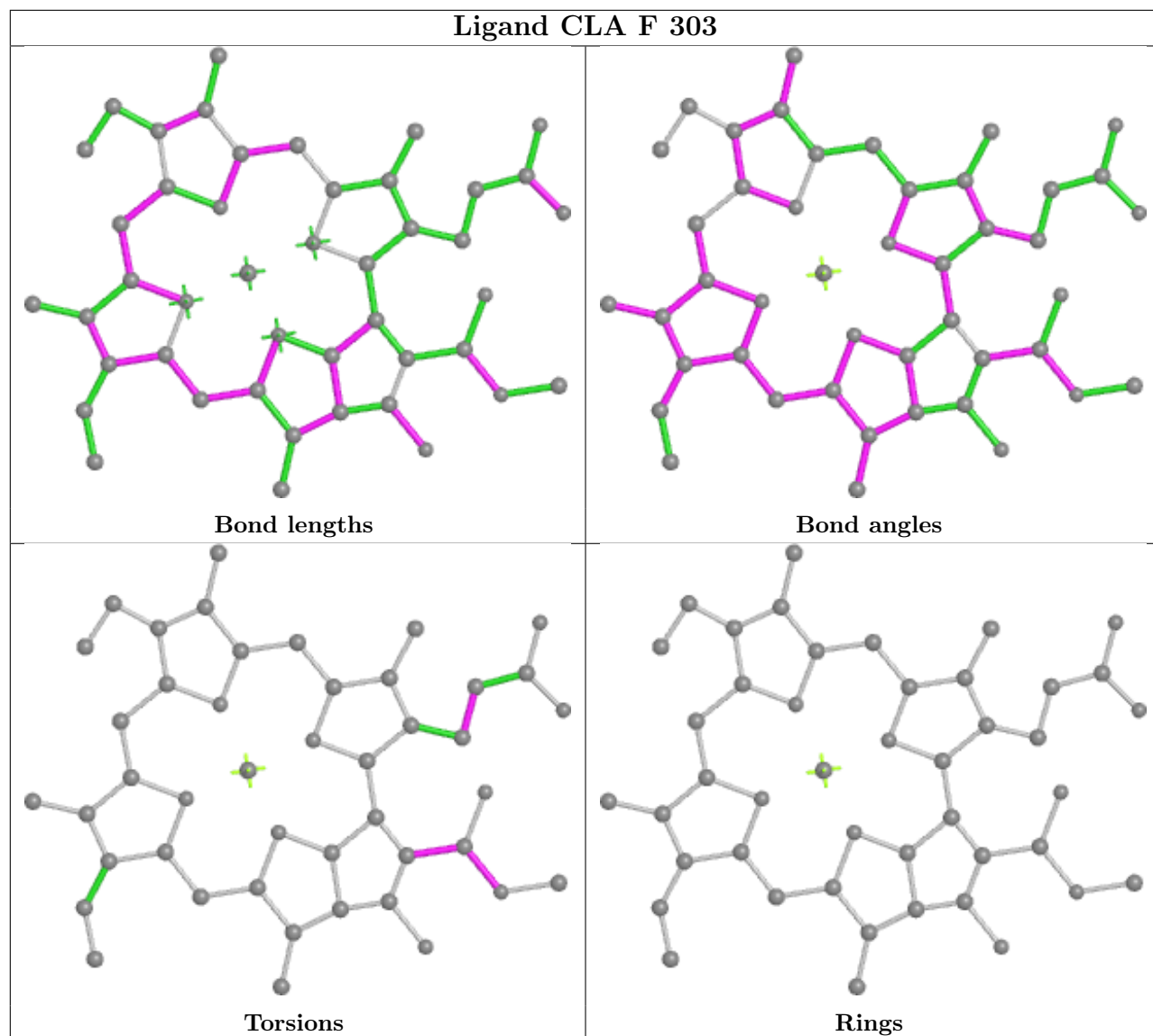


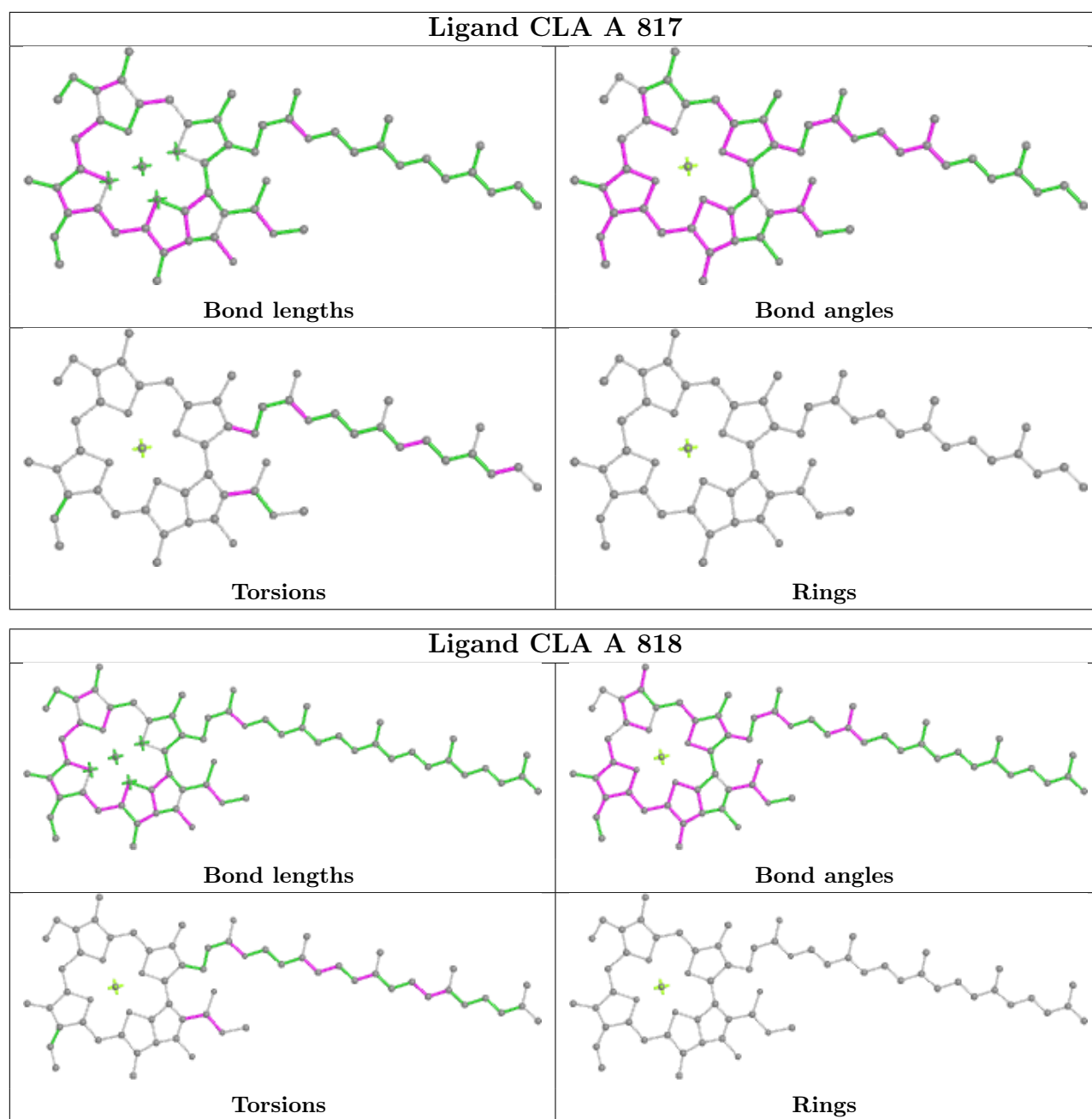


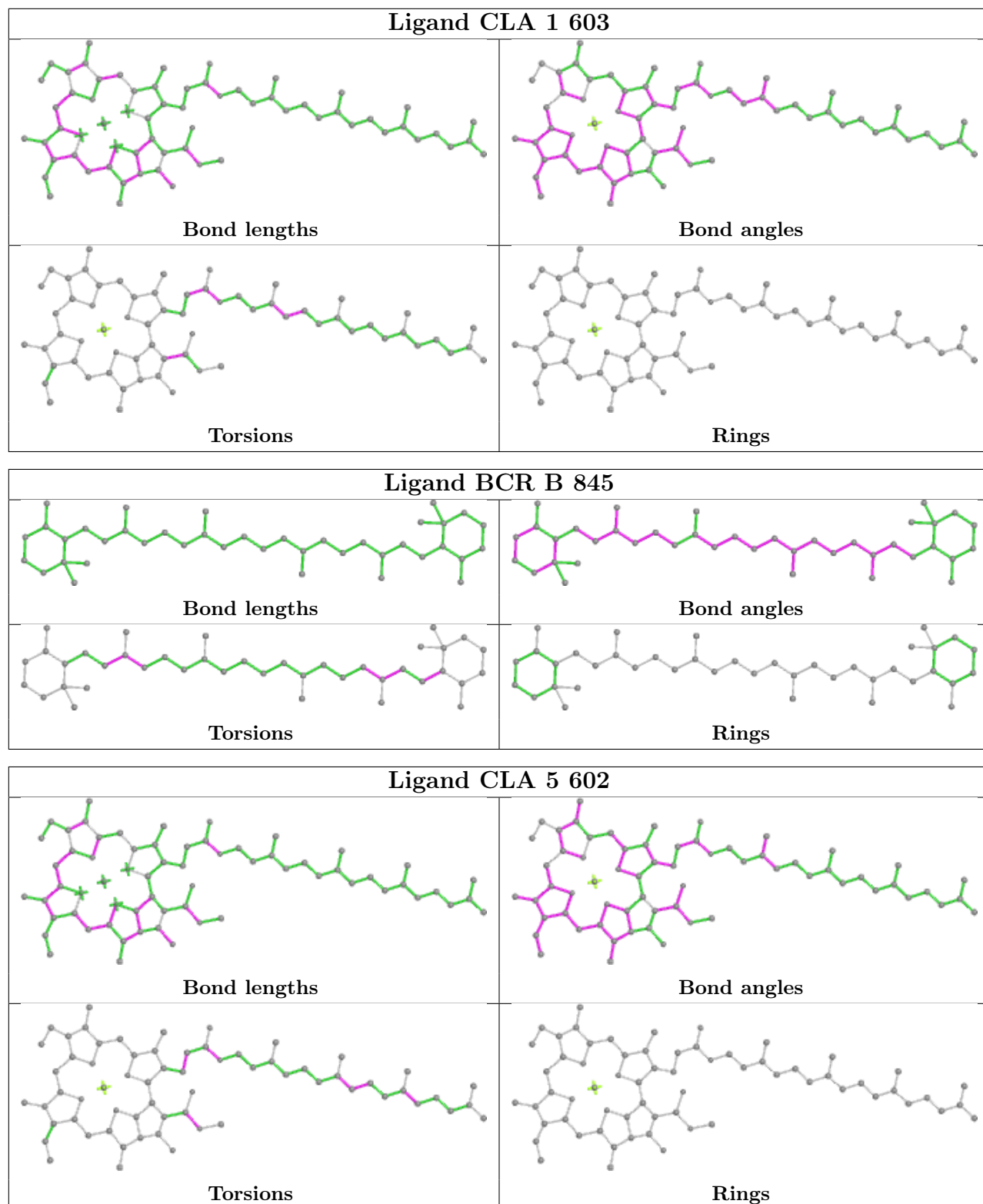


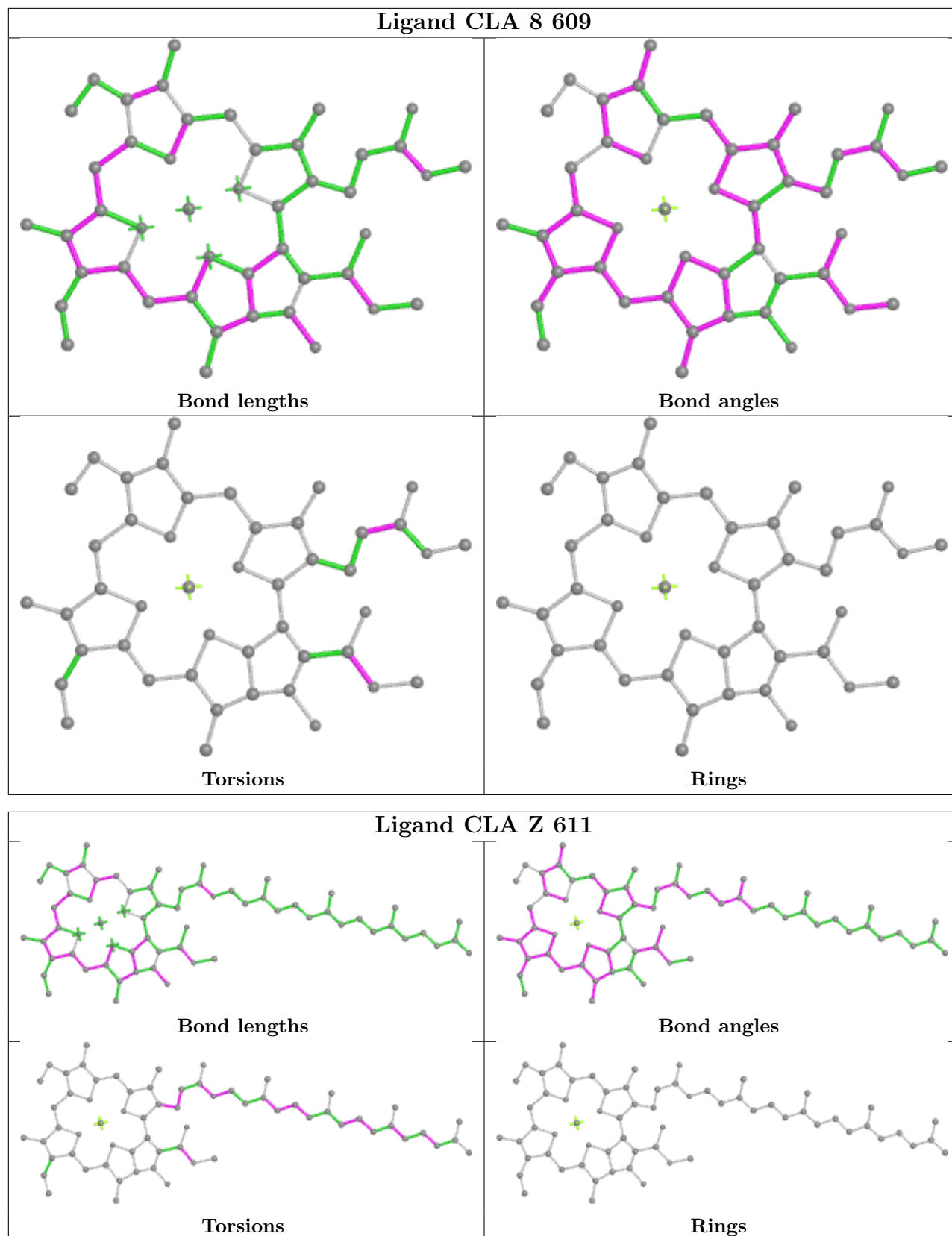


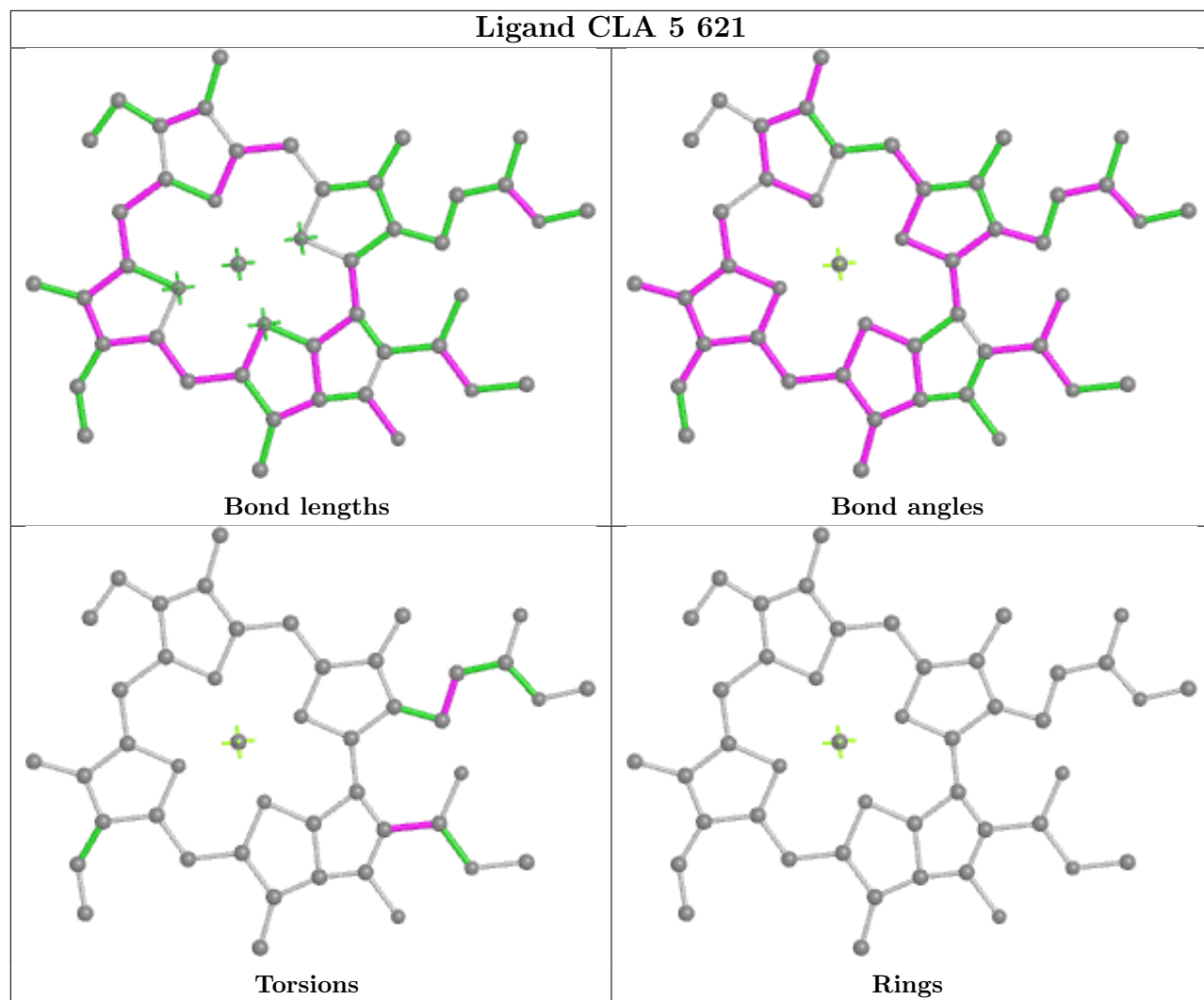


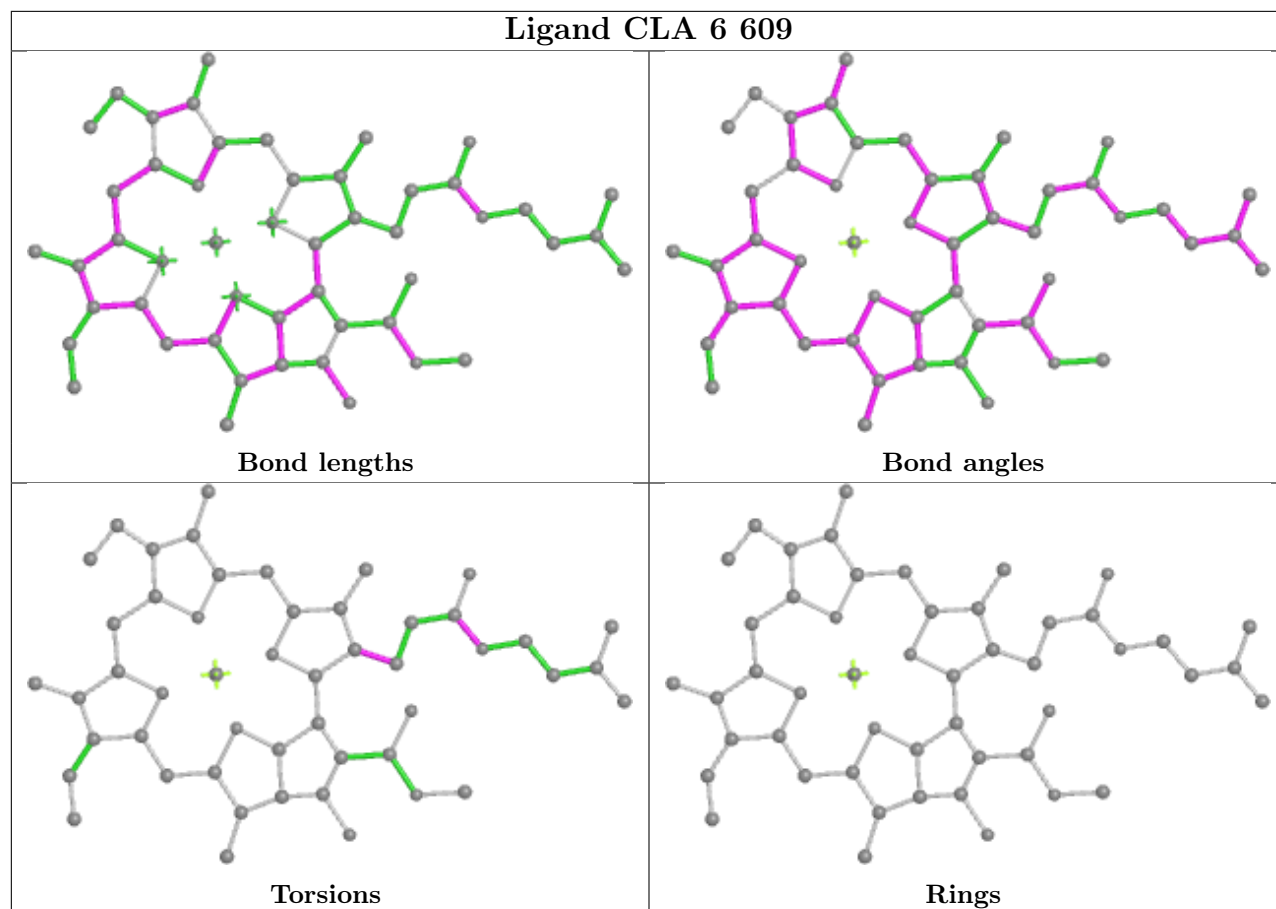


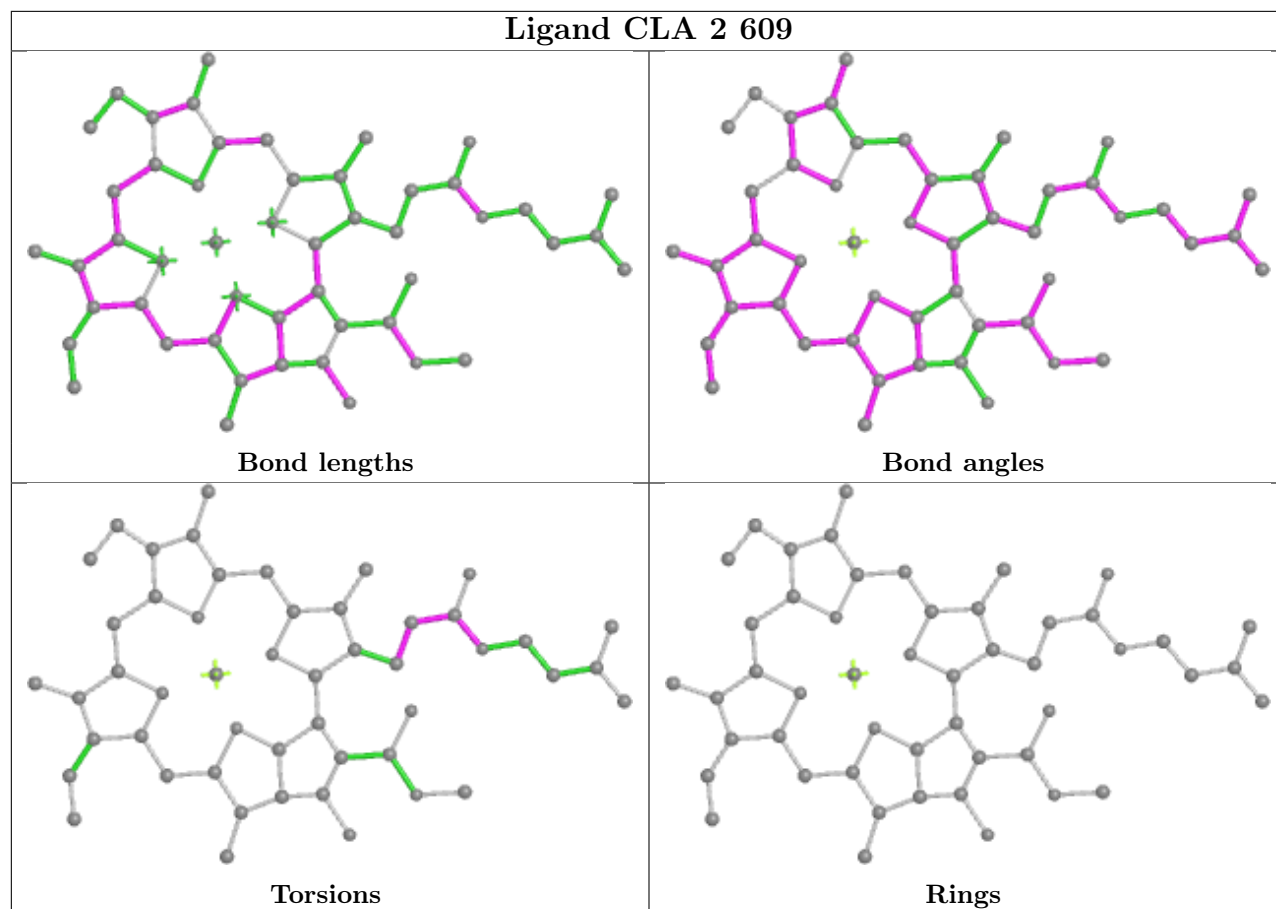


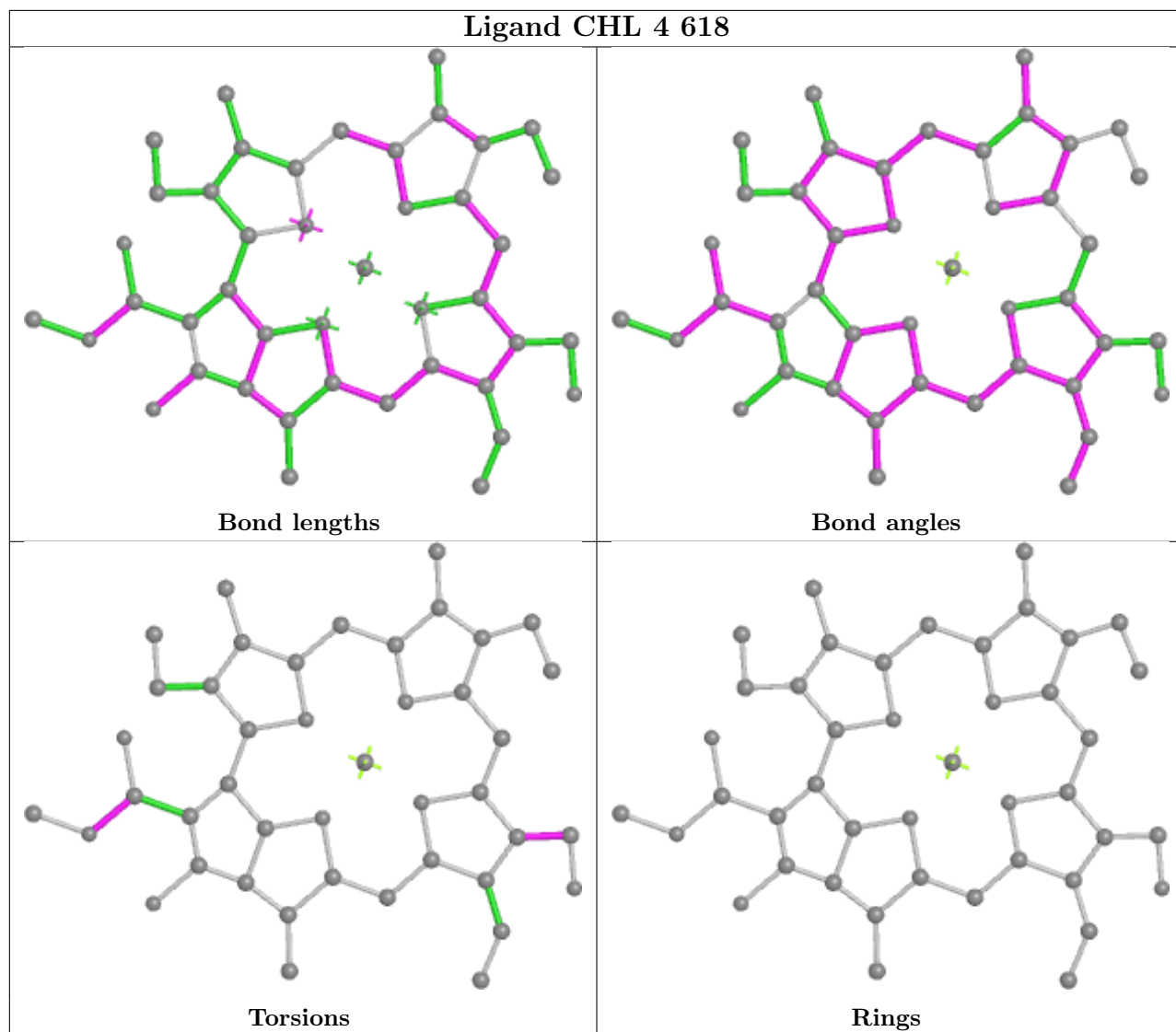


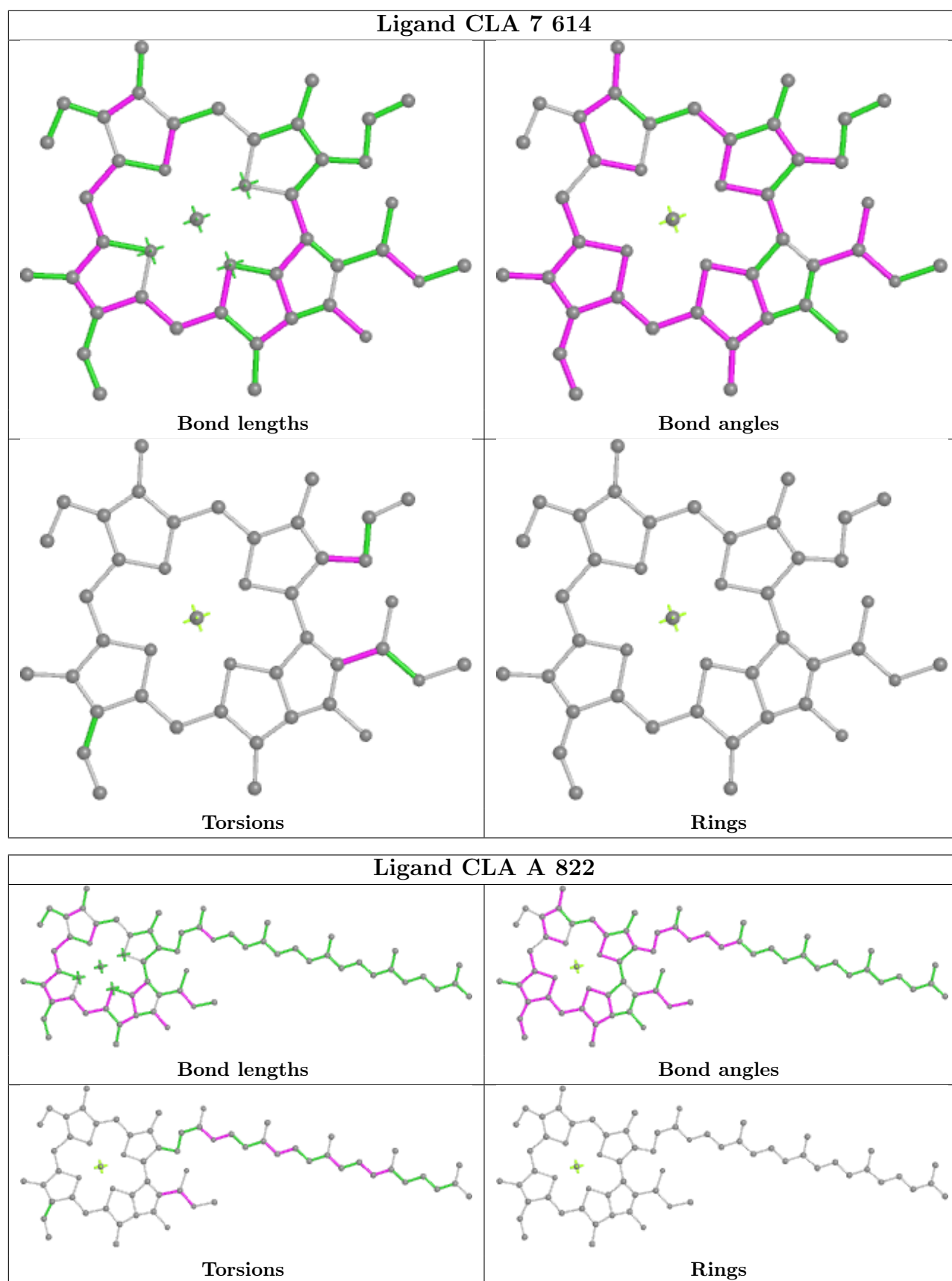


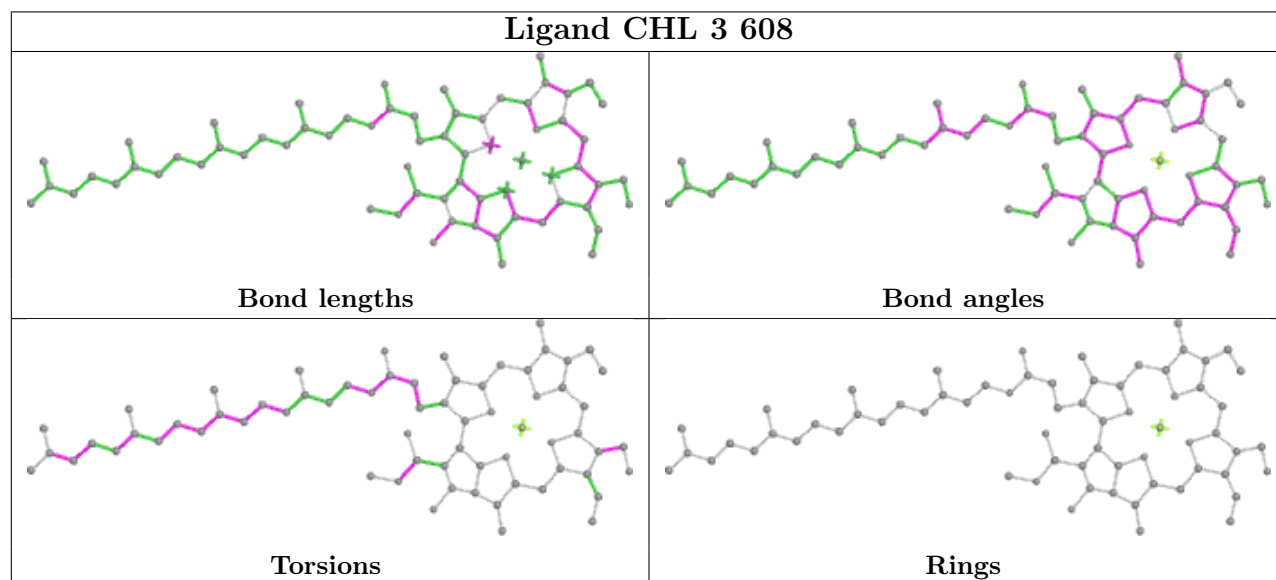
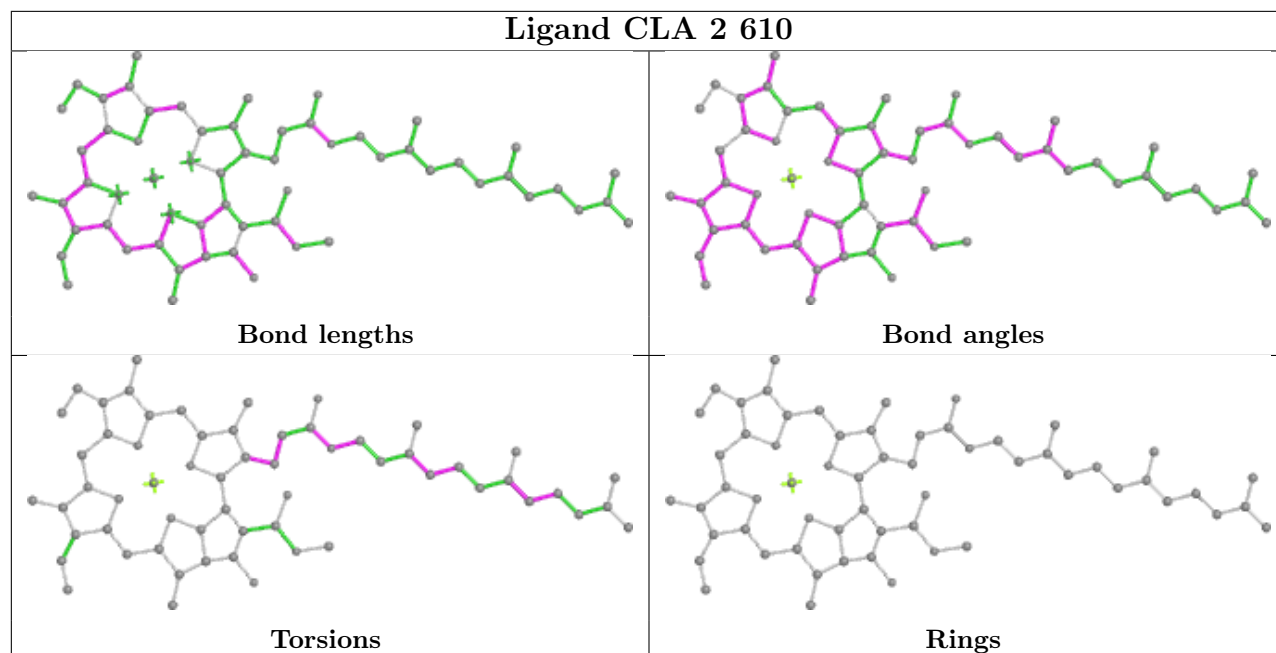


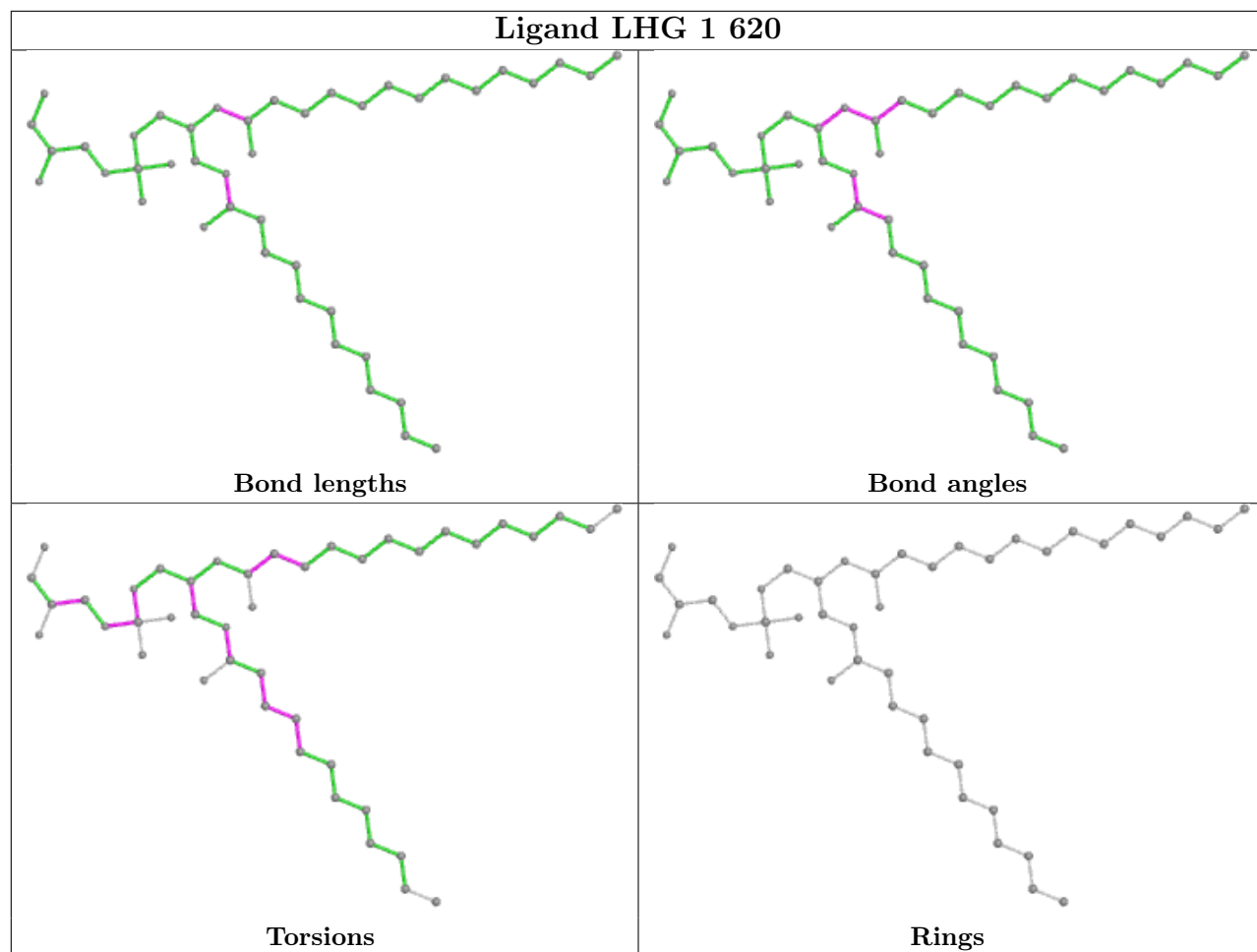


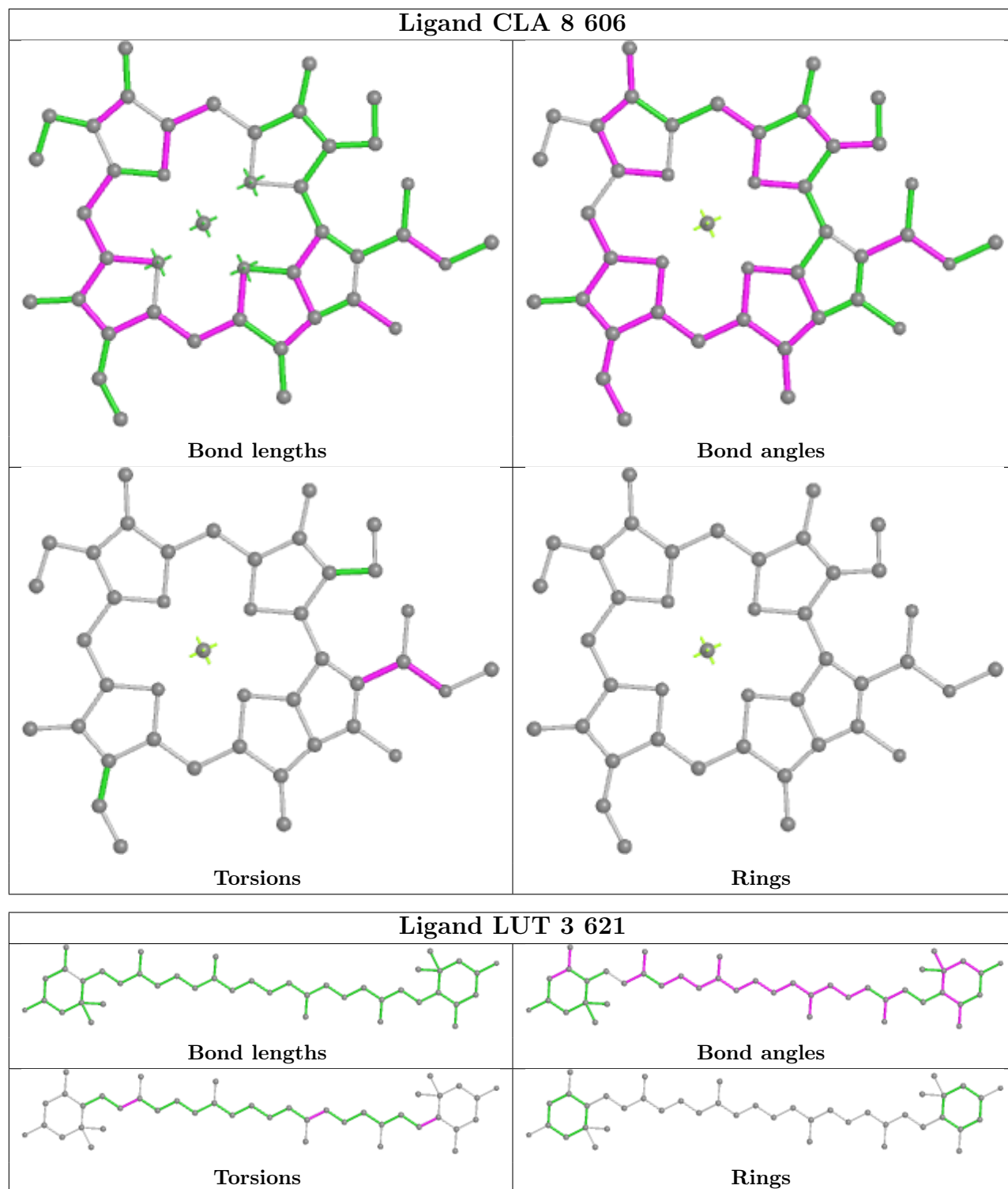


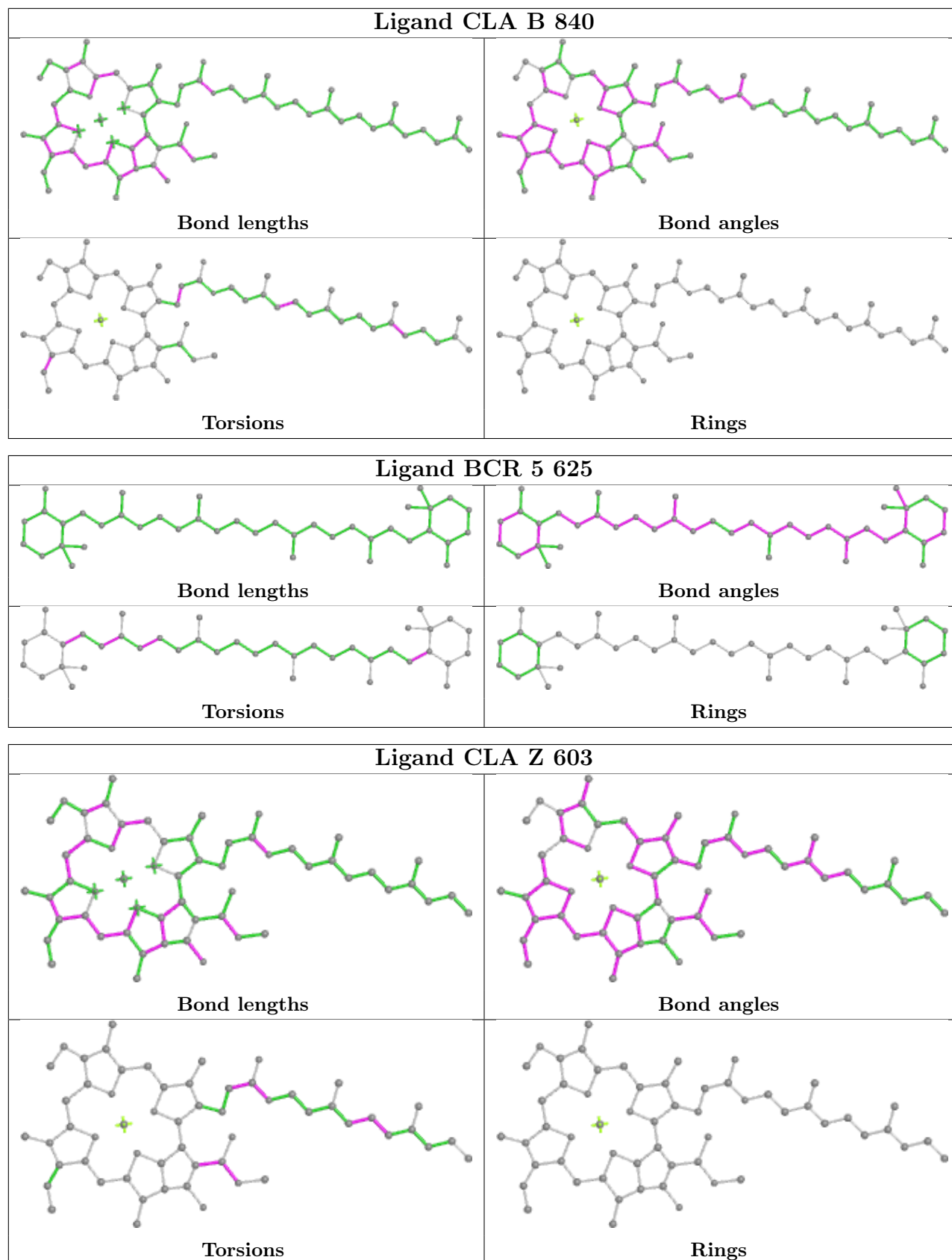


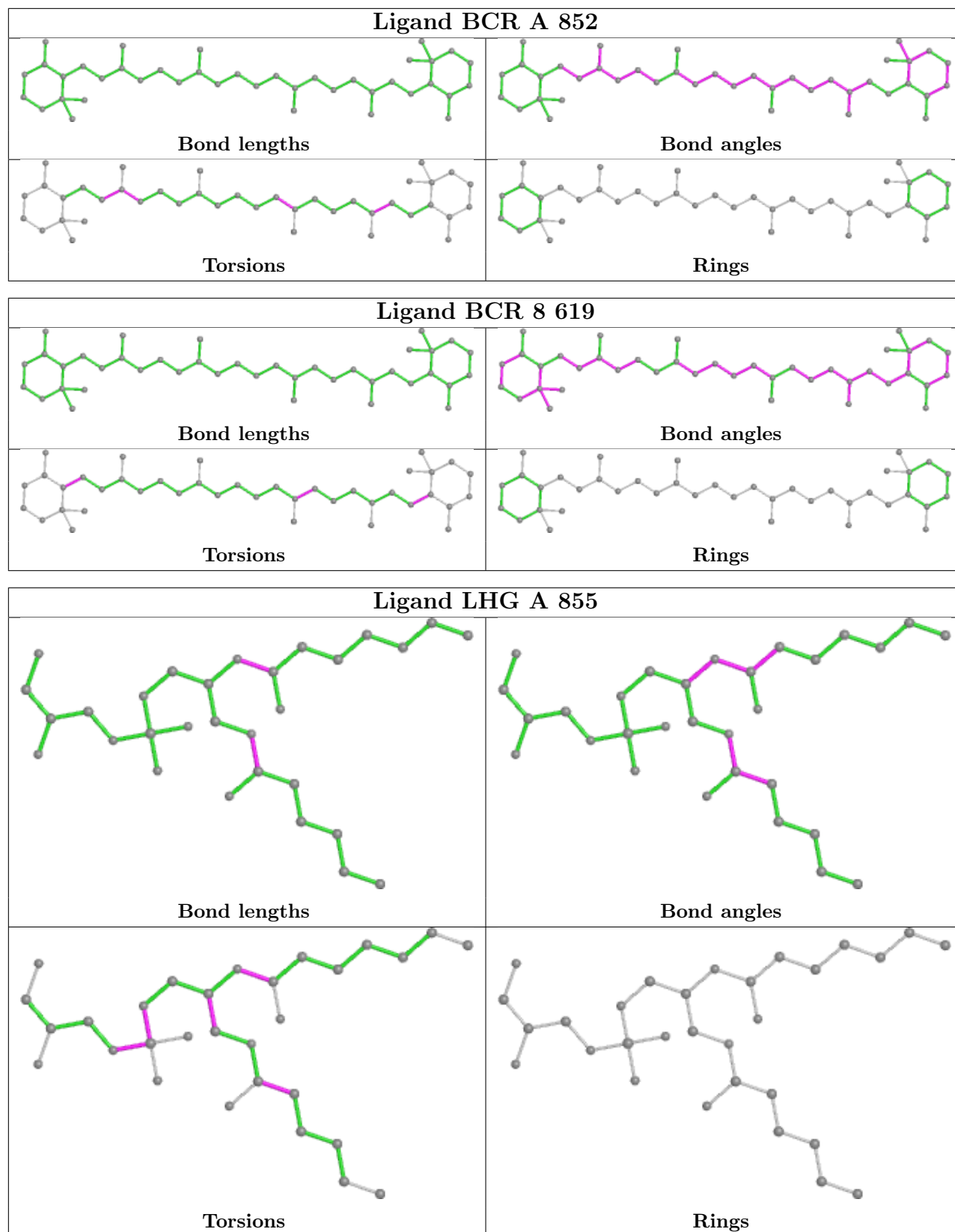


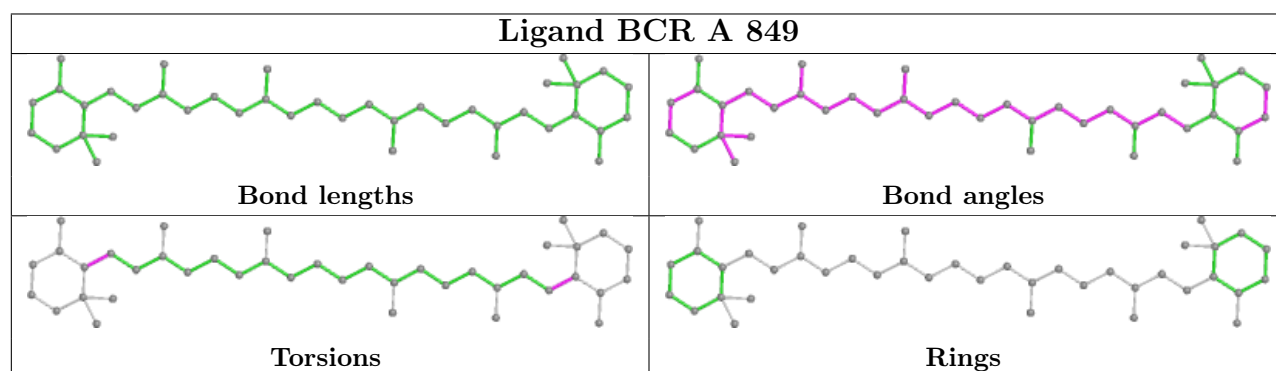
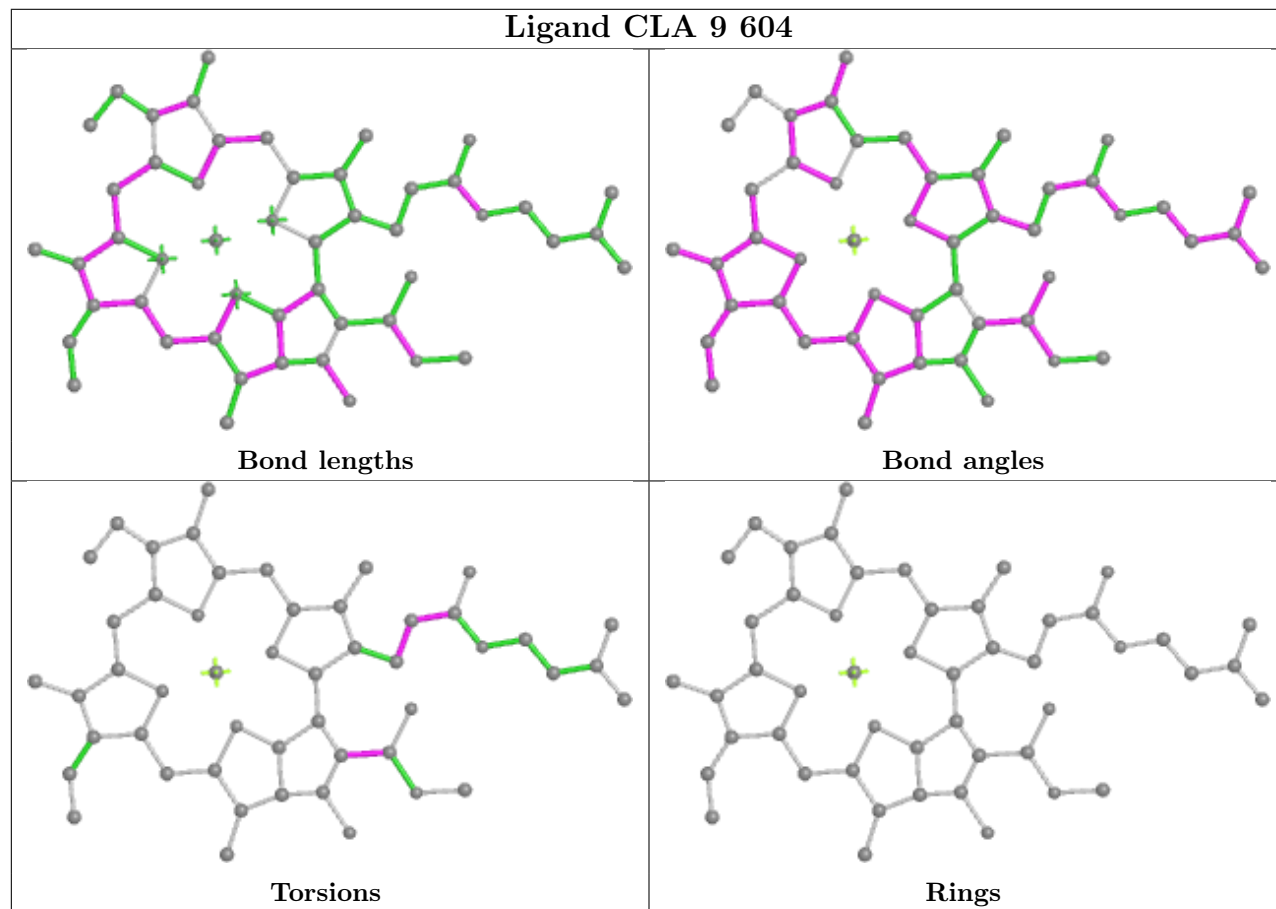
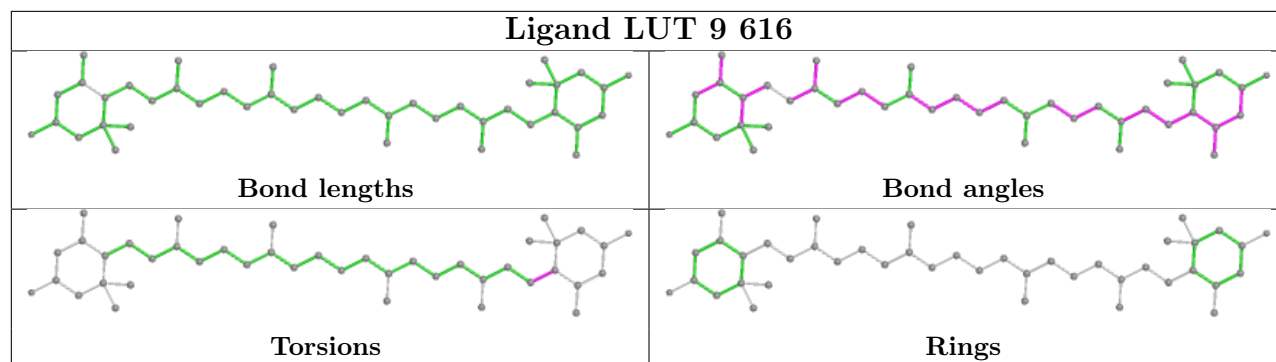


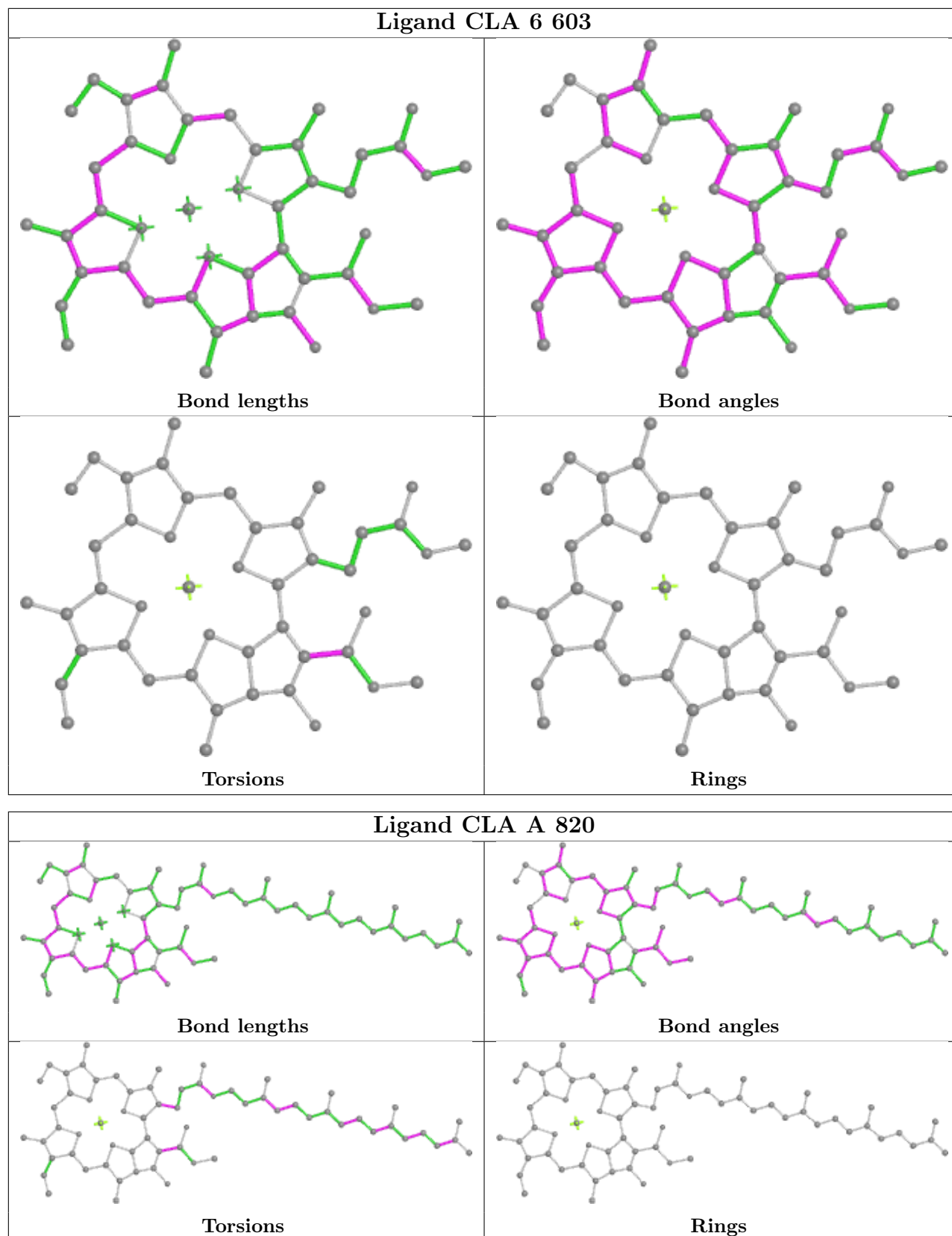




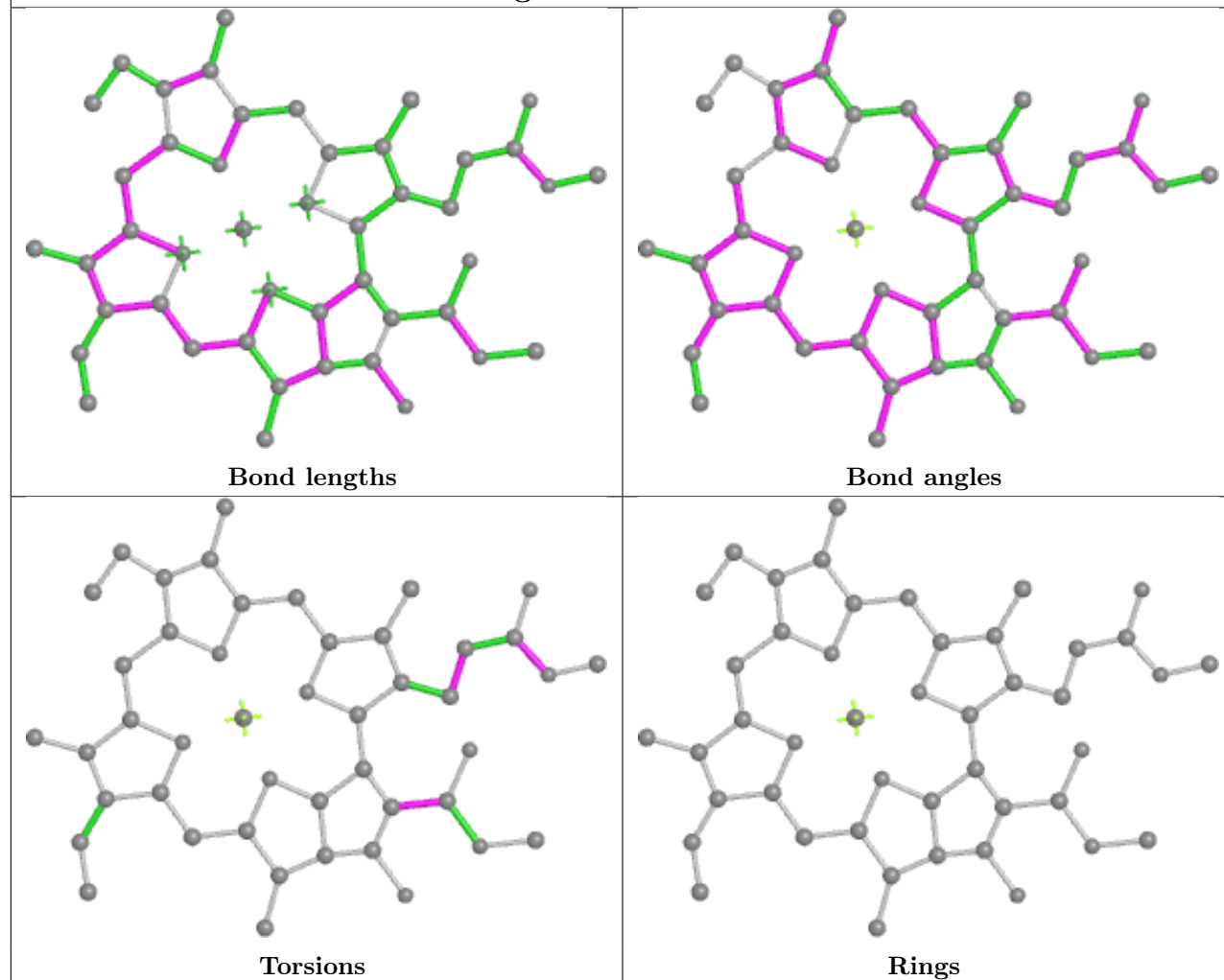




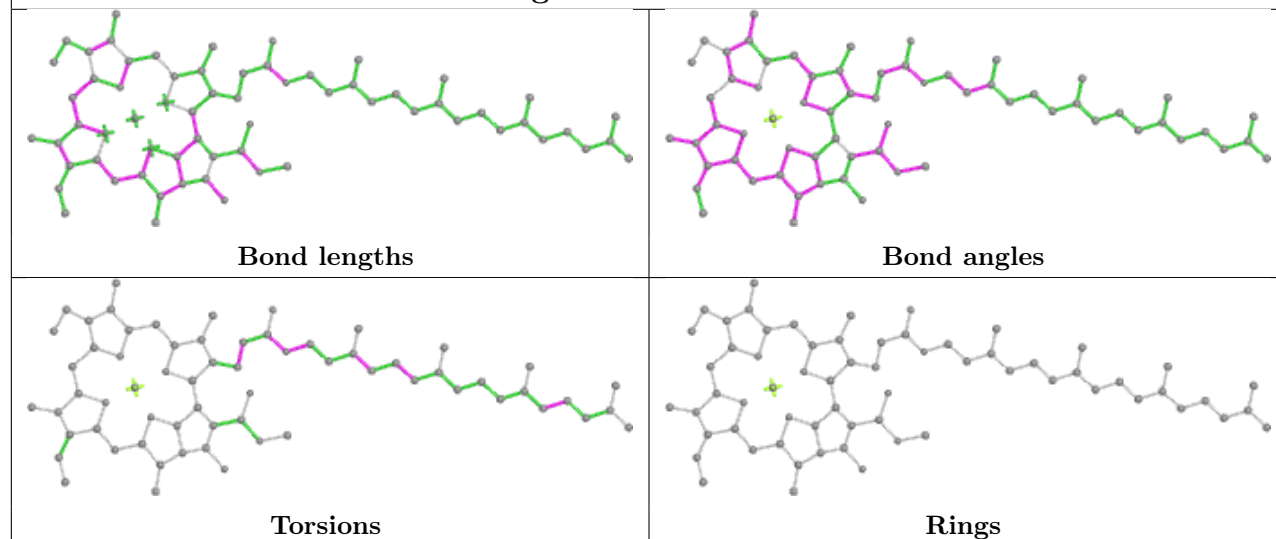


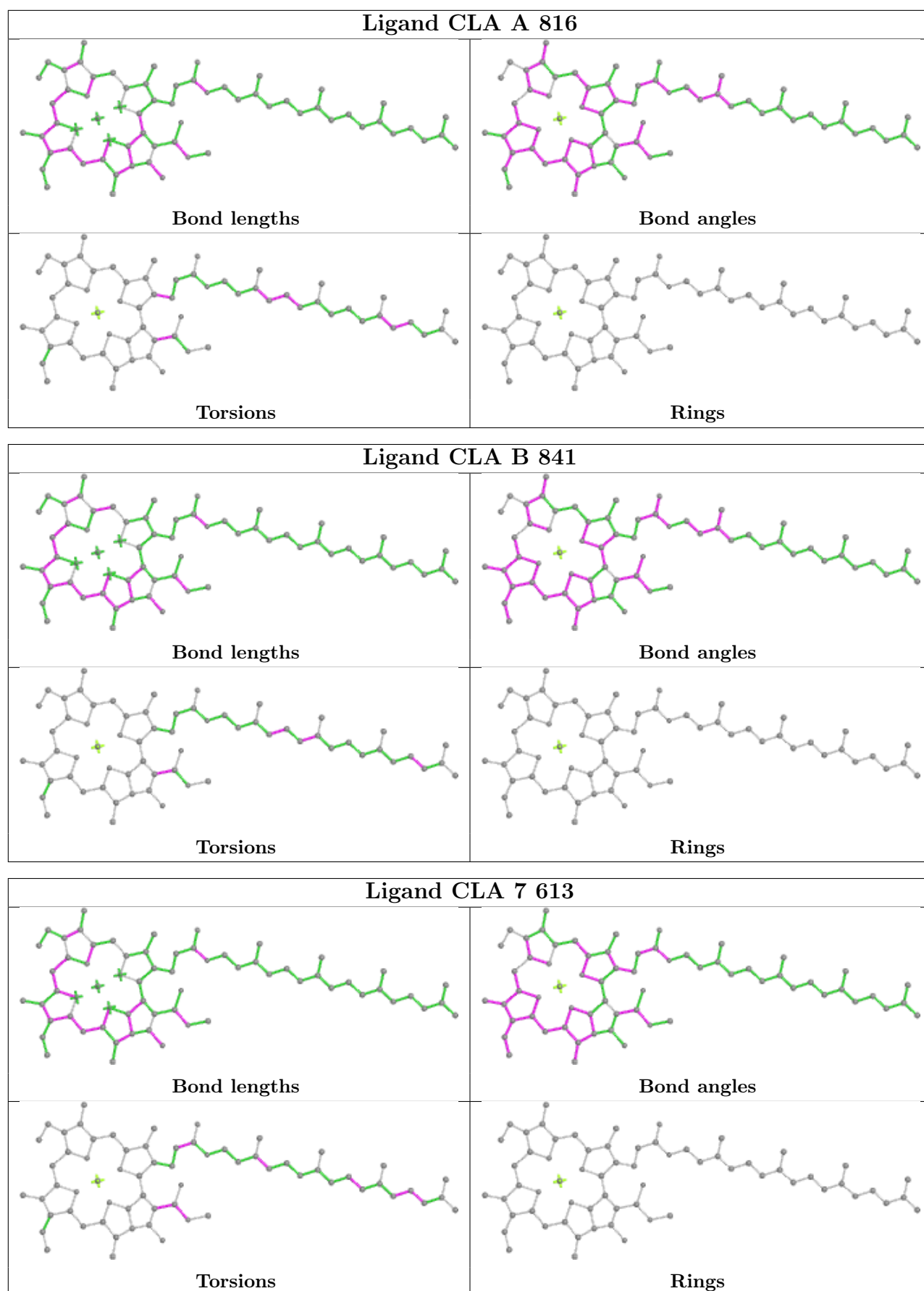


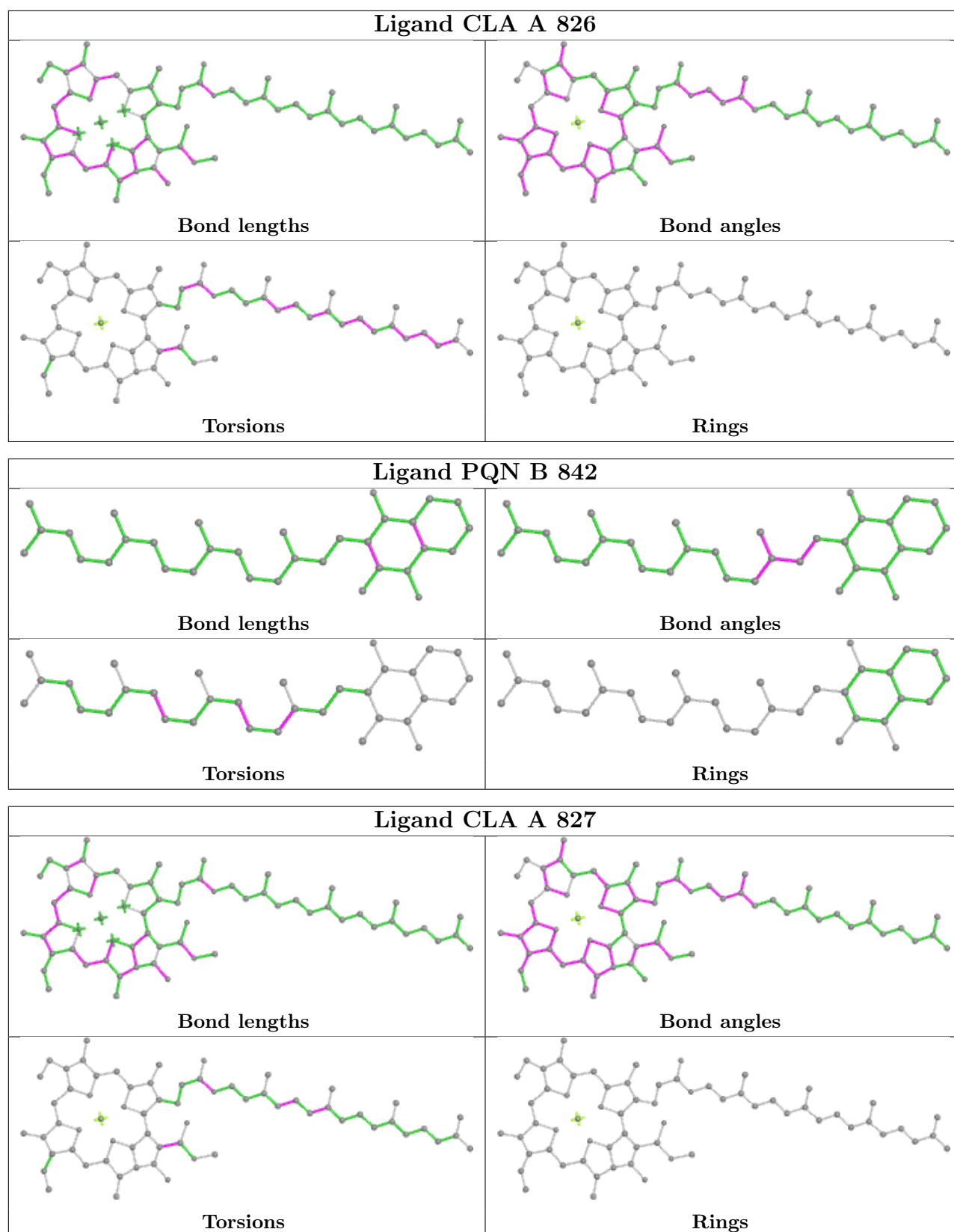
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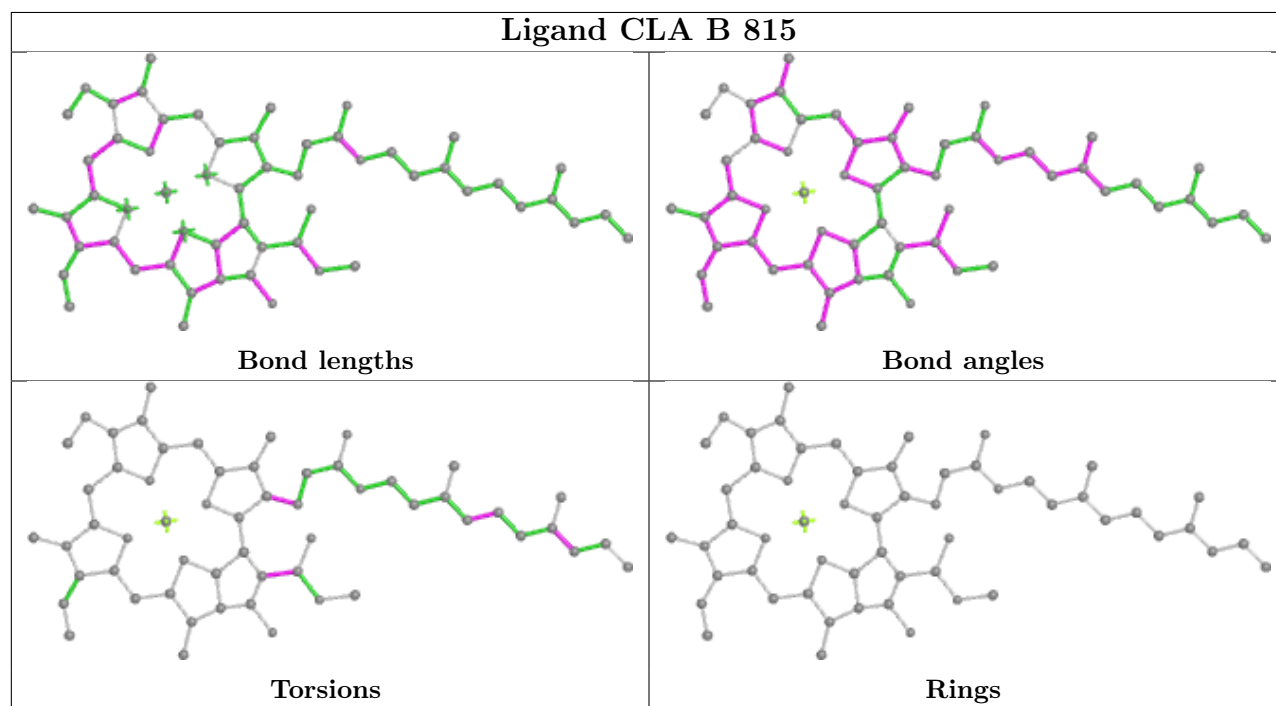
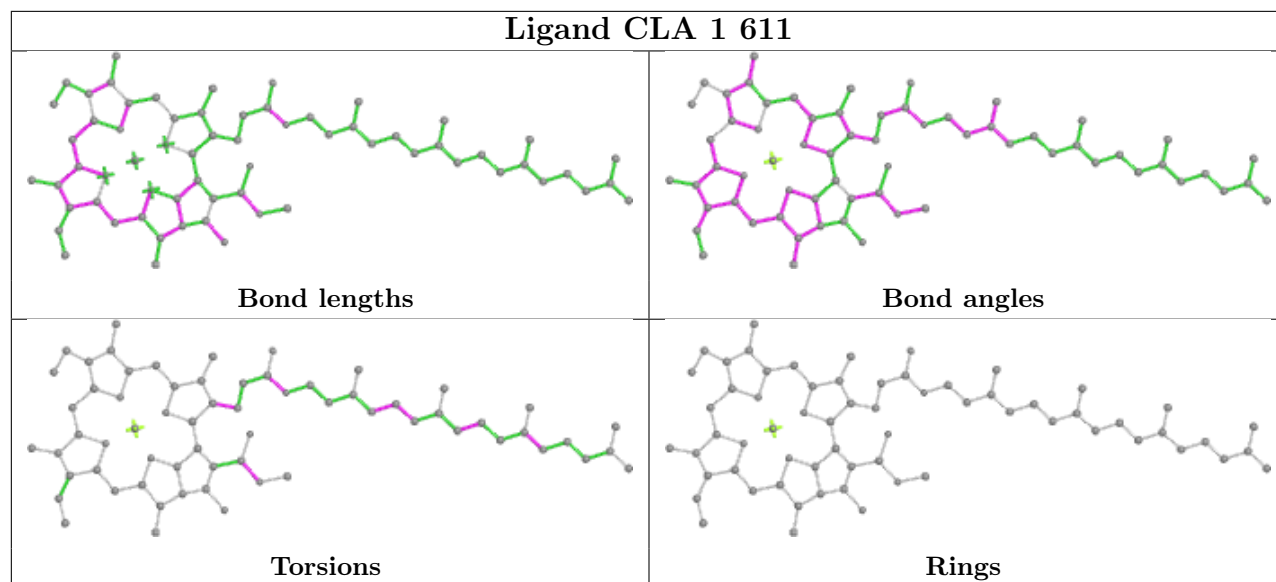


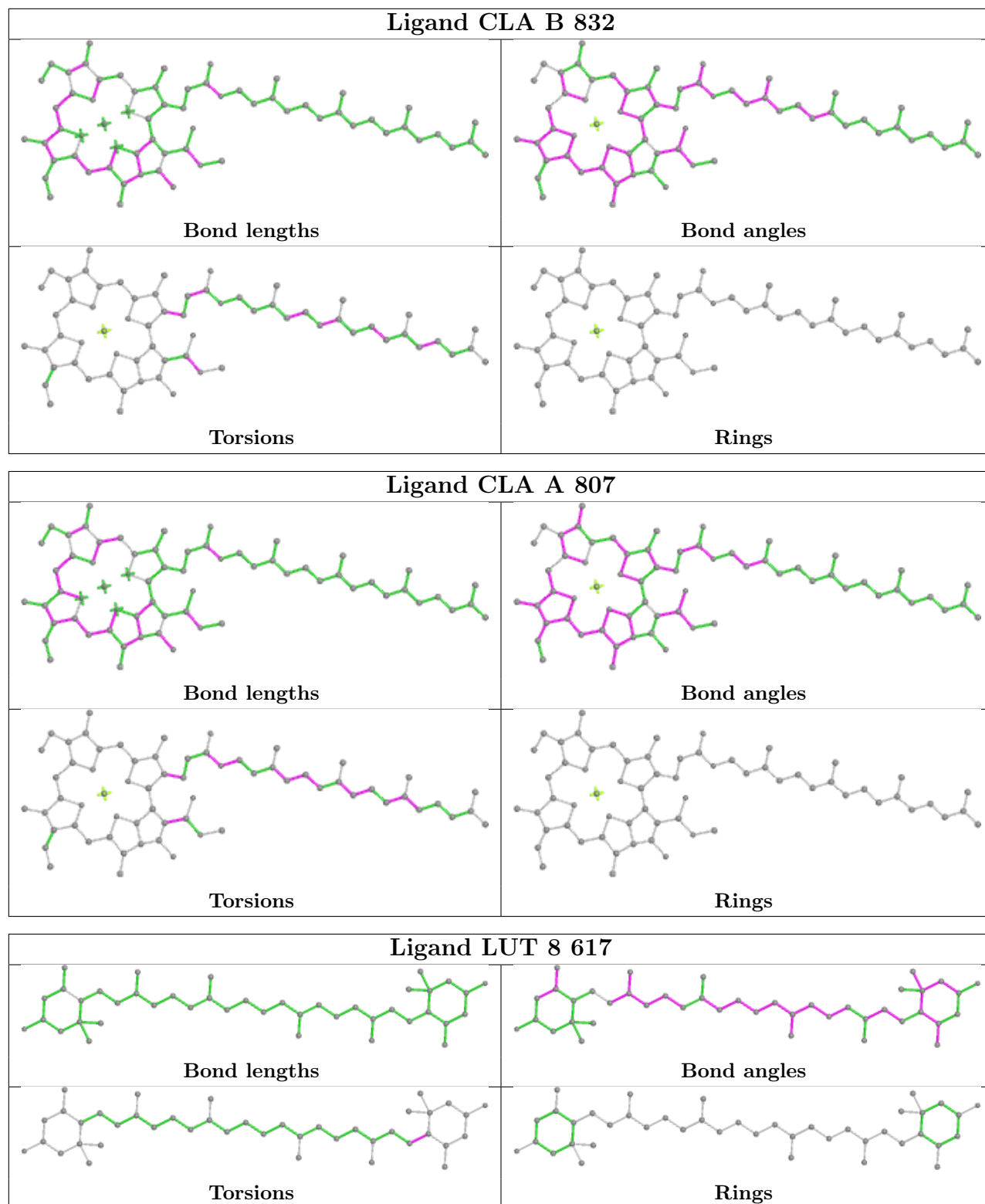
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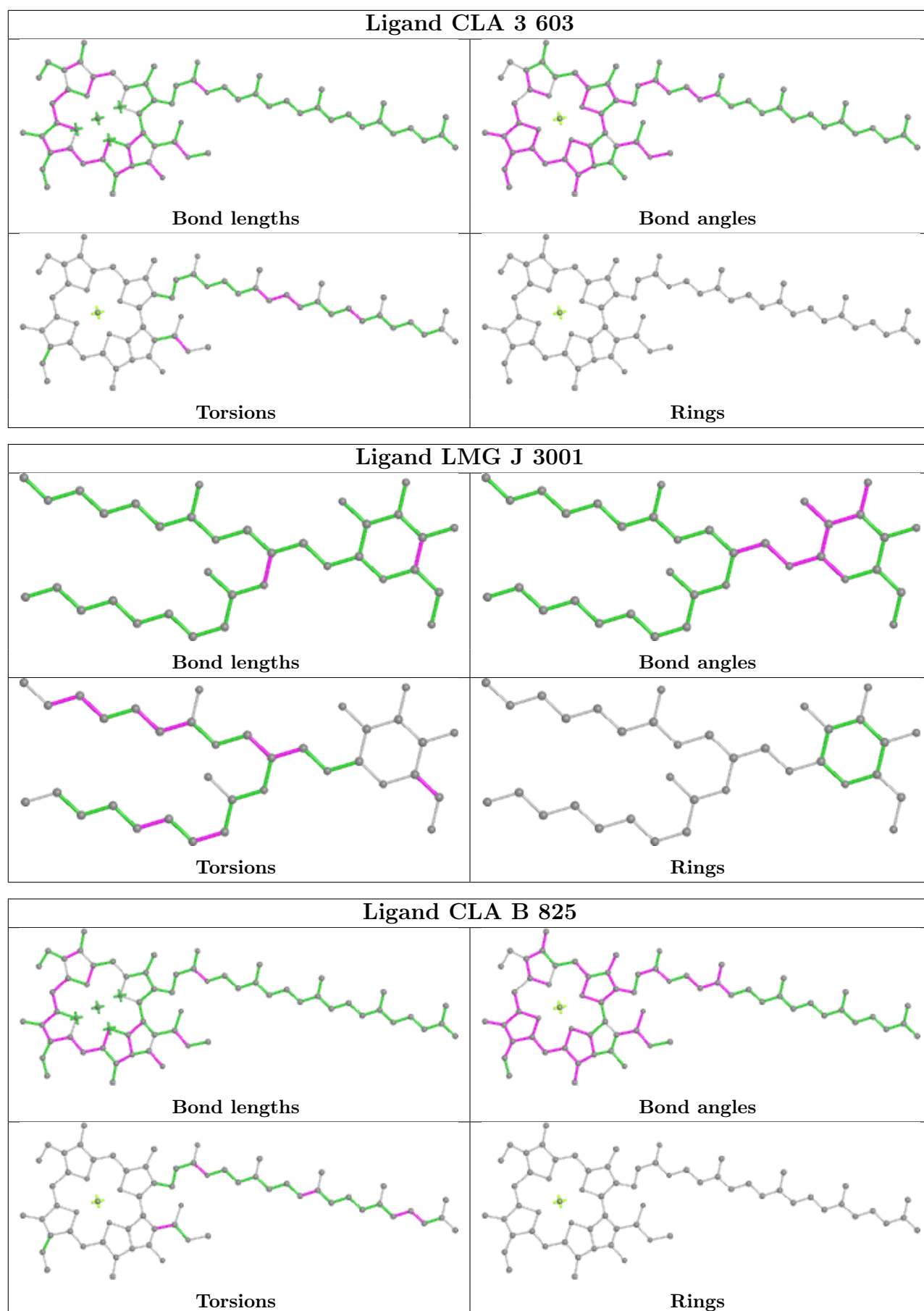


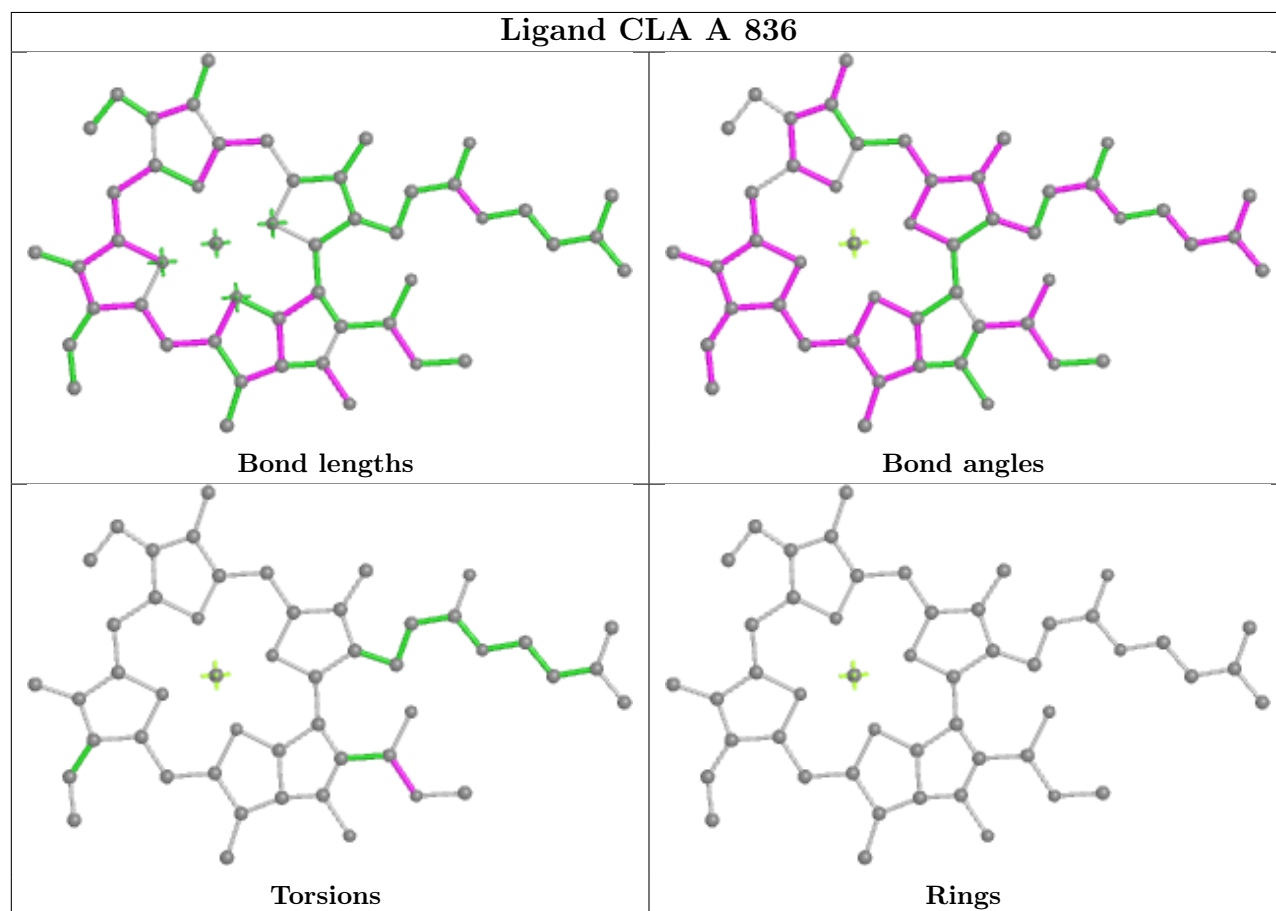
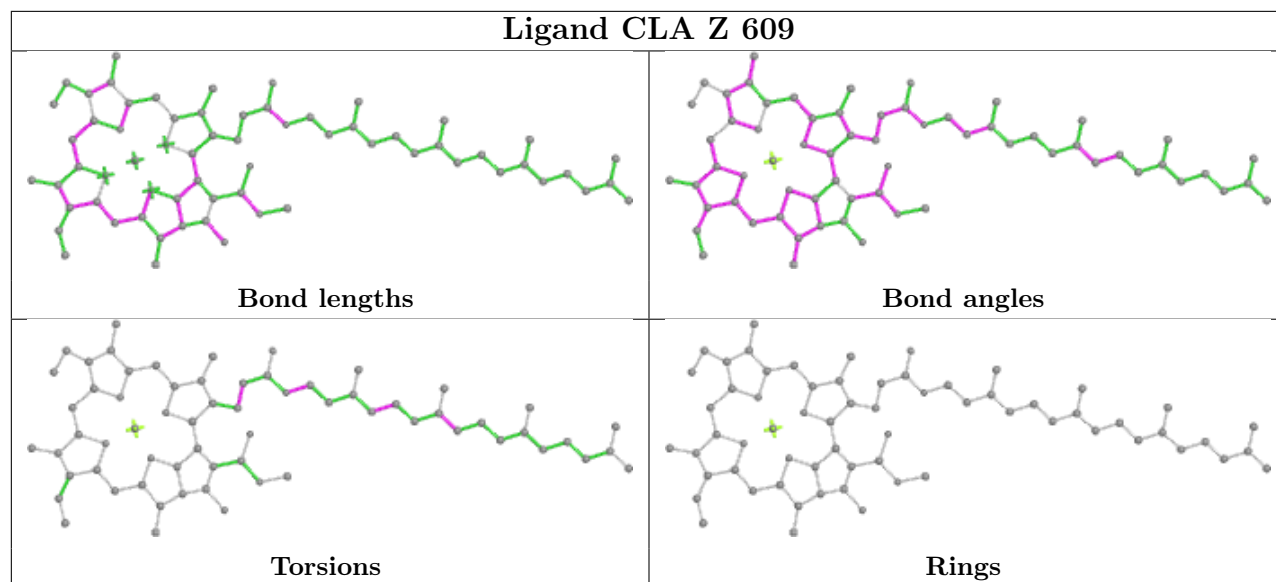


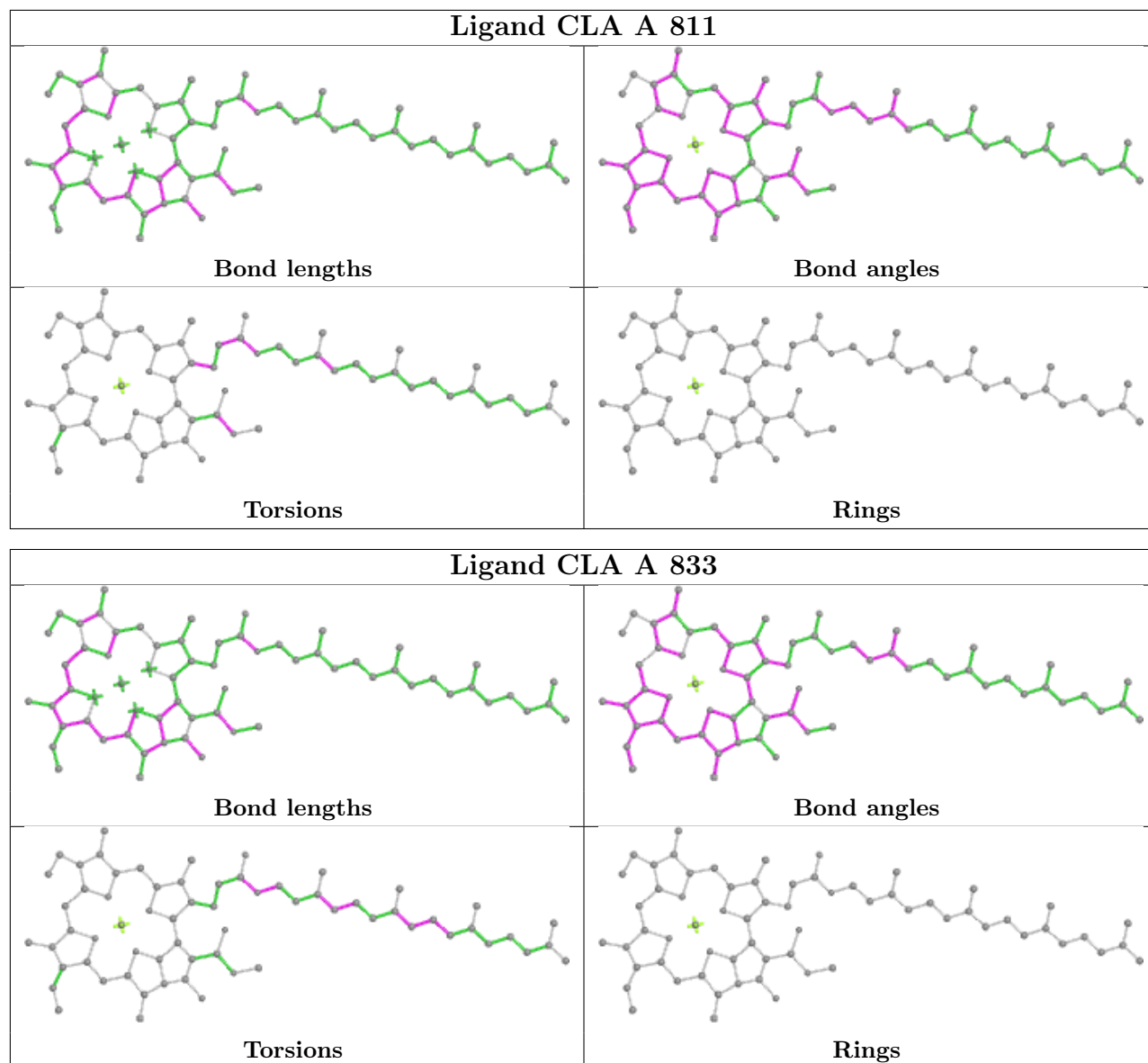


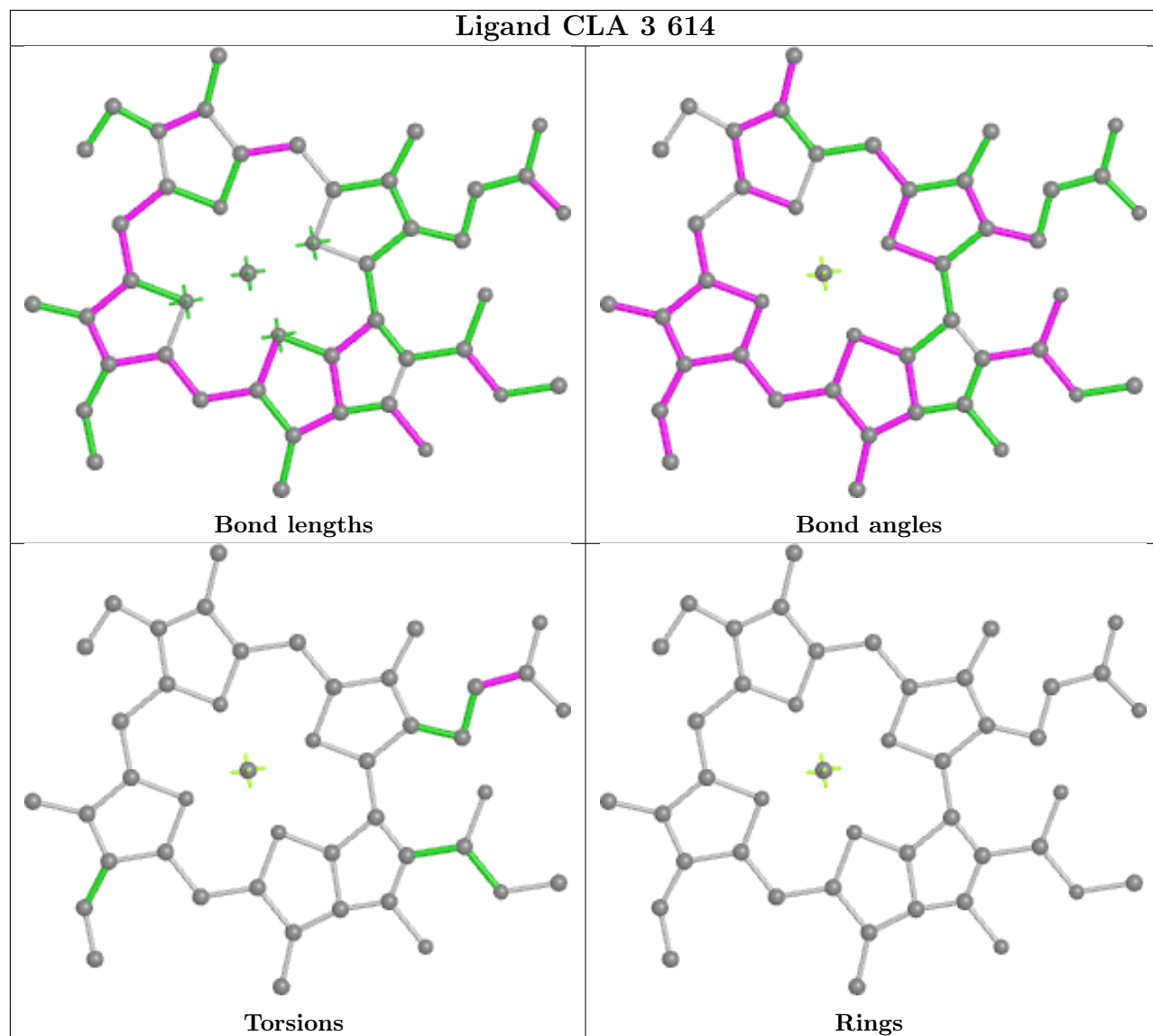


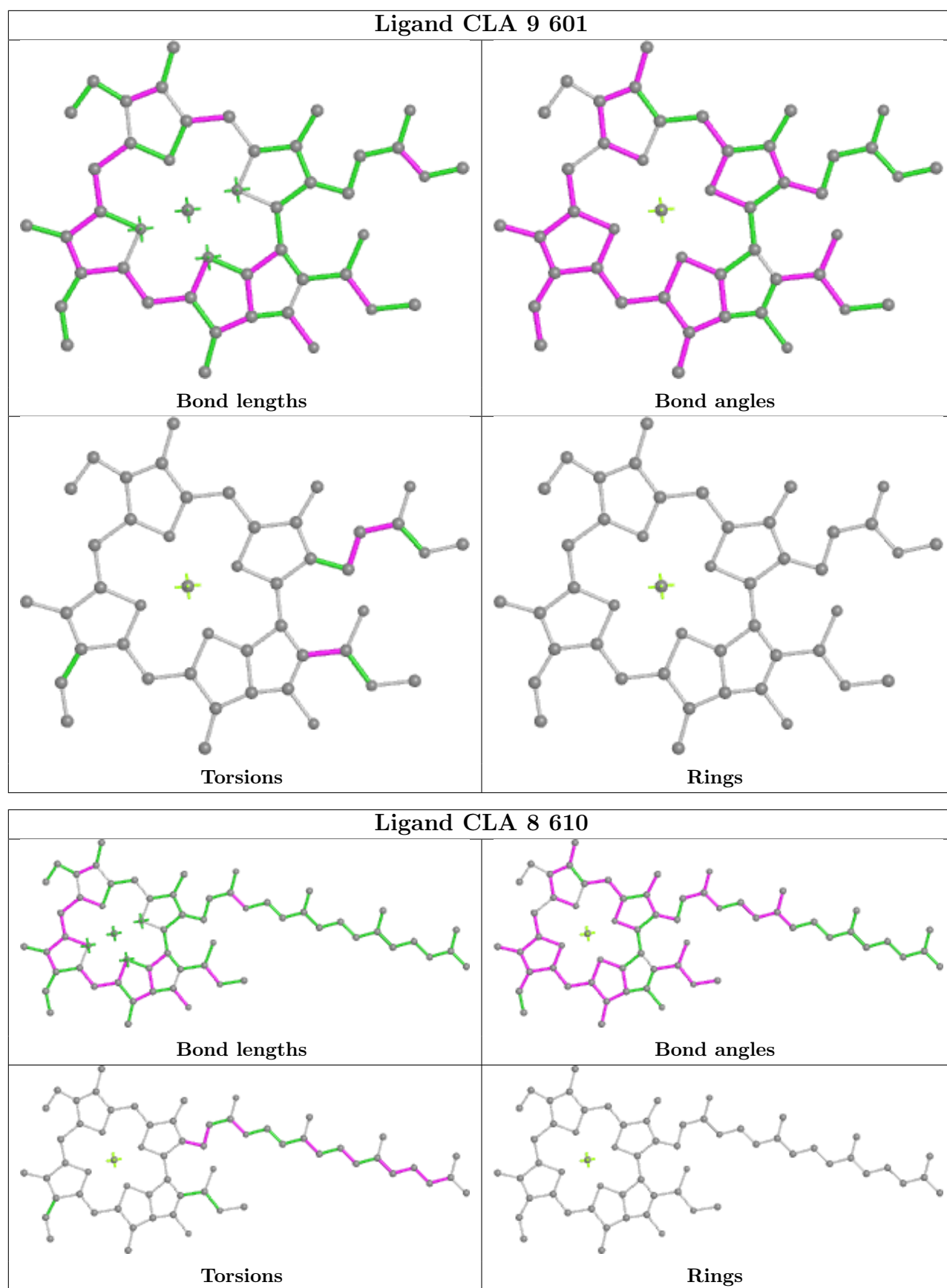


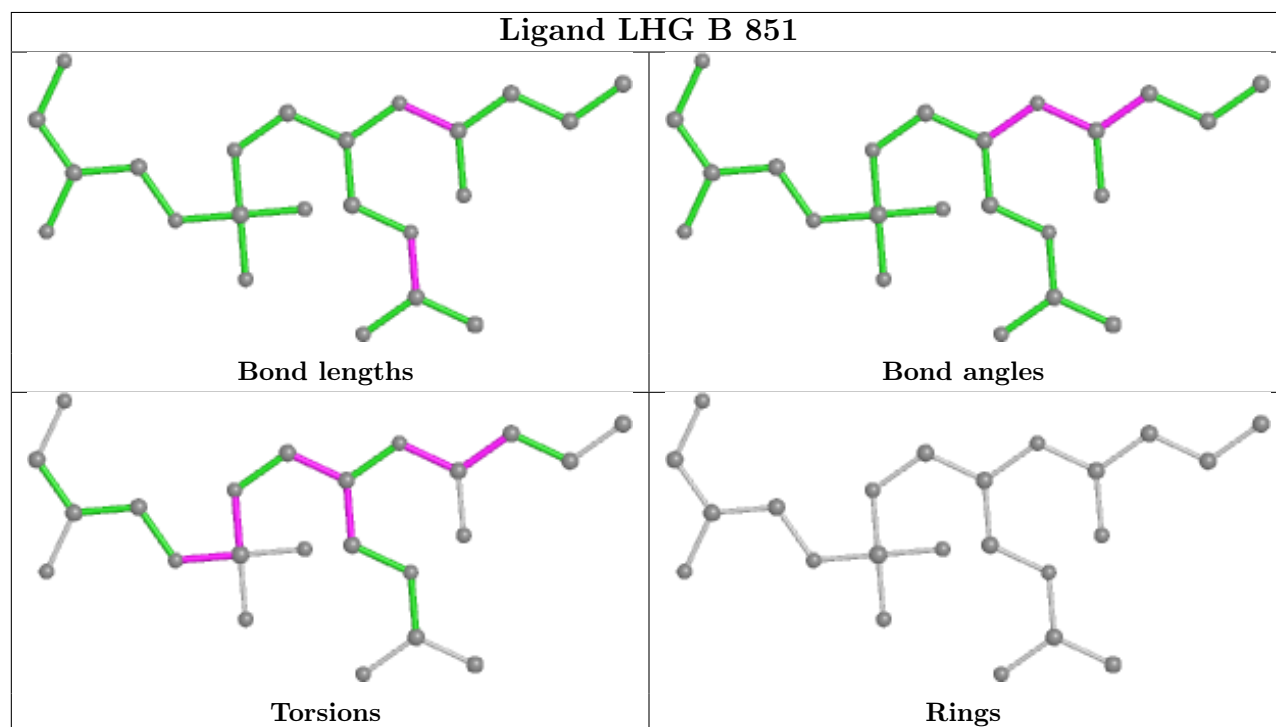
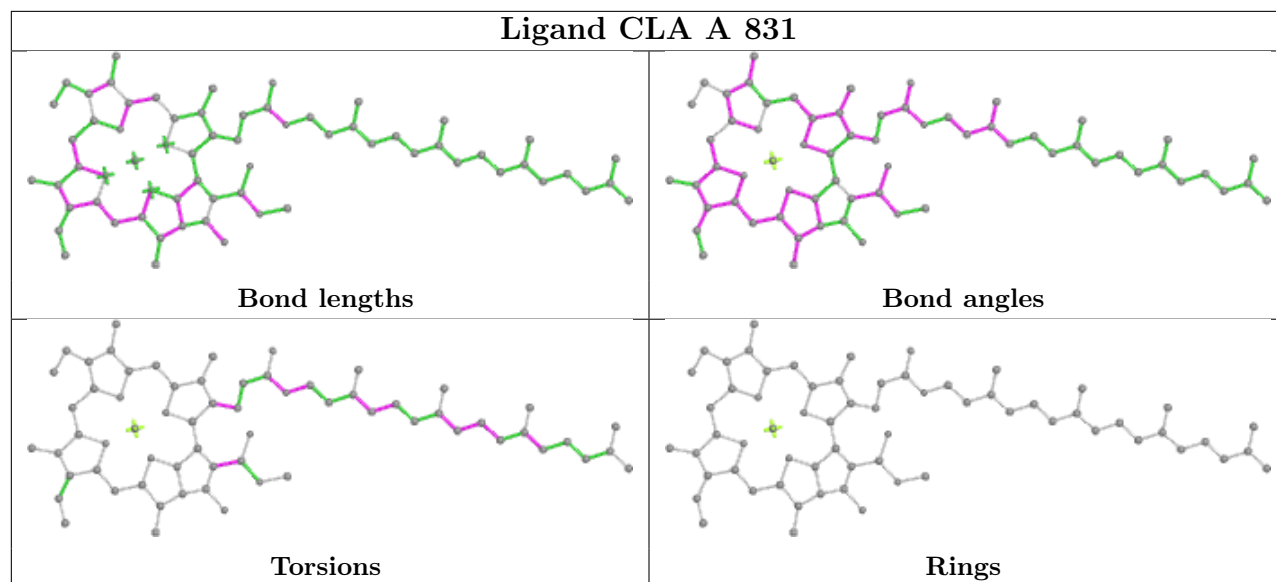


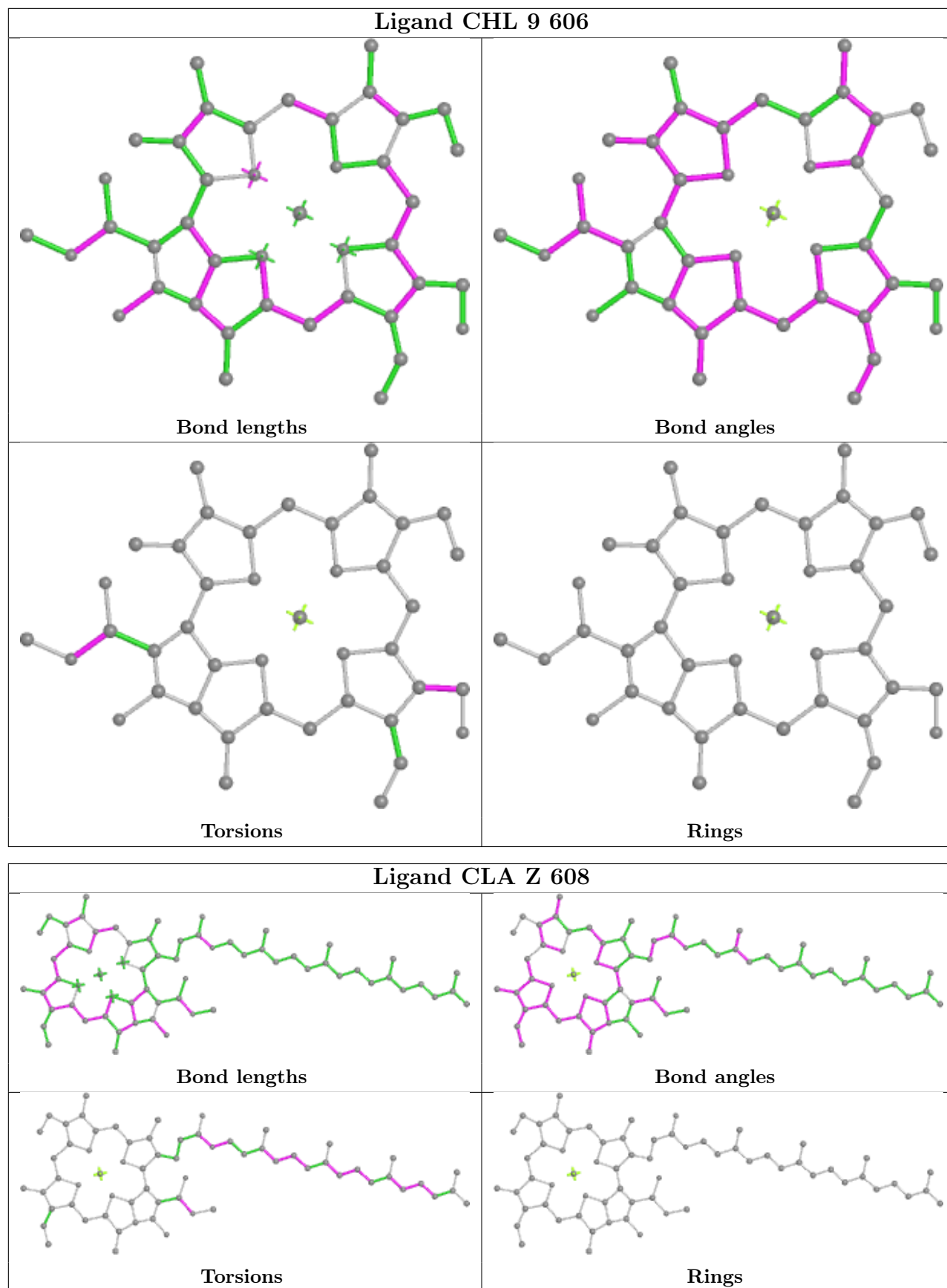


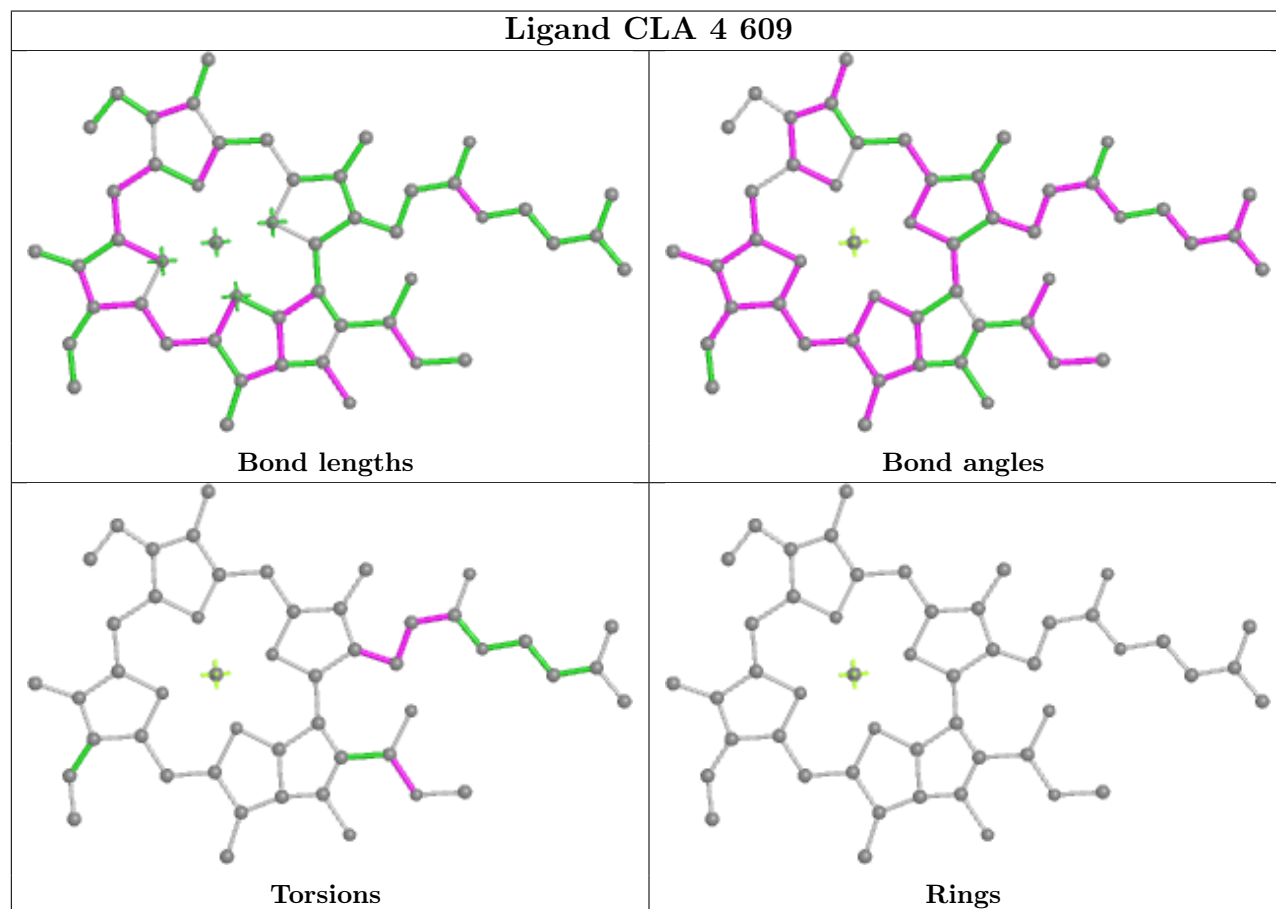
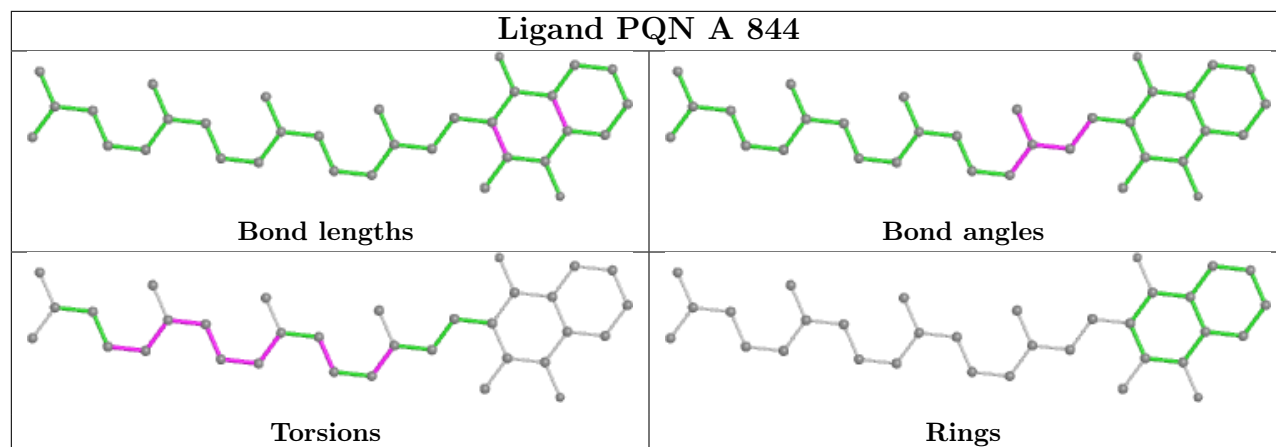


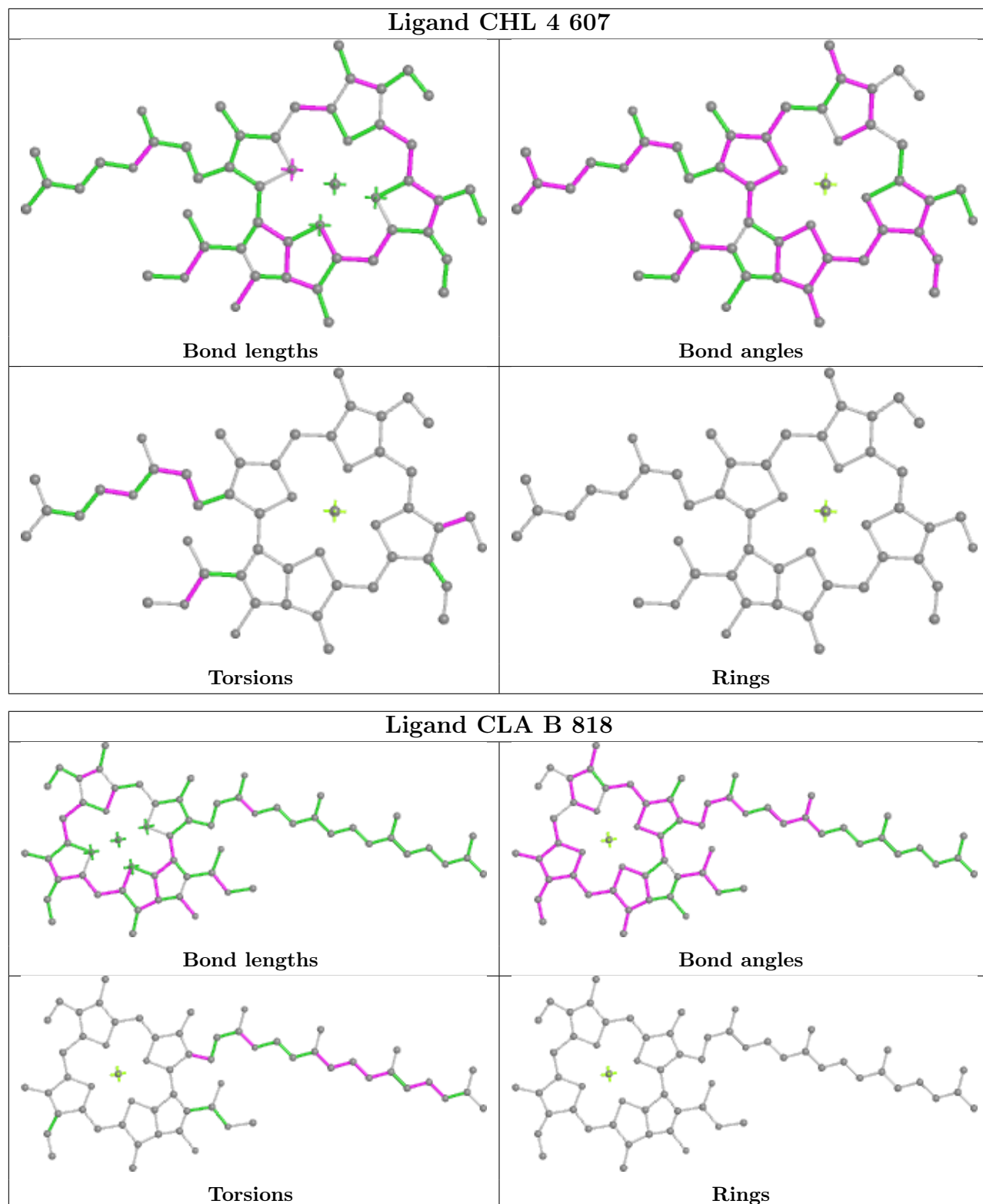


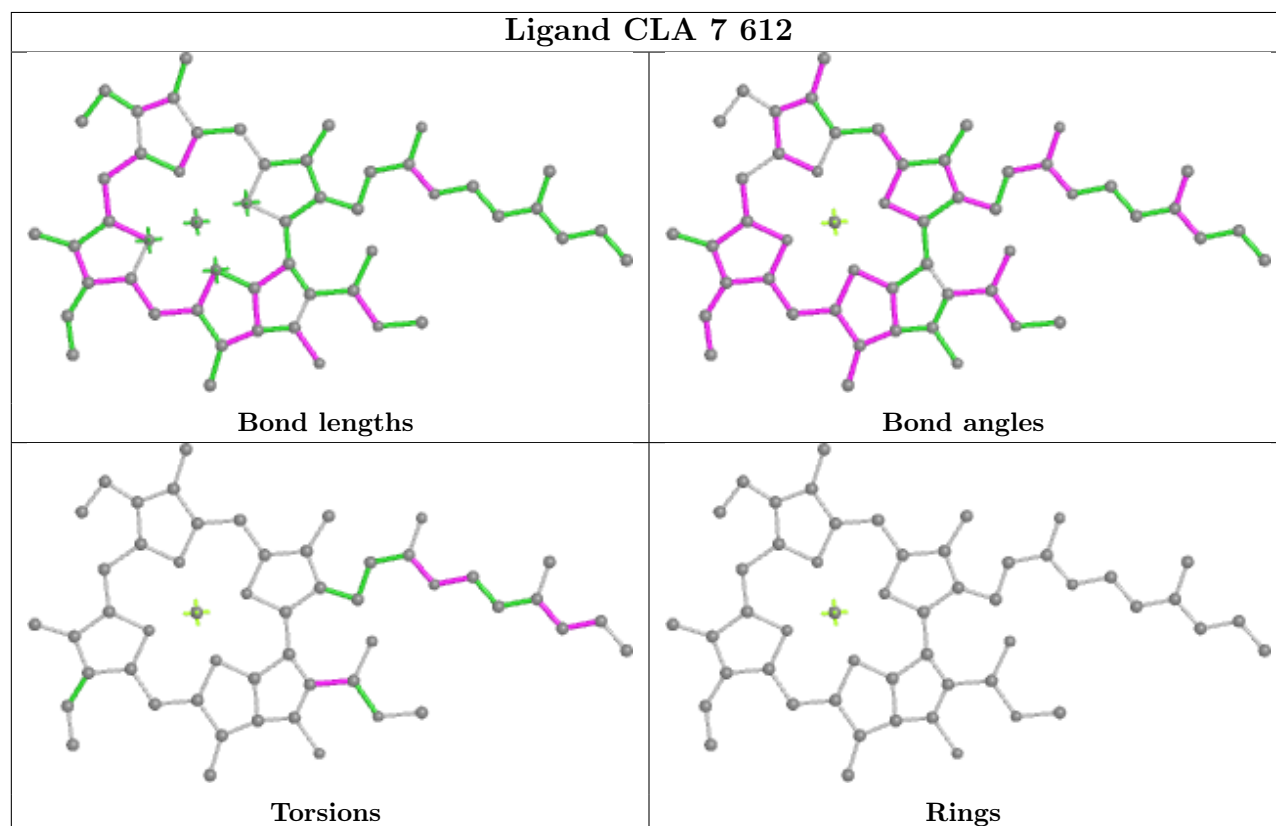
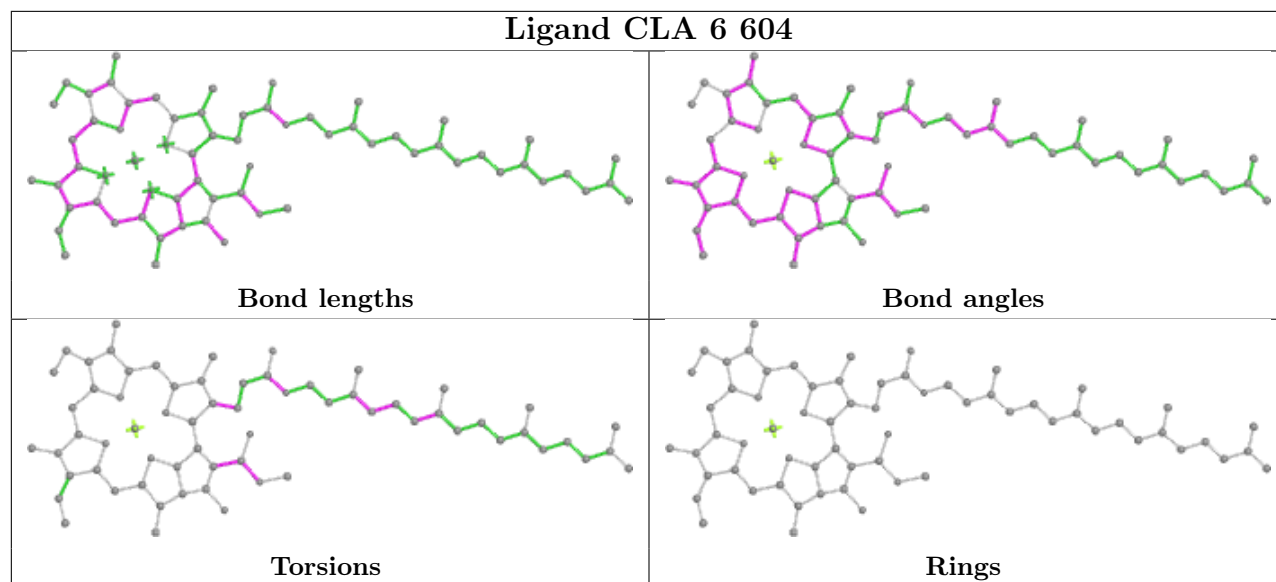


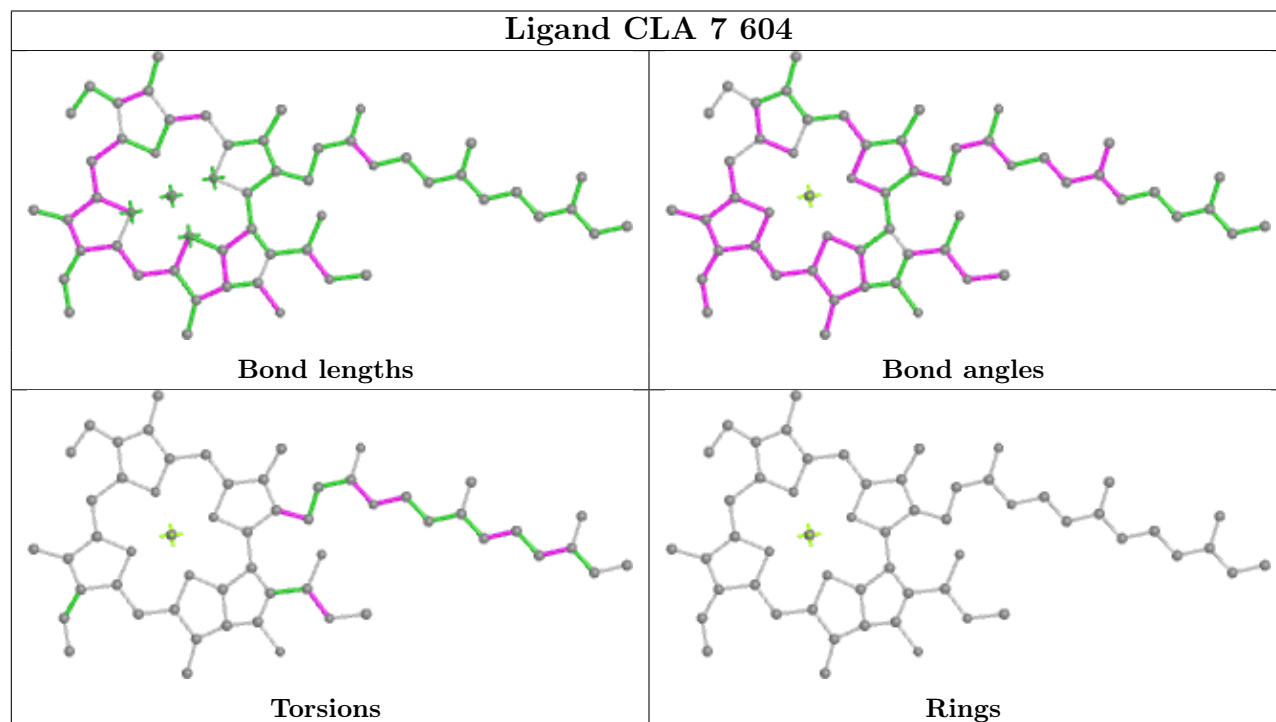
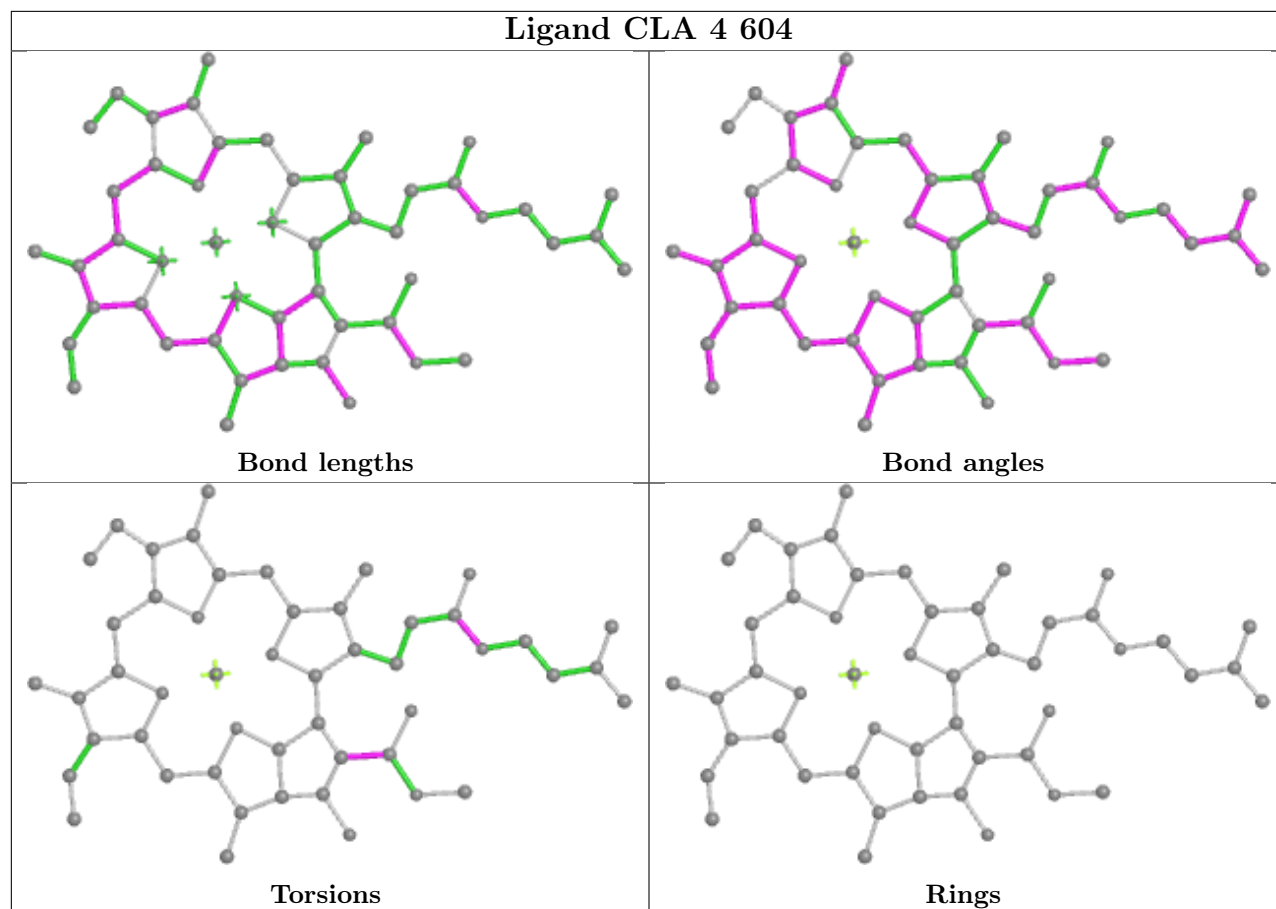


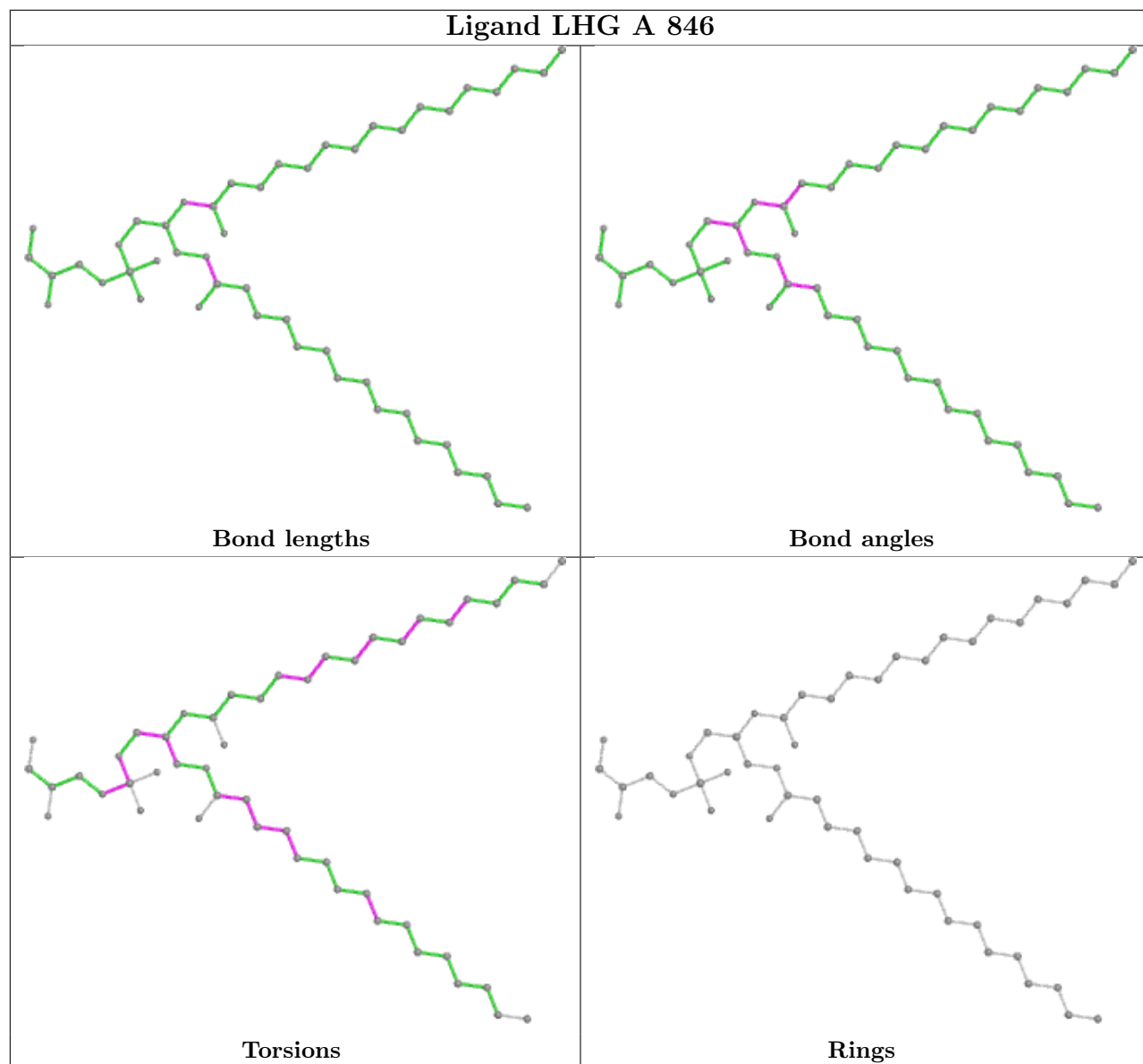


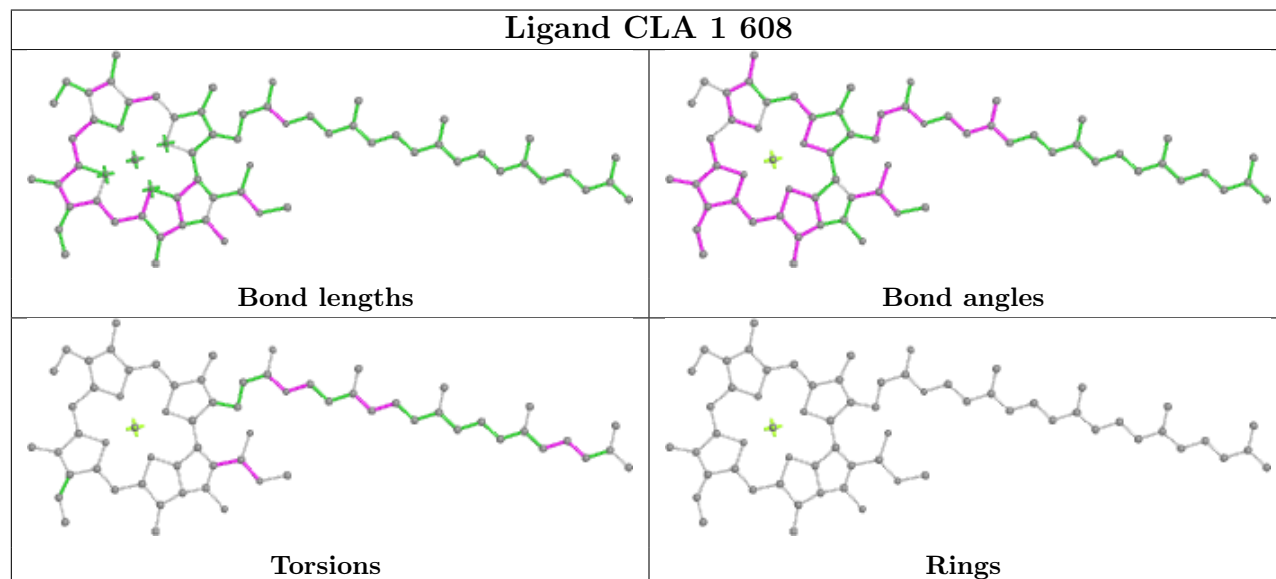
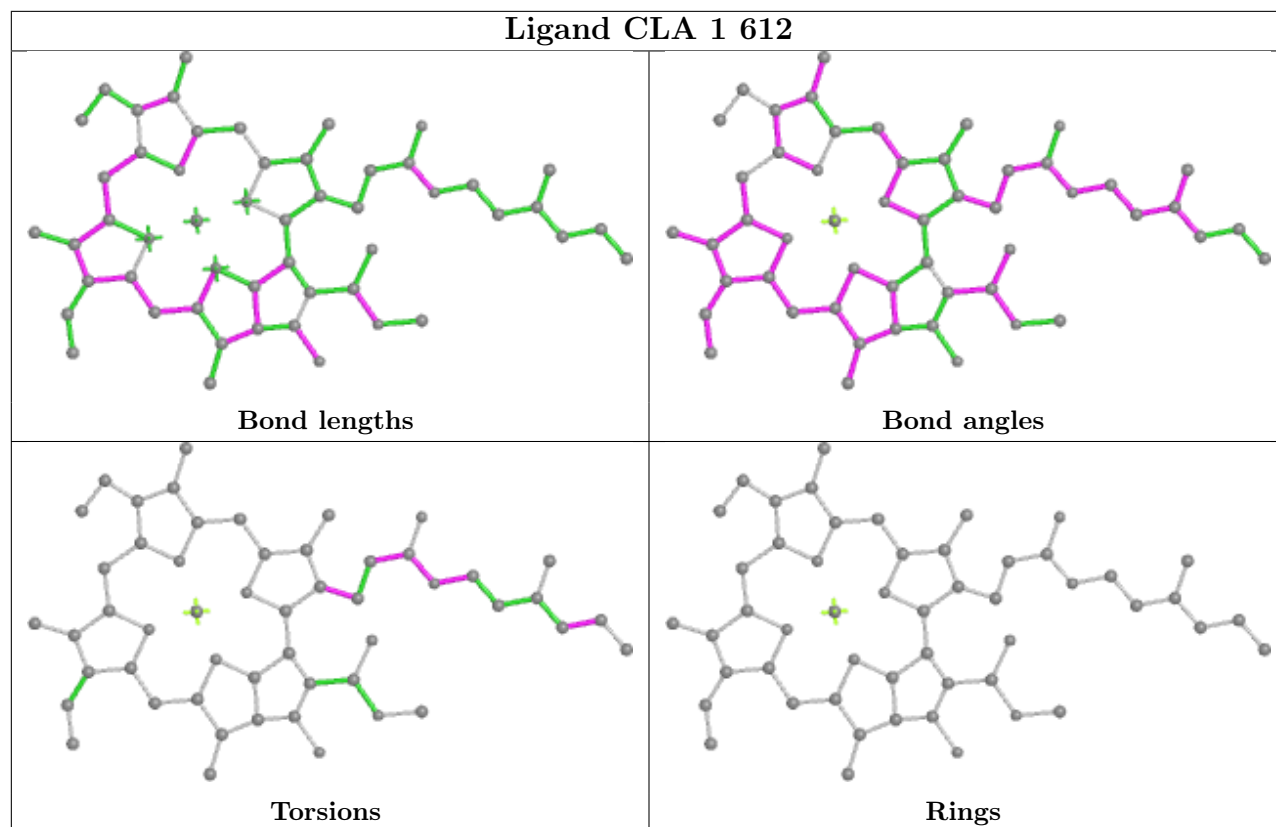


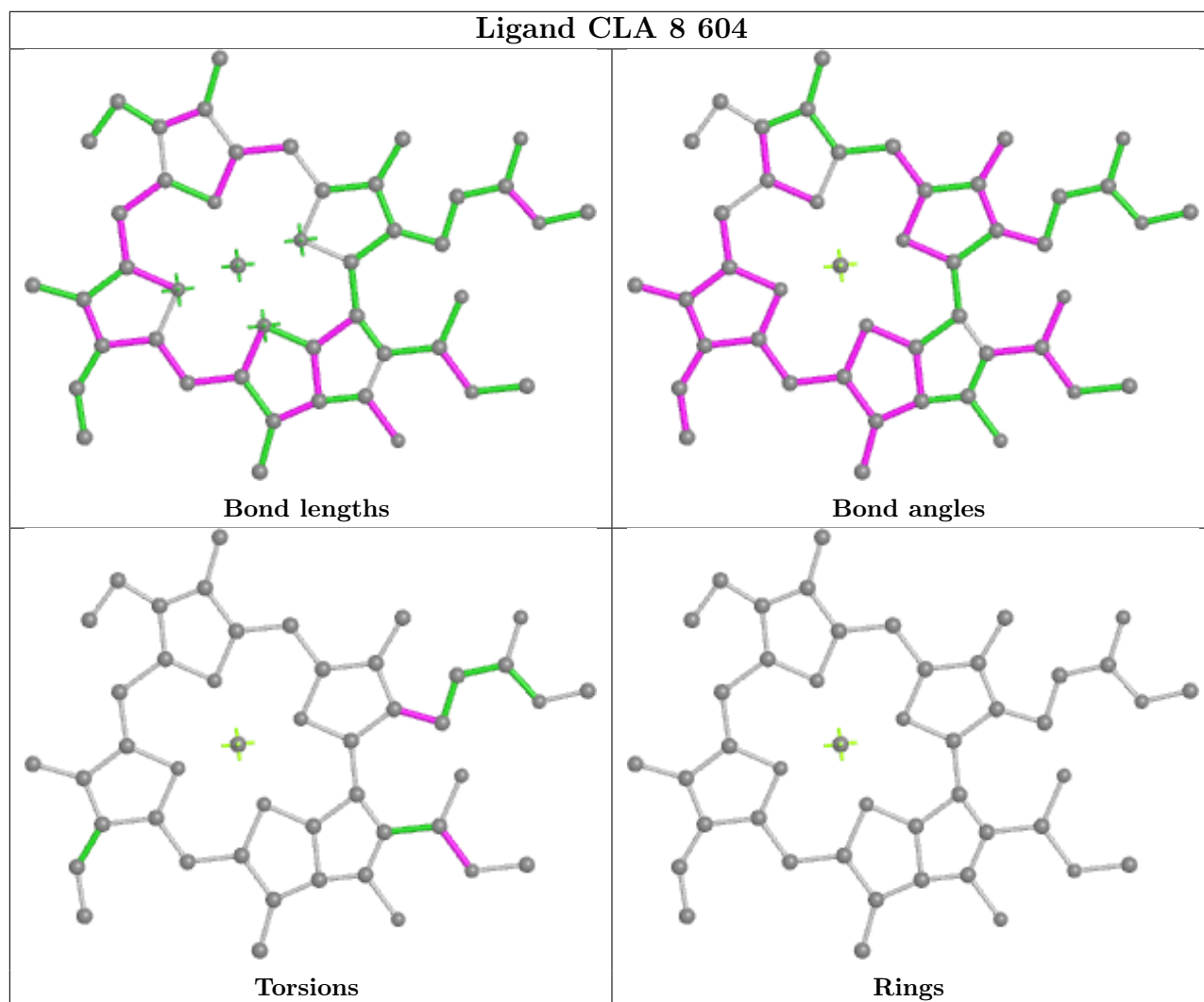
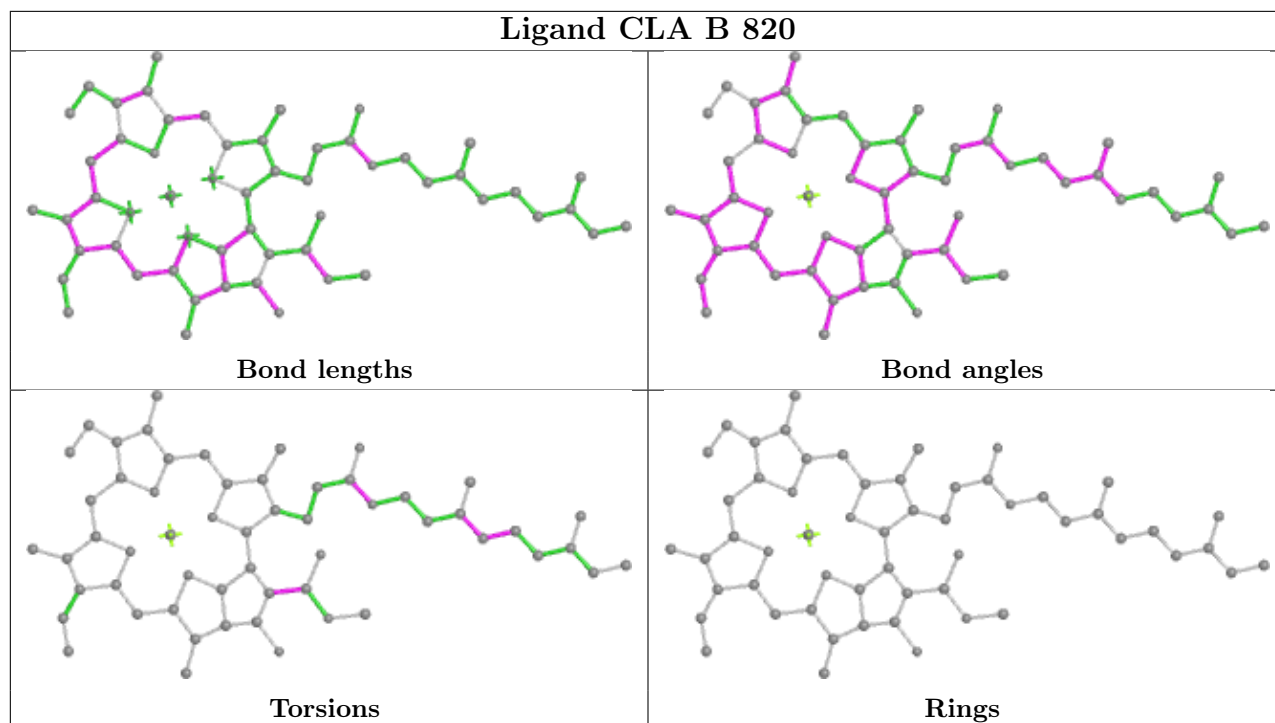


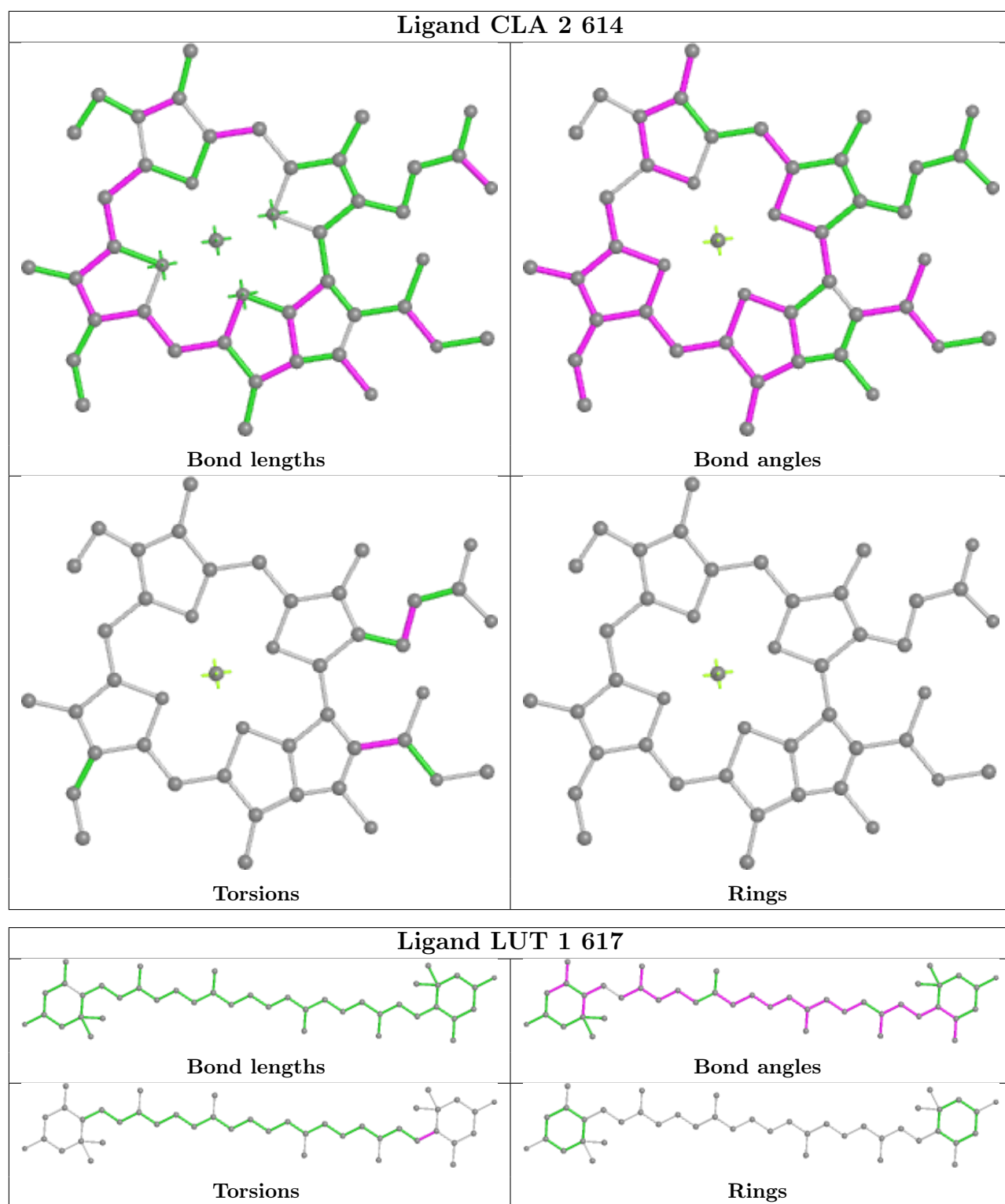


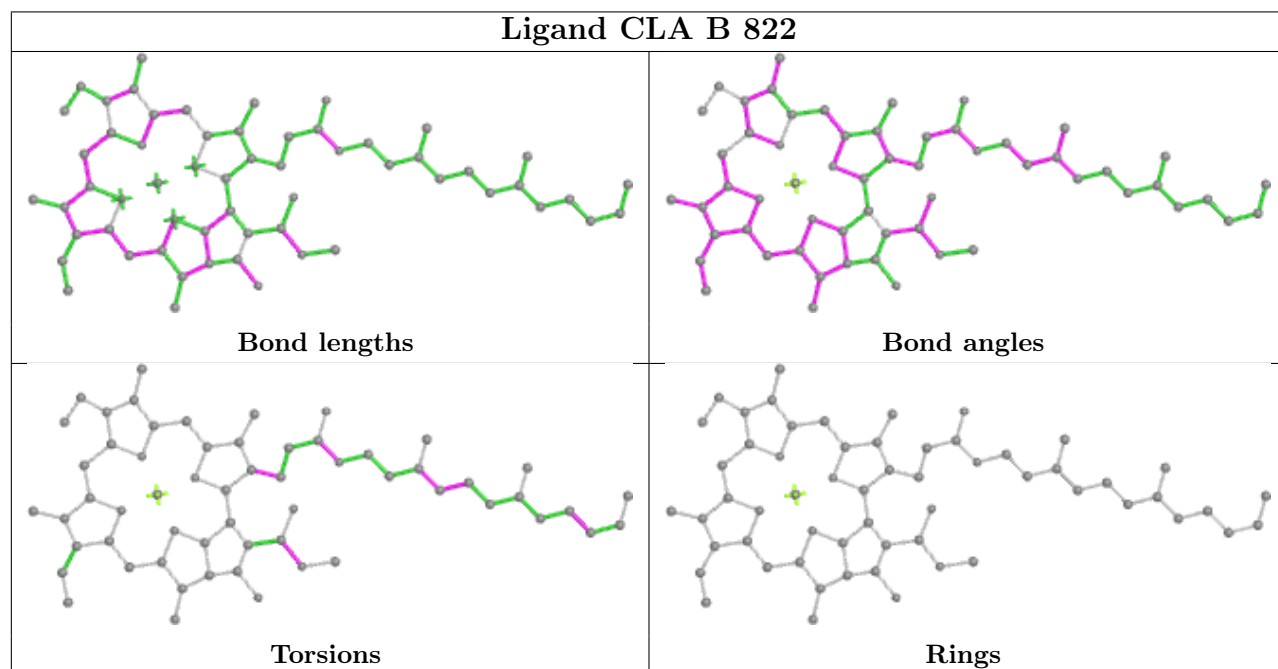
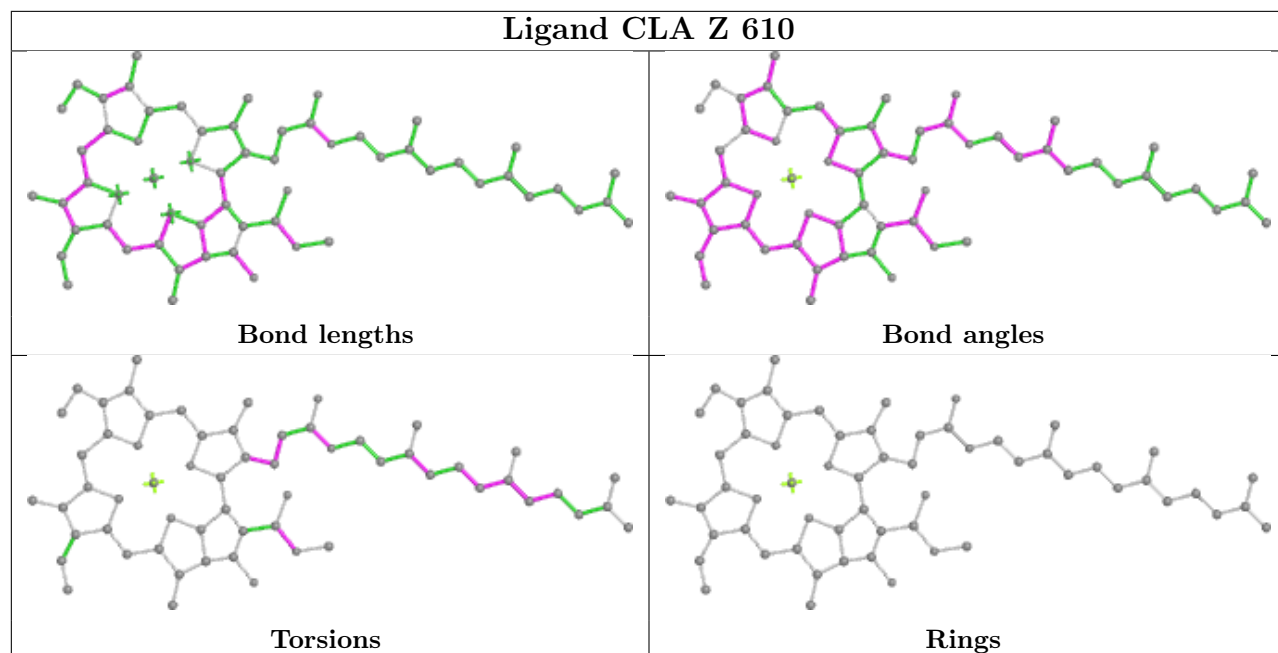


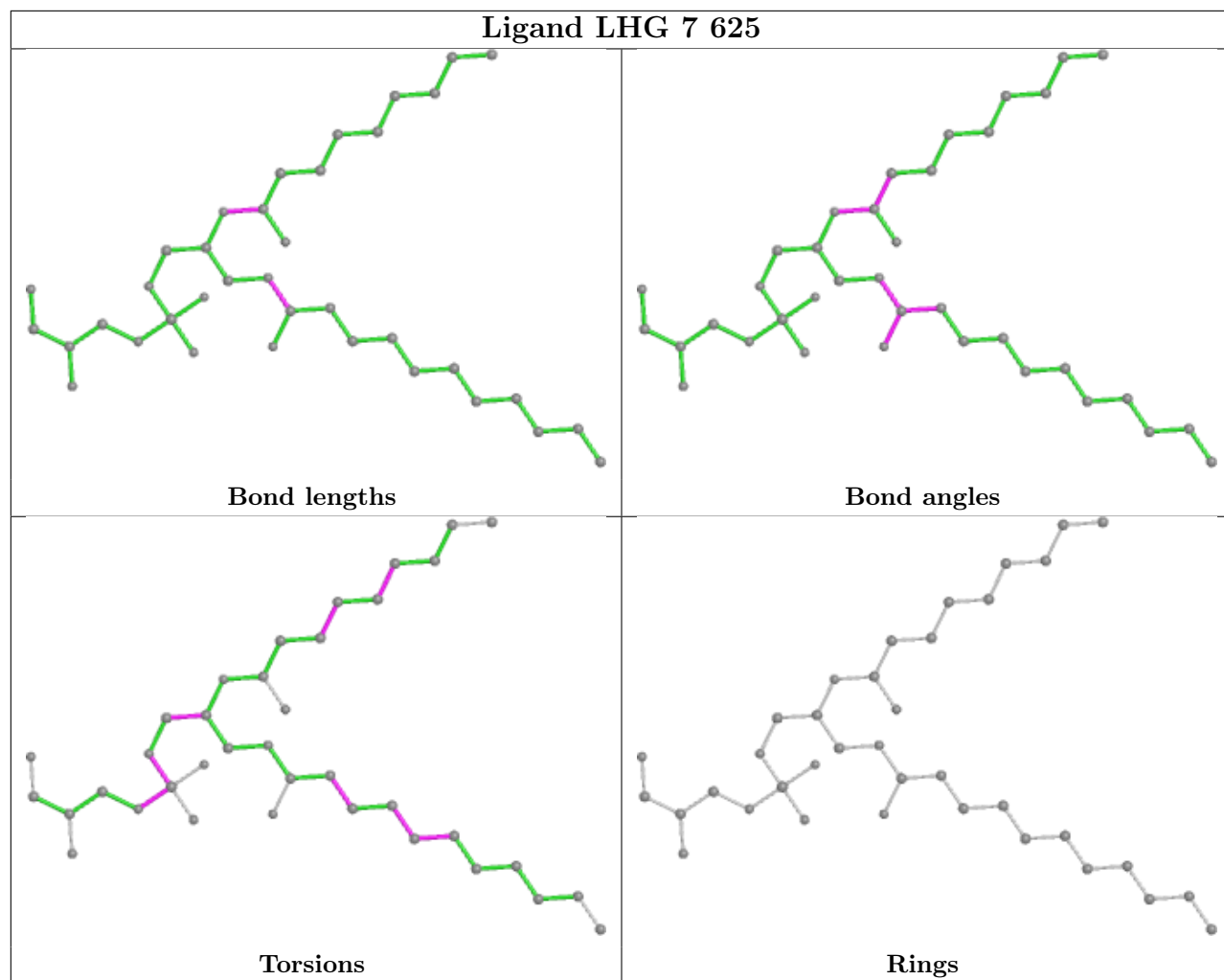


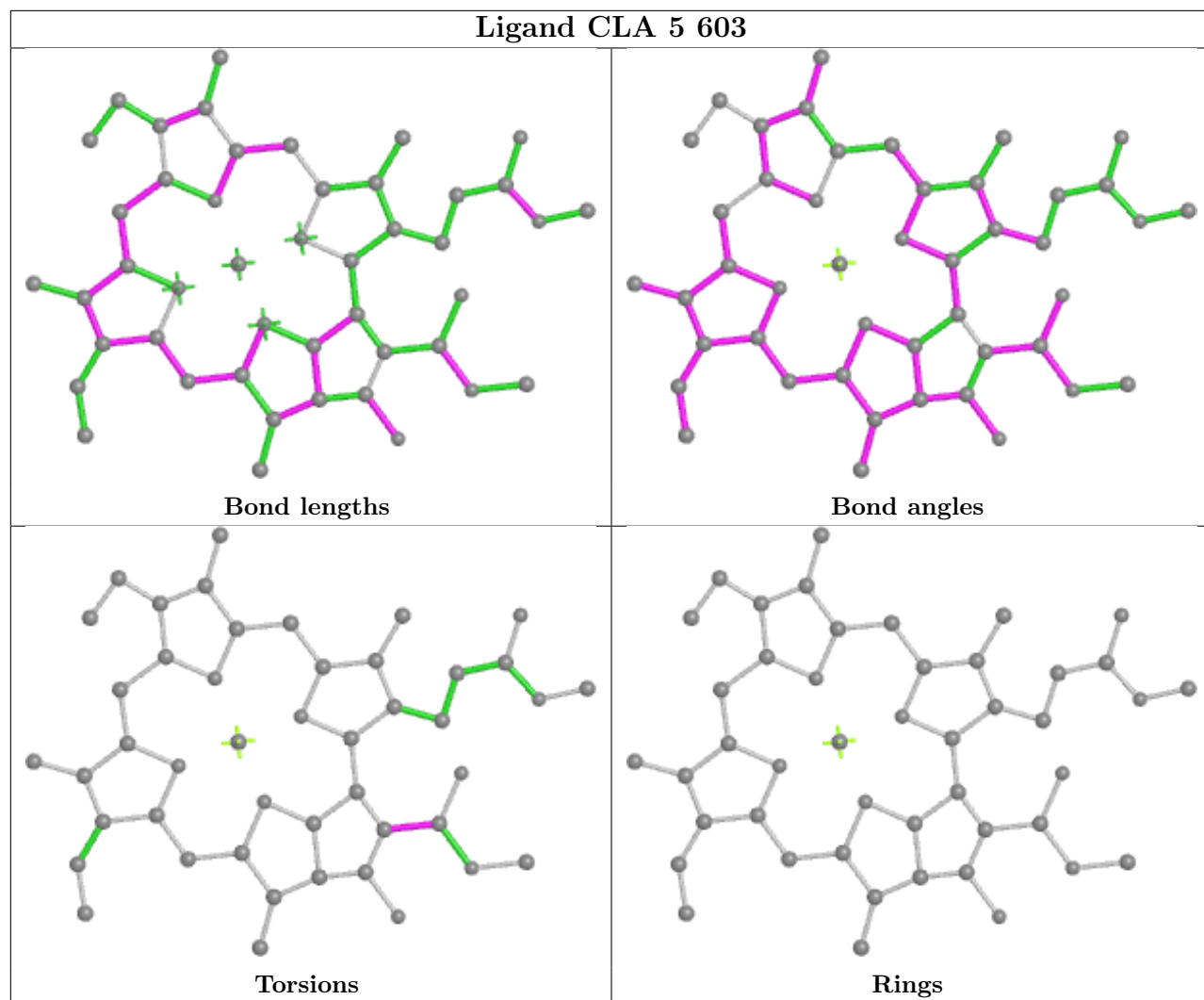


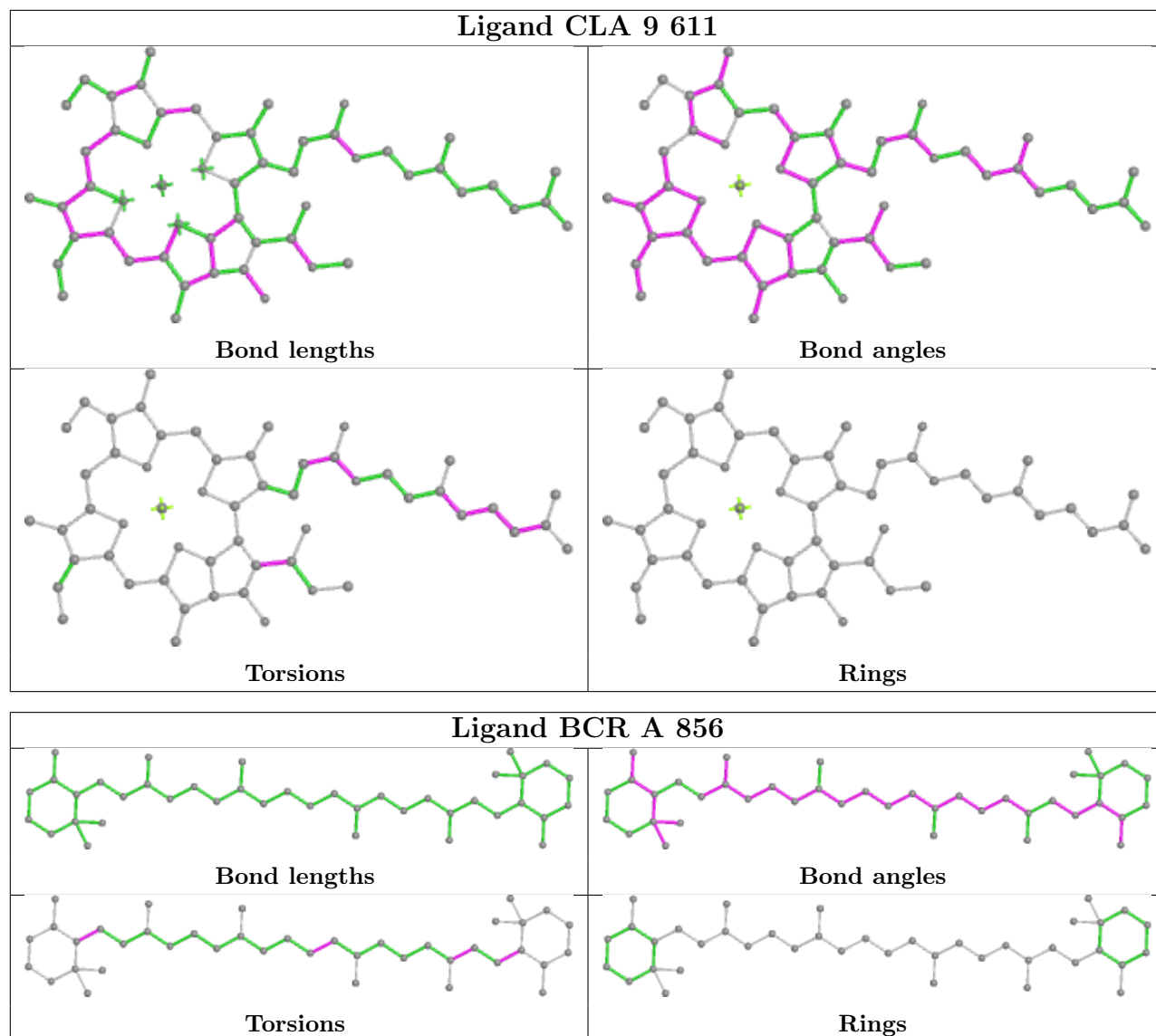


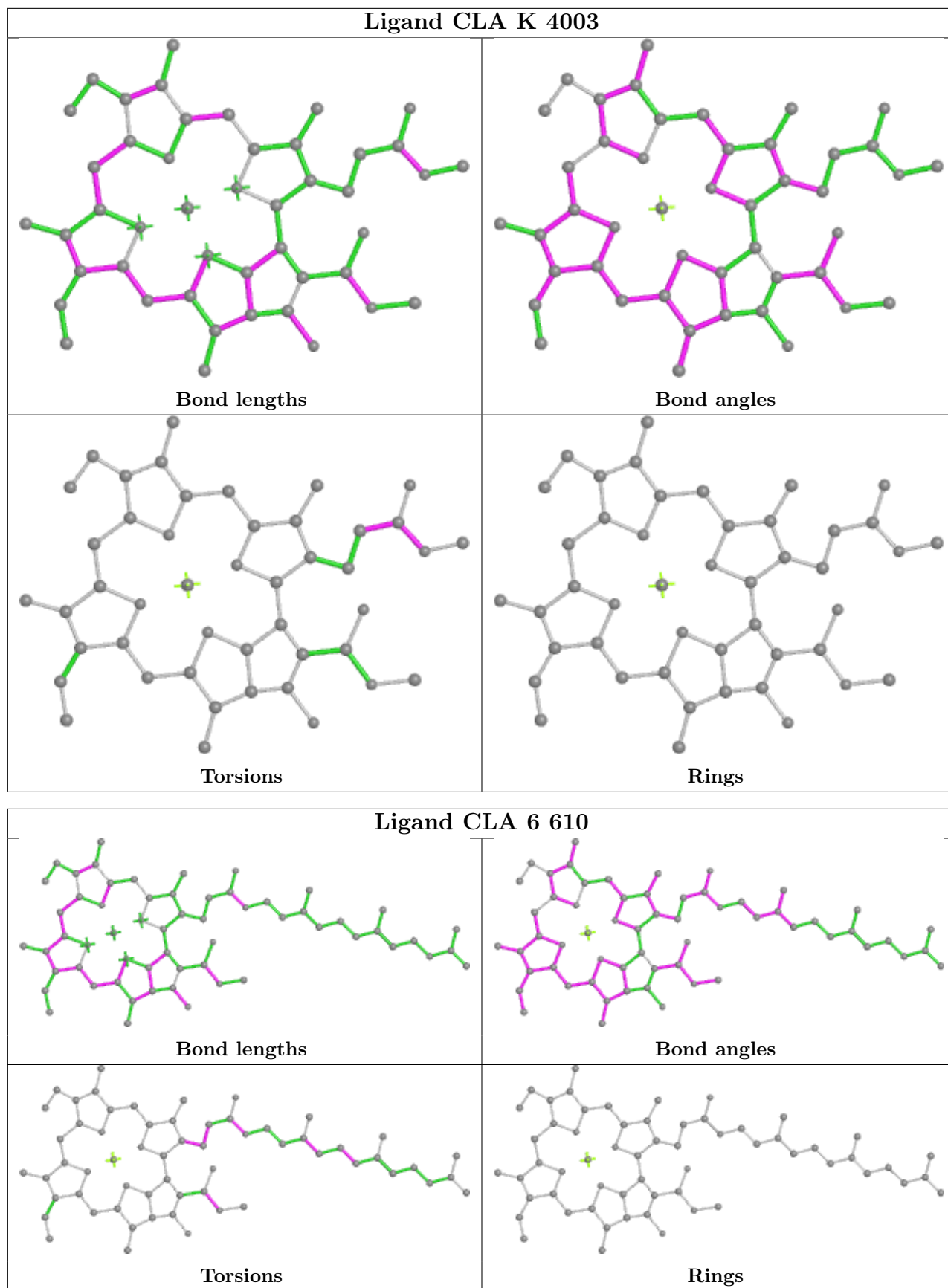


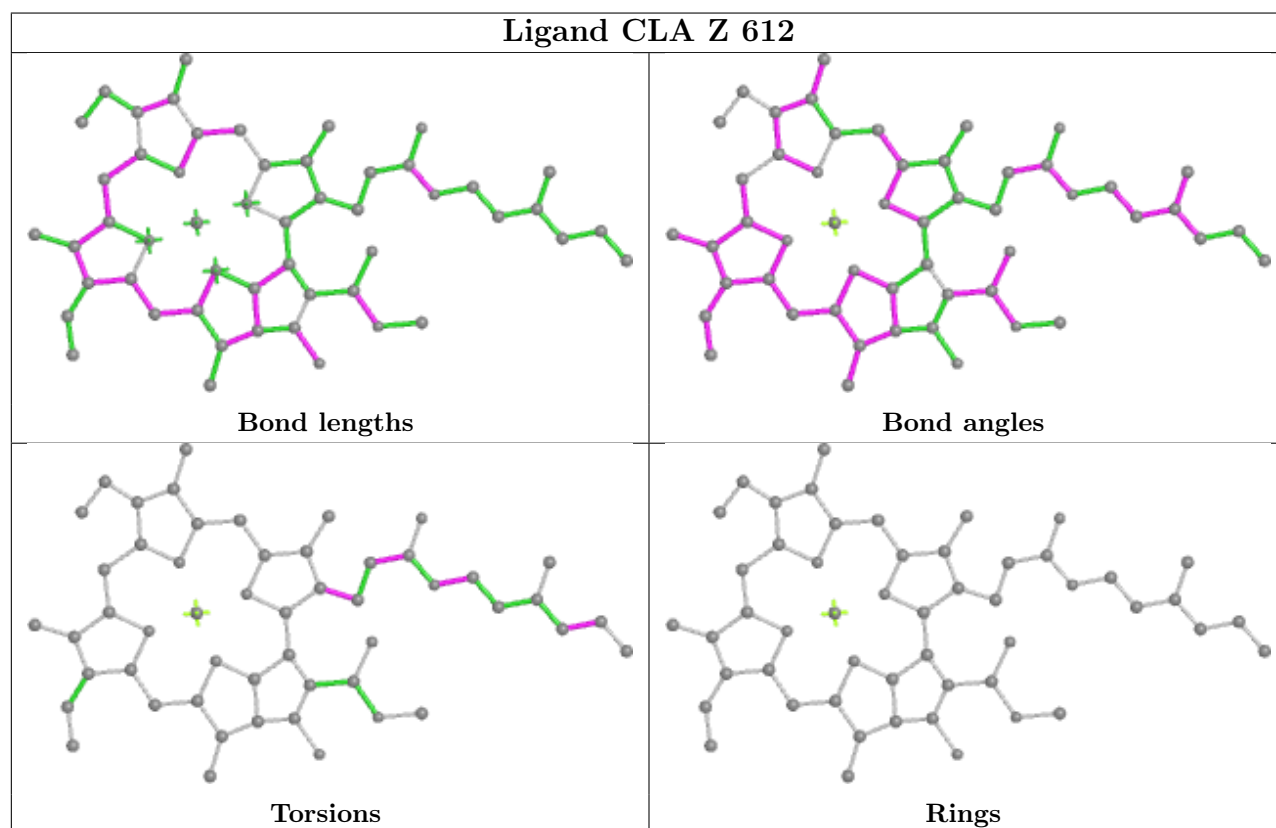
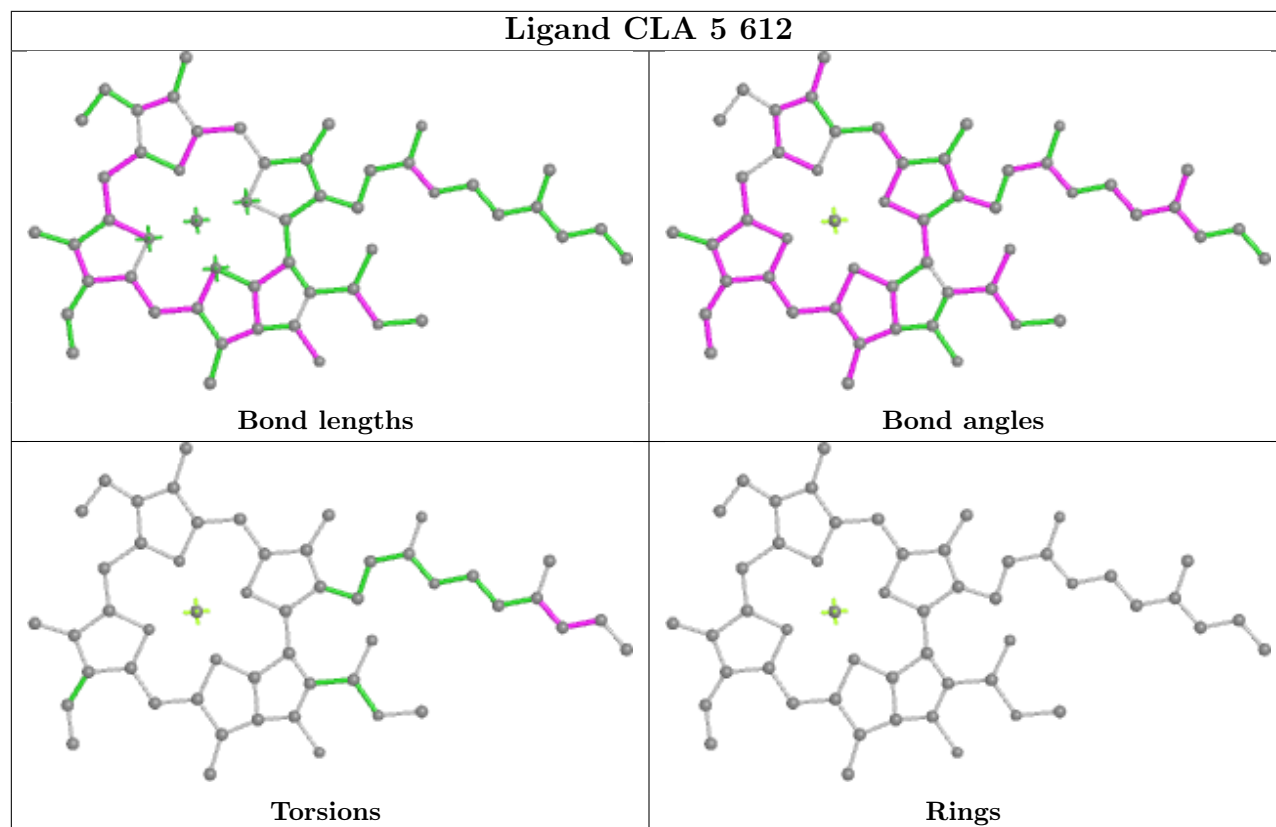


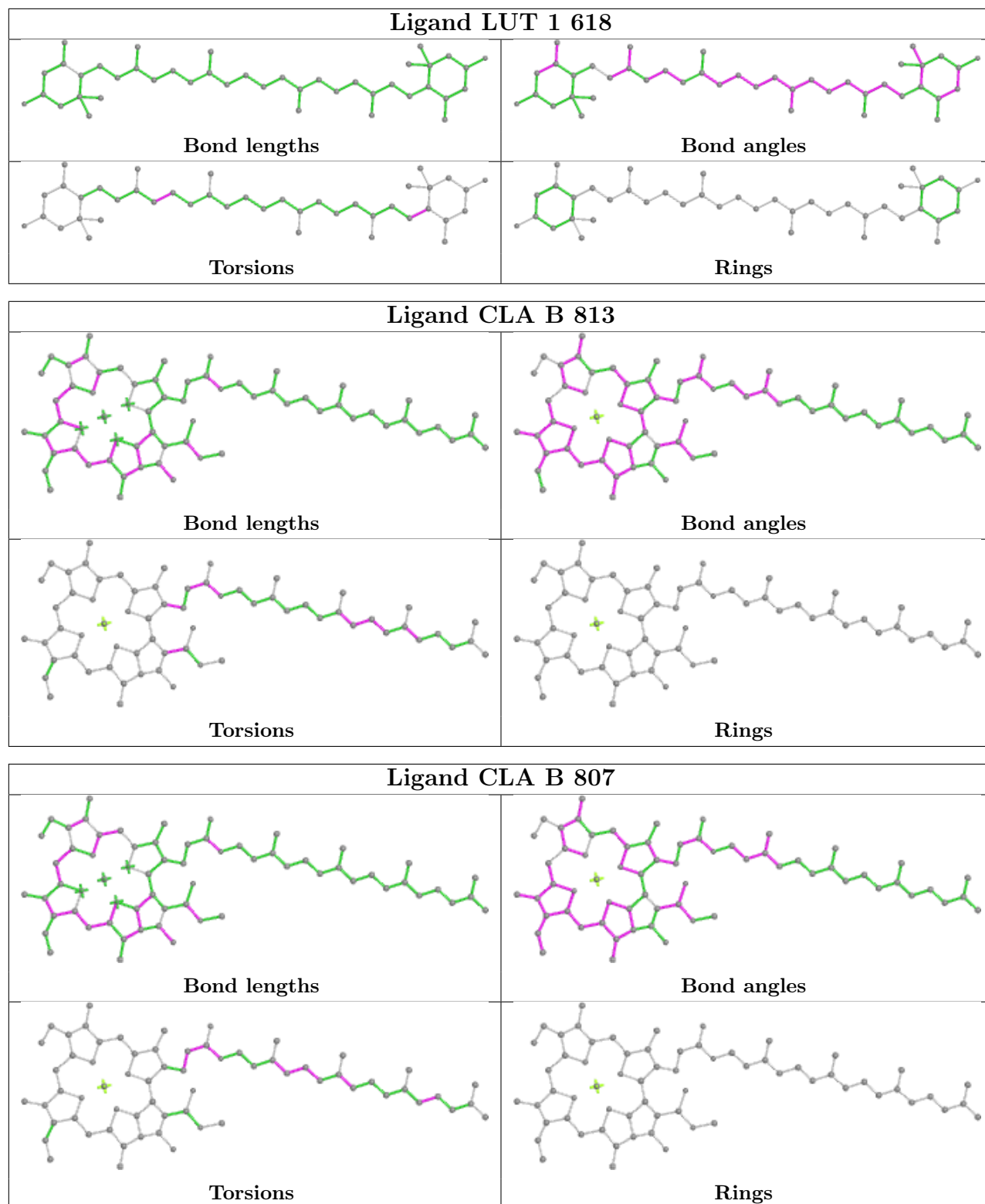


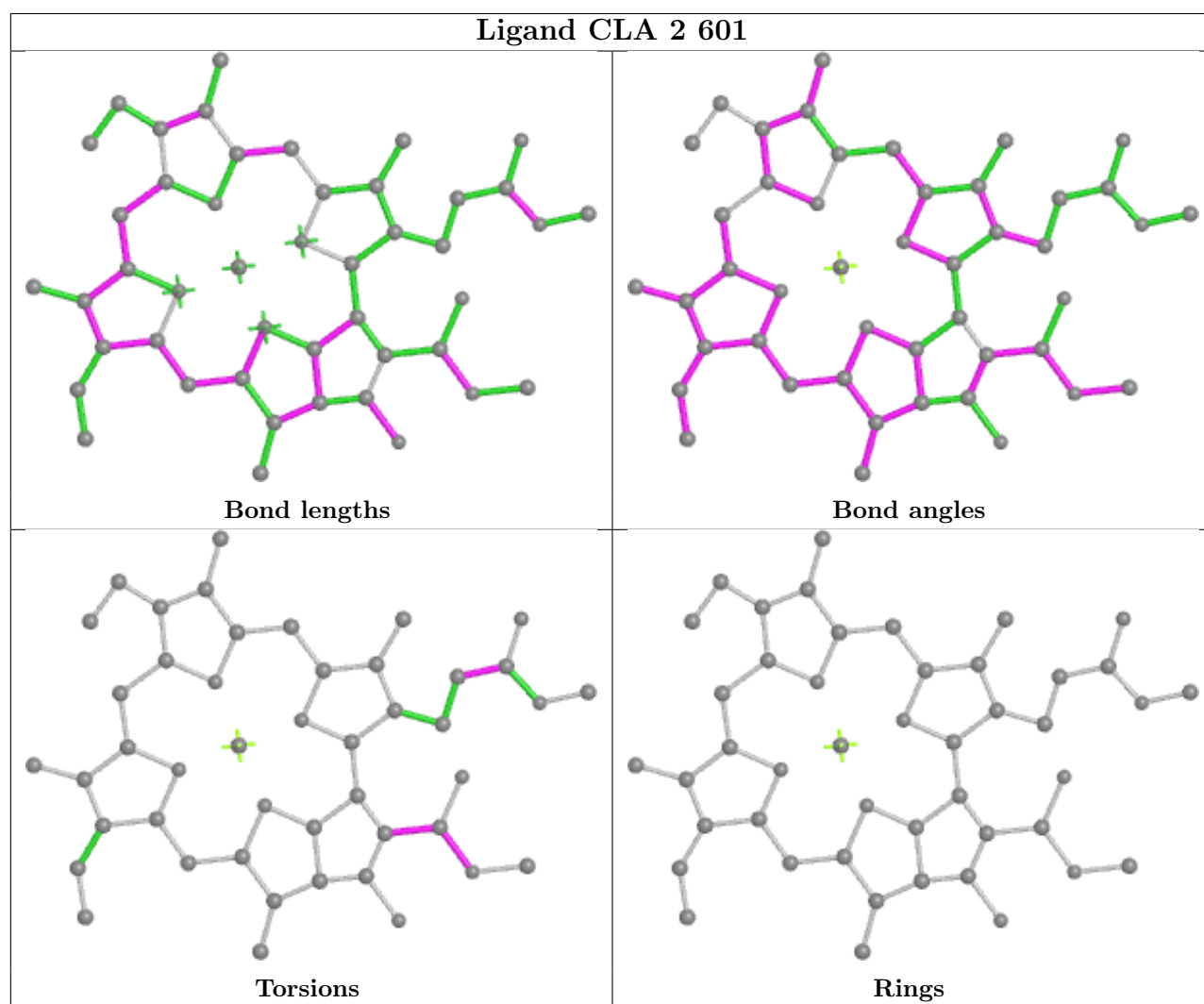
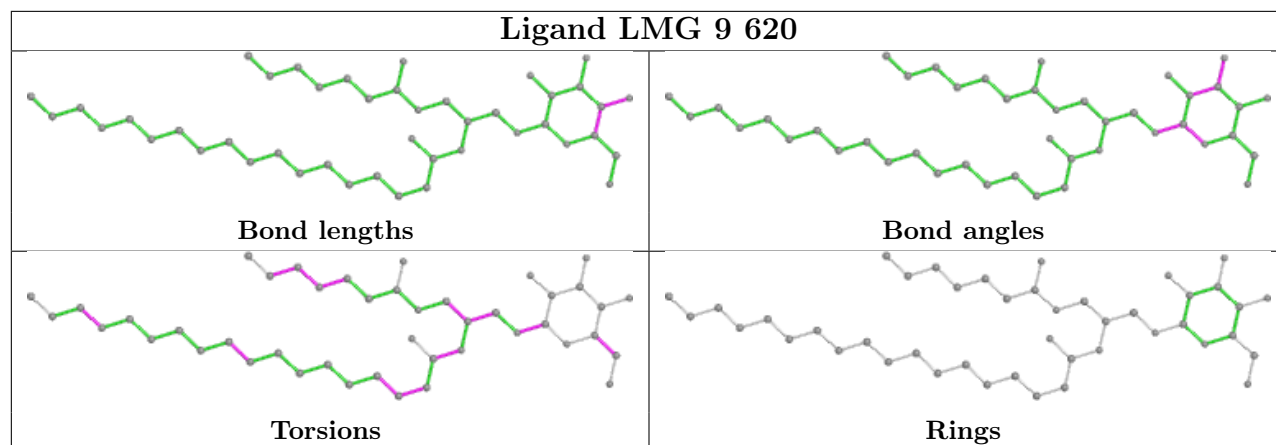


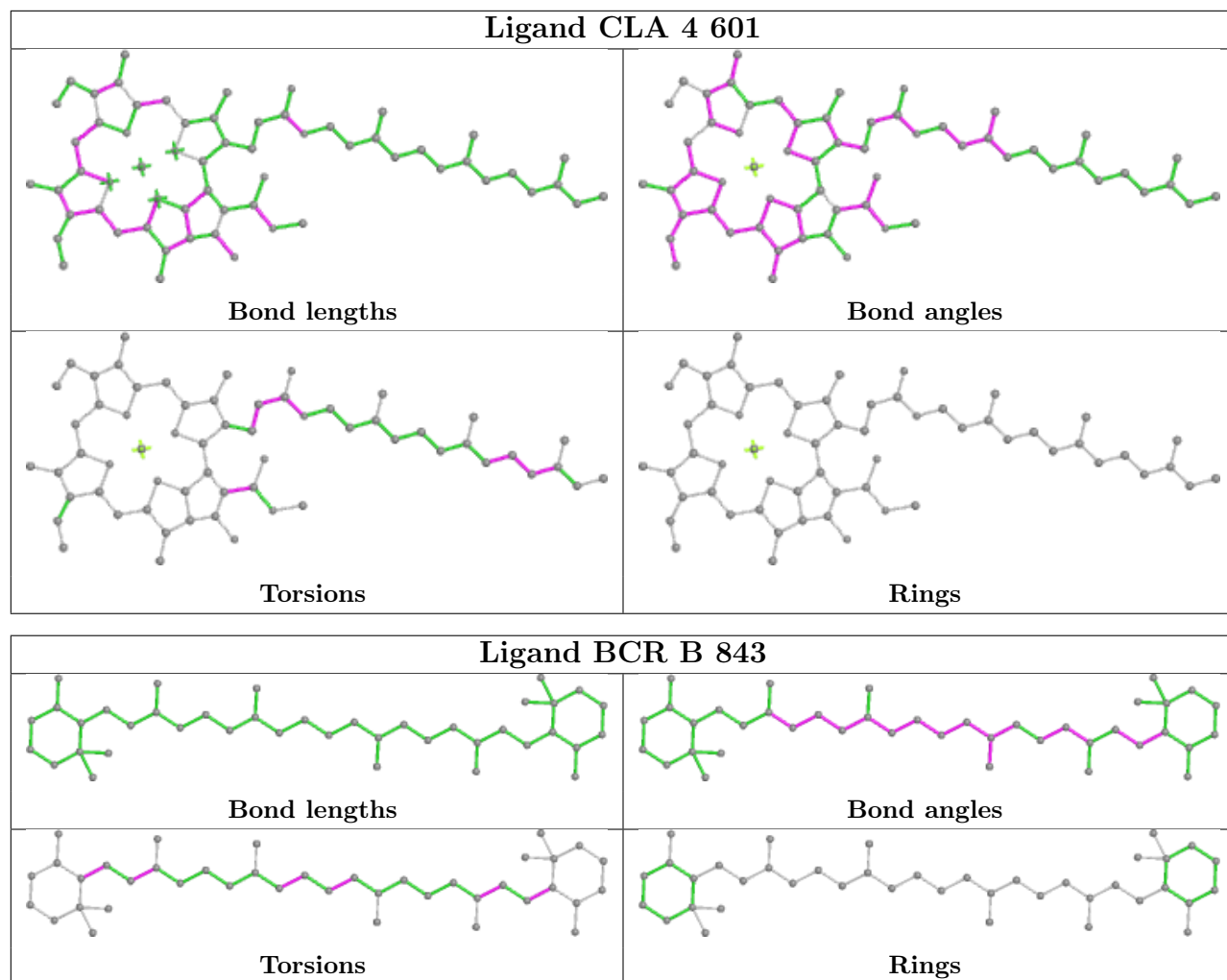


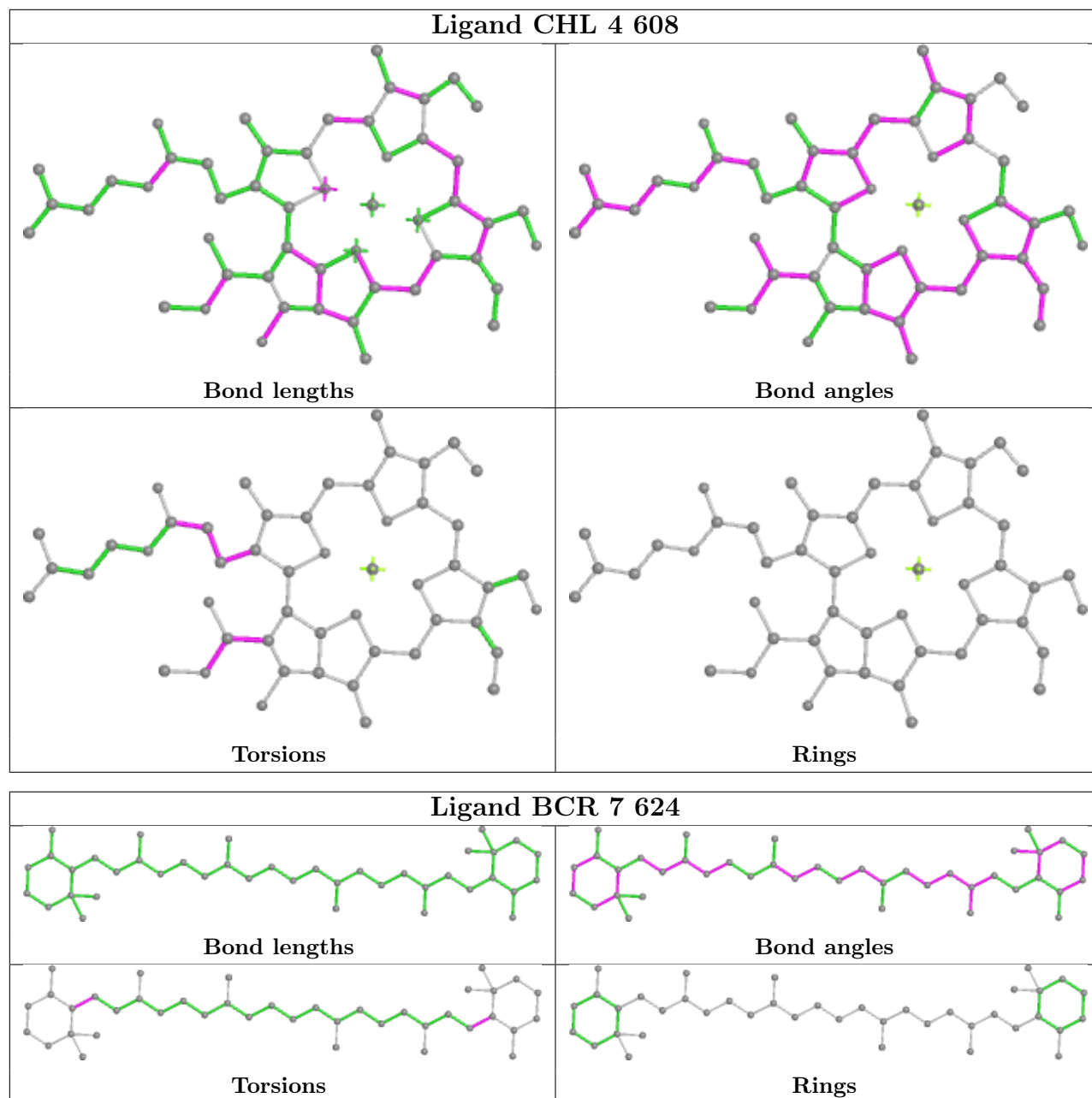


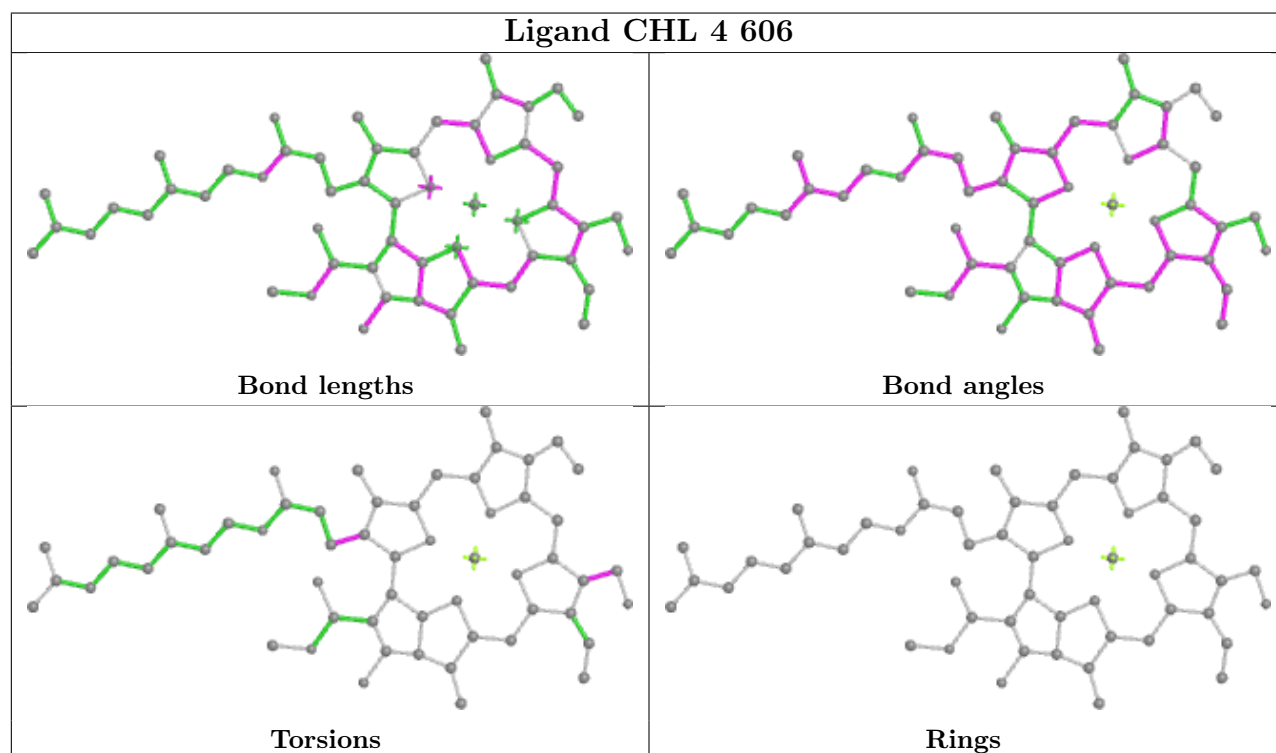
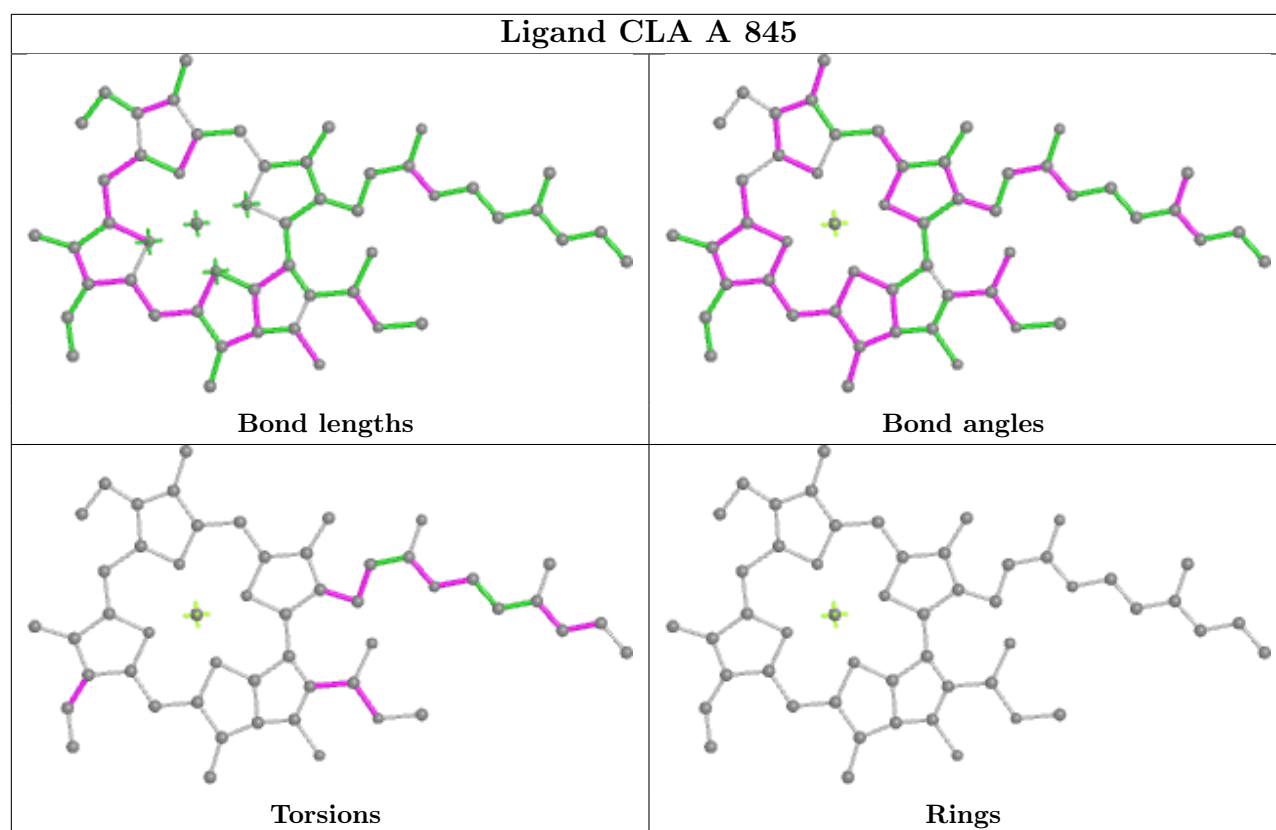


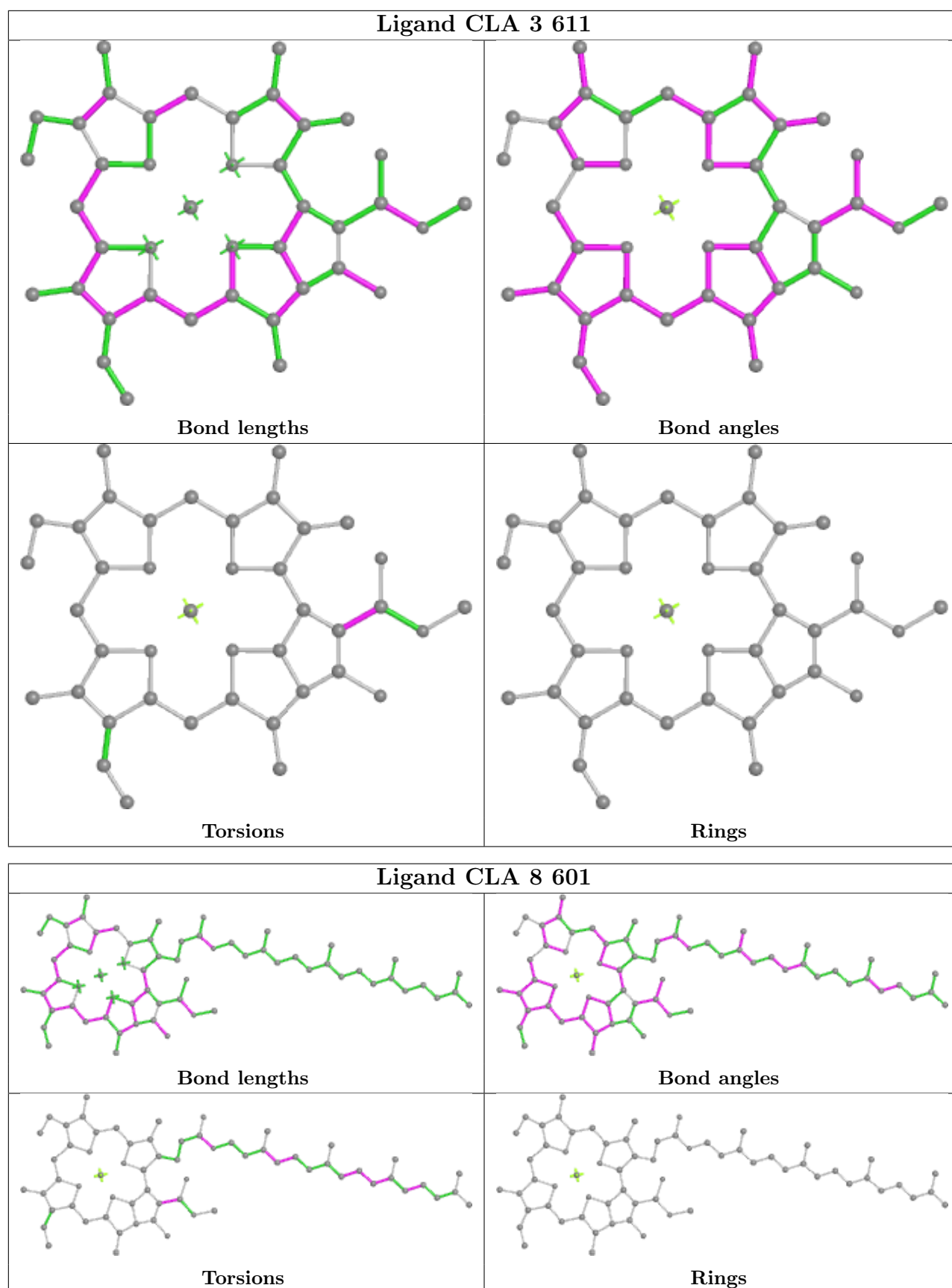


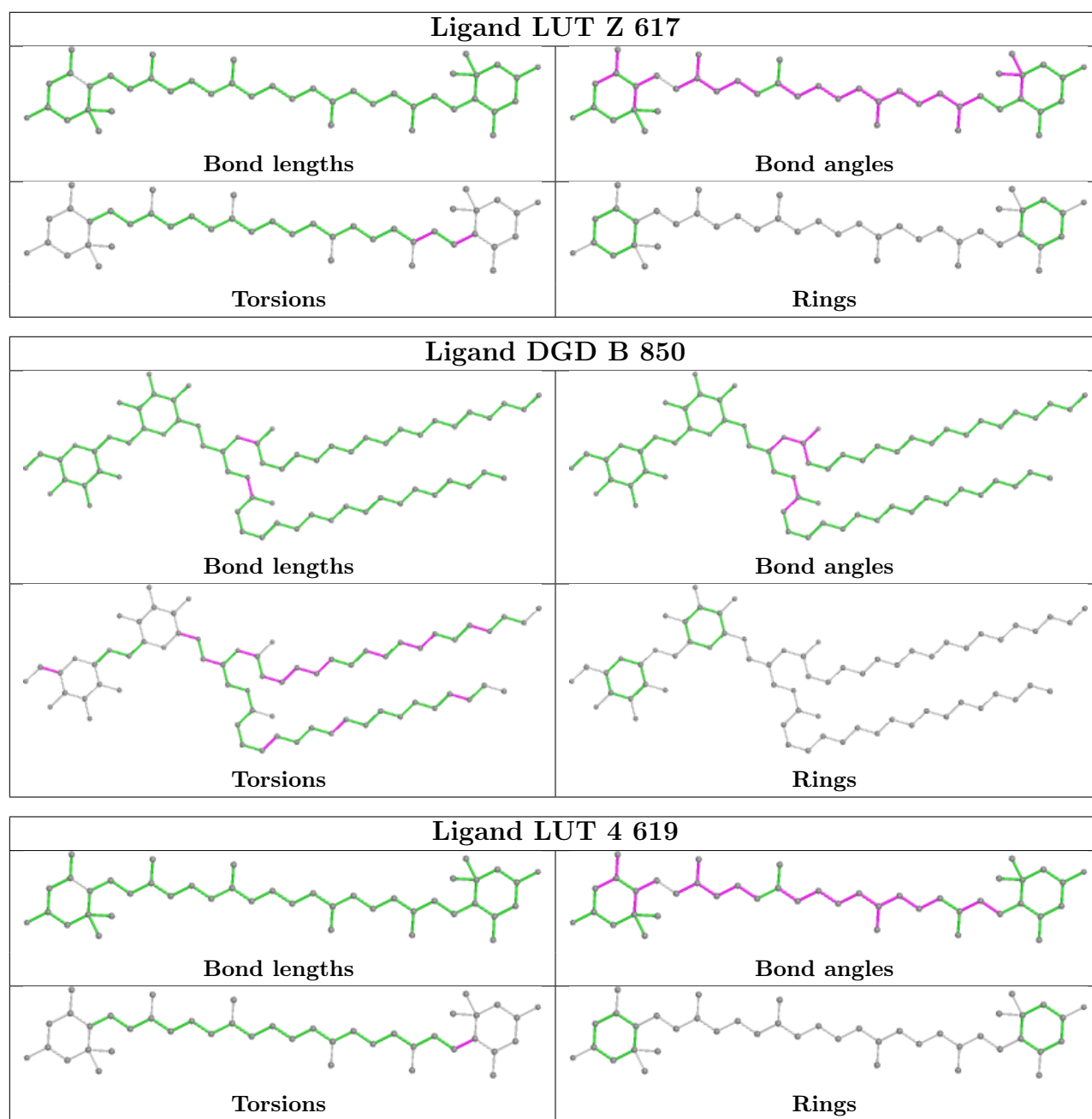


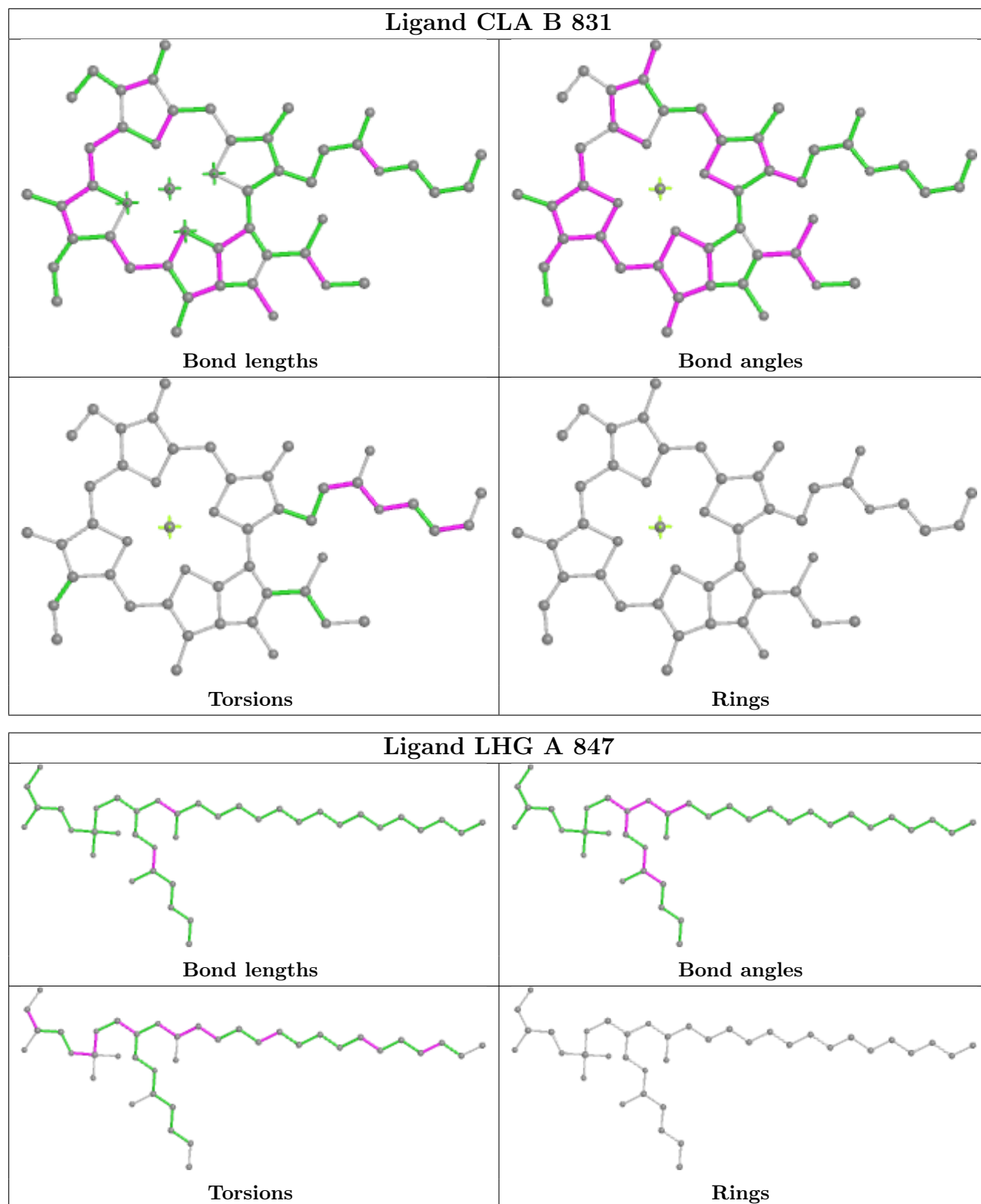


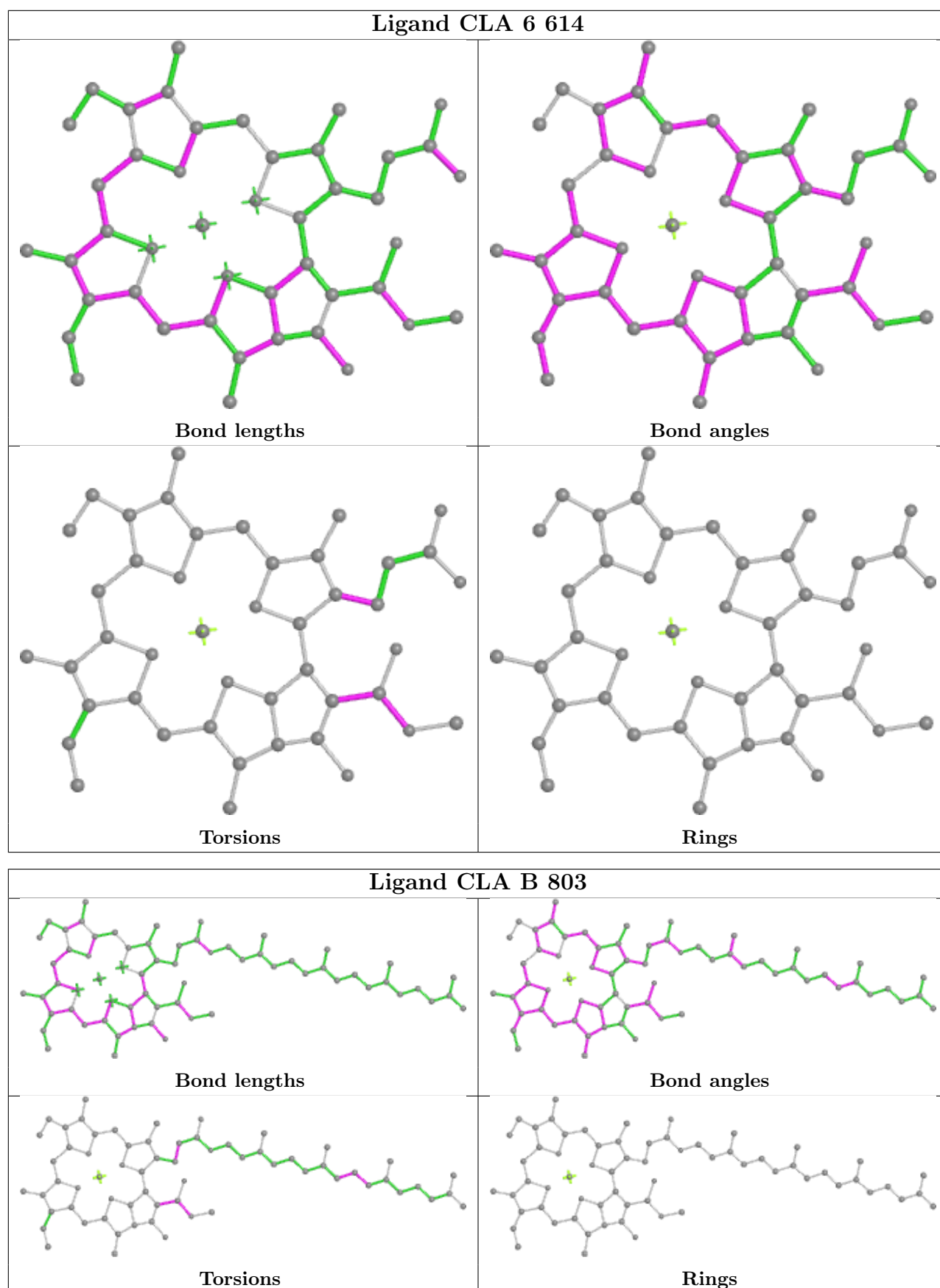


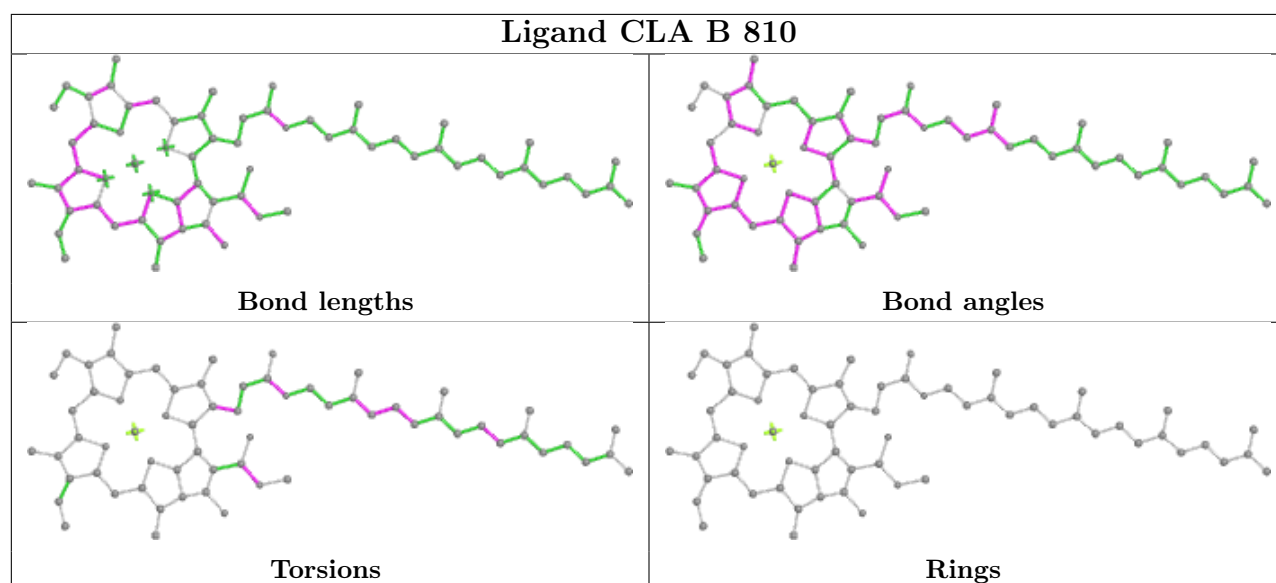
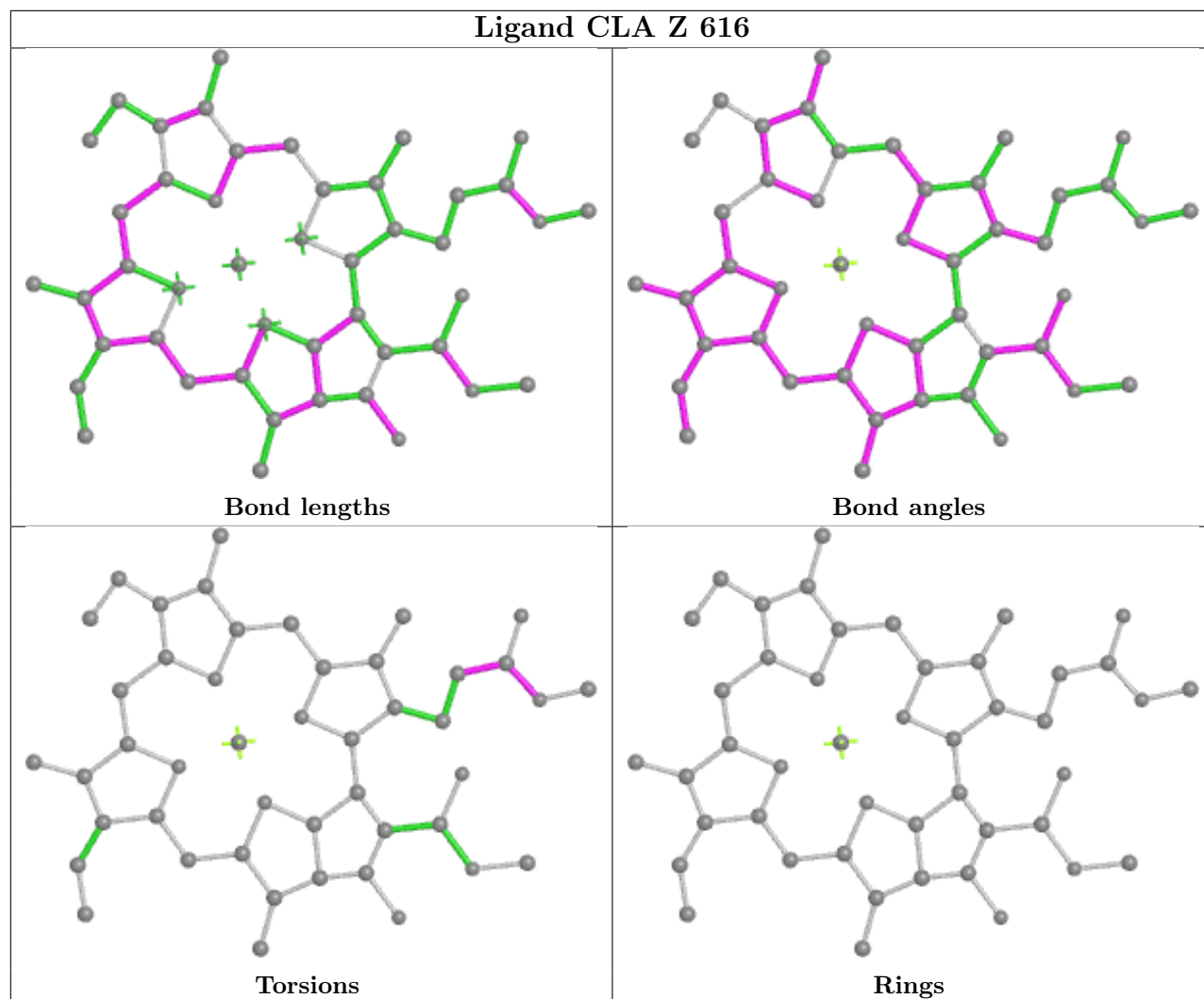


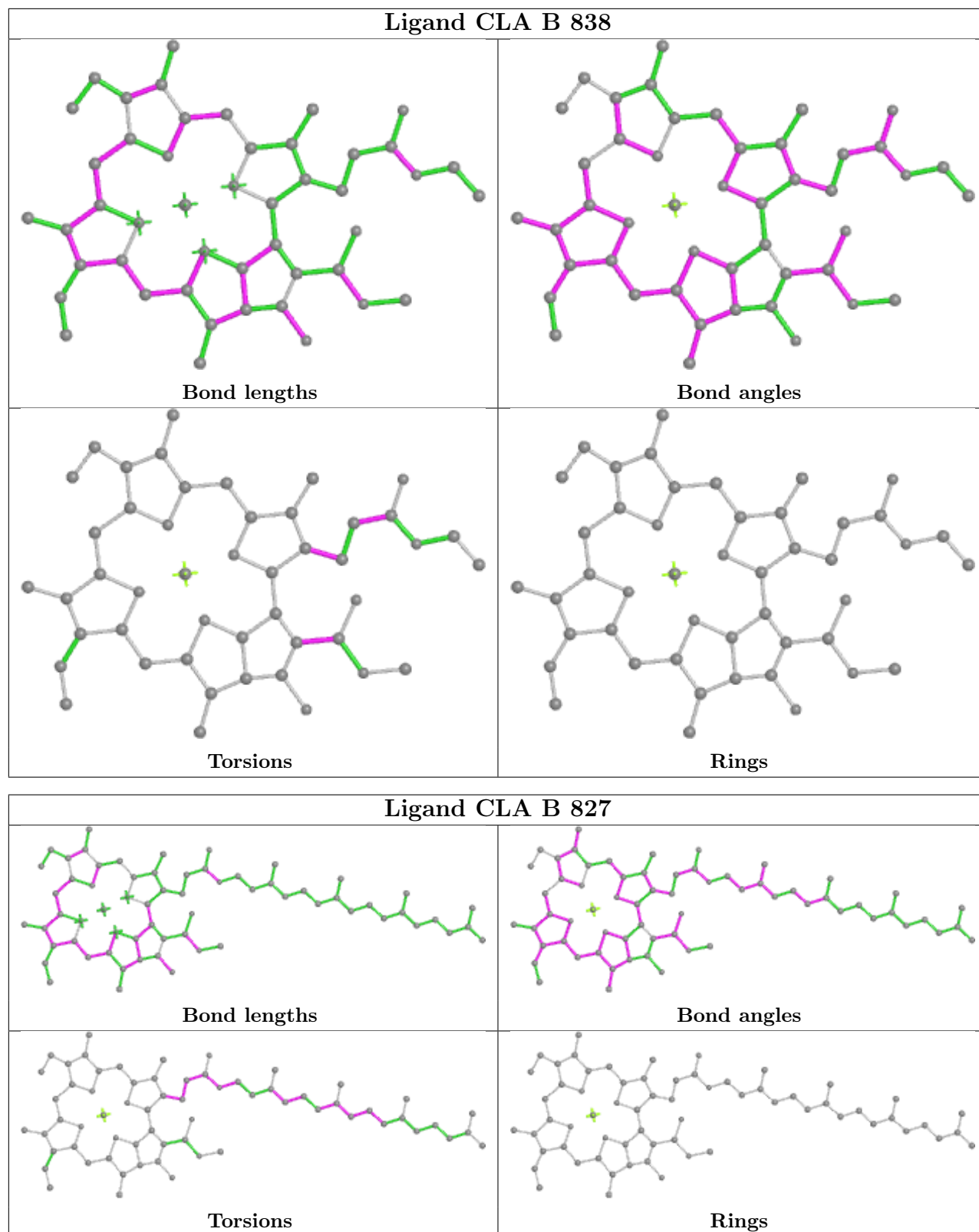


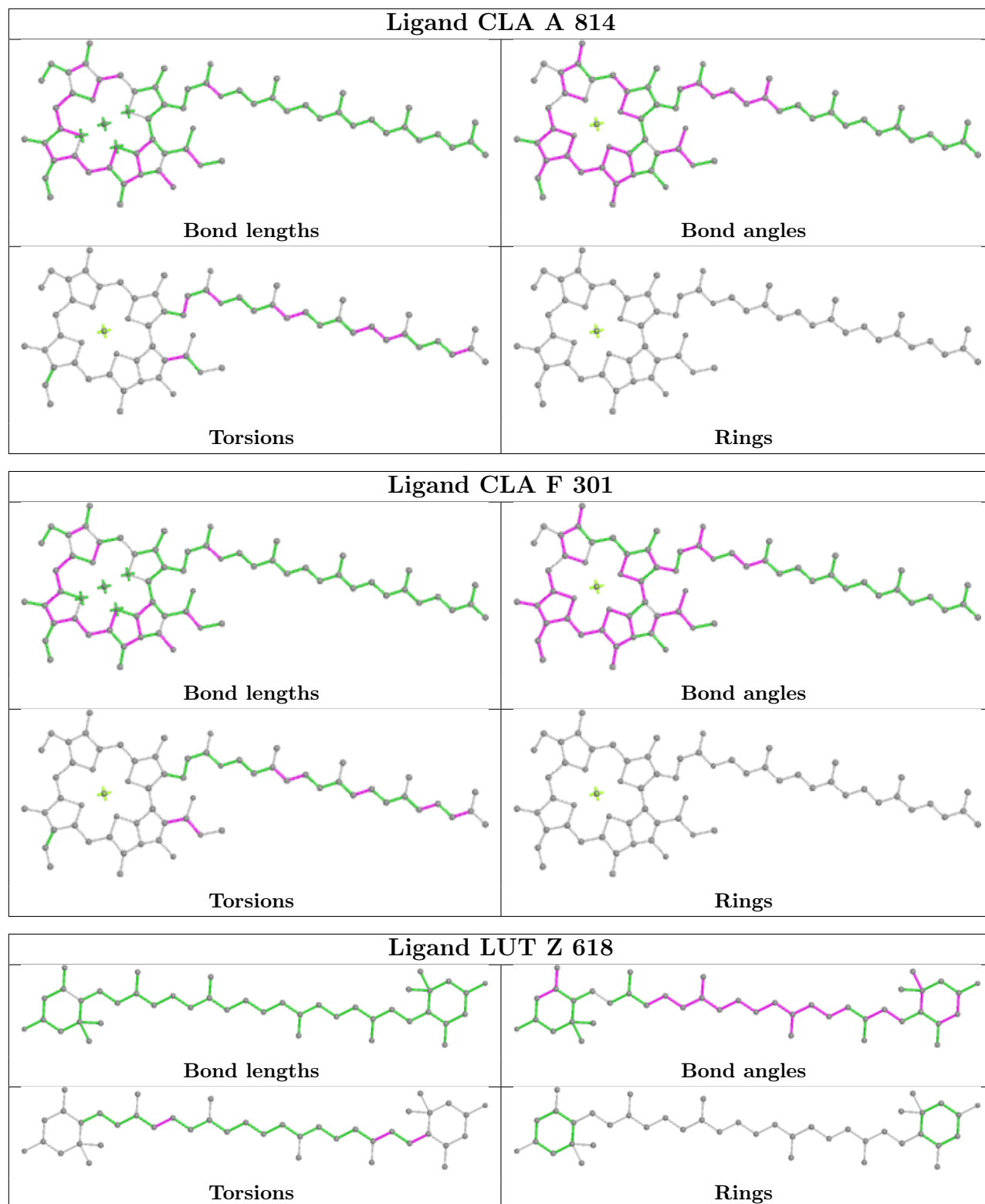


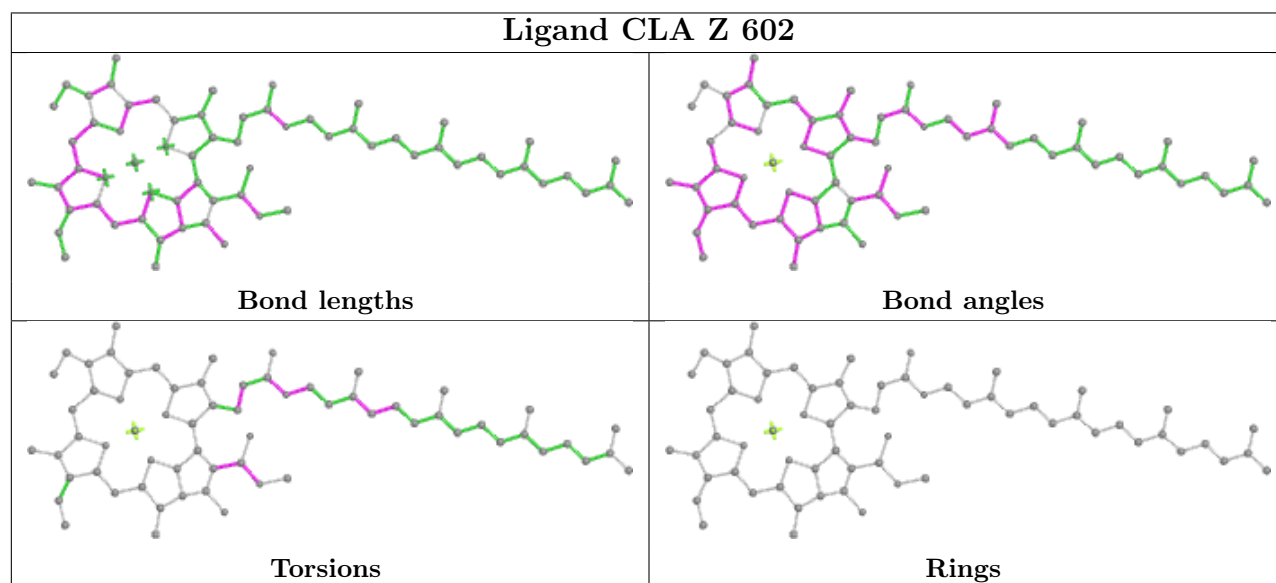
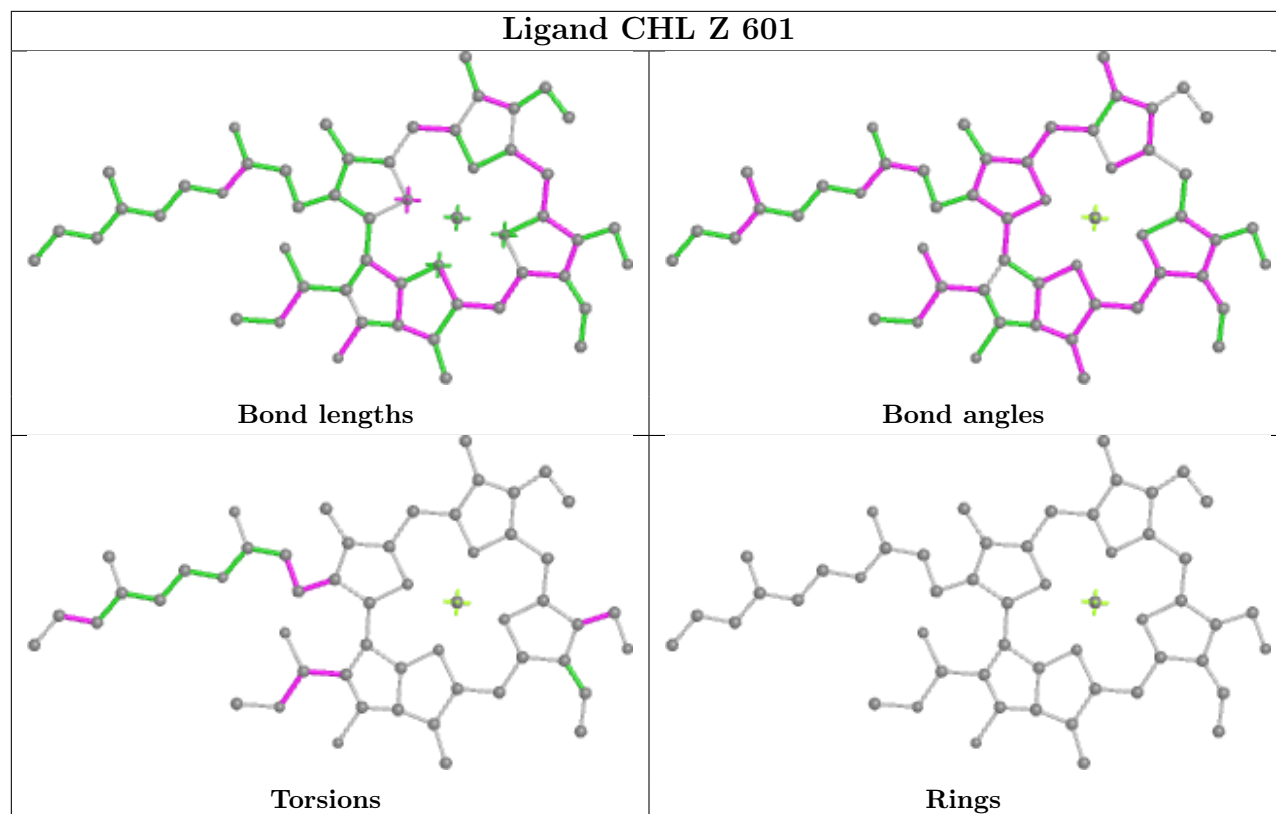


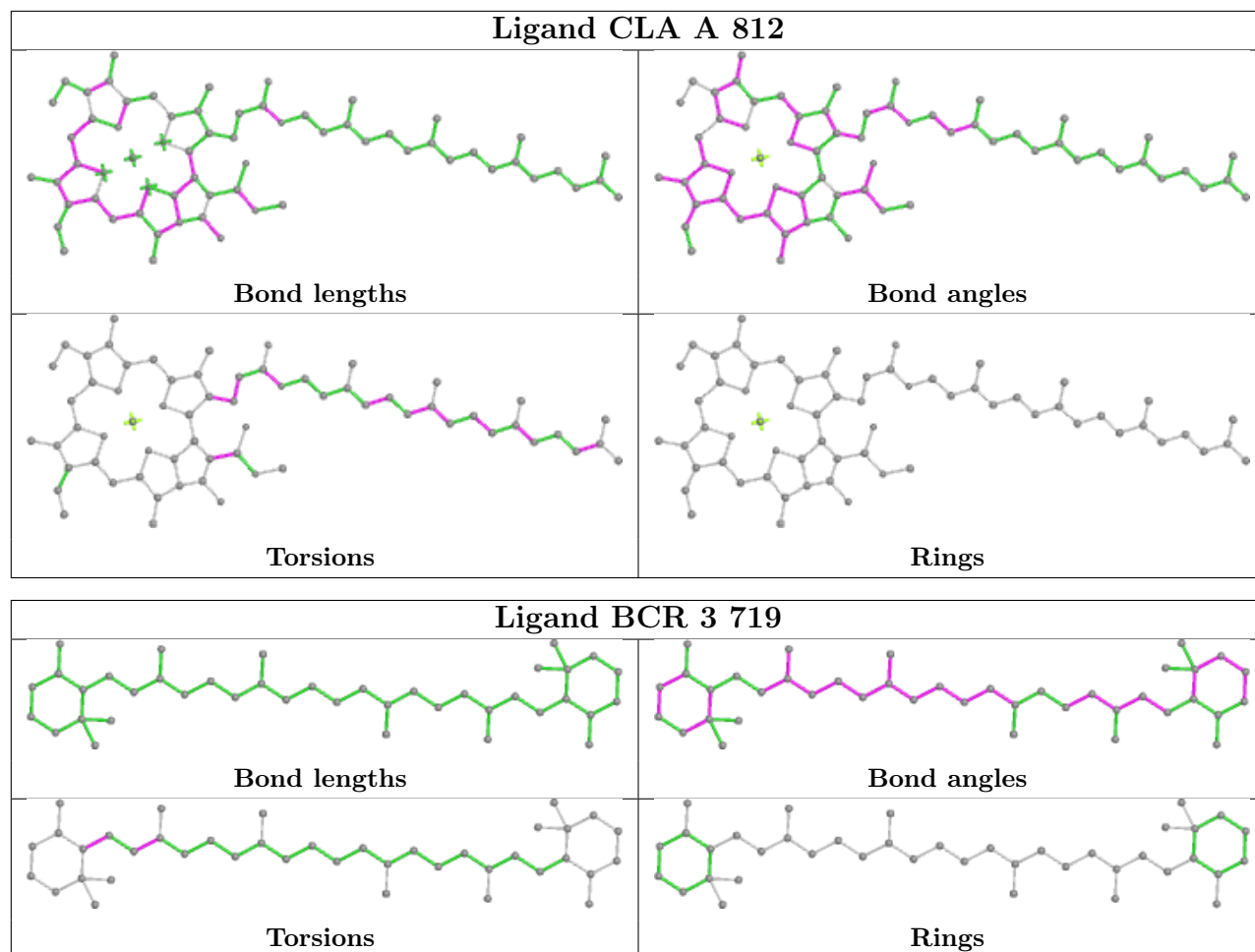


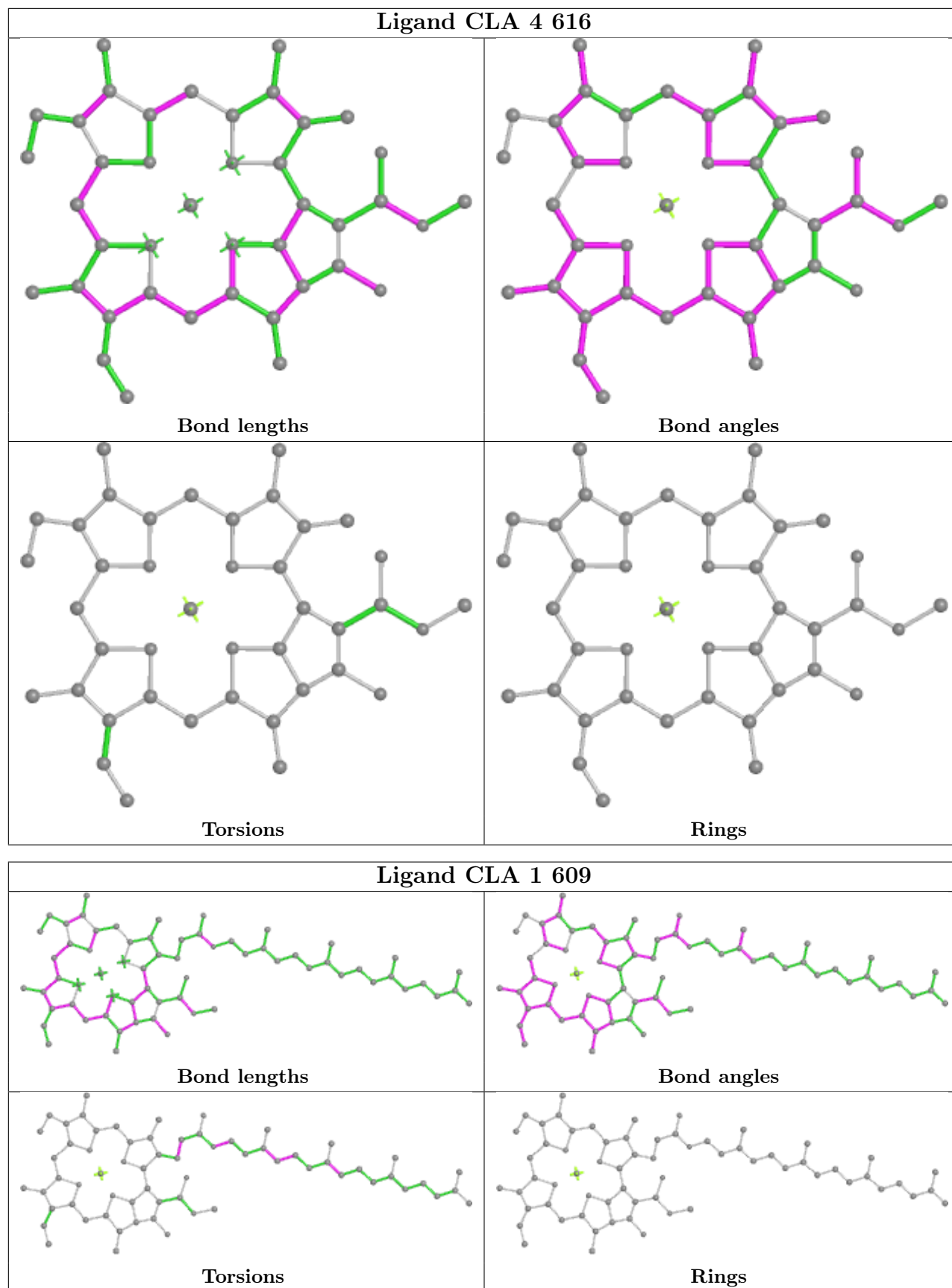


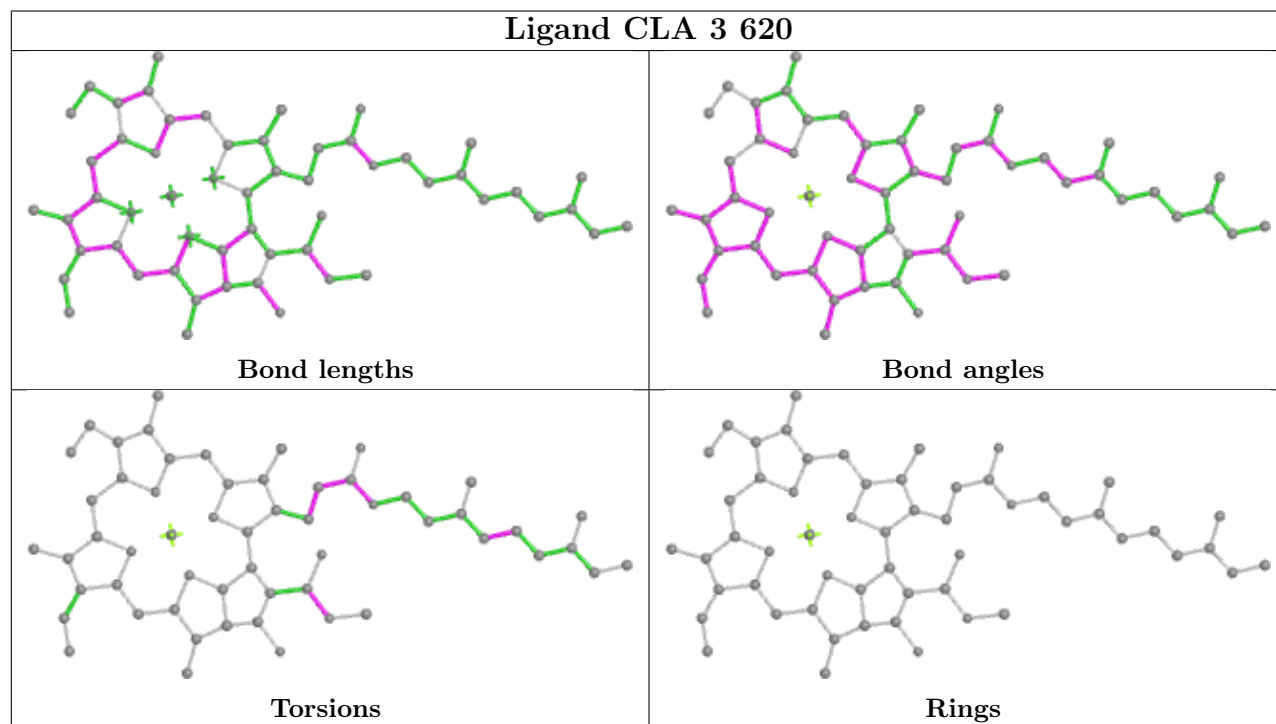
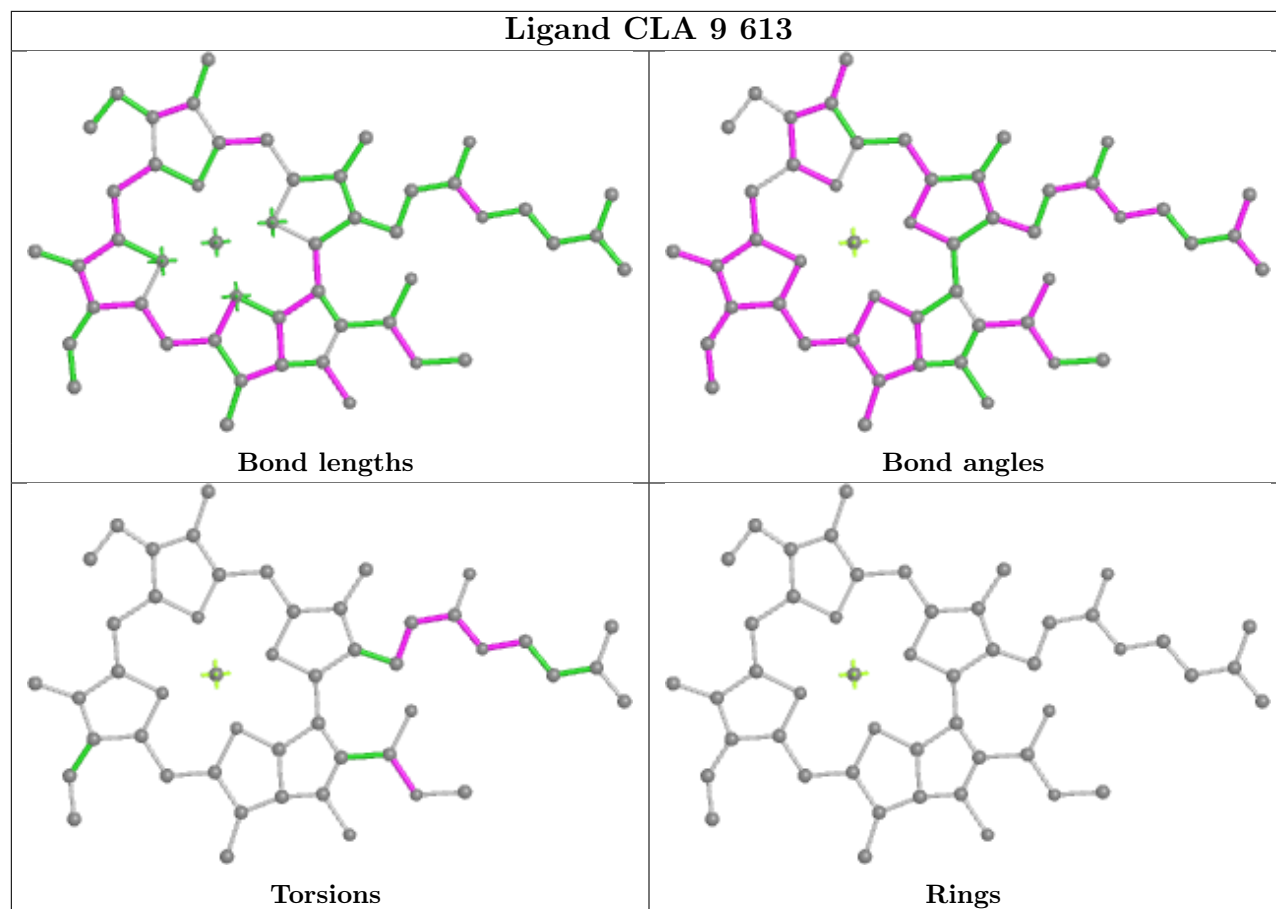


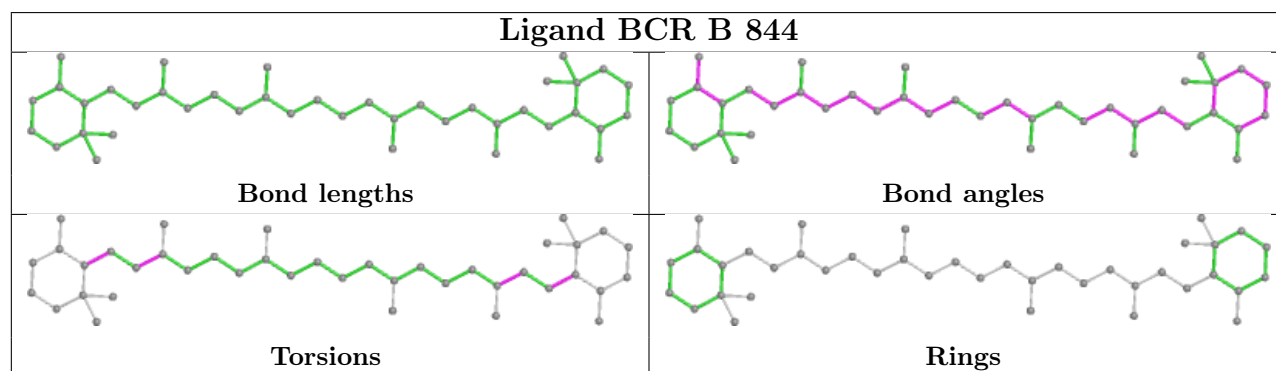
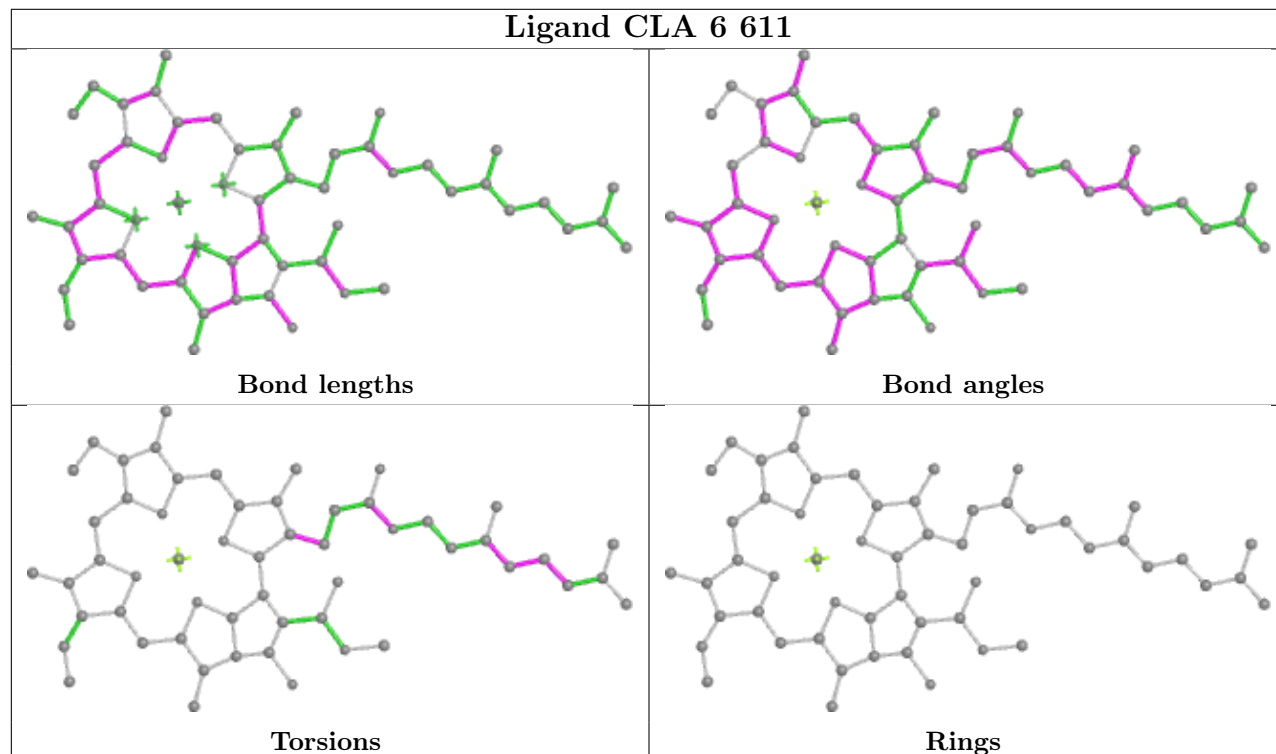
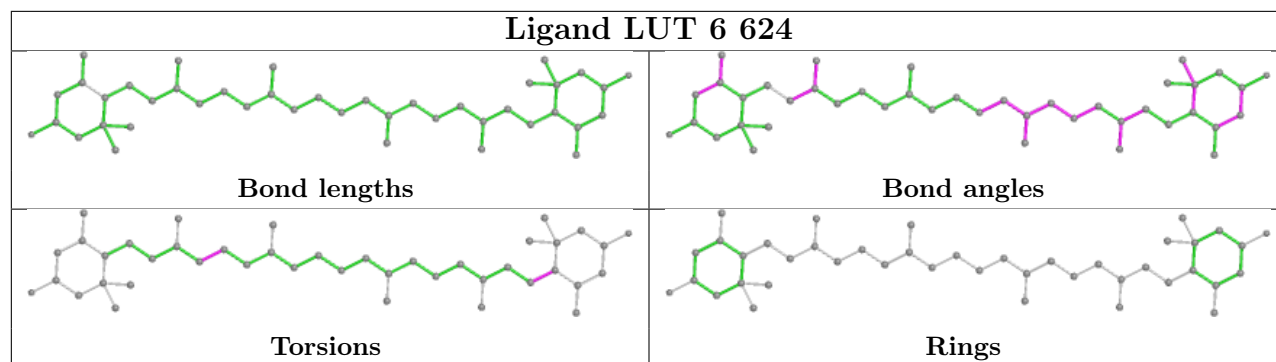


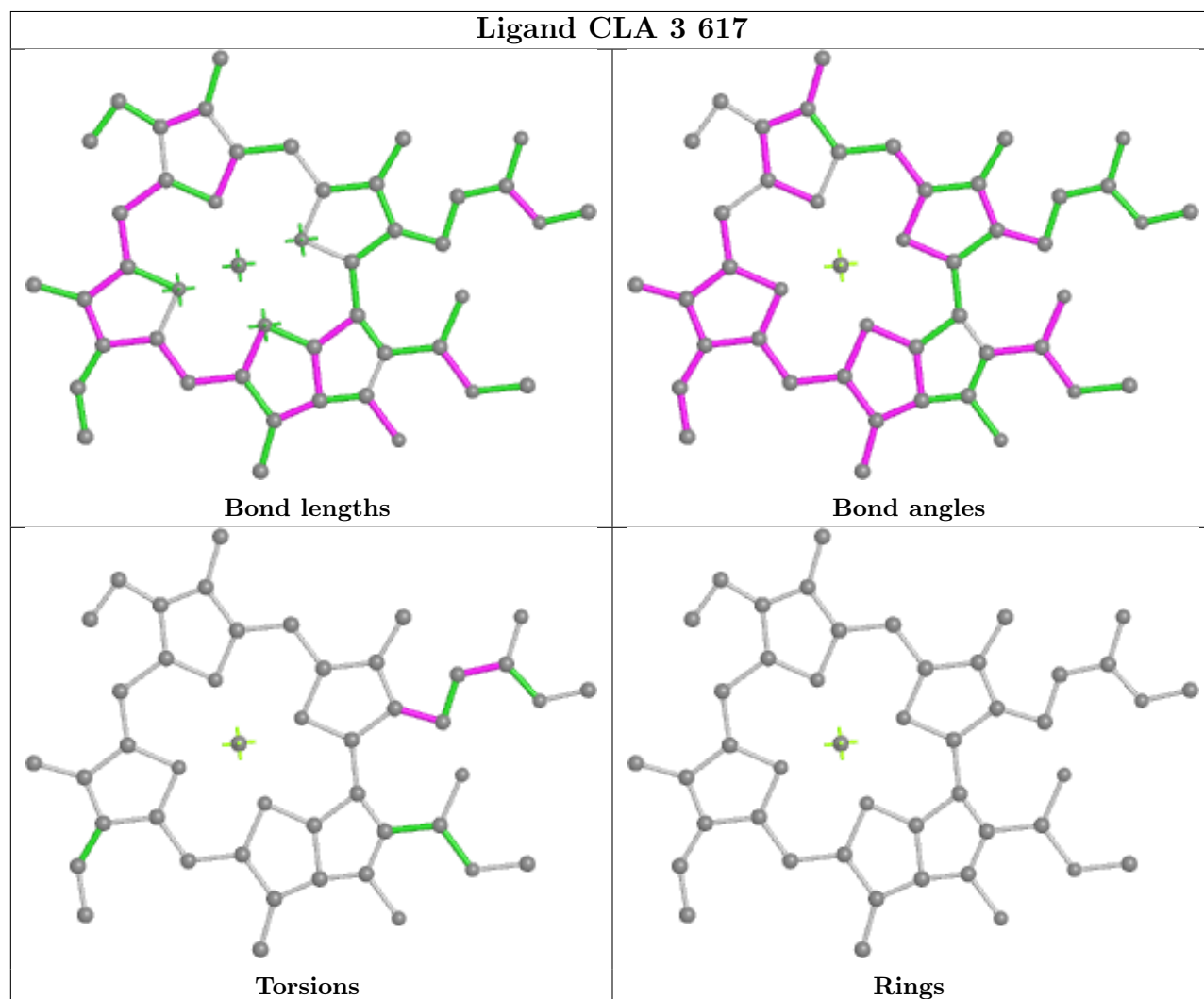
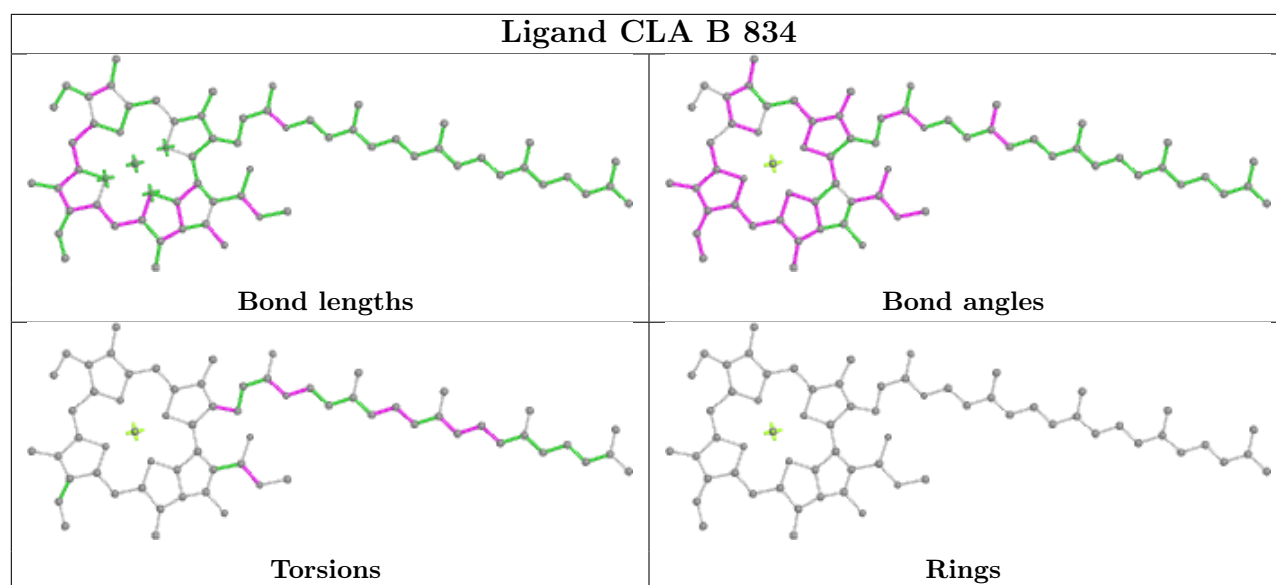


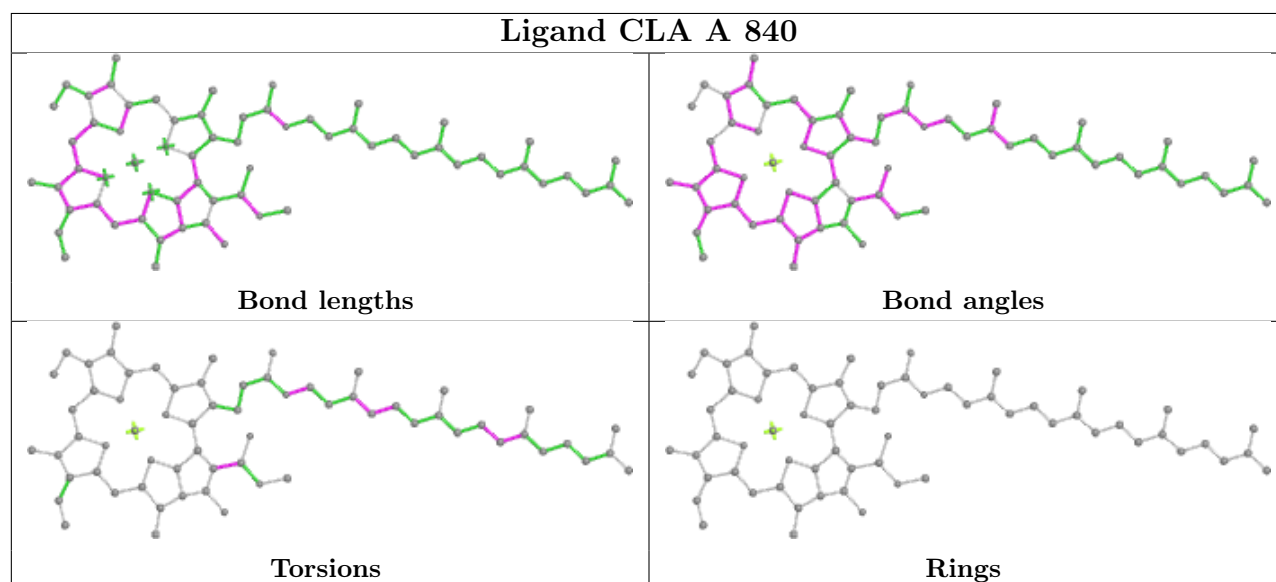
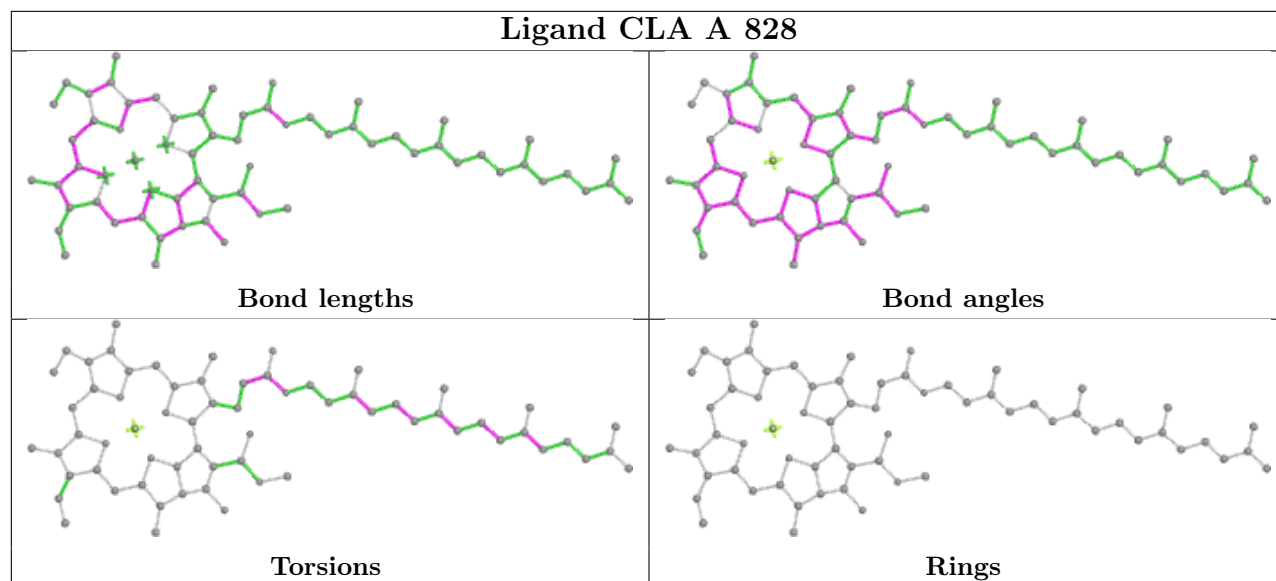
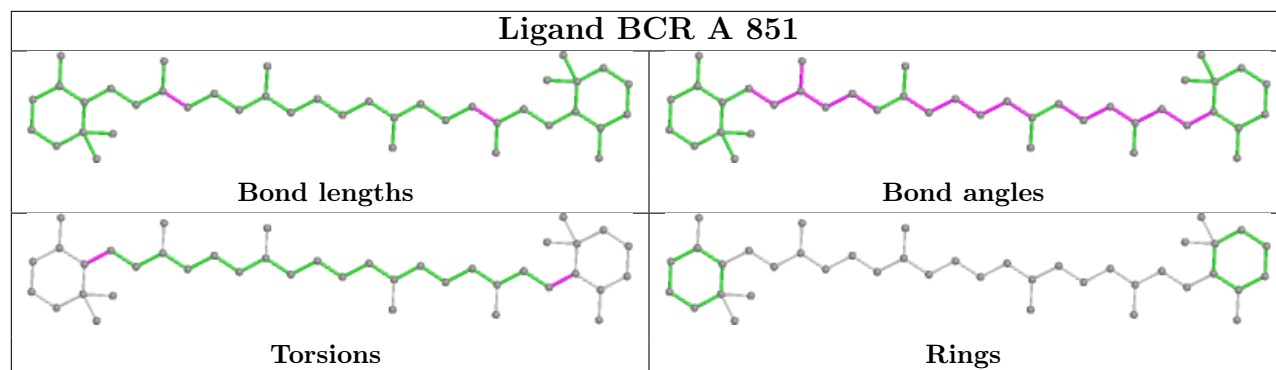


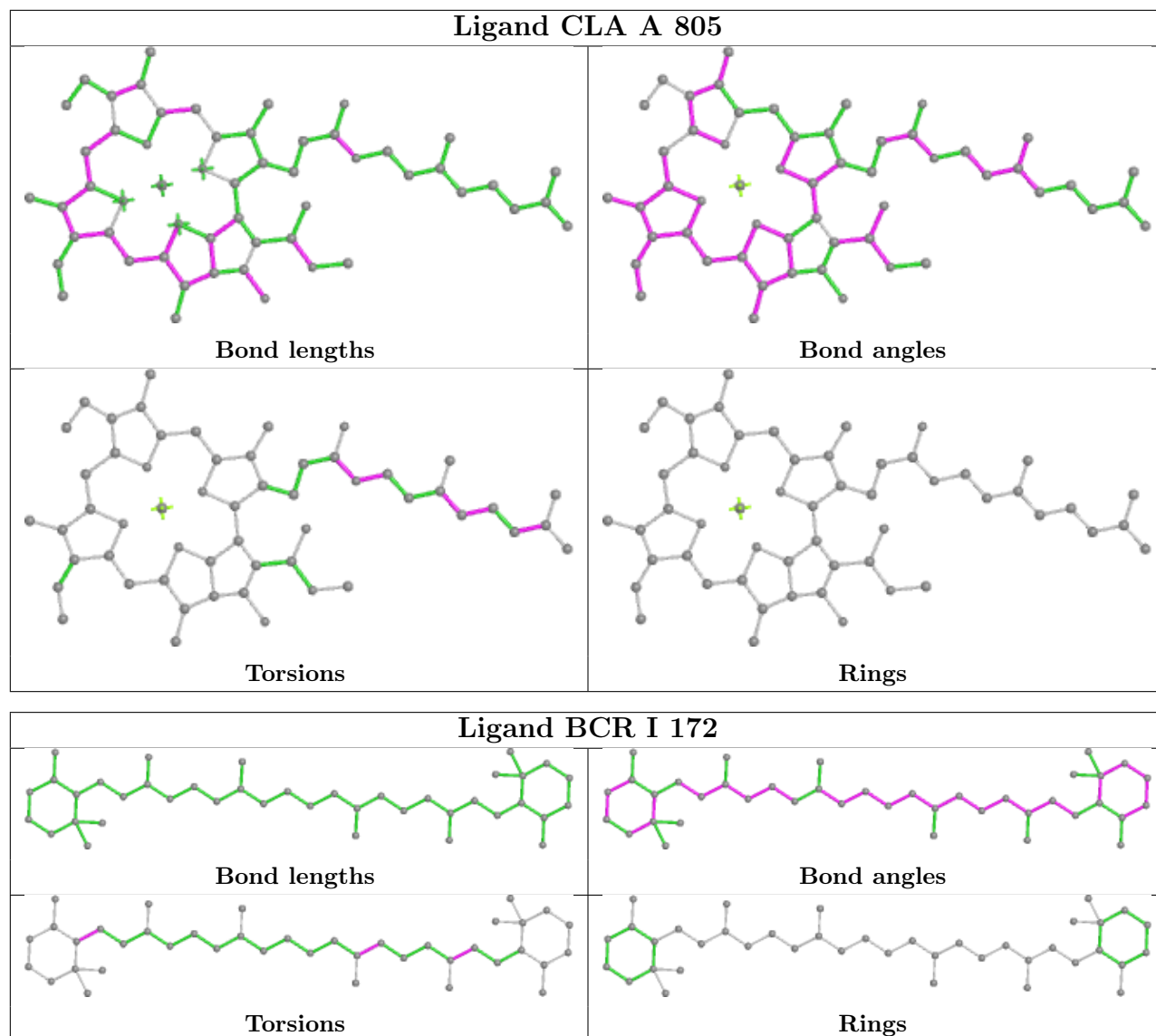


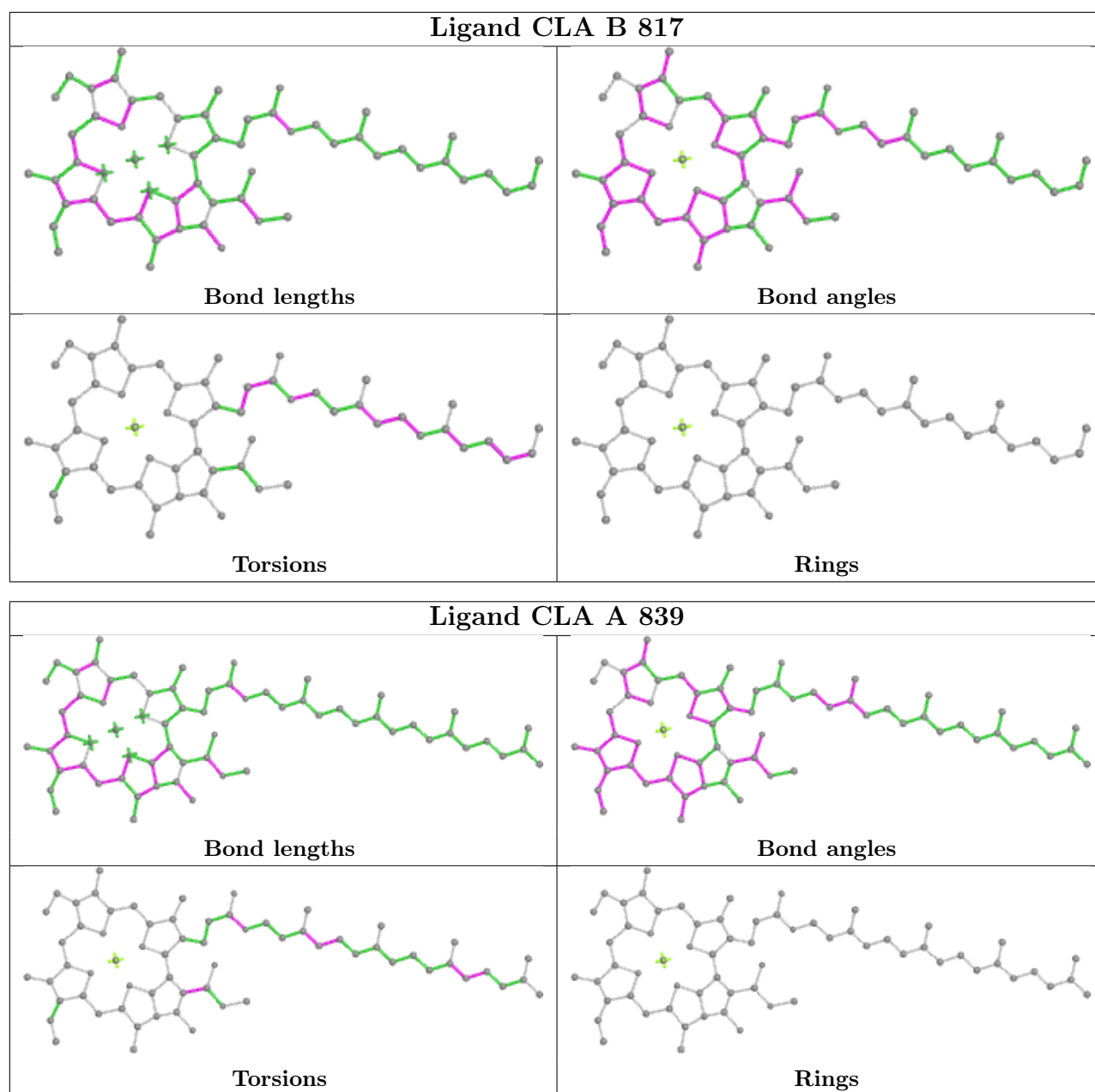


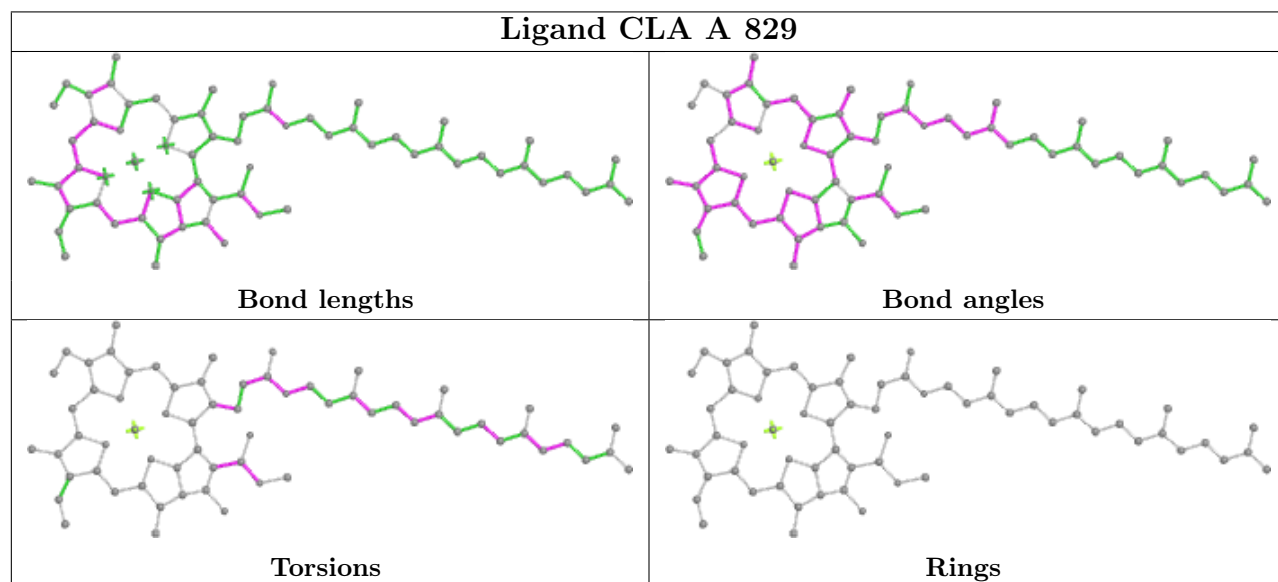
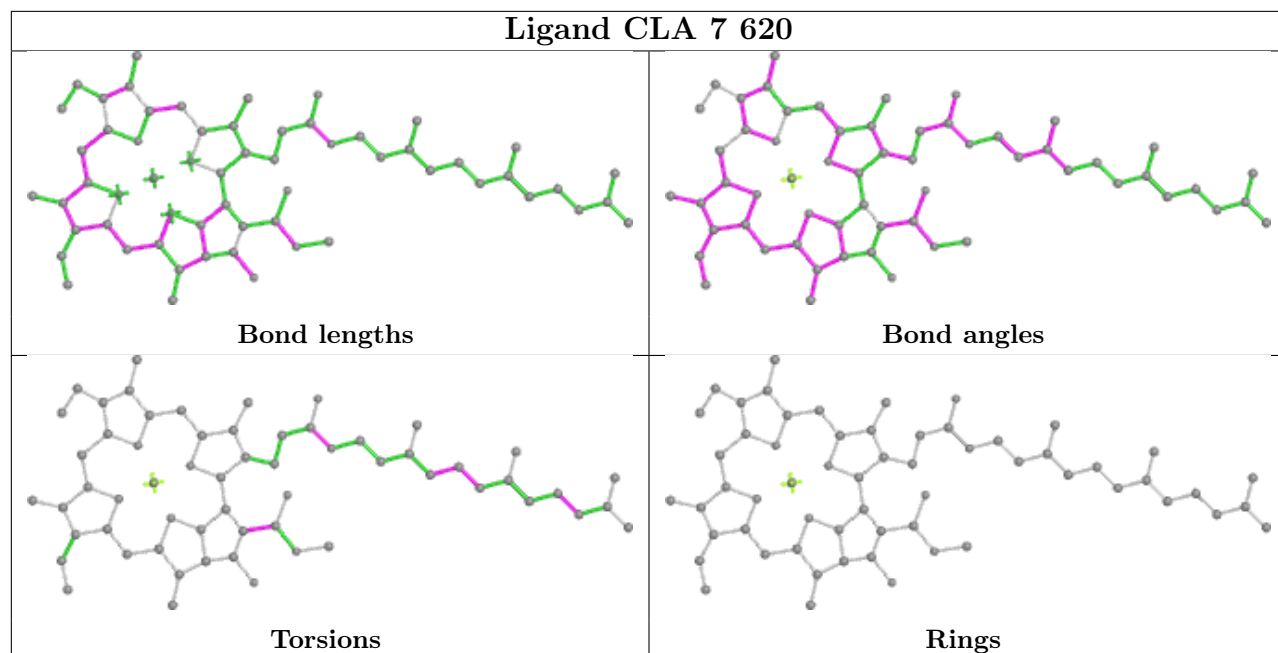


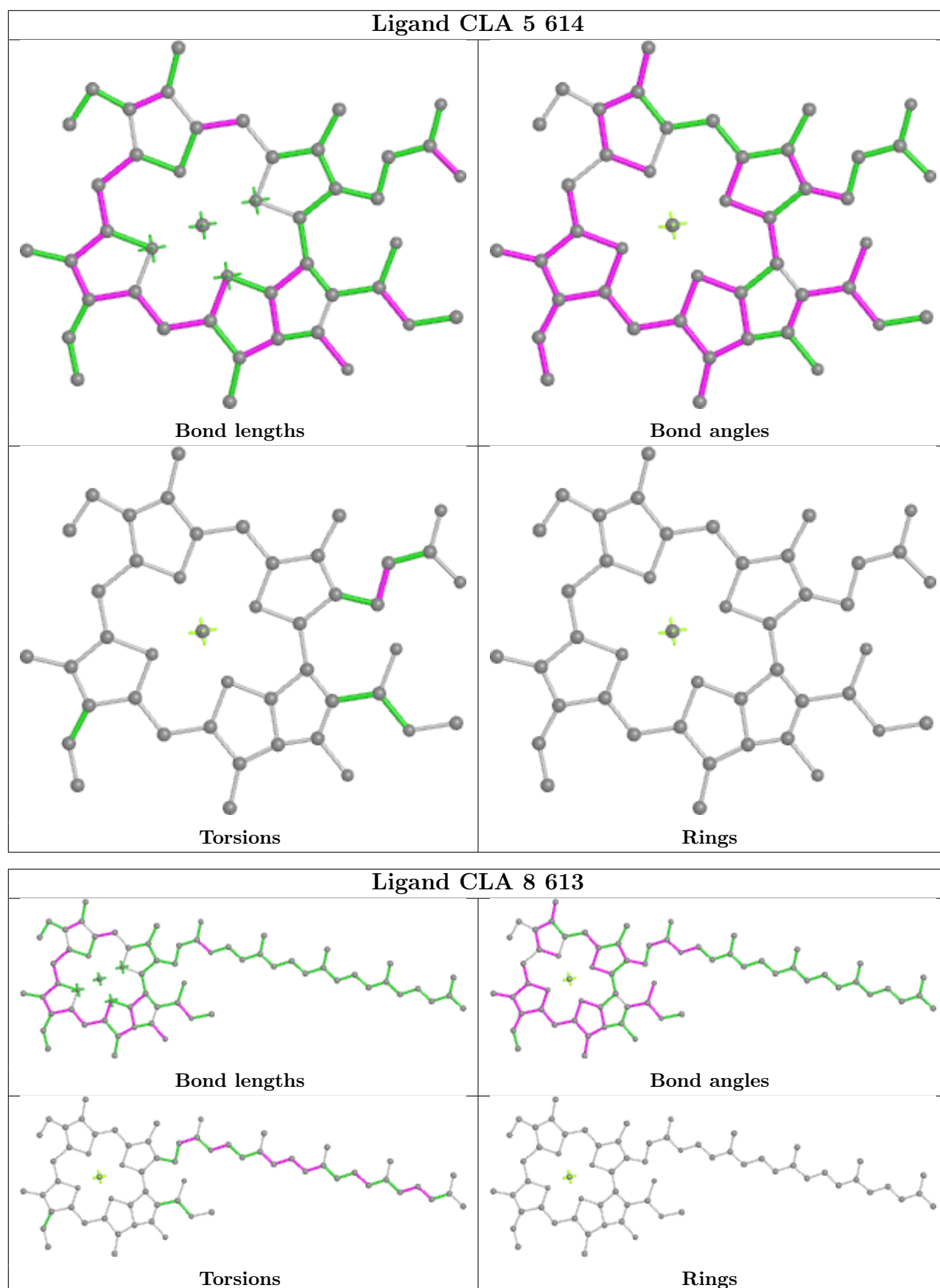


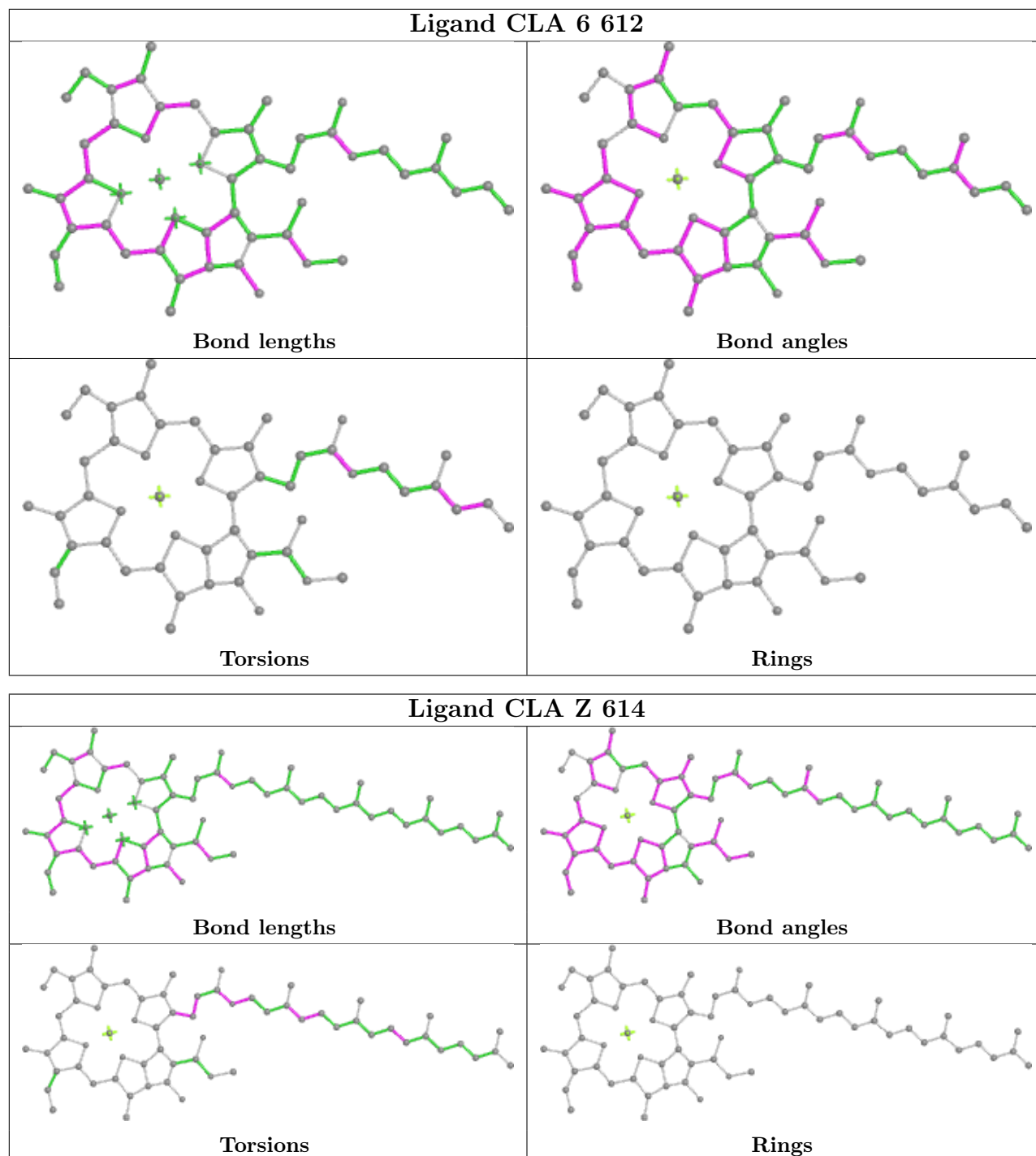


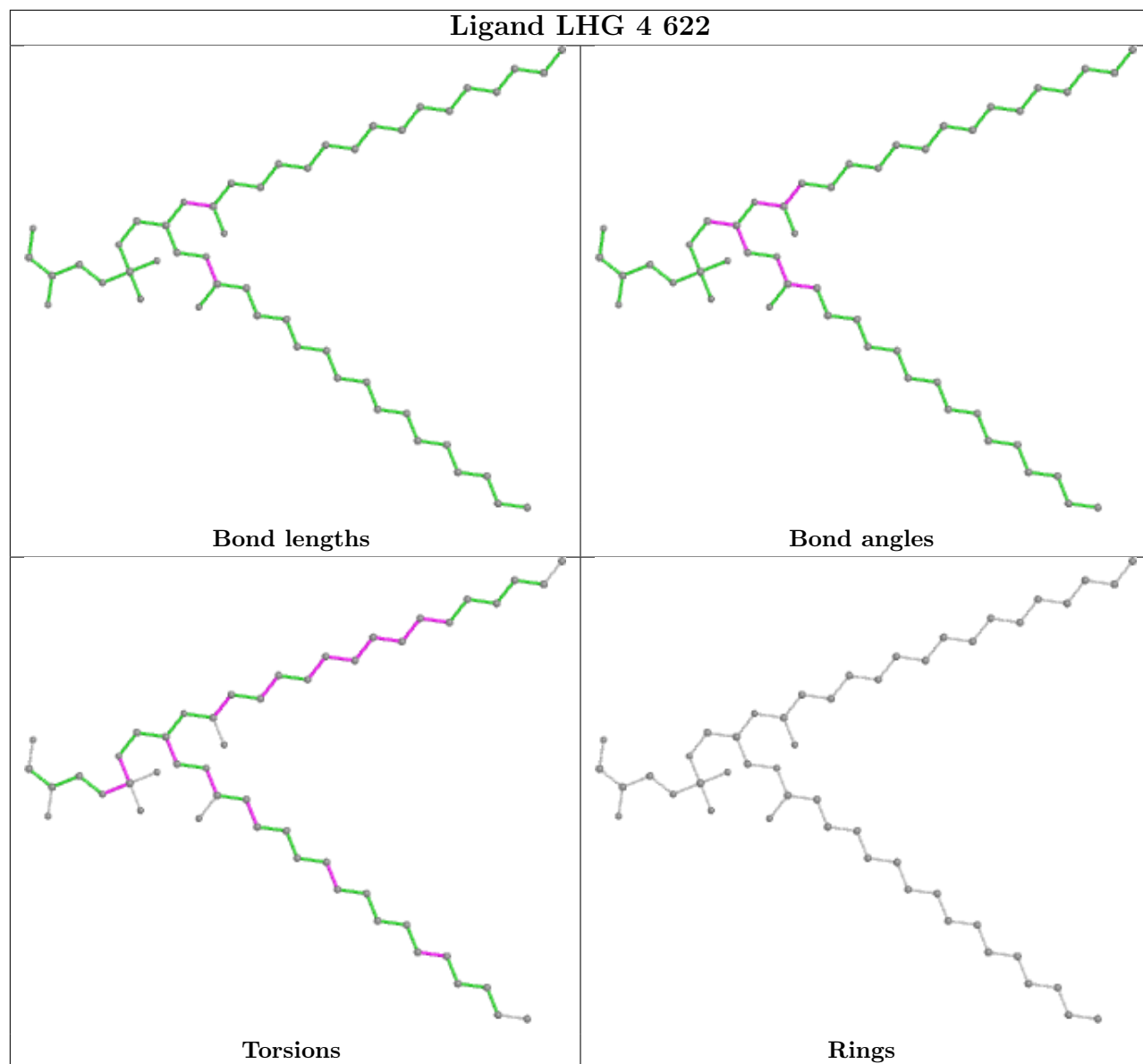


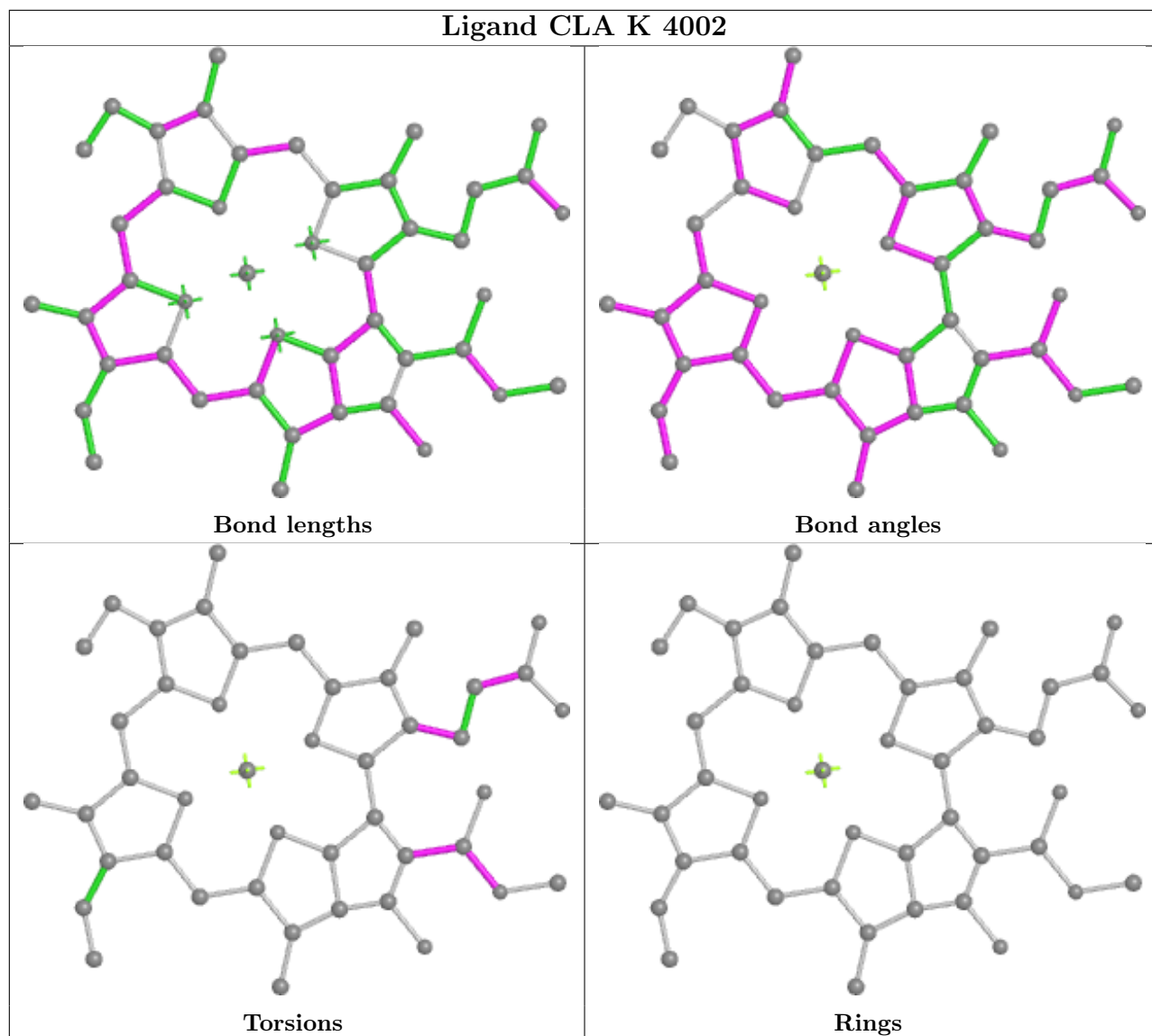


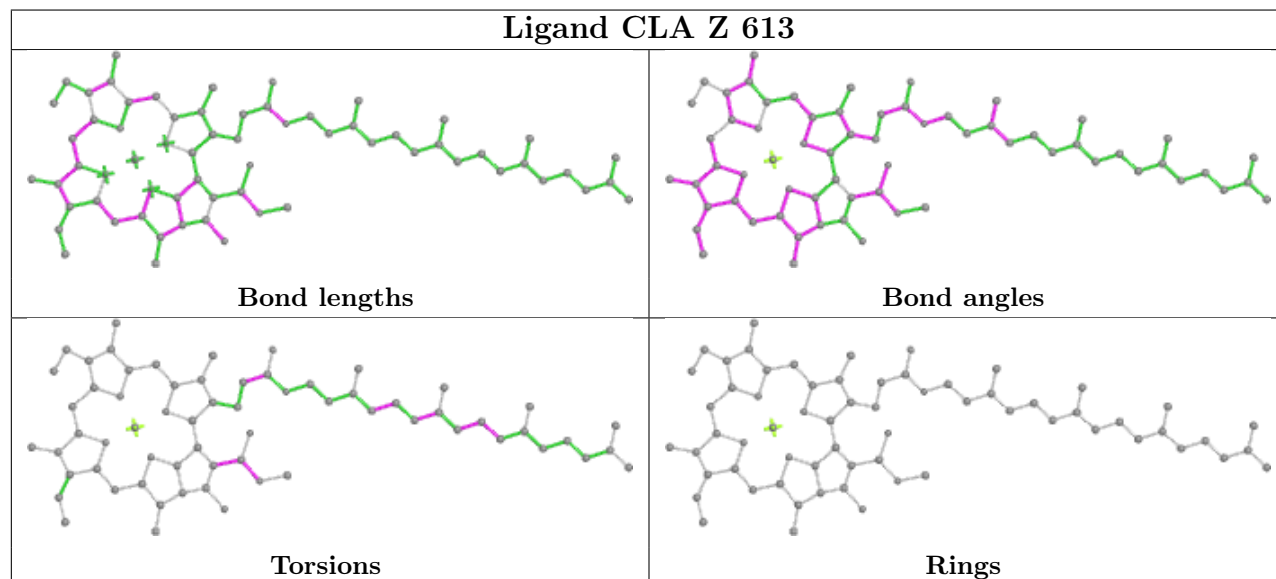
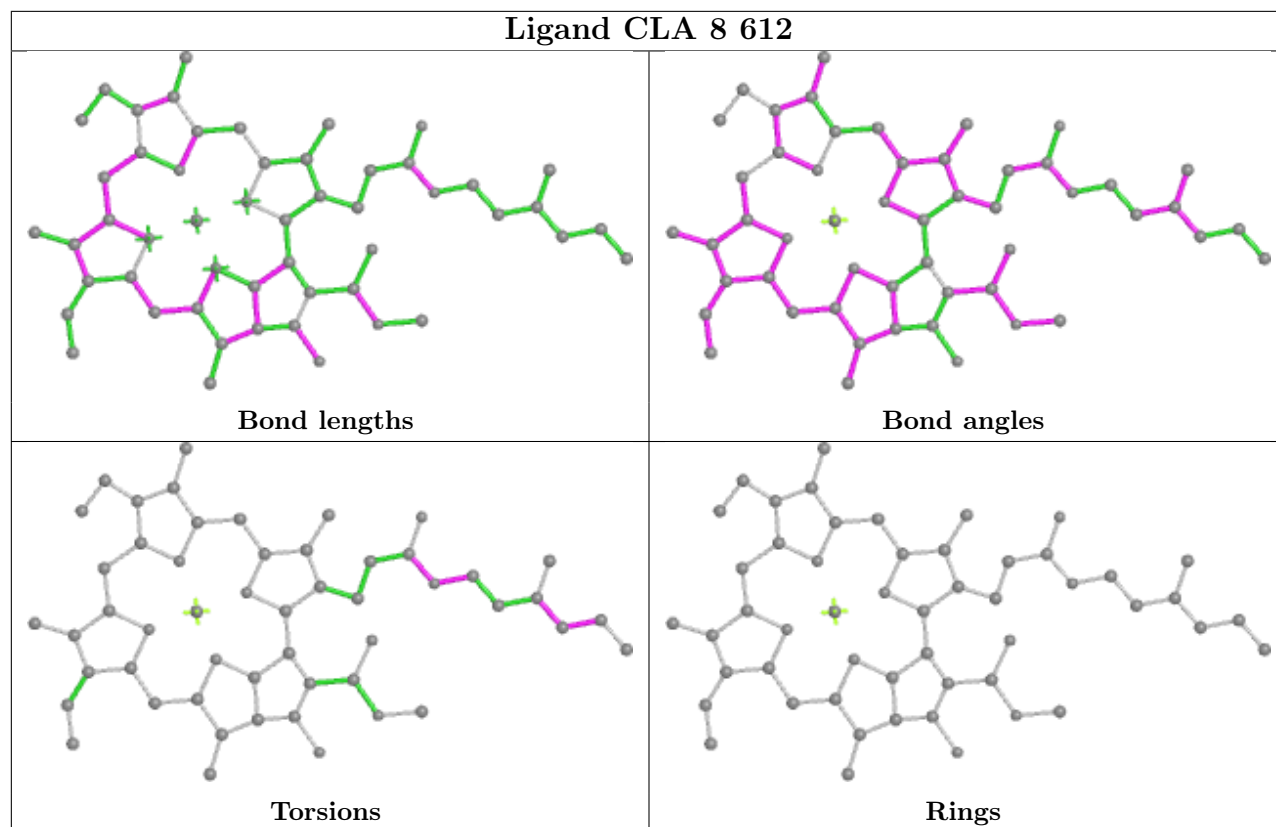


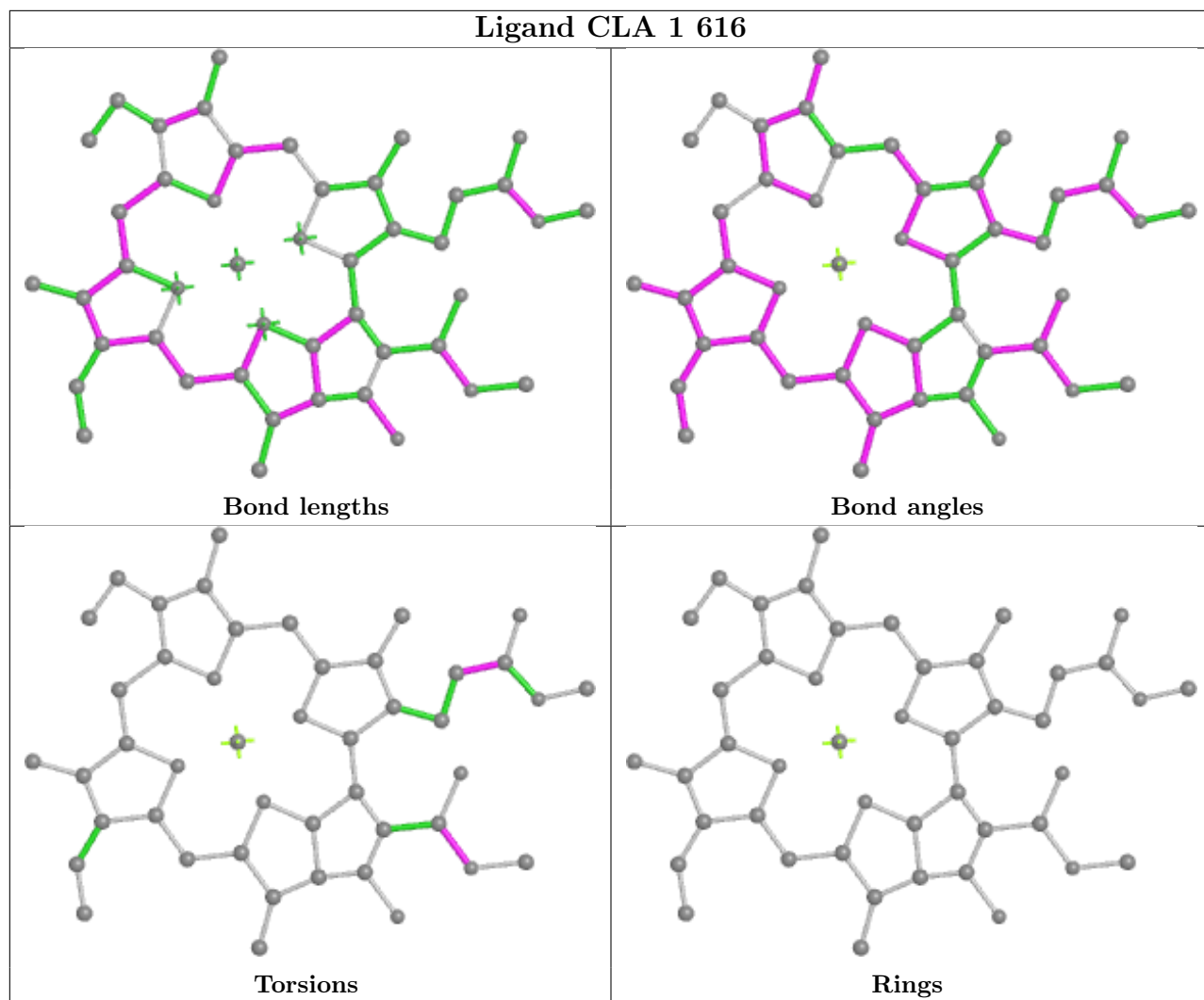


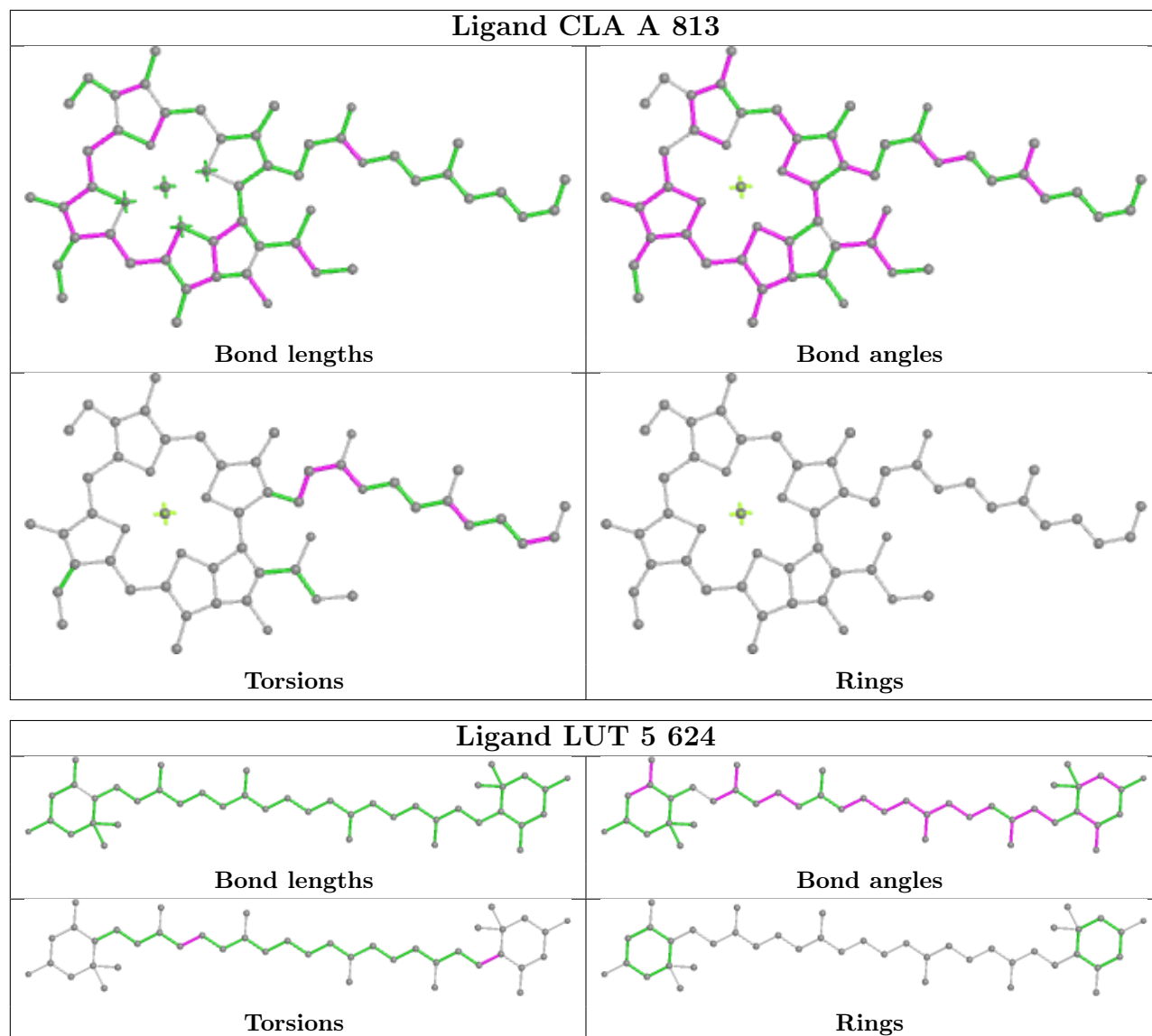


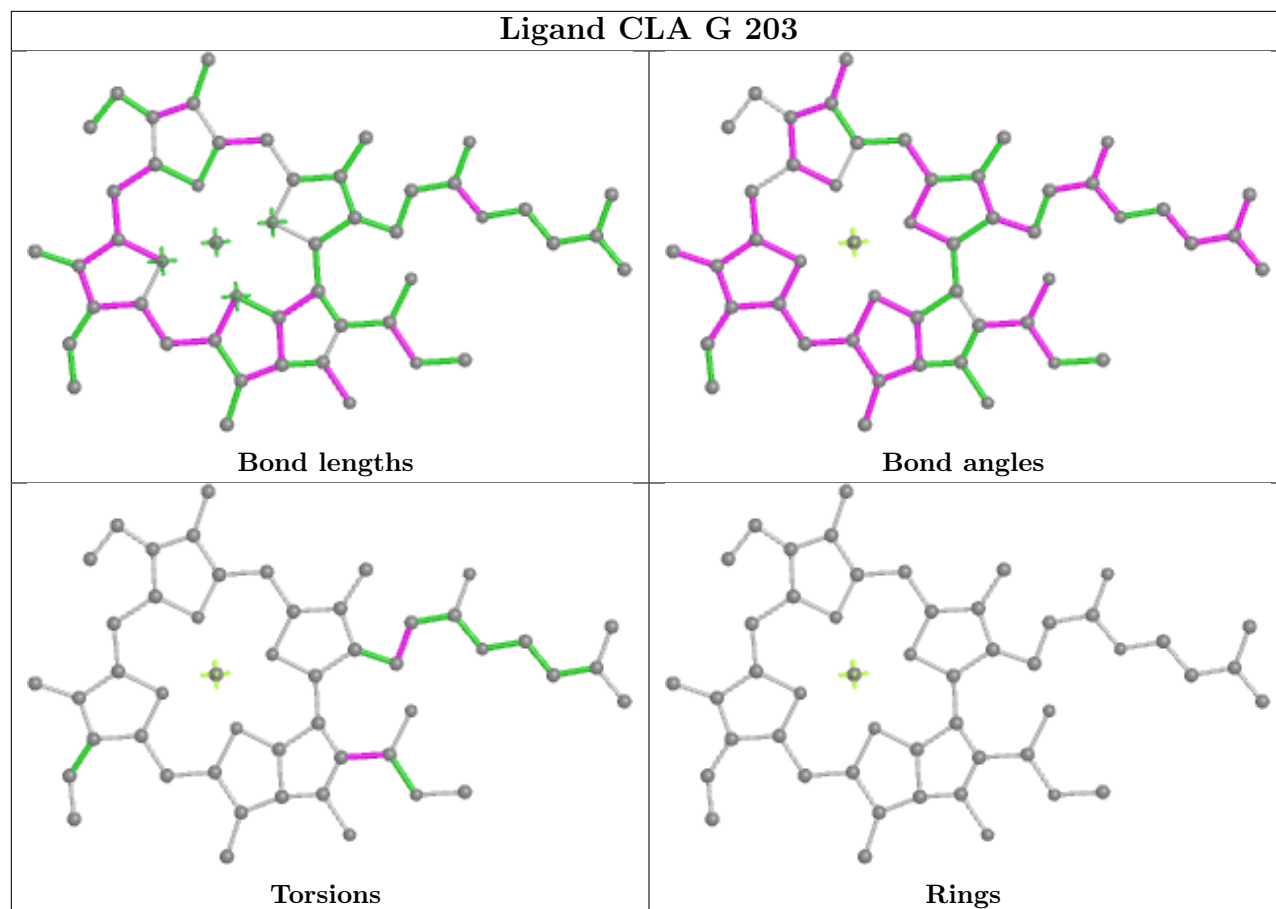


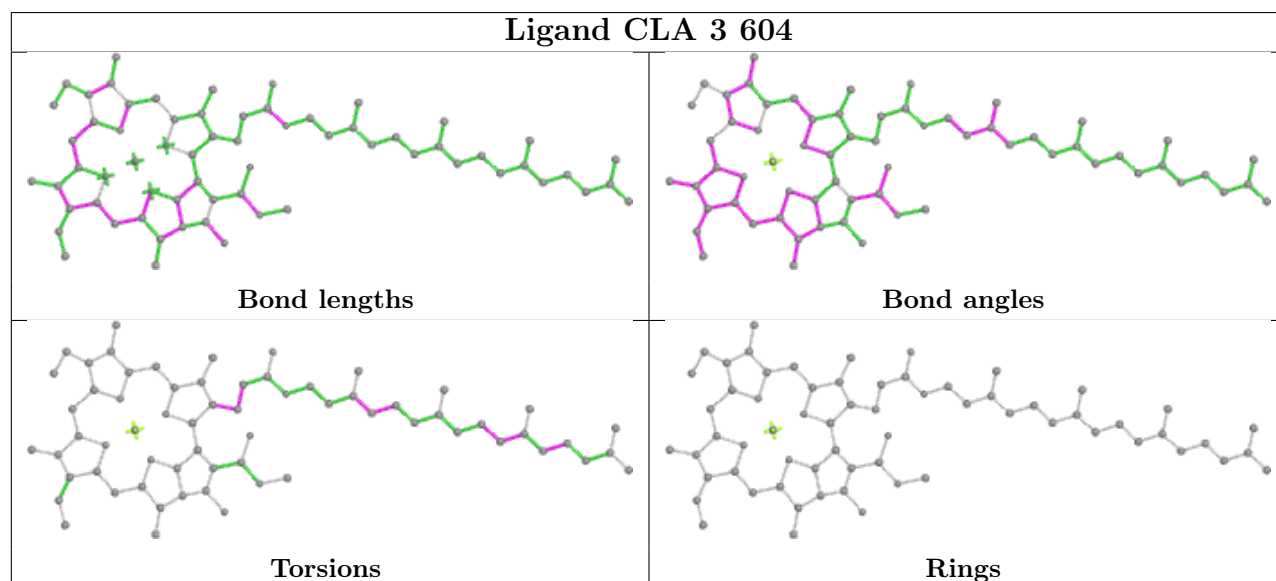
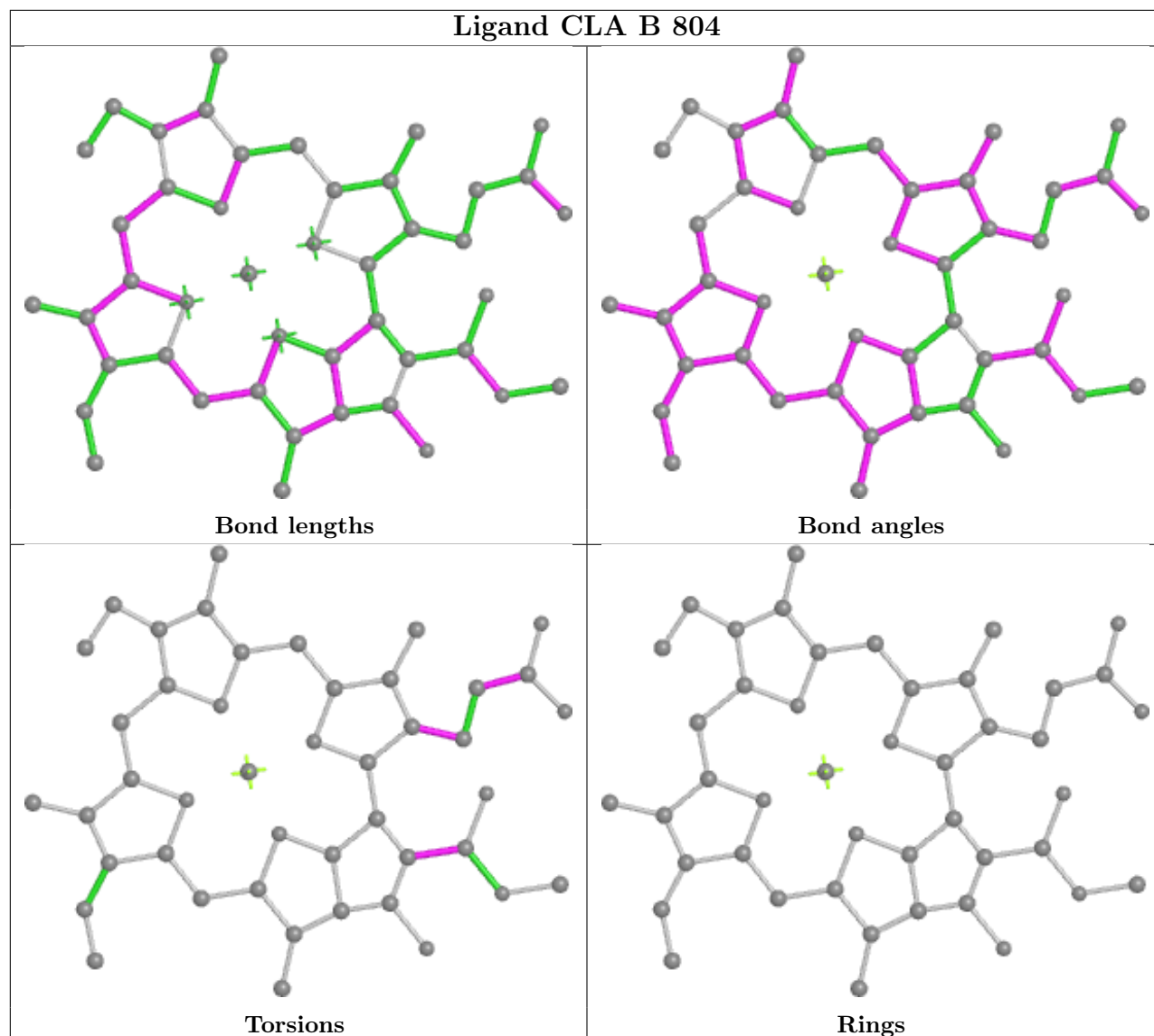


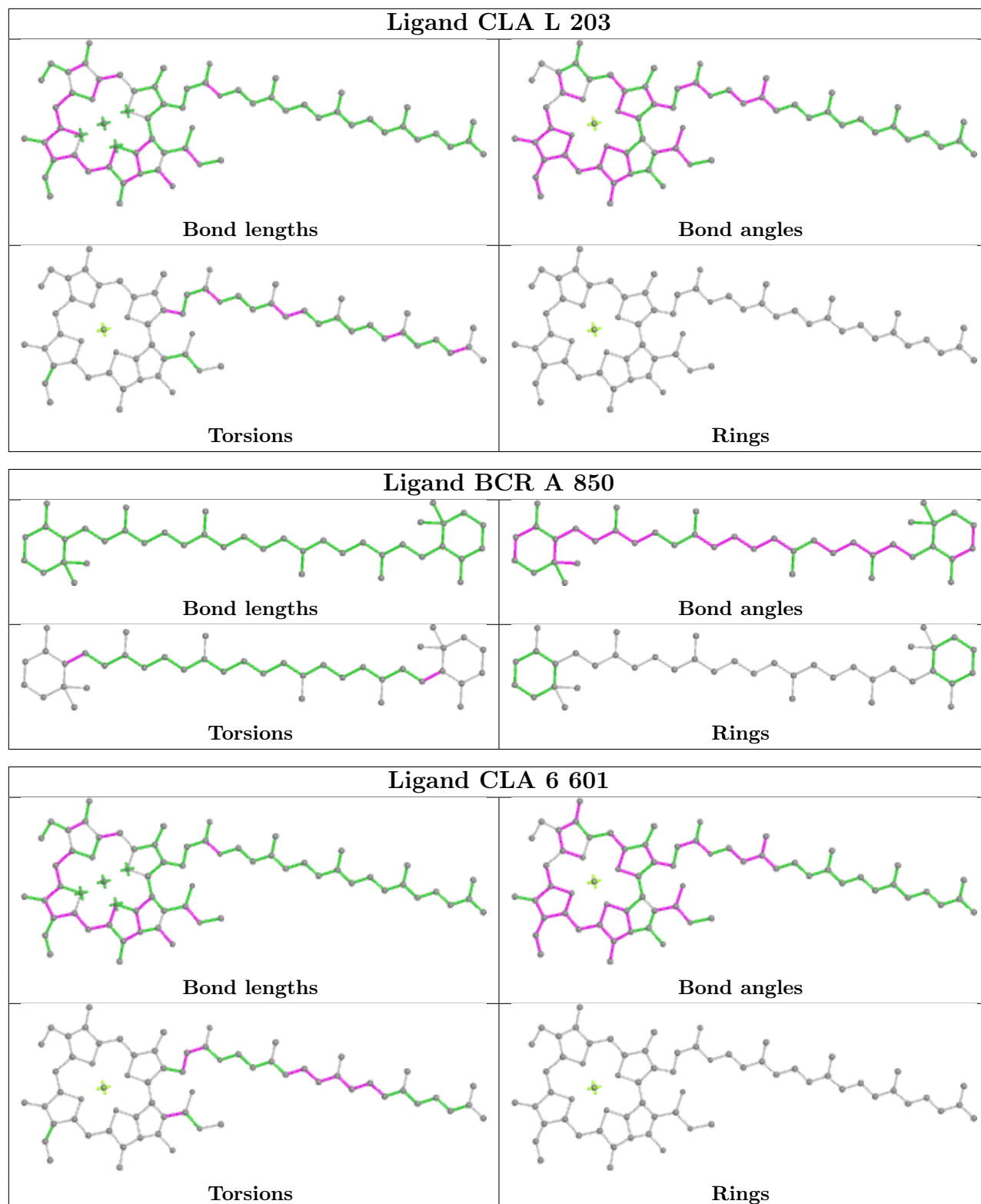


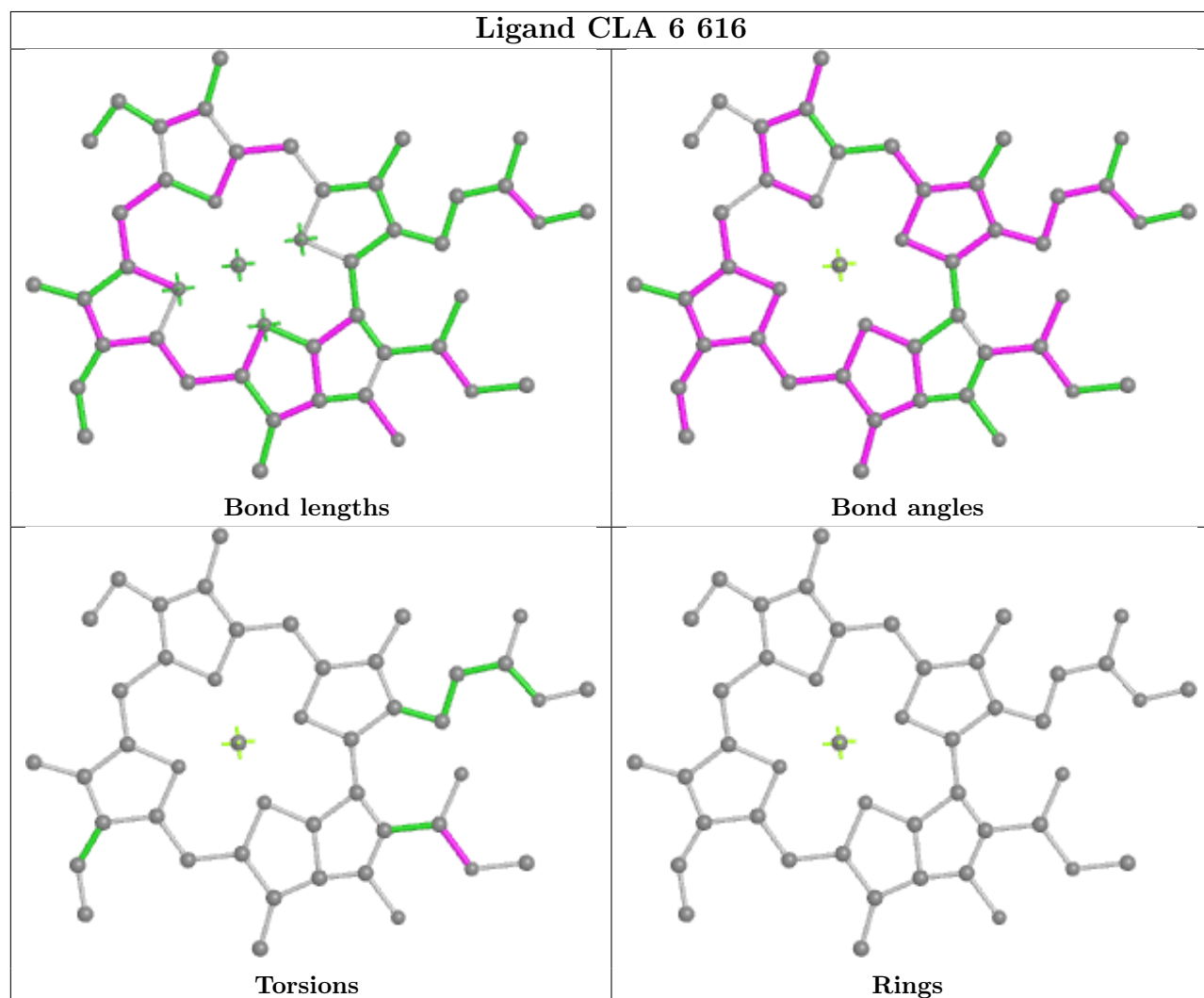
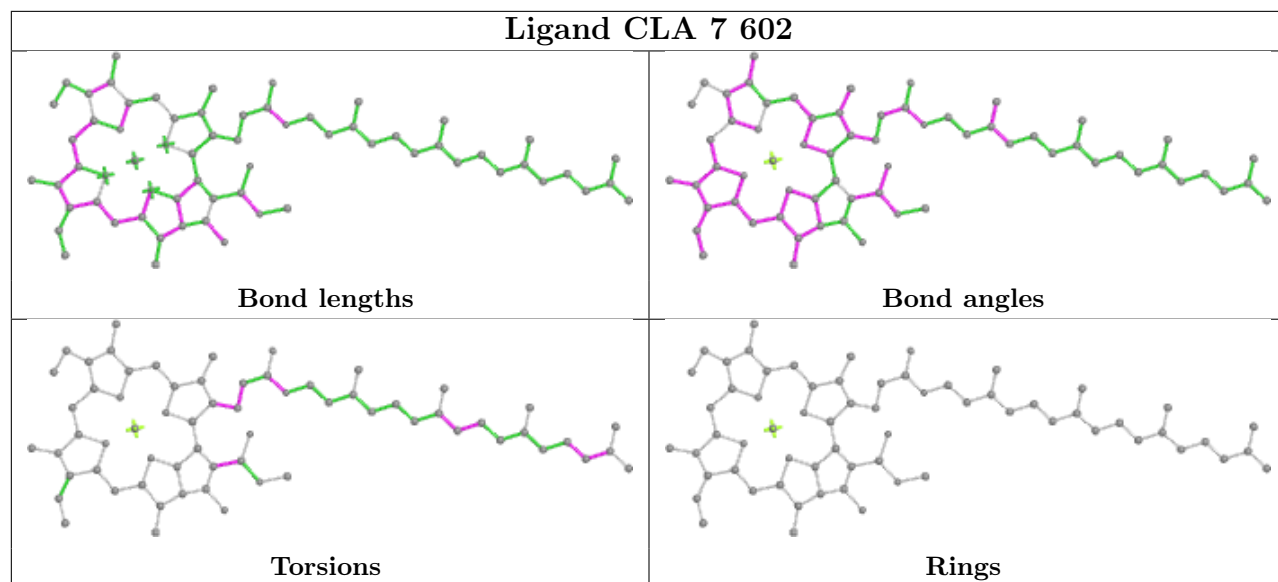


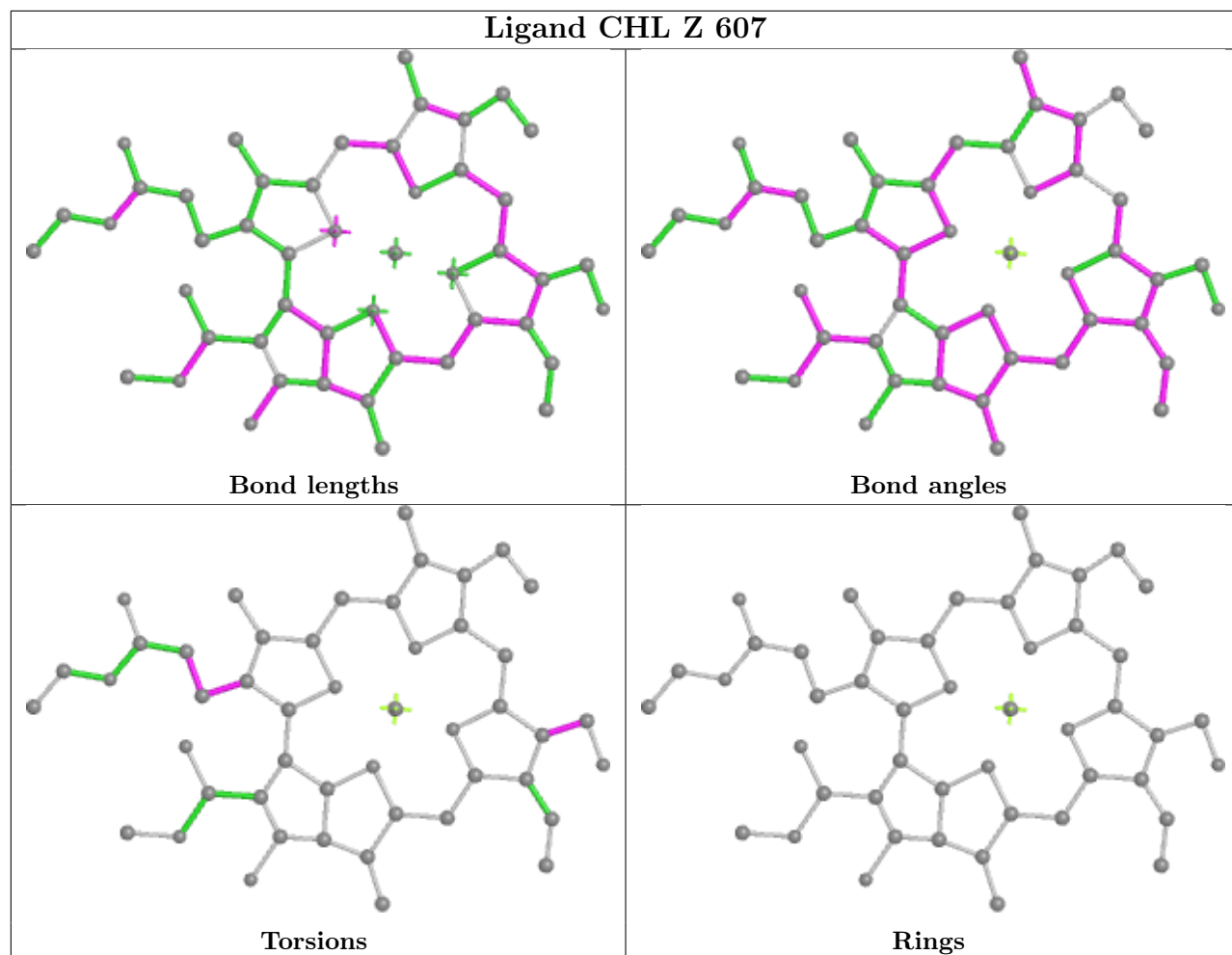


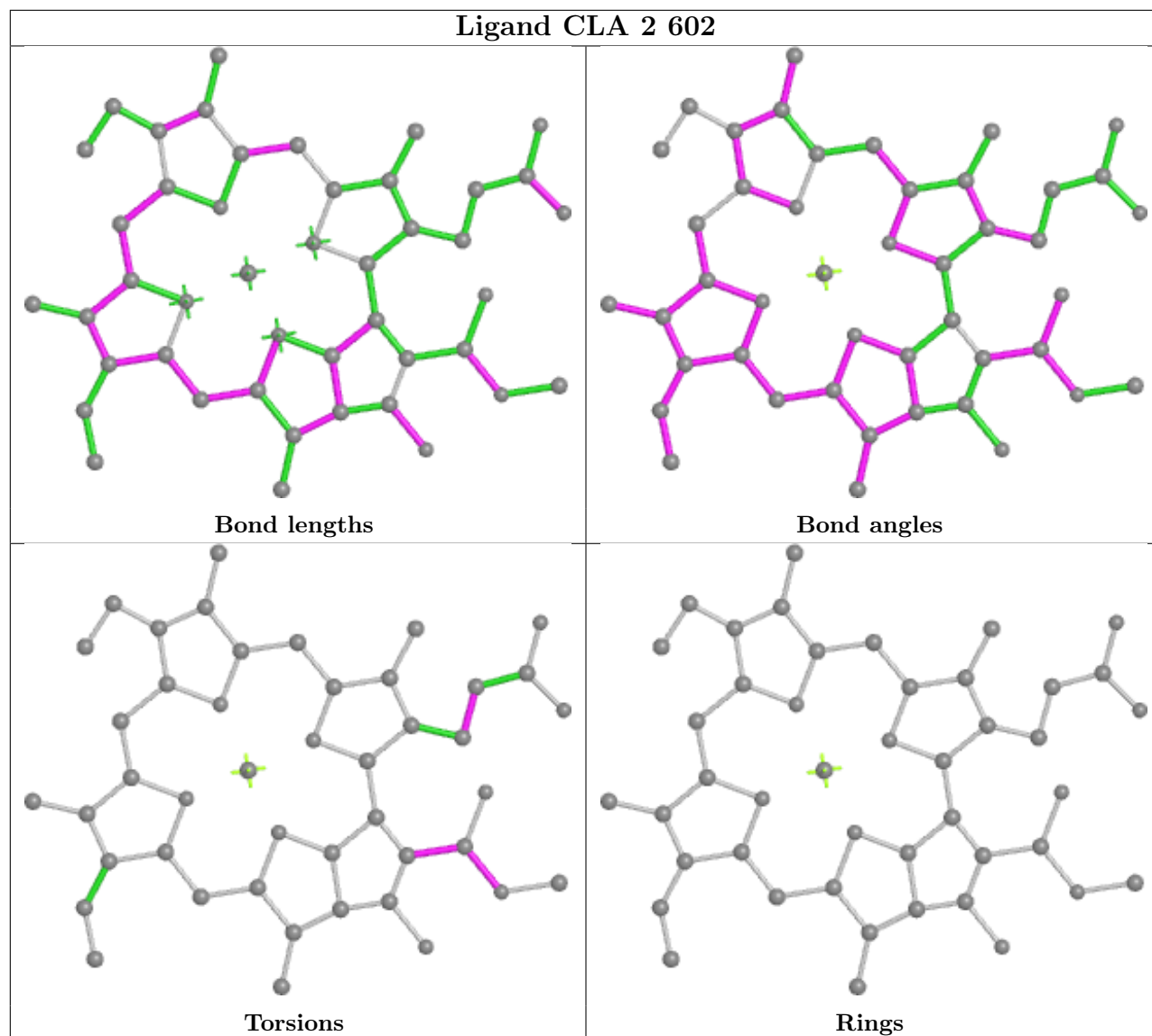


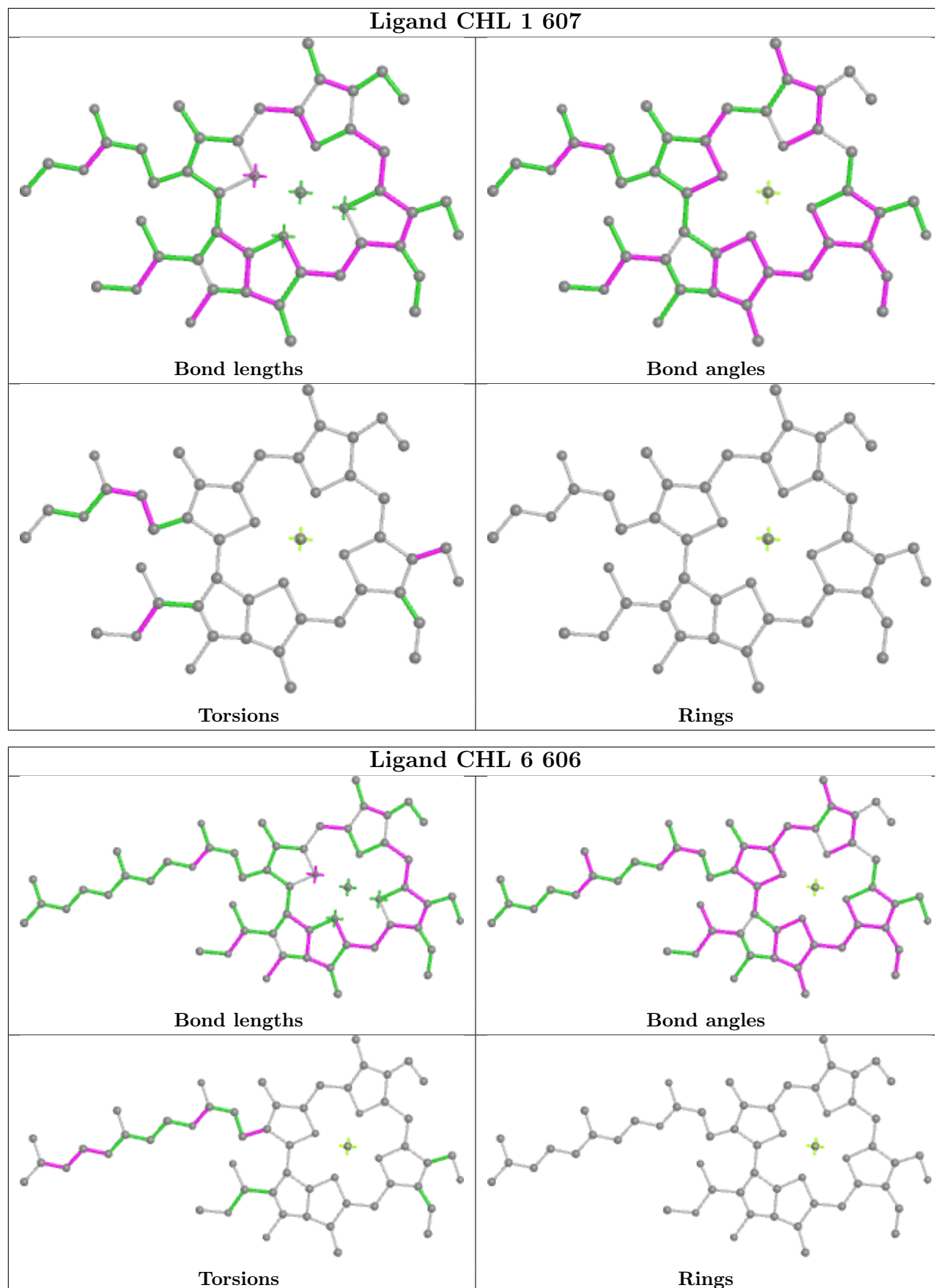


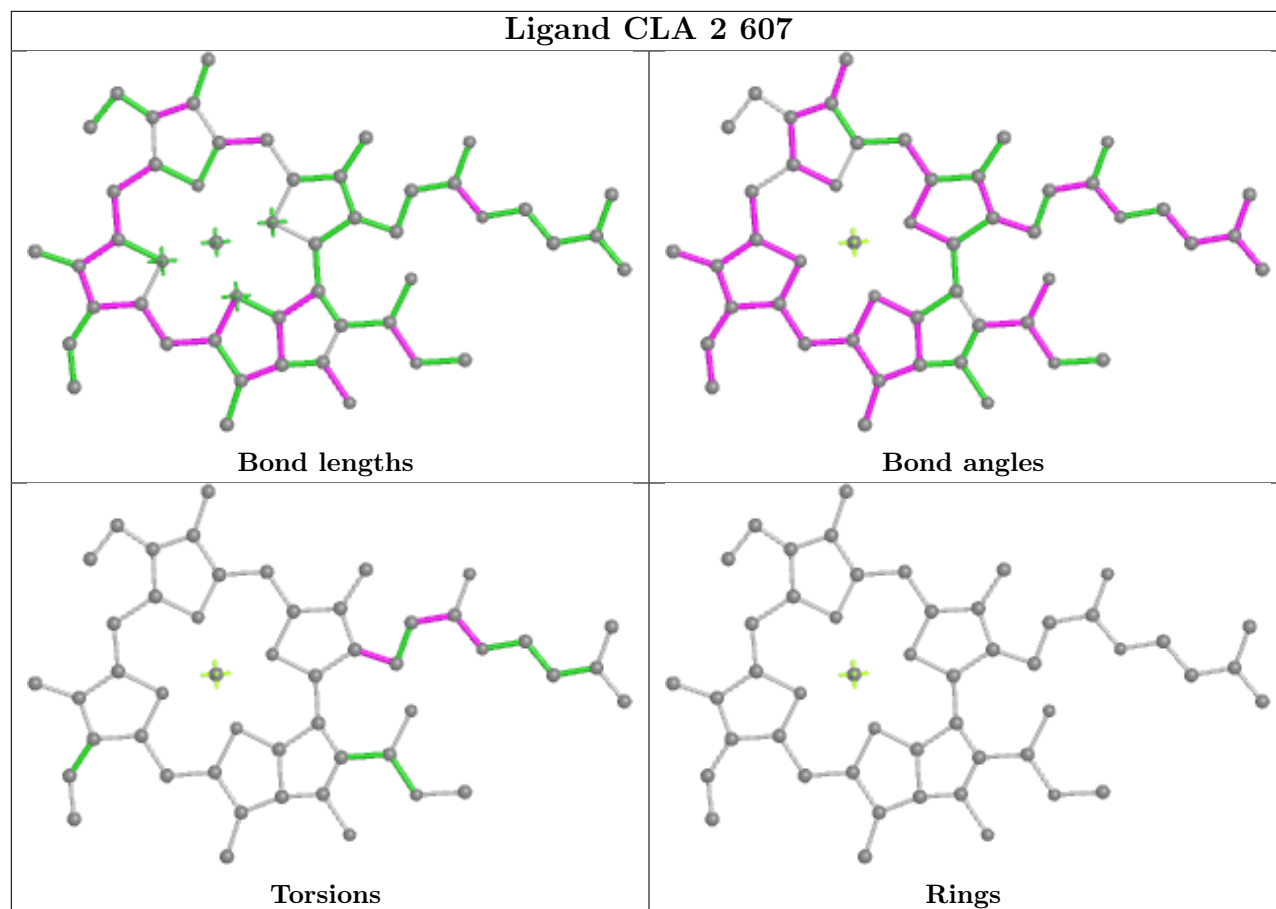


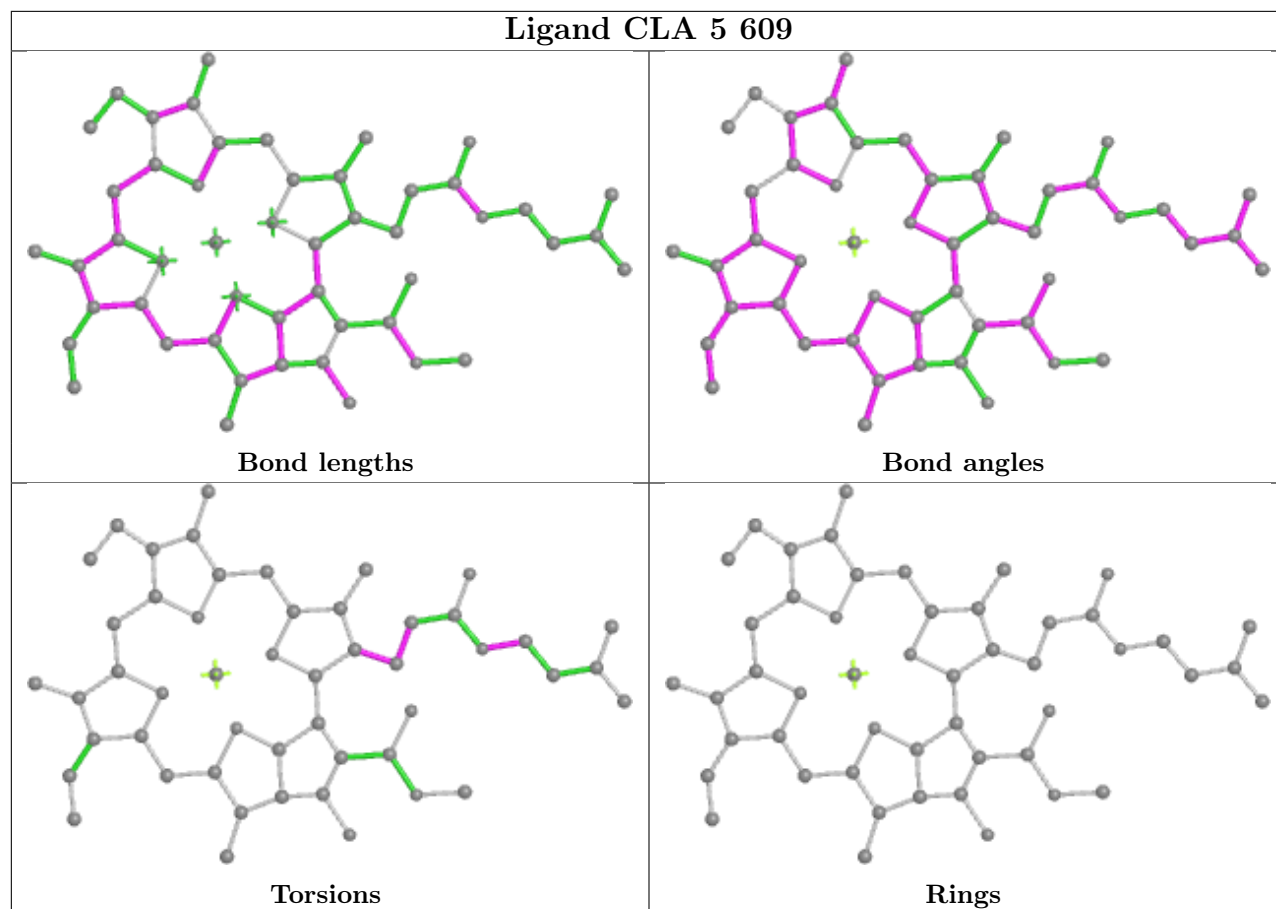


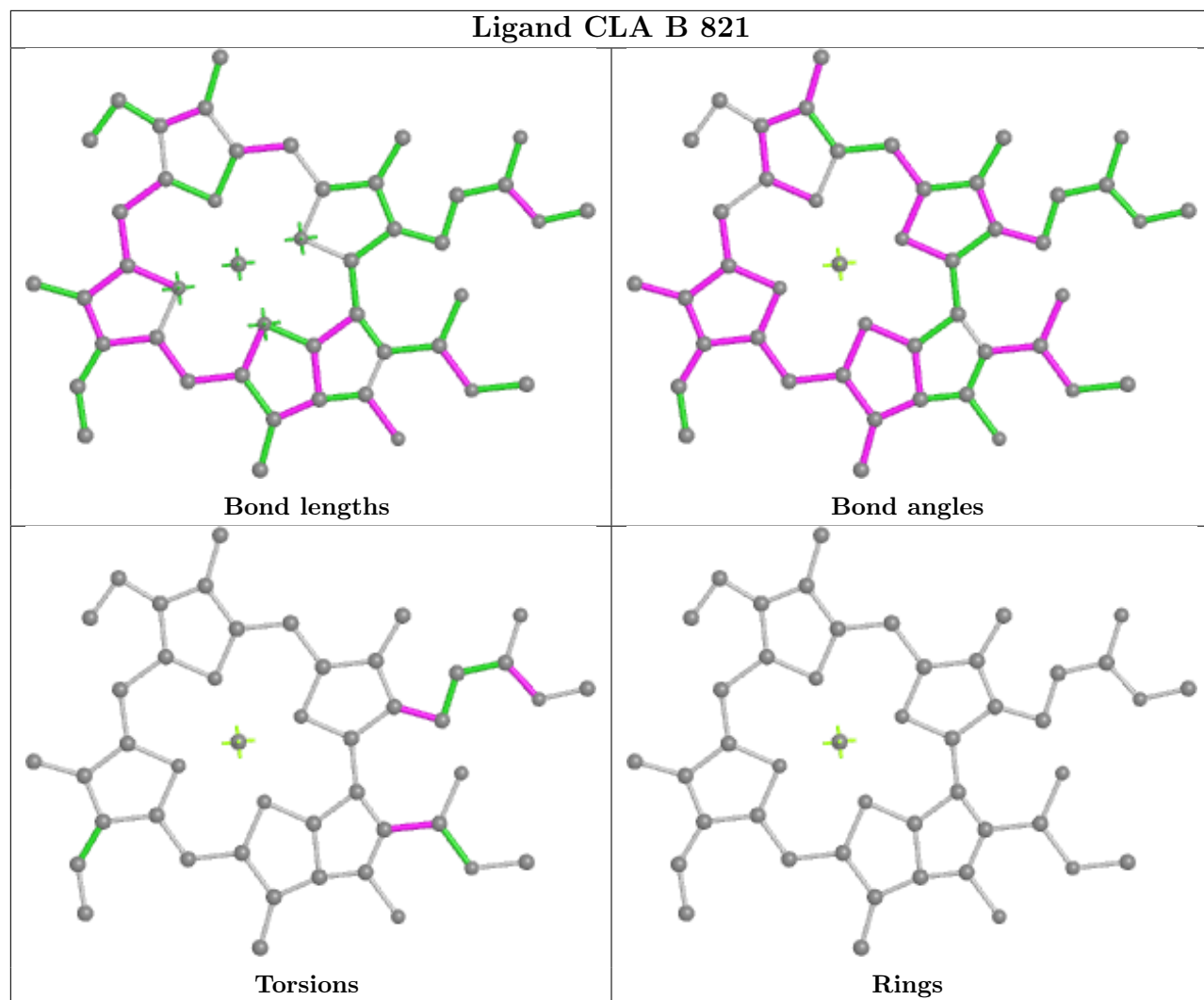


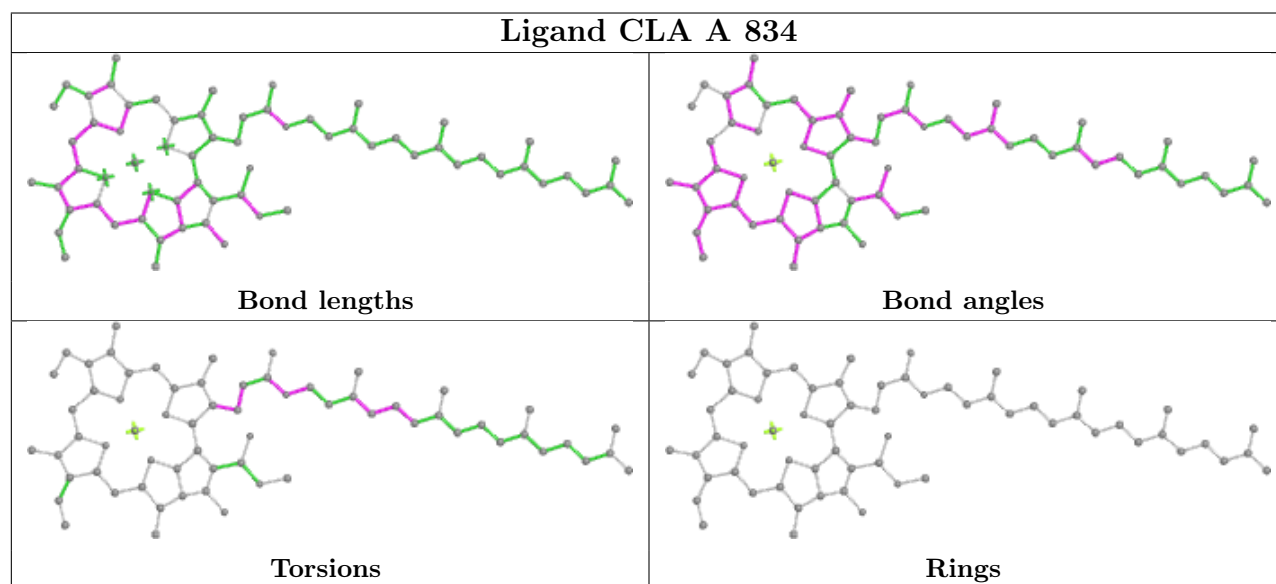
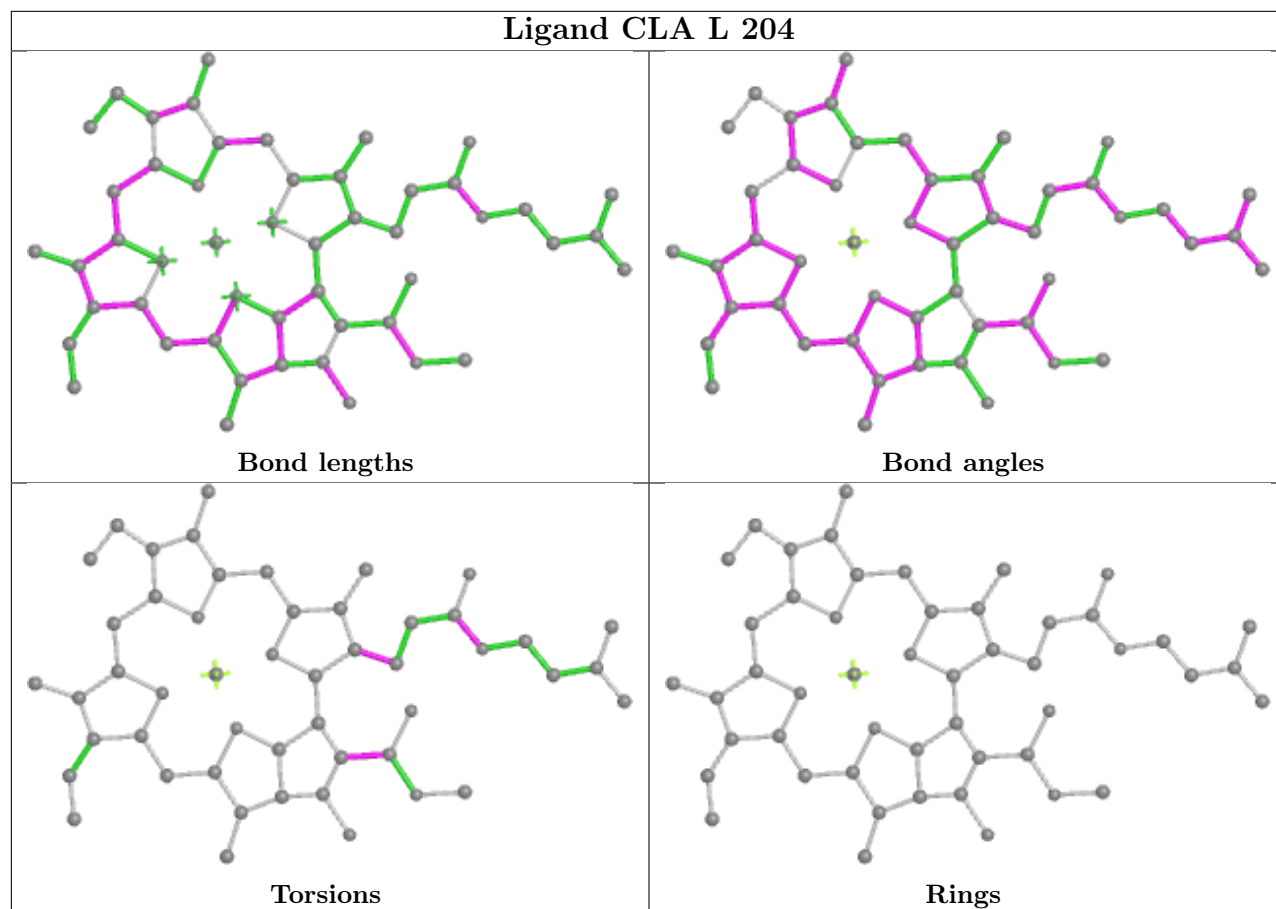


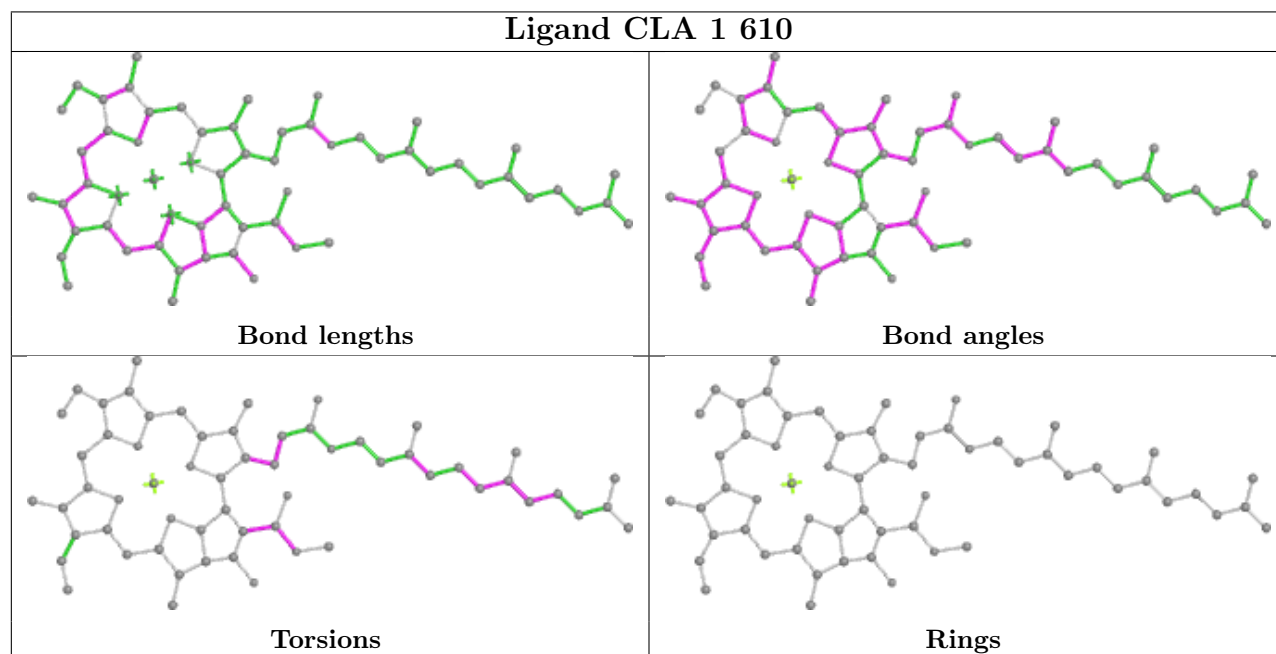
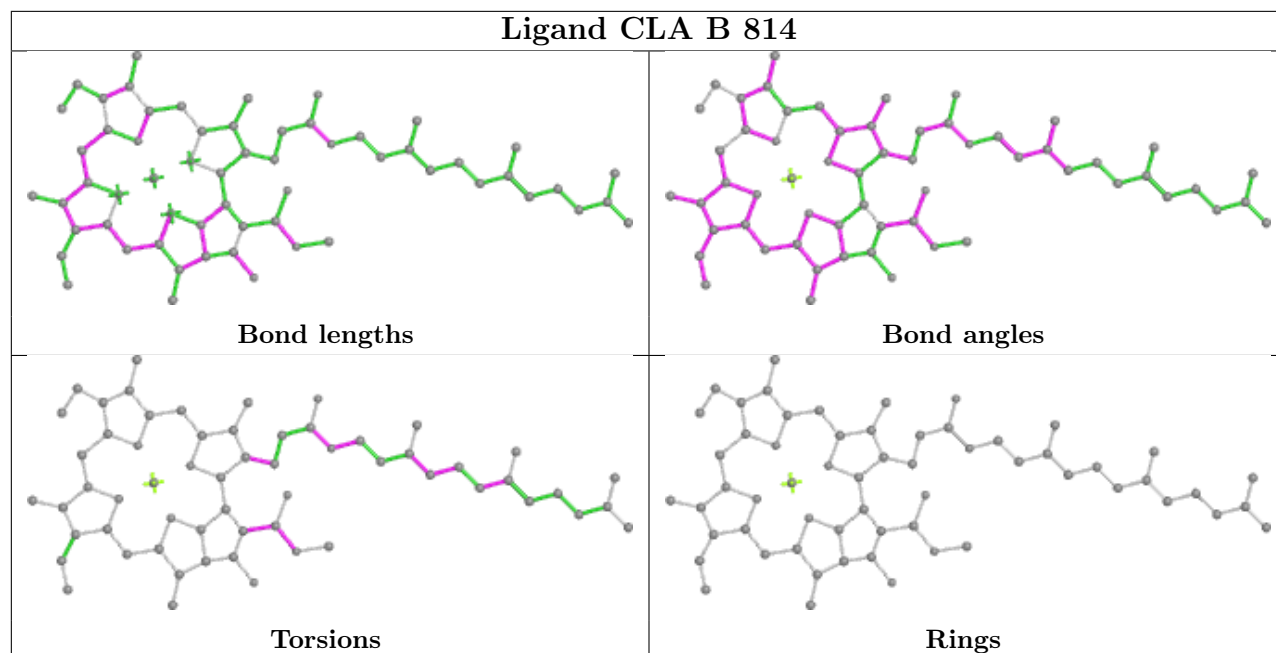


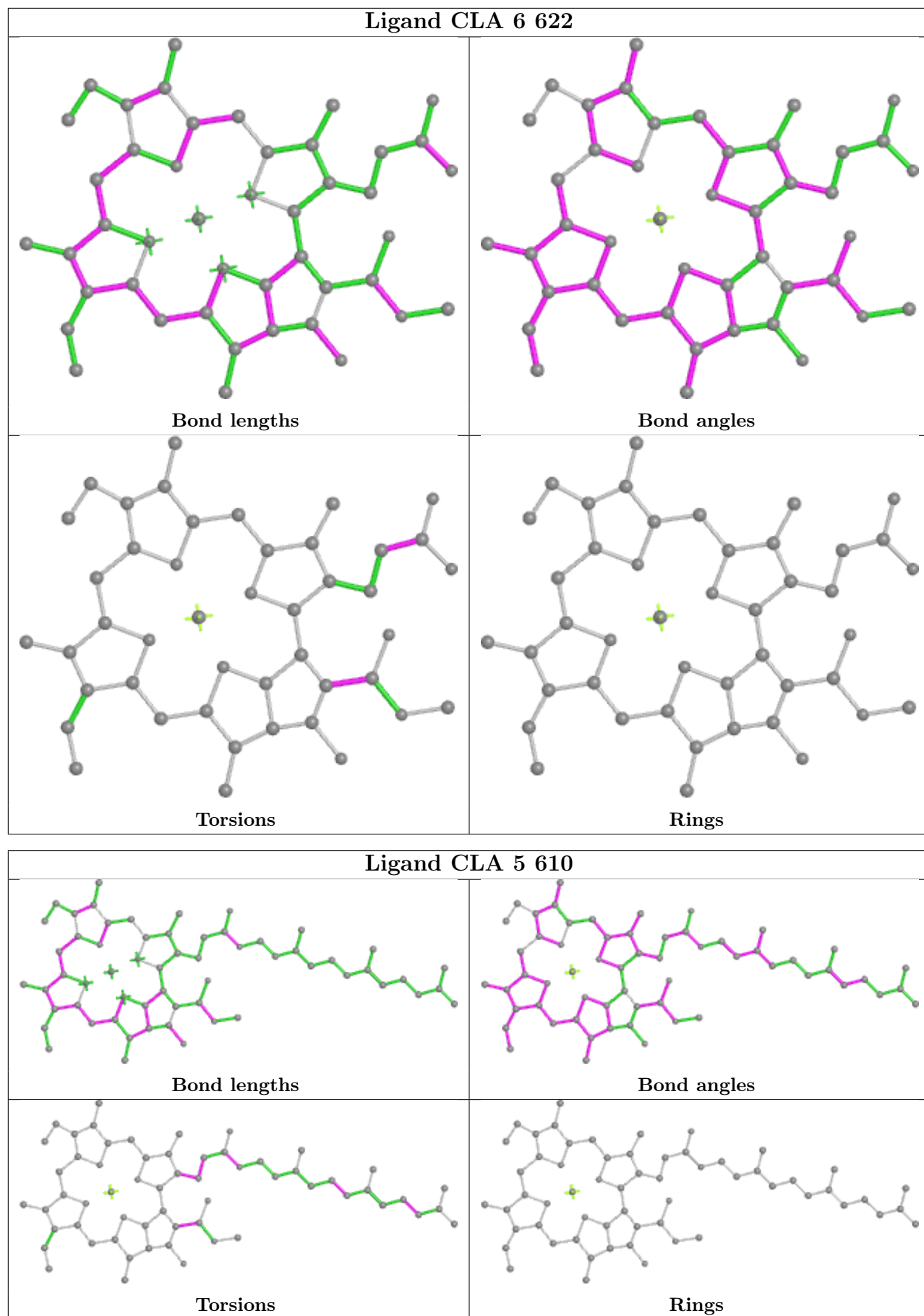


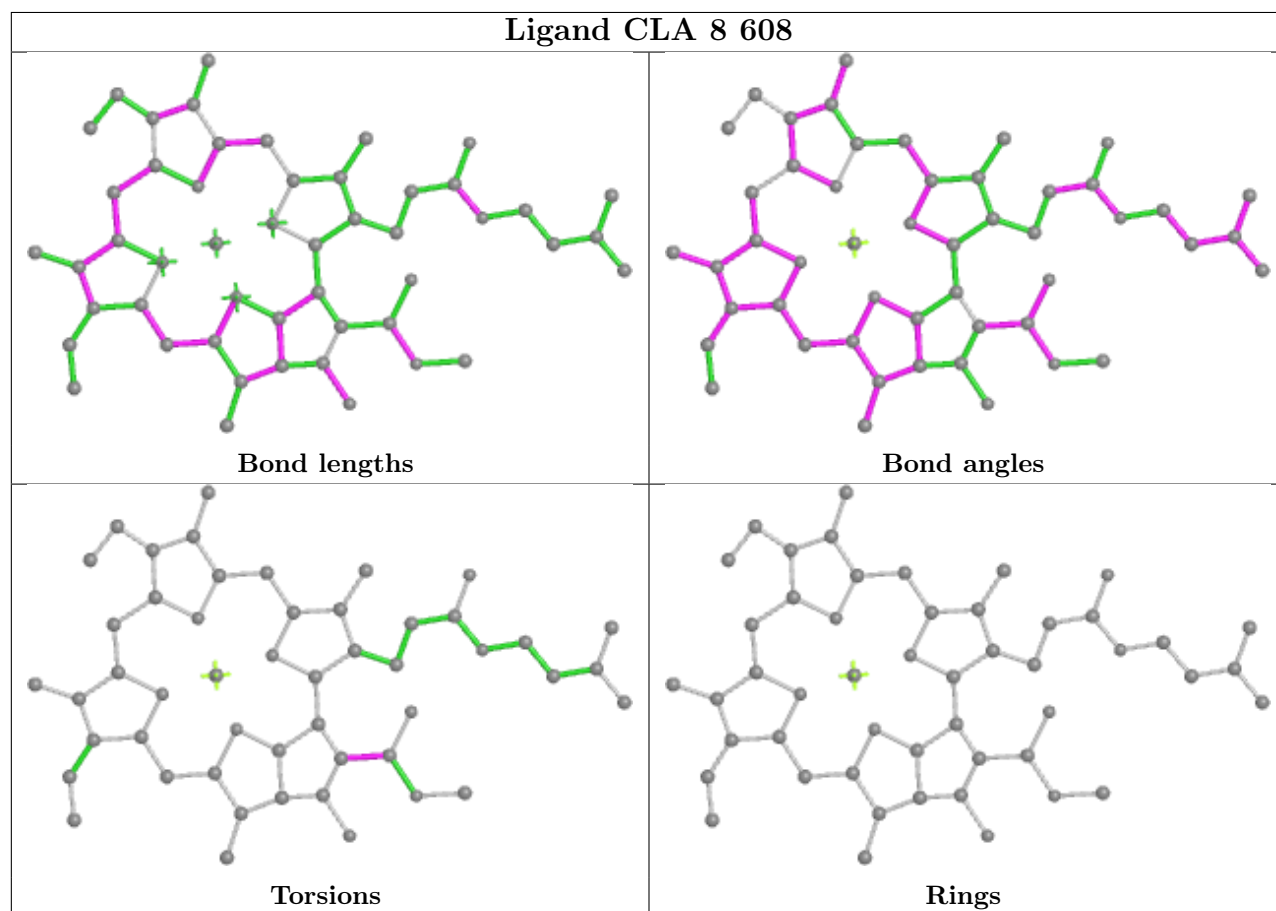
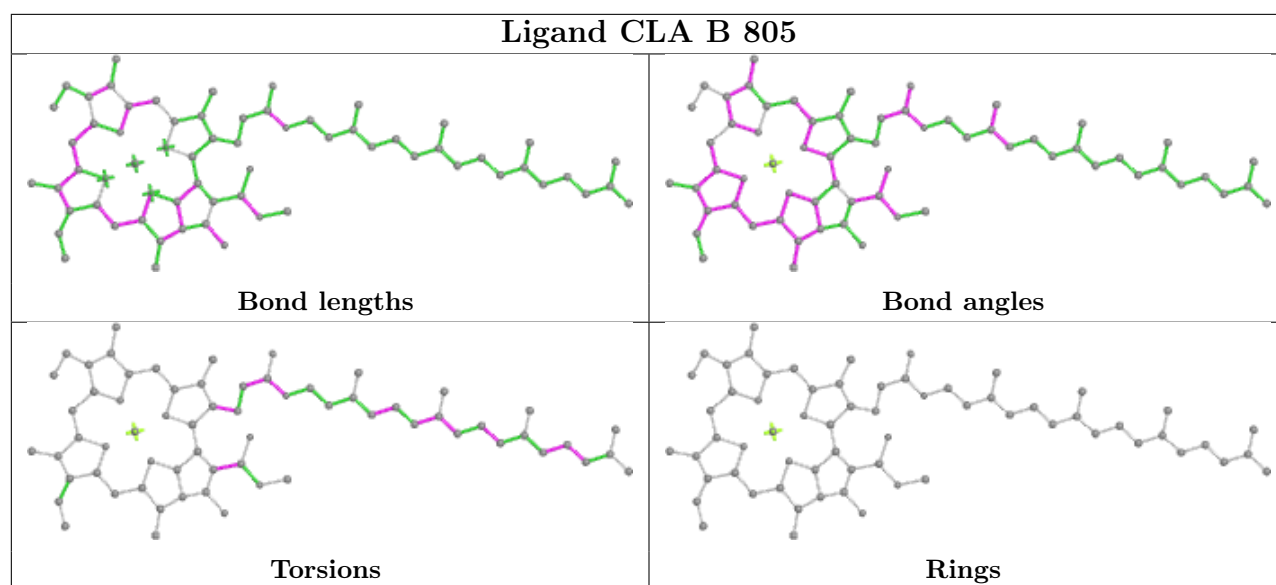


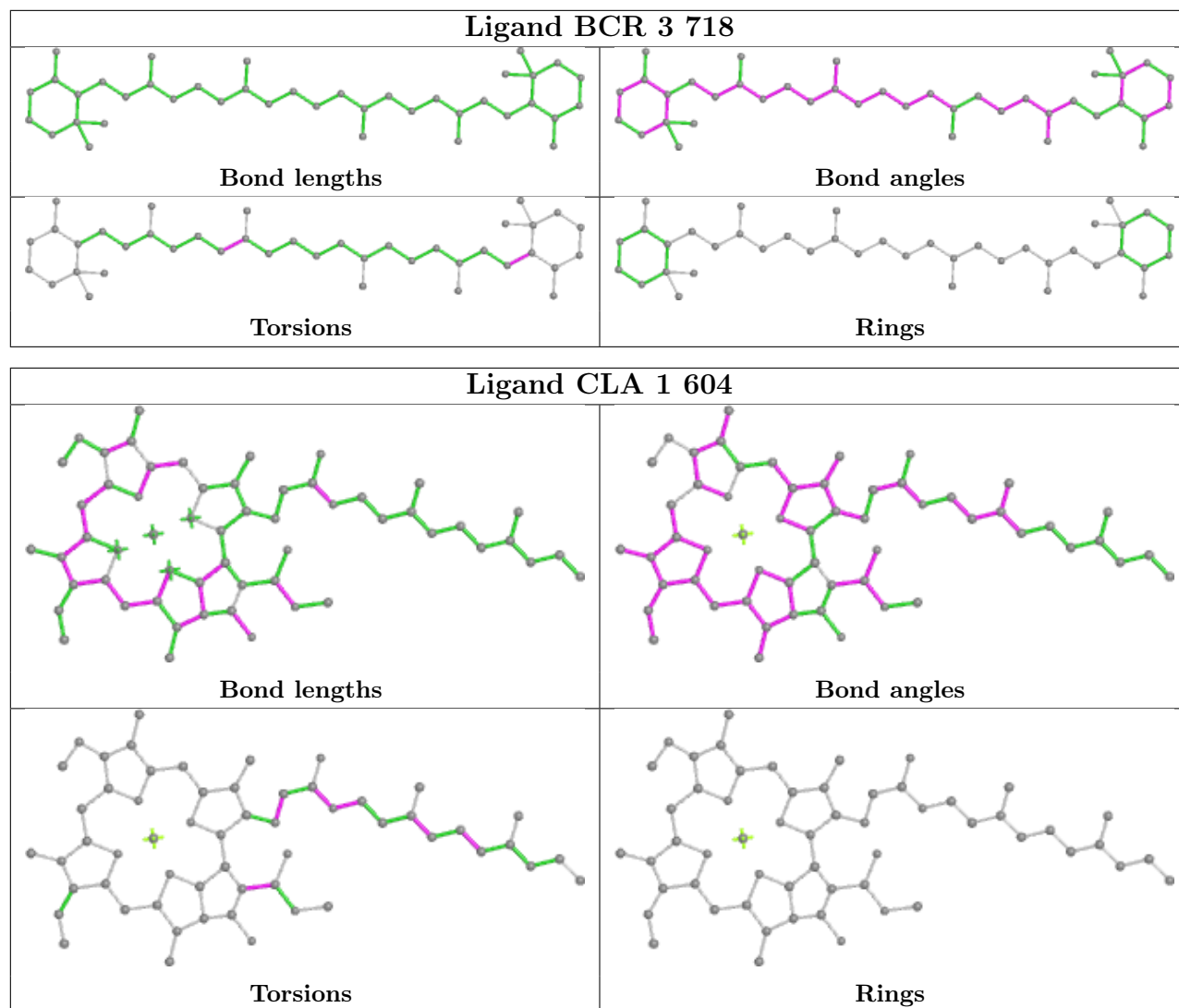


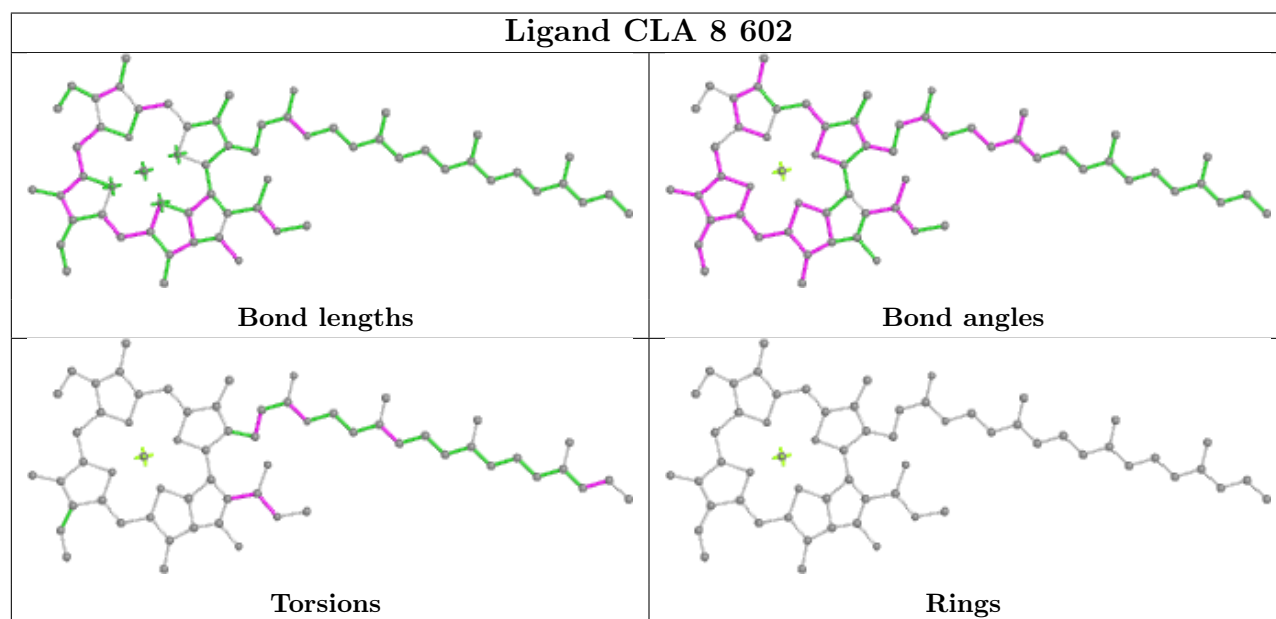
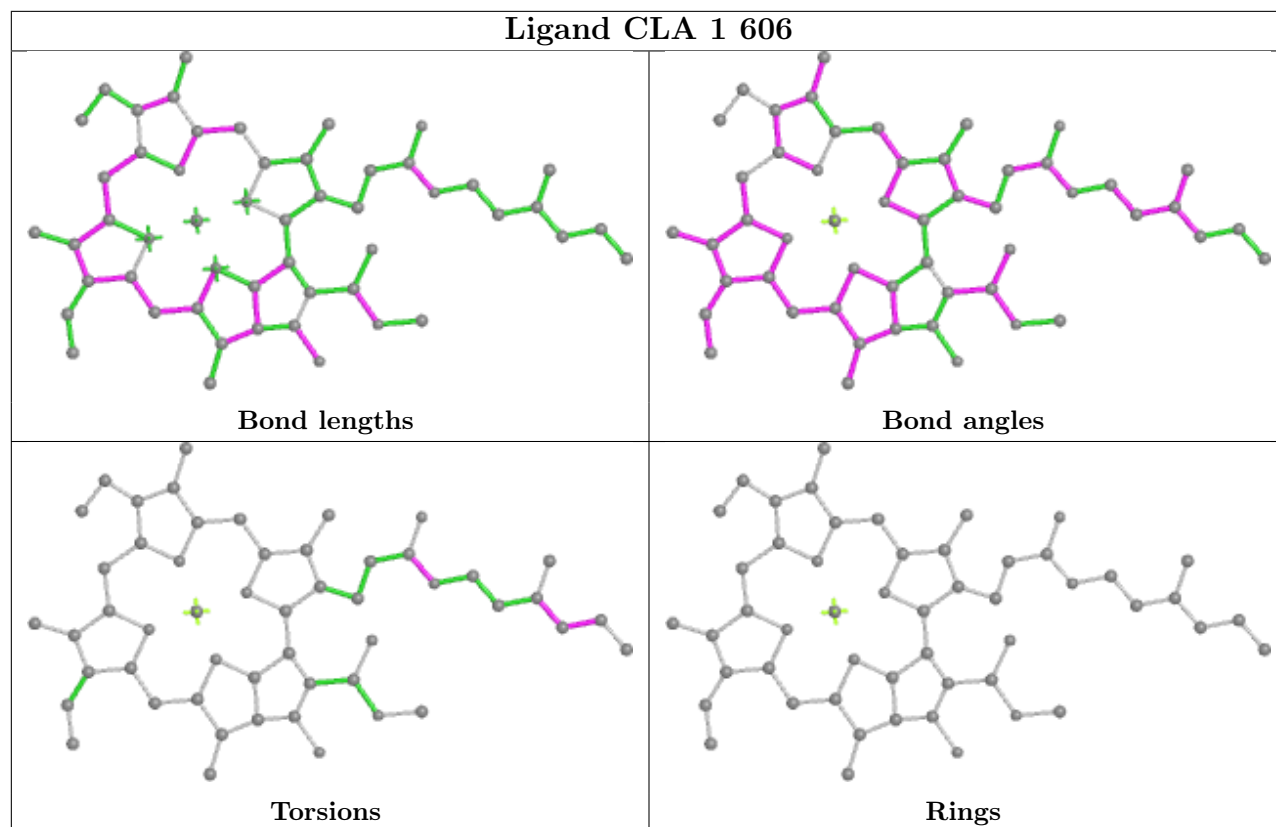


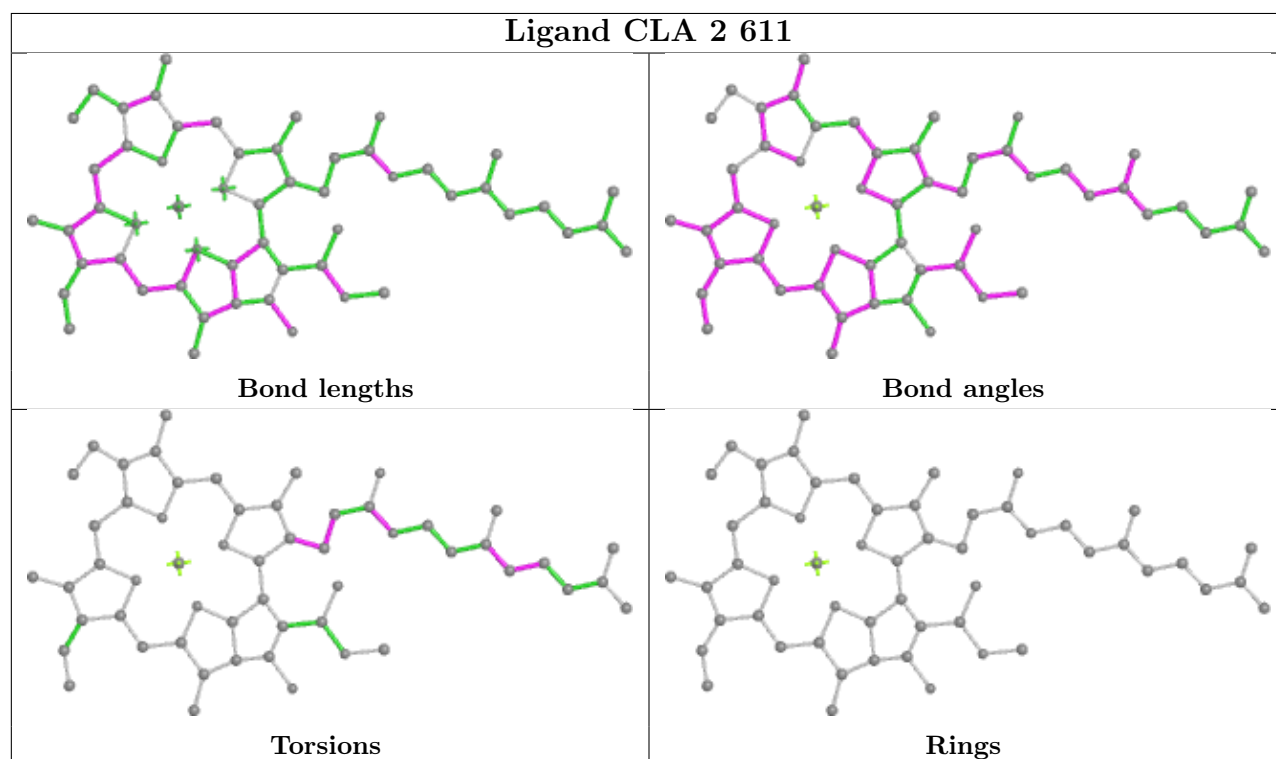
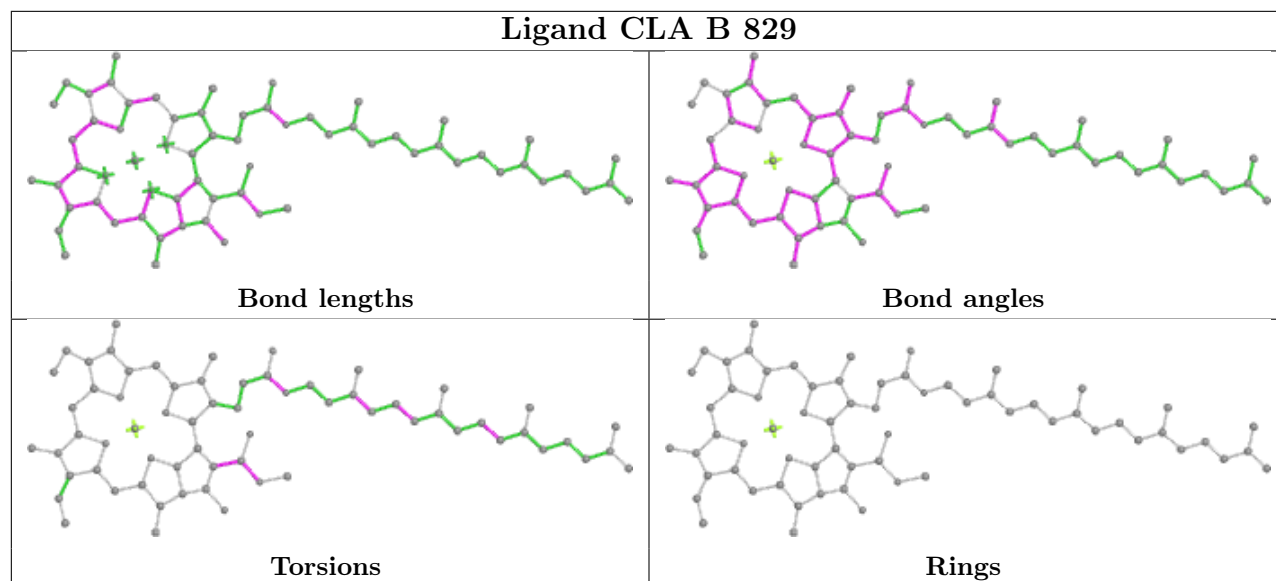
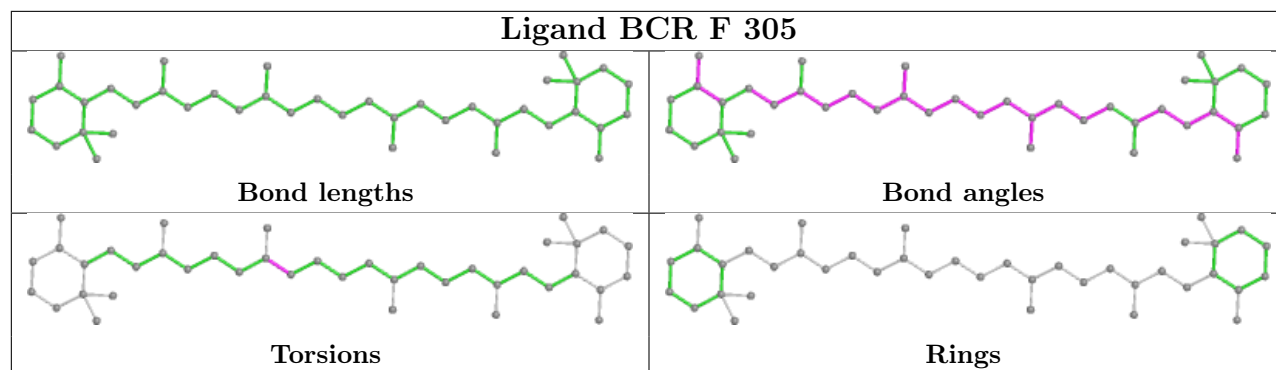


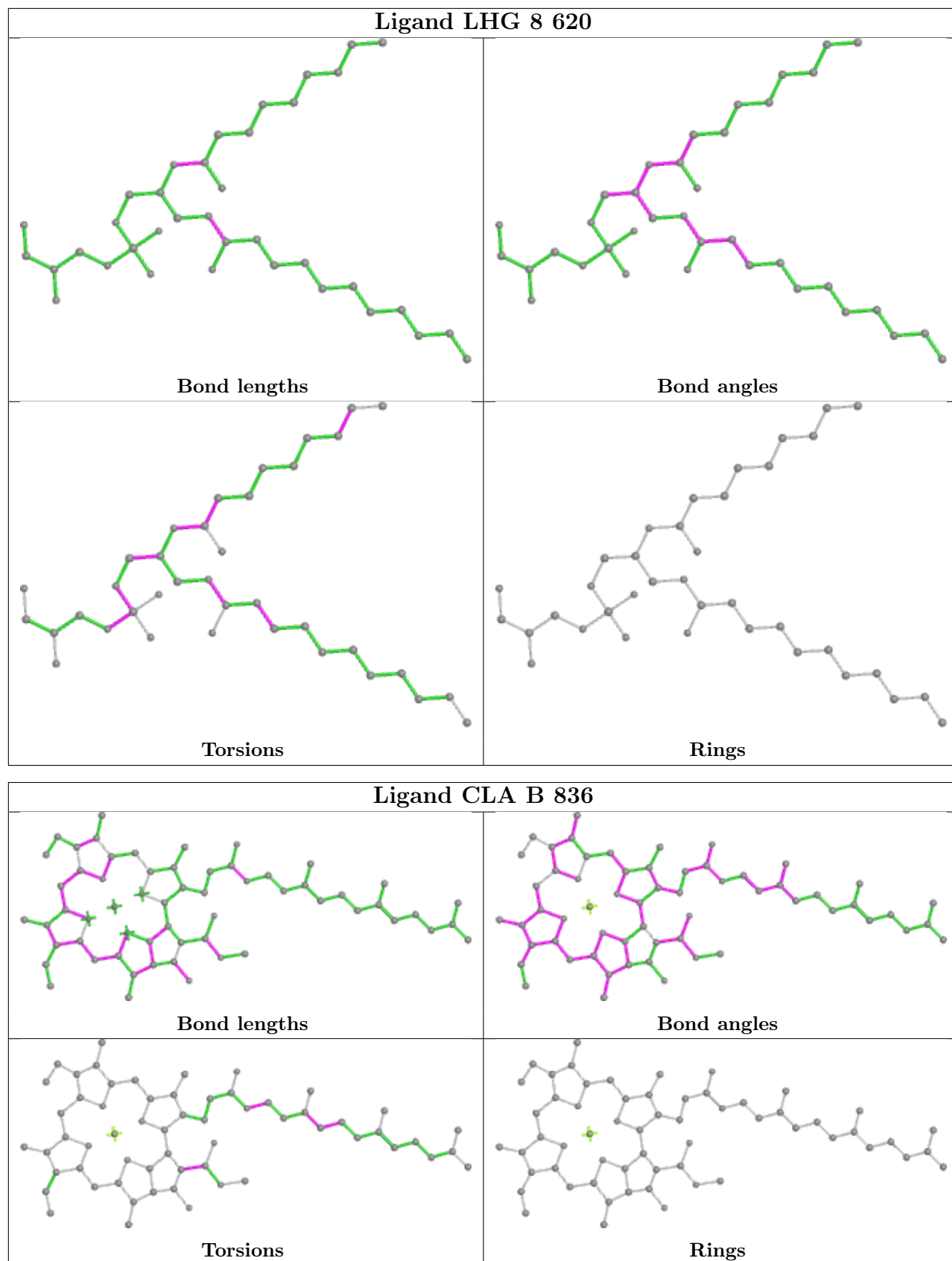


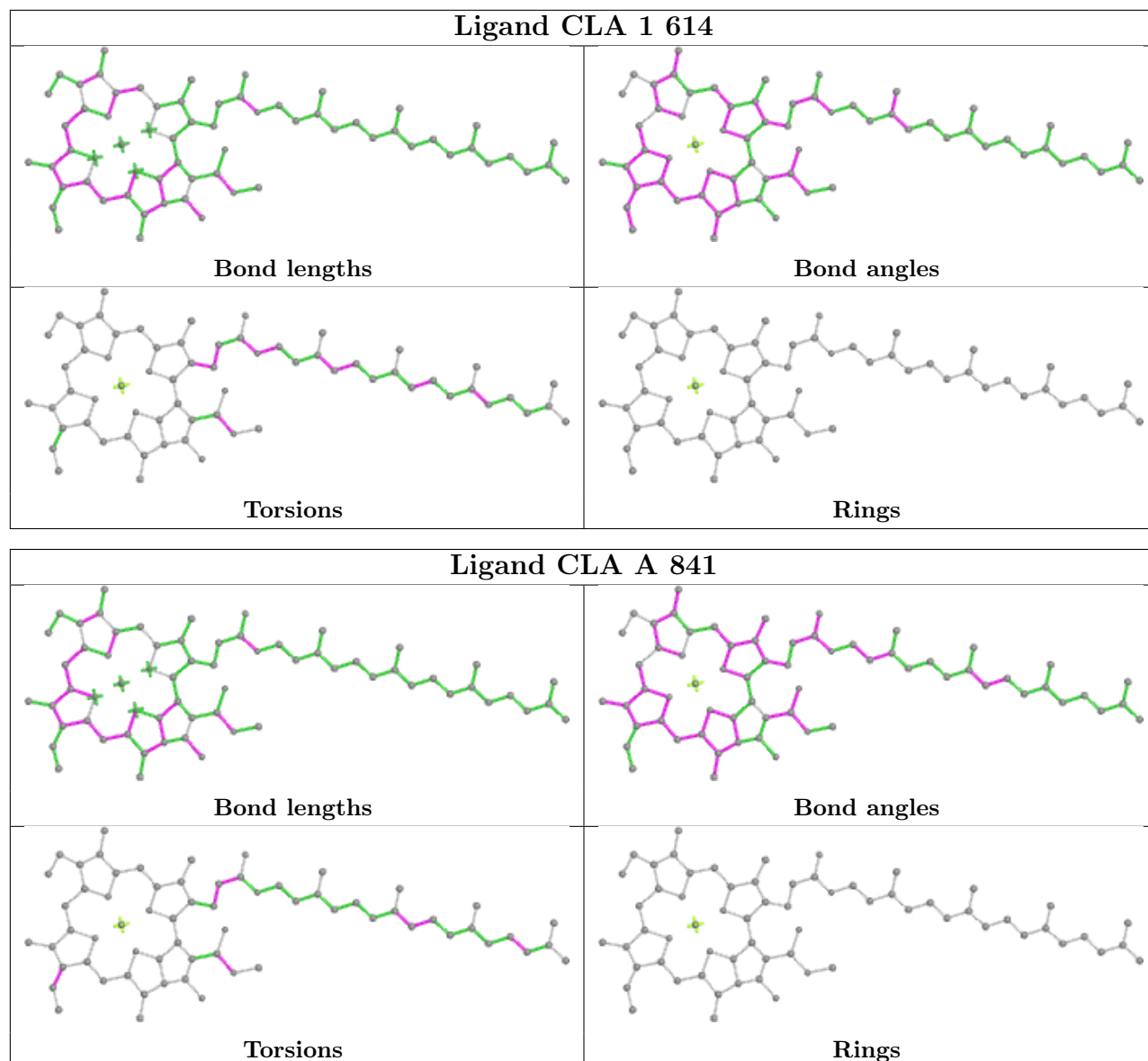


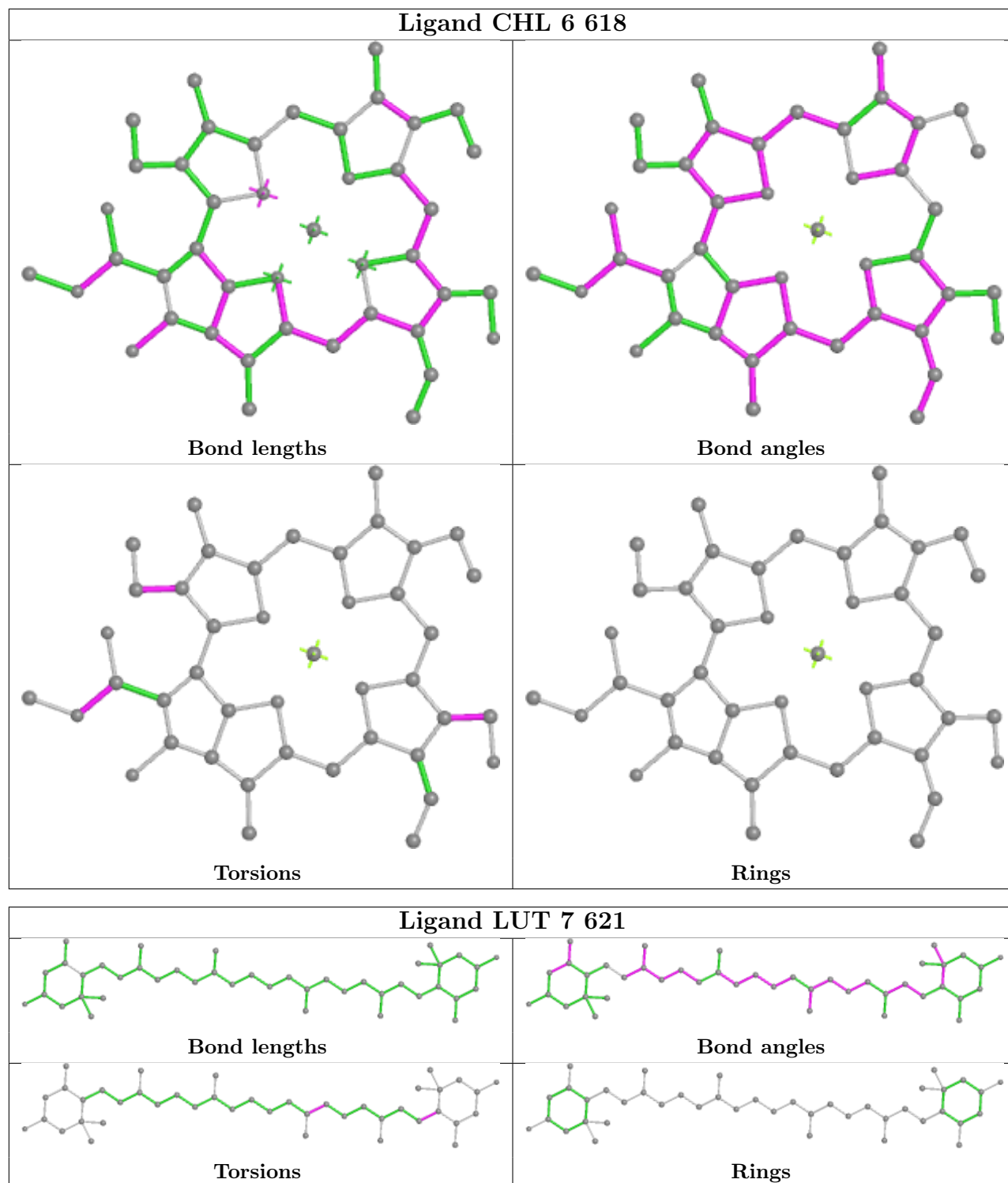


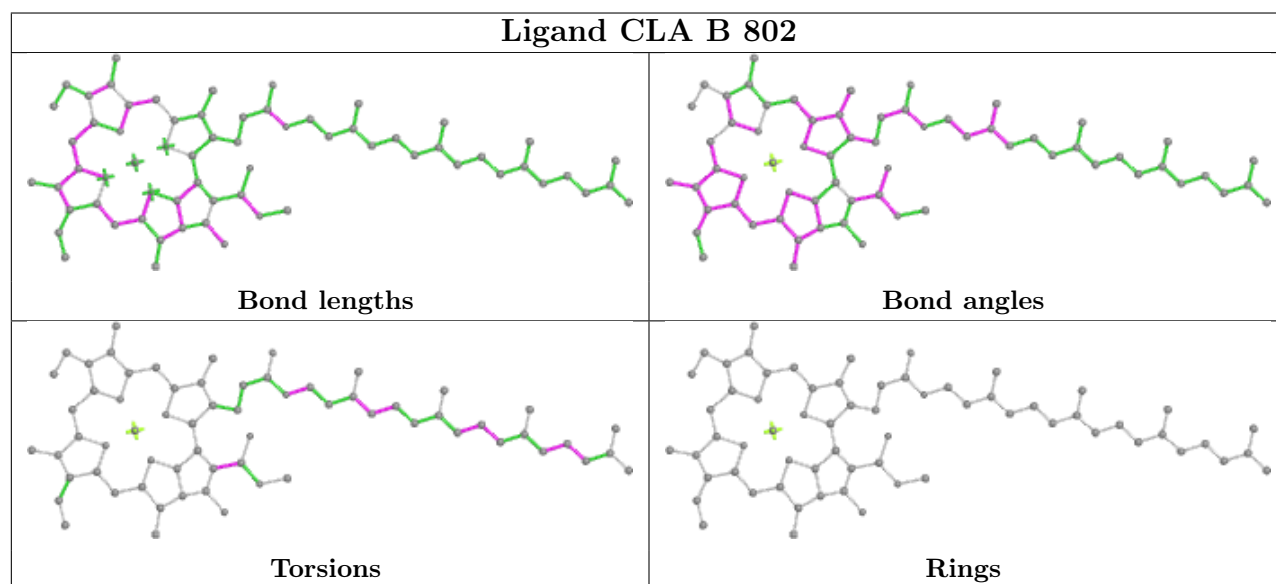
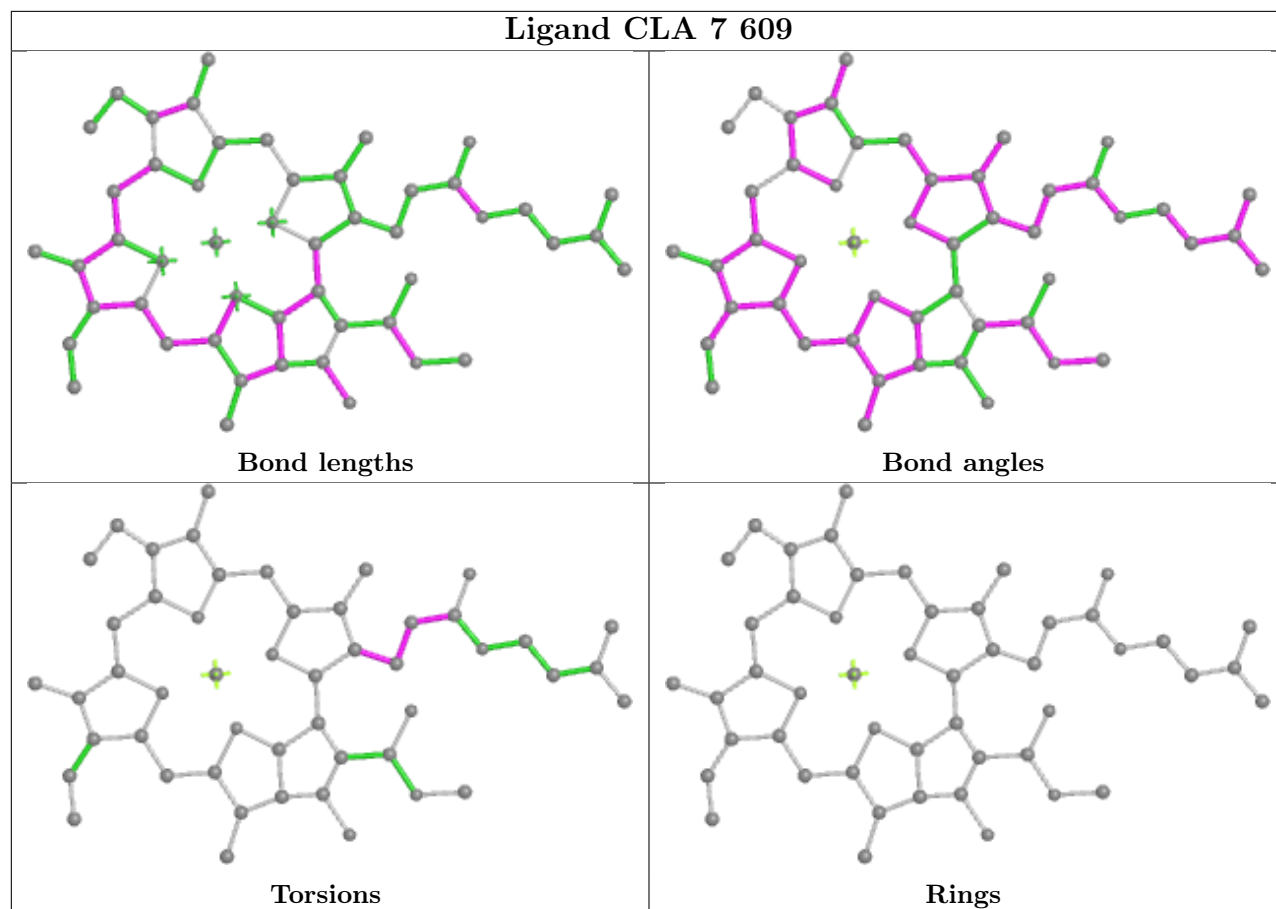


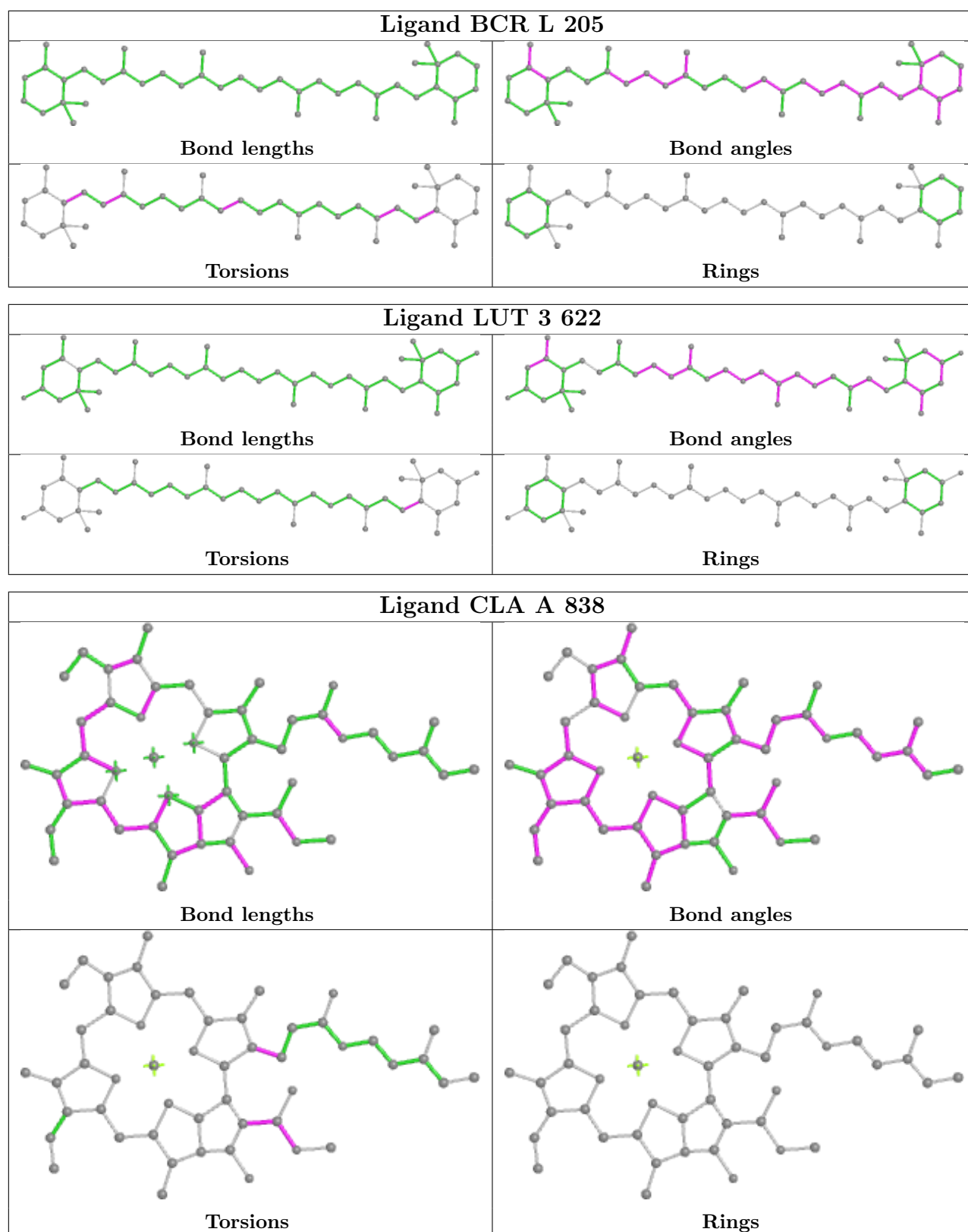


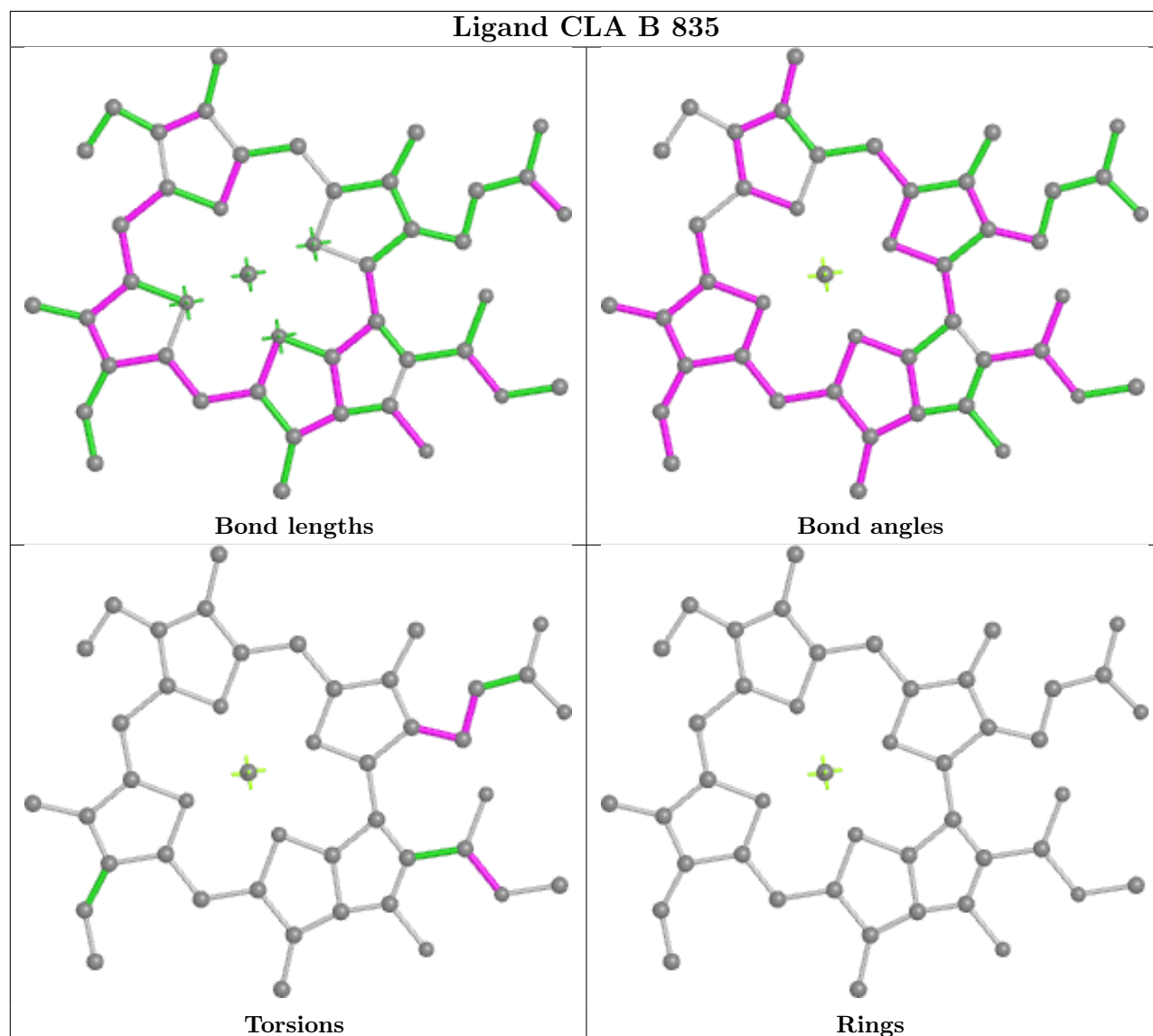
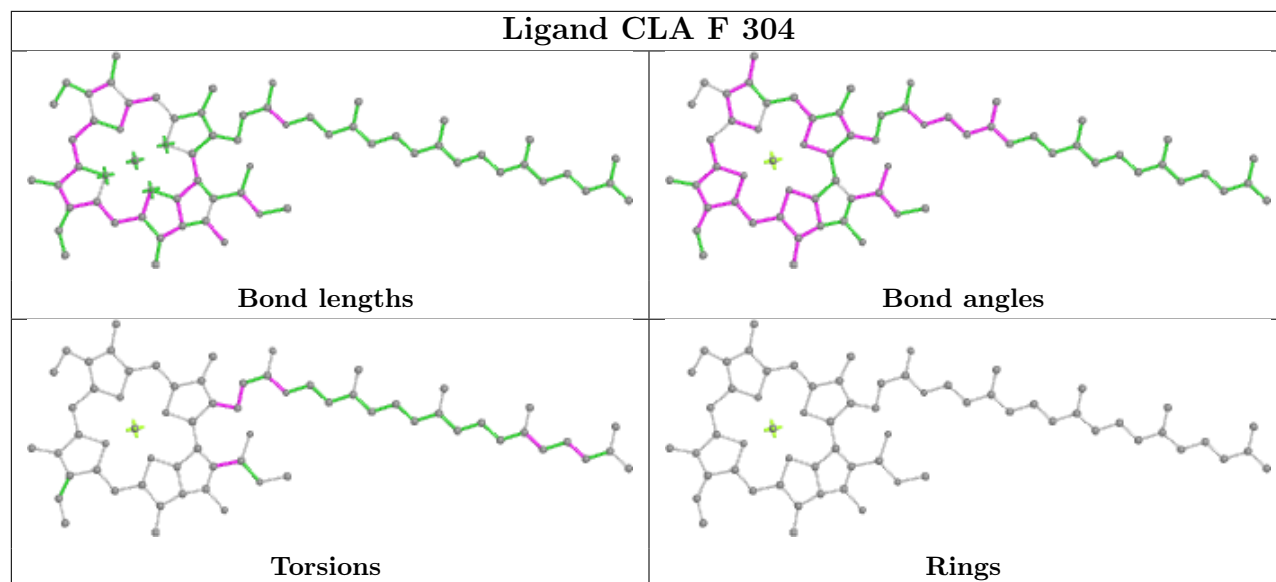


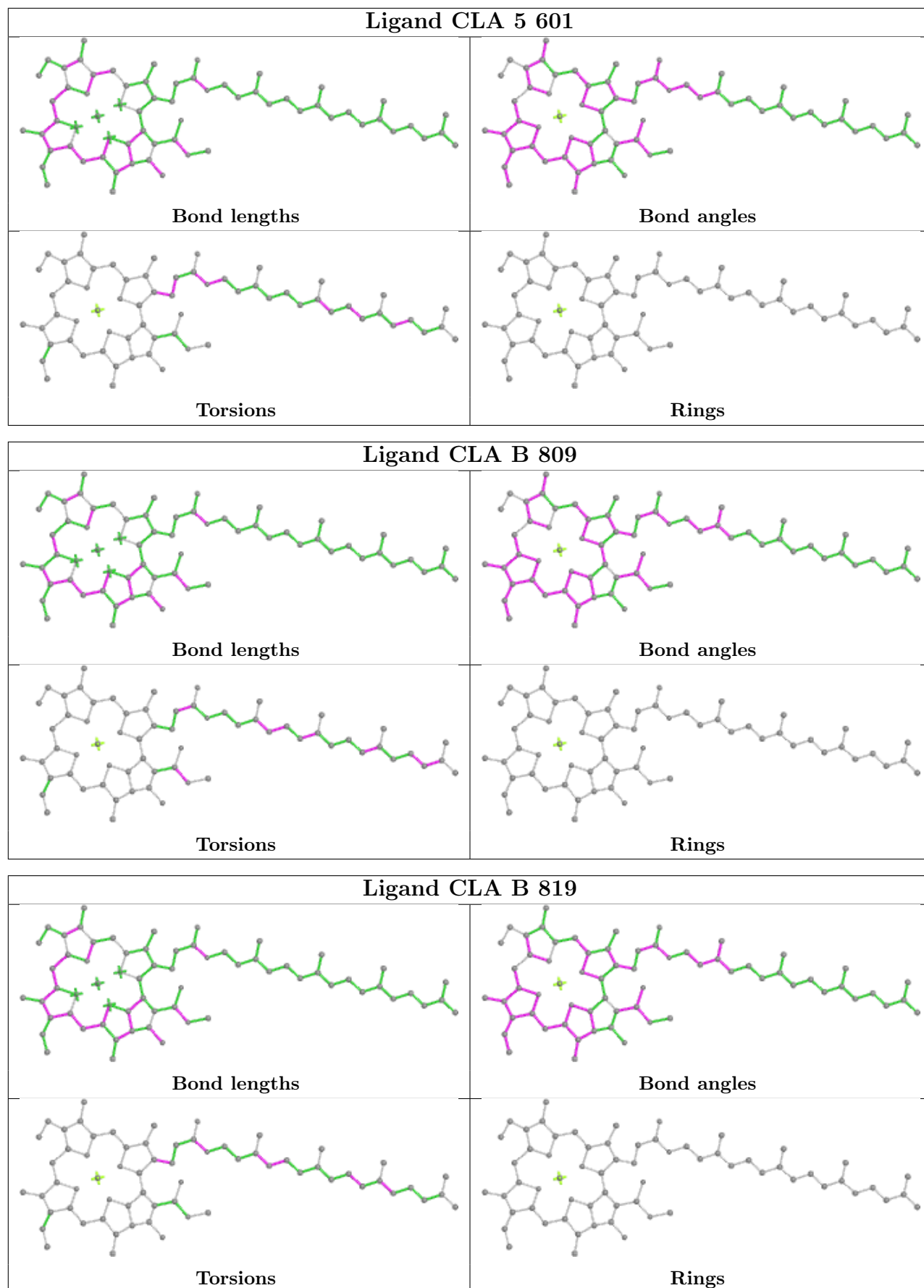


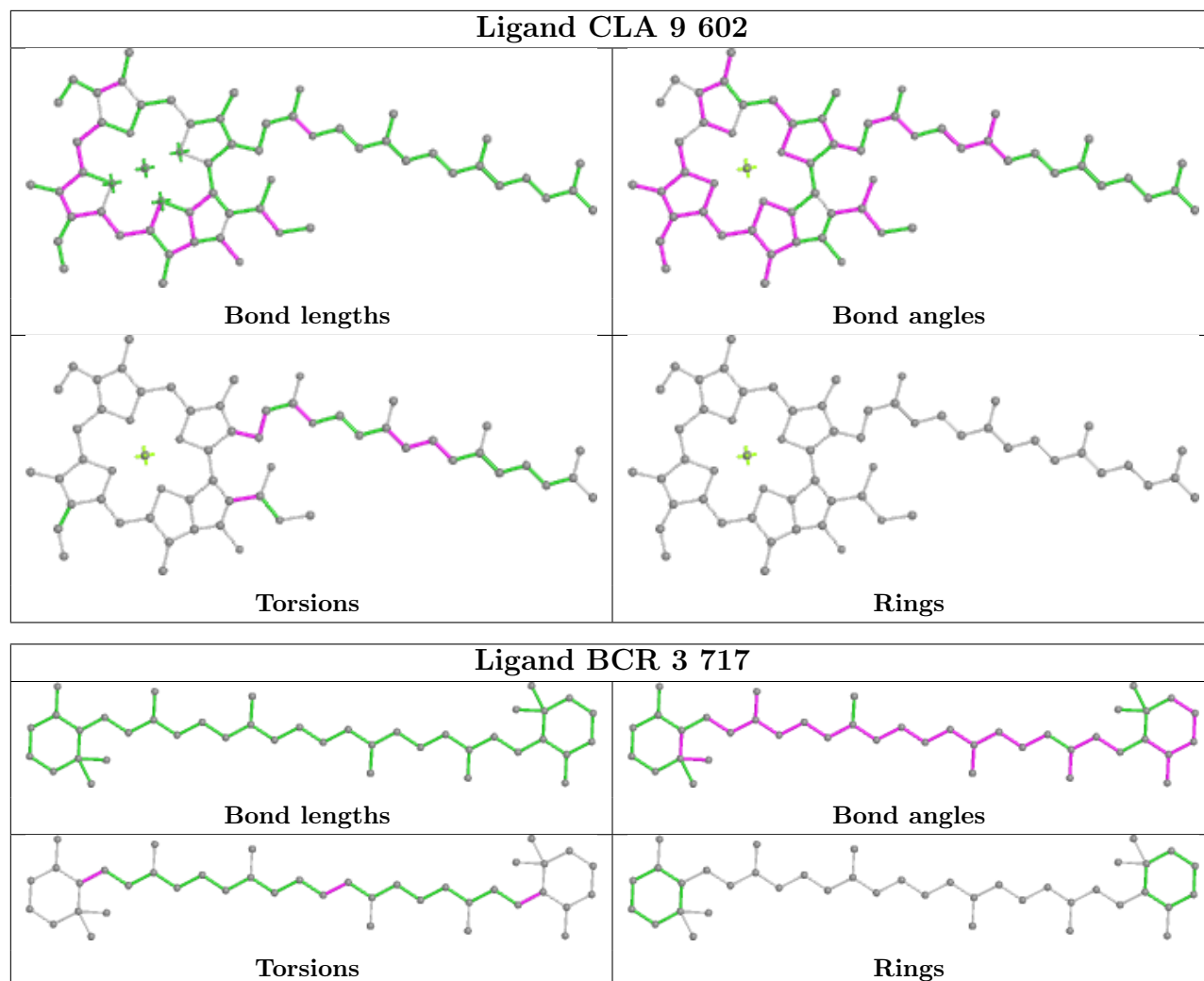


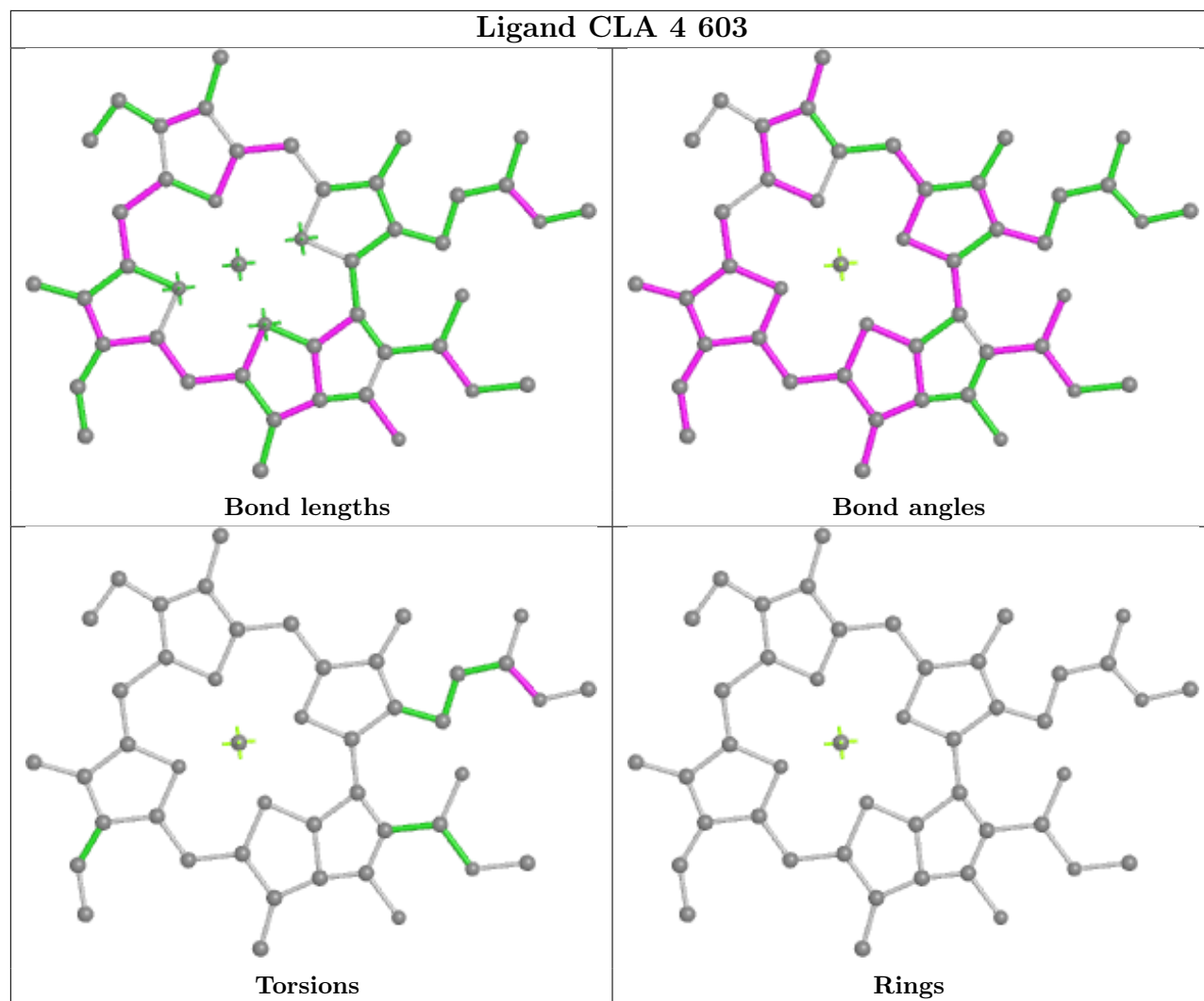


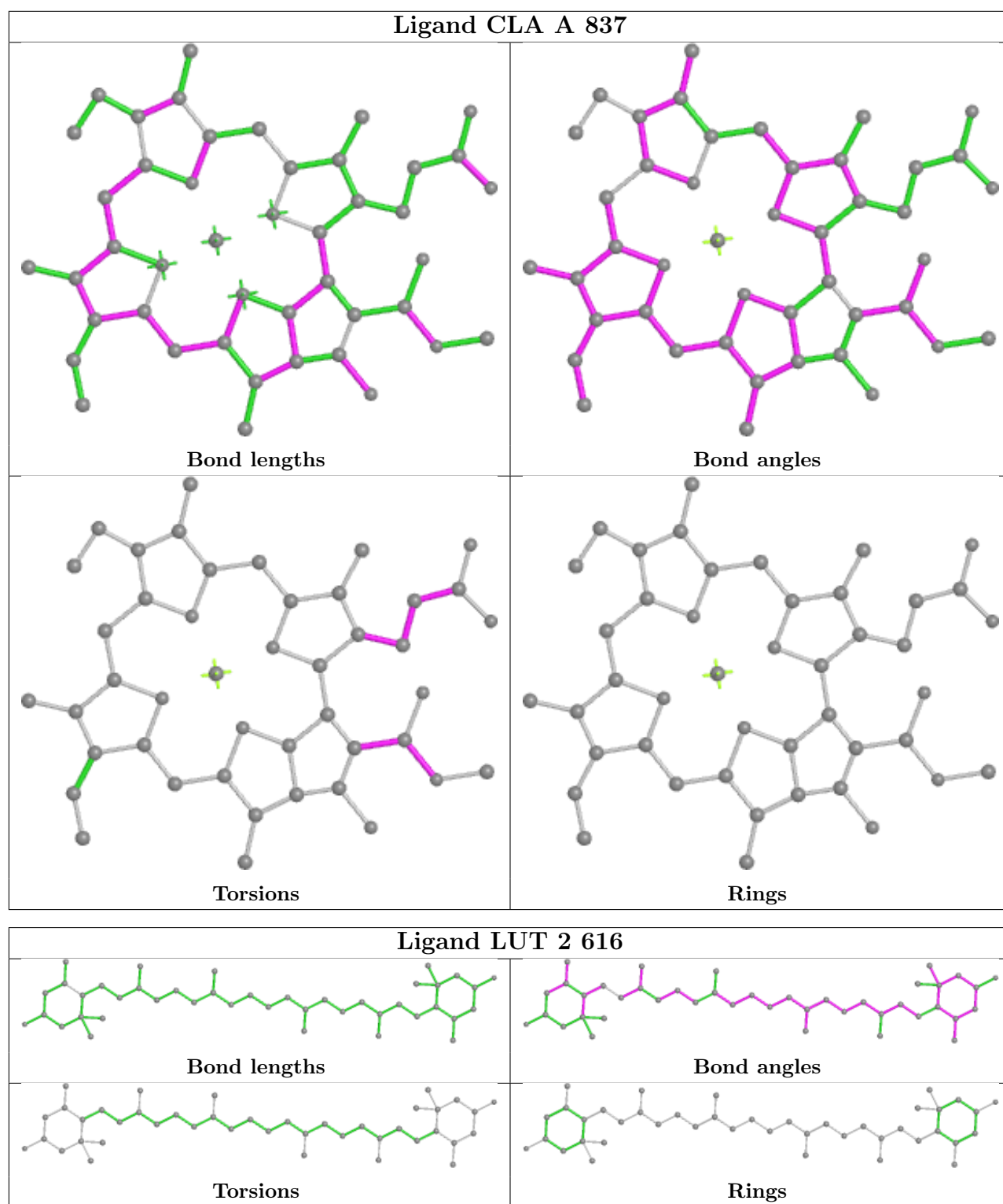


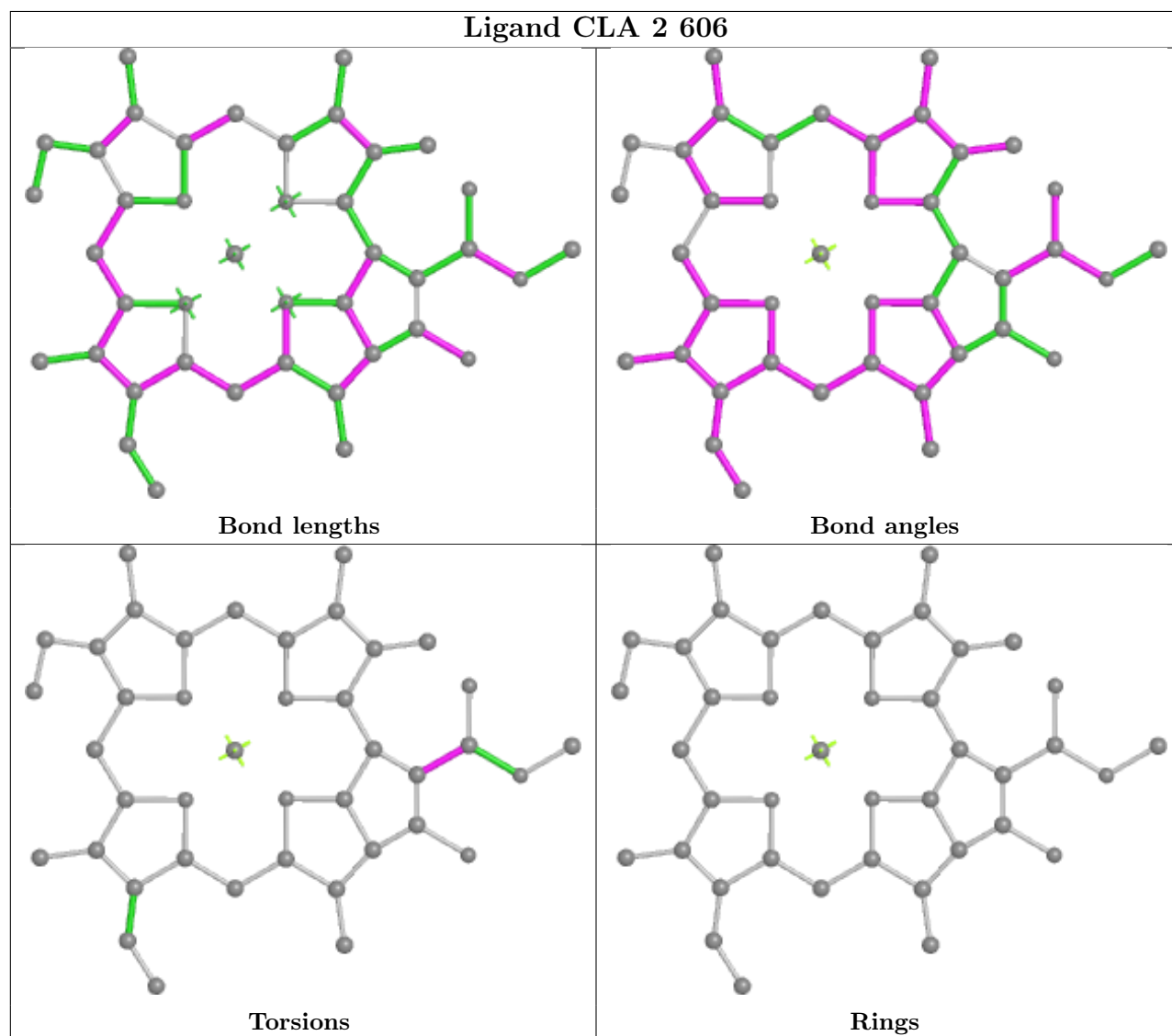
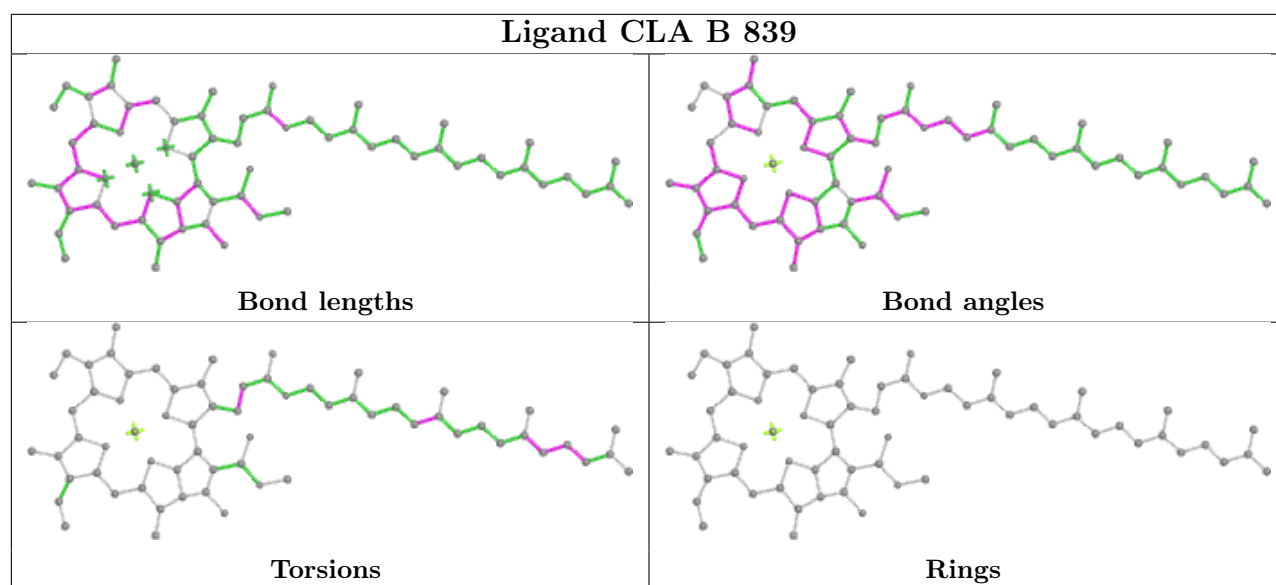


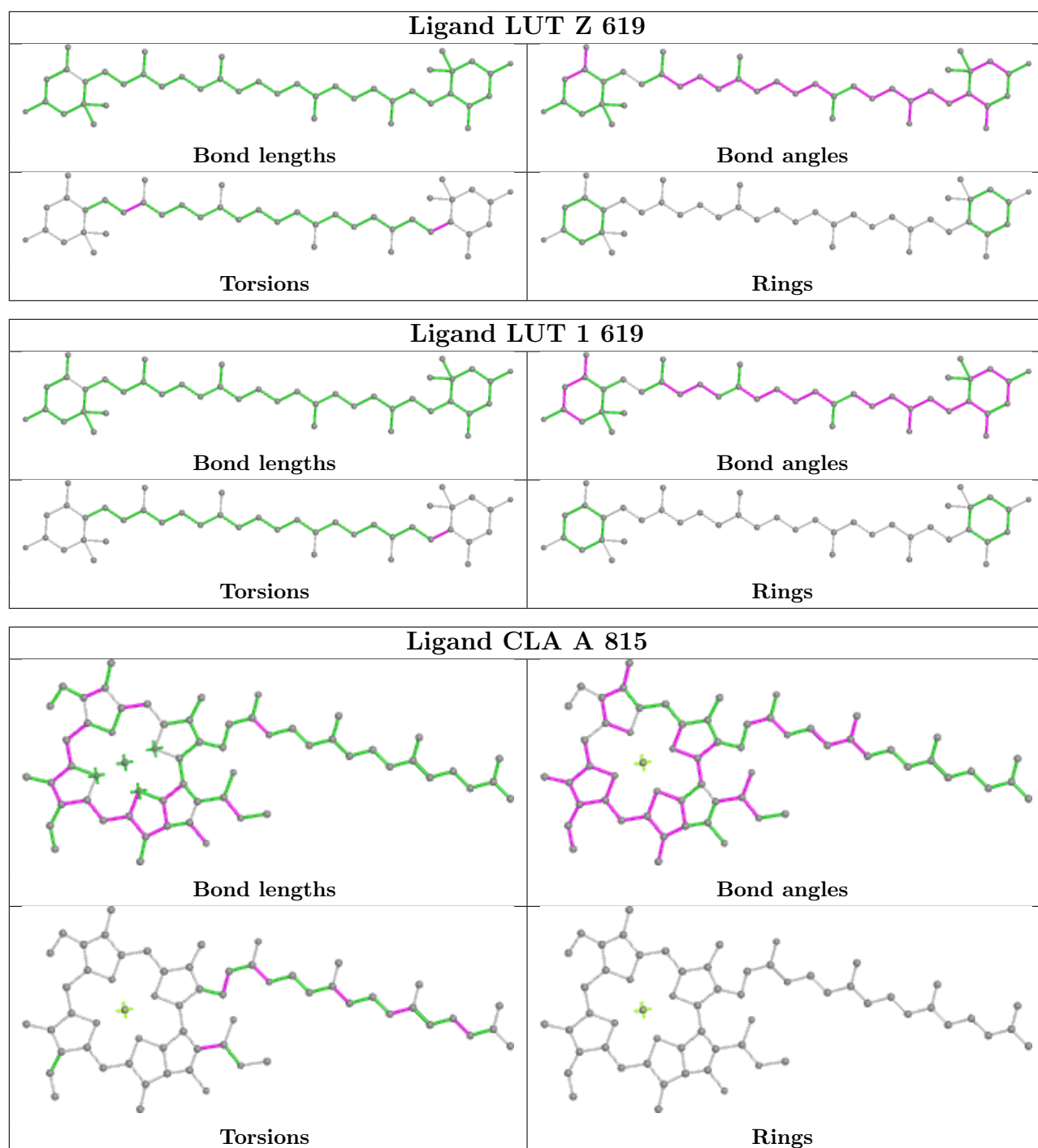


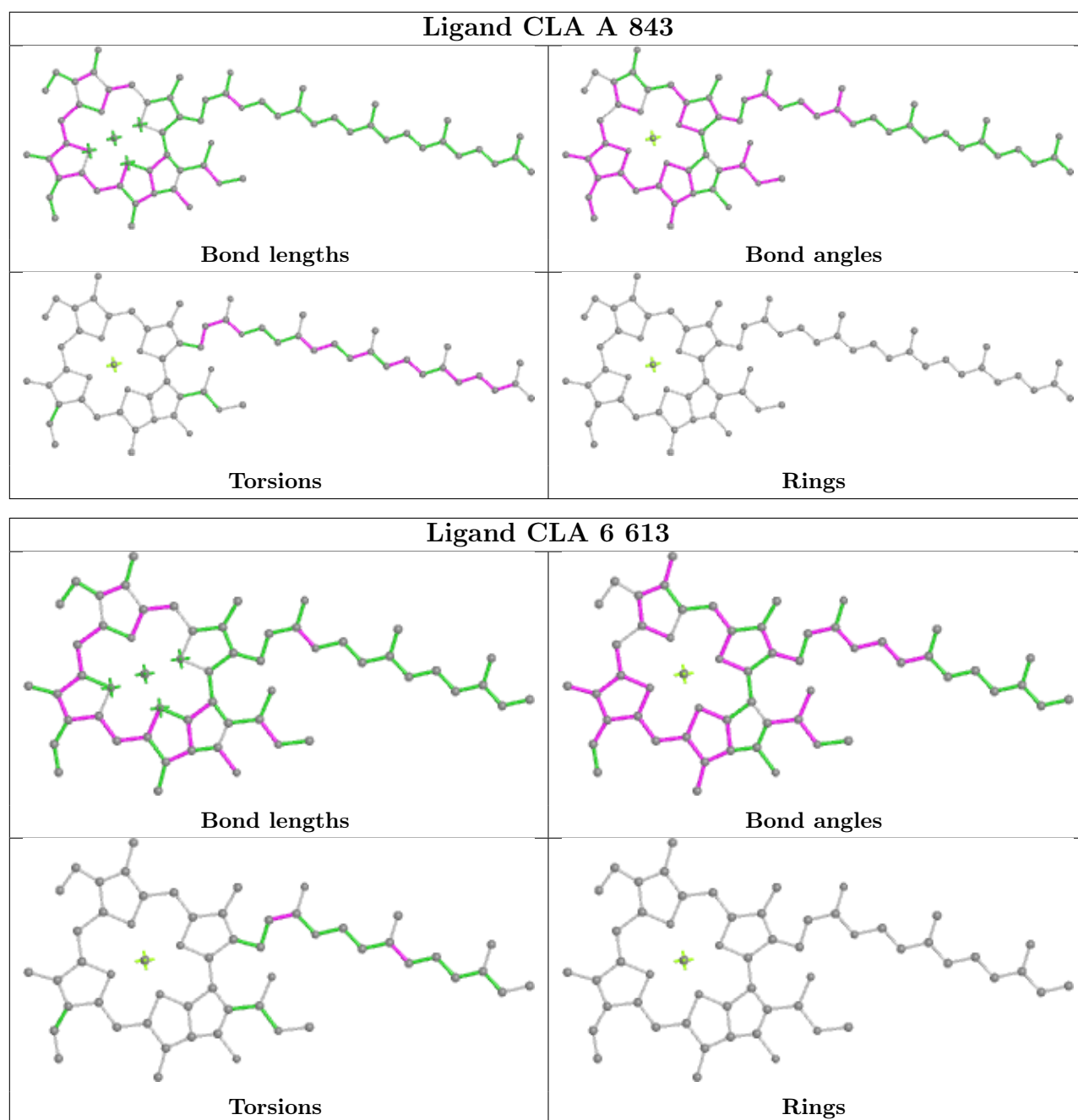












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

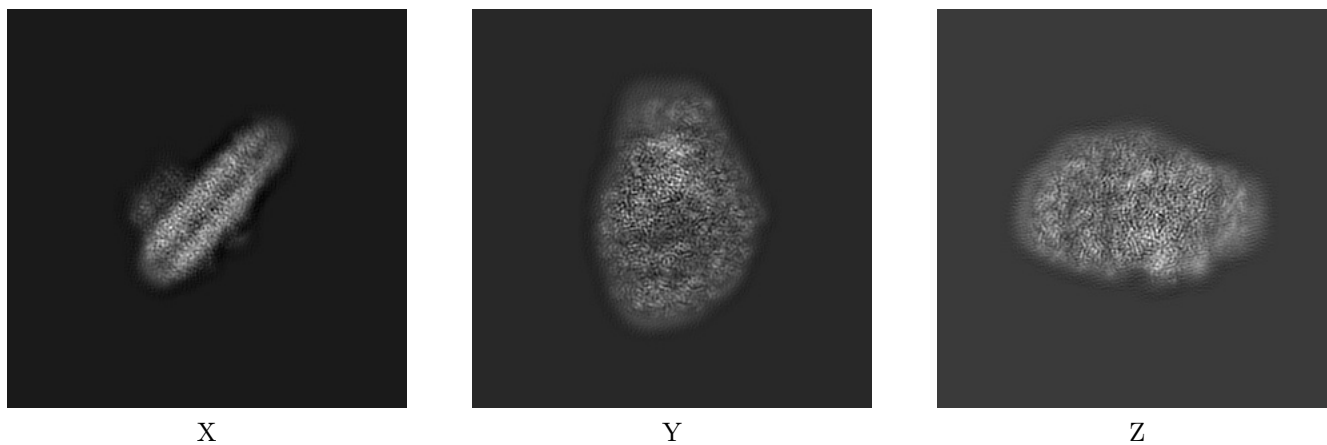
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9853. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

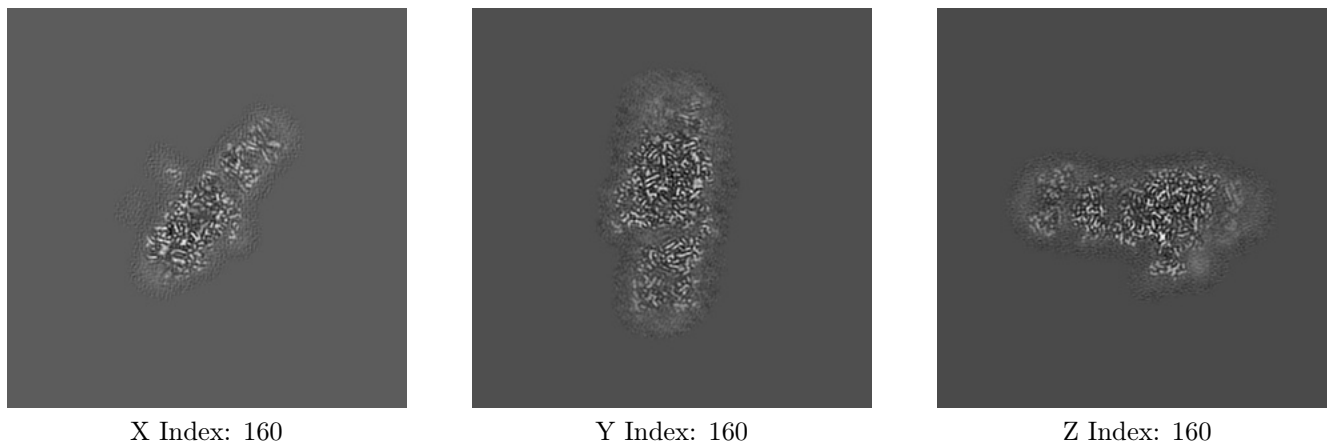
6.1.1 Primary map



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

6.2 Central slices [i](#)

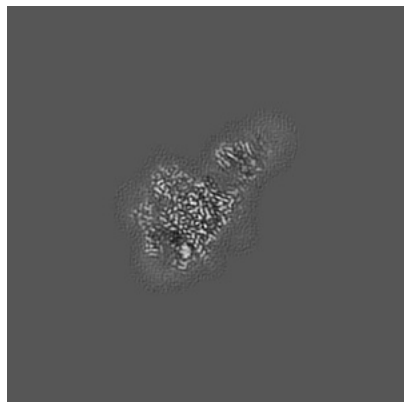
6.2.1 Primary map



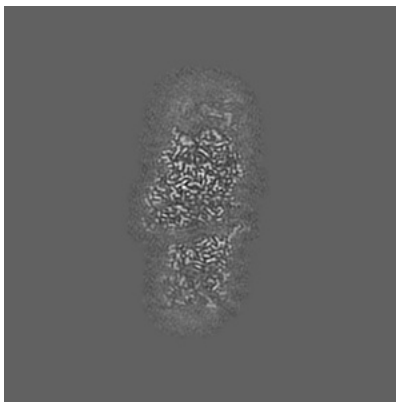
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

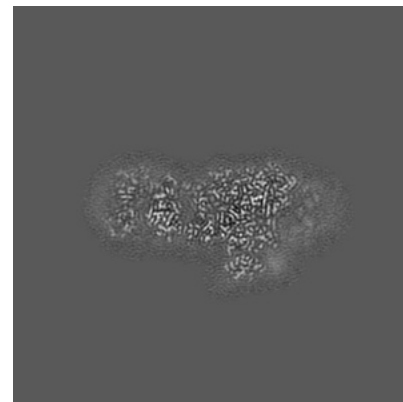
6.3.1 Primary map



X Index: 175



Y Index: 158



Z Index: 157

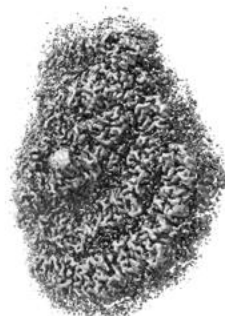
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

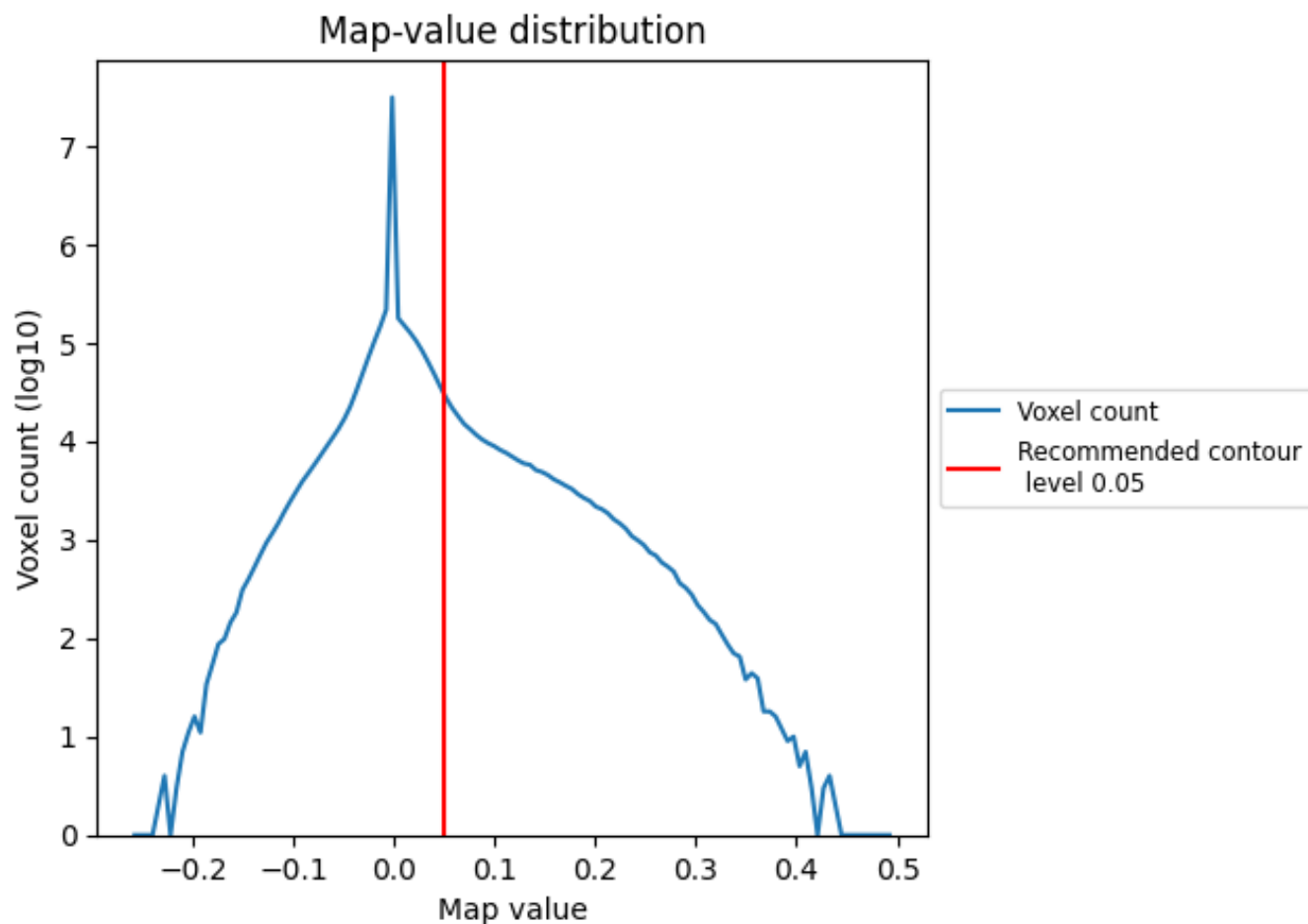
6.5 Mask visualisation

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

7 Map analysis [i](#)

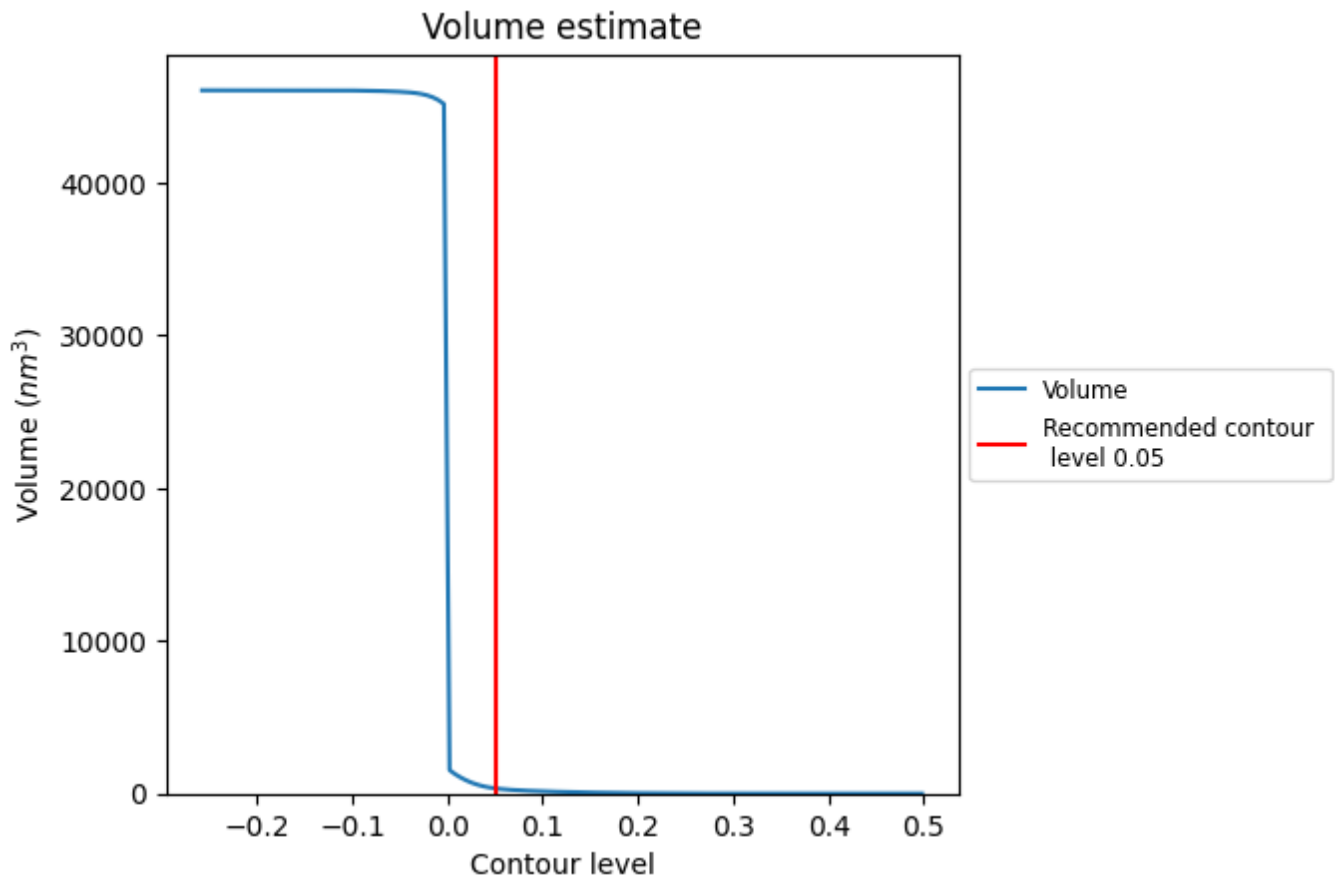
This section contains the results of statistical analysis of the map.

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.

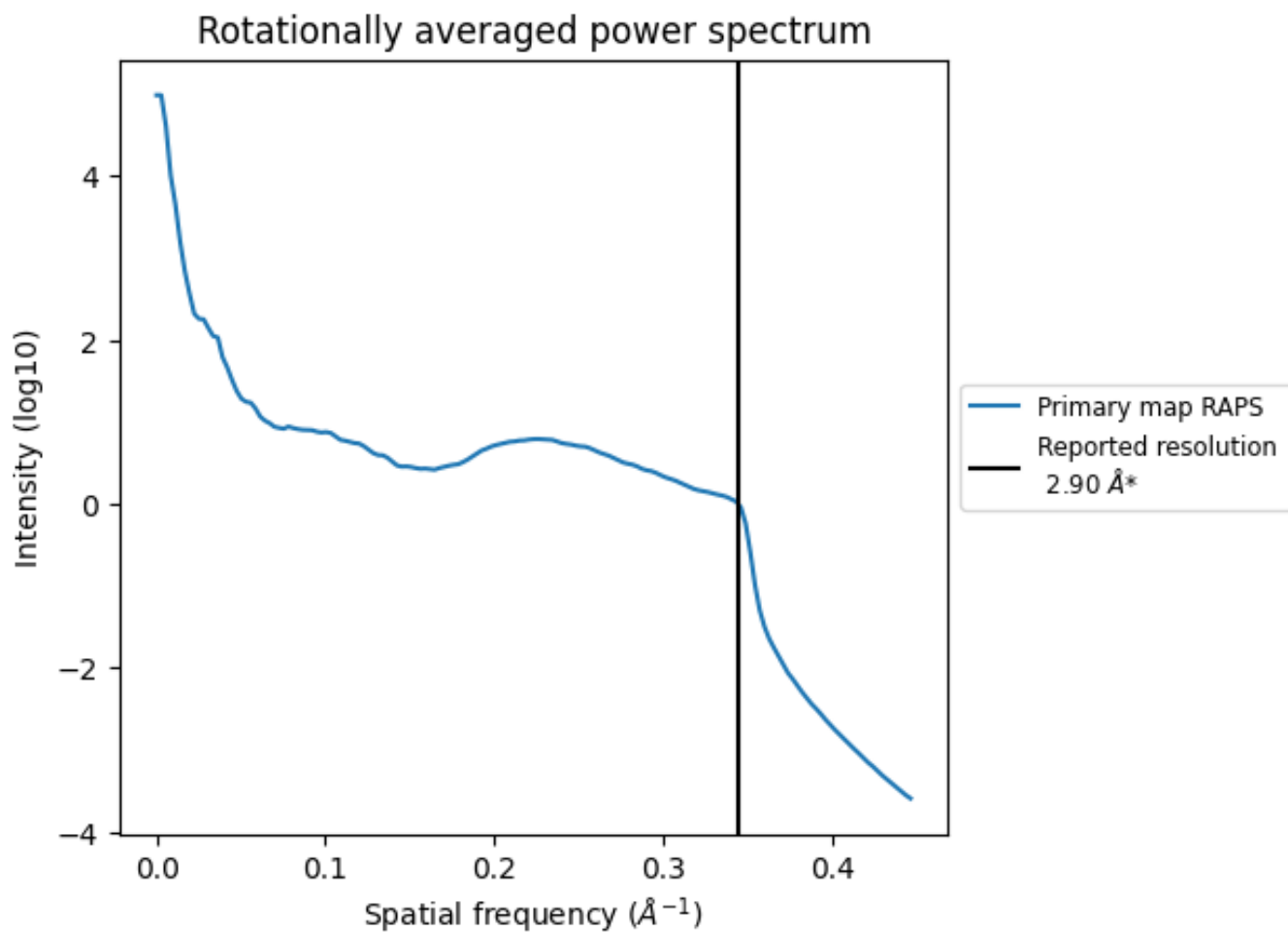
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 342 nm³; this corresponds to an approximate mass of 309 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.345\AA^{-1}

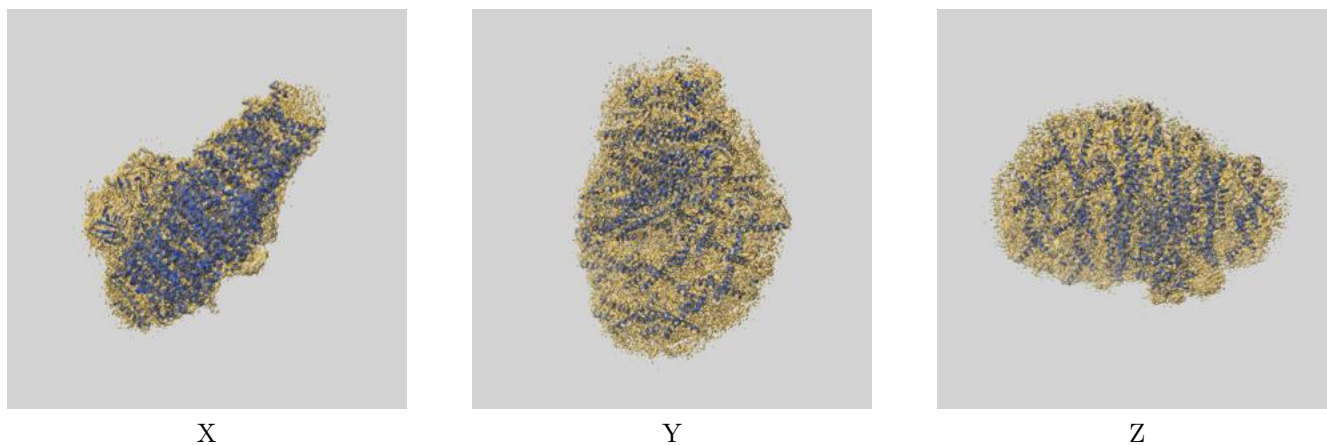
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

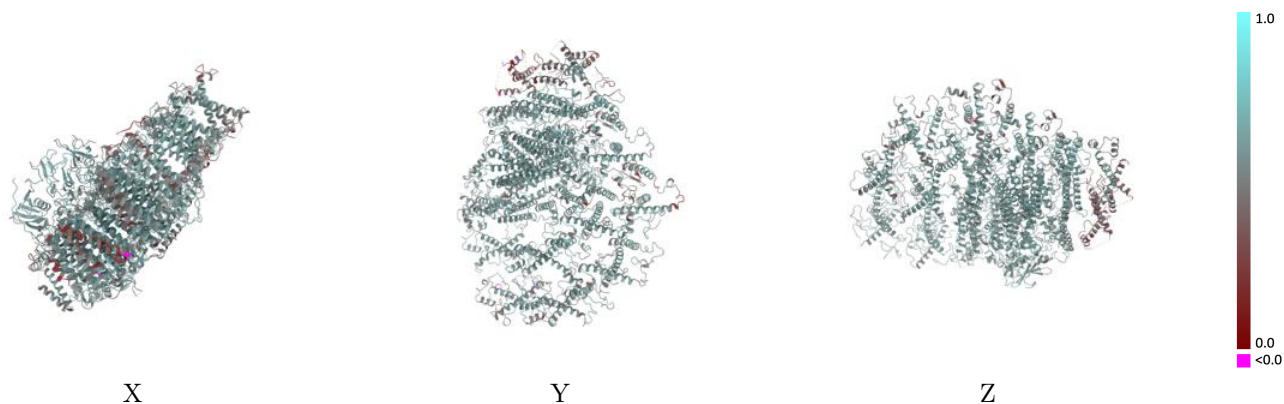
This section contains information regarding the fit between EMDB map EMD-9853 and PDB model 6JO5. Per-residue inclusion information can be found in section 3 on page 33.

9.1 Map-model overlay [i](#)



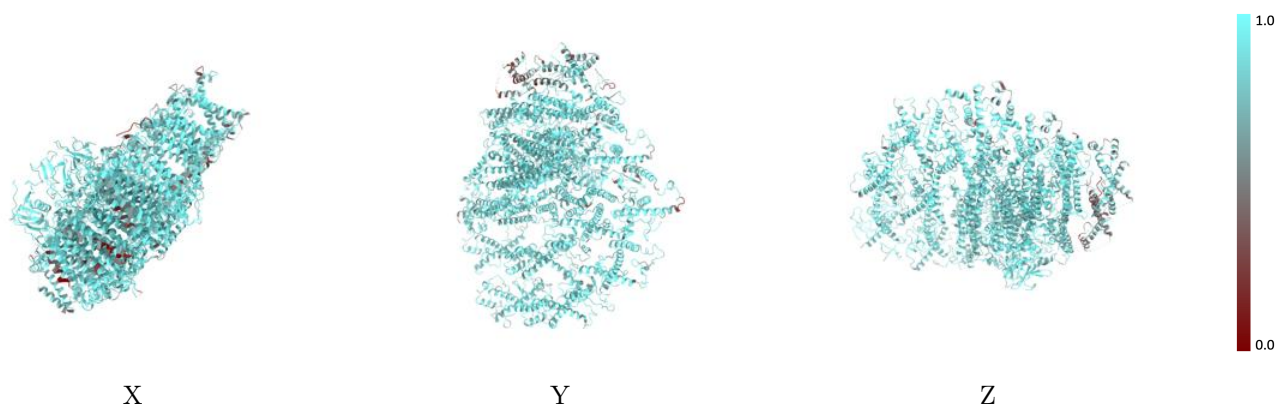
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



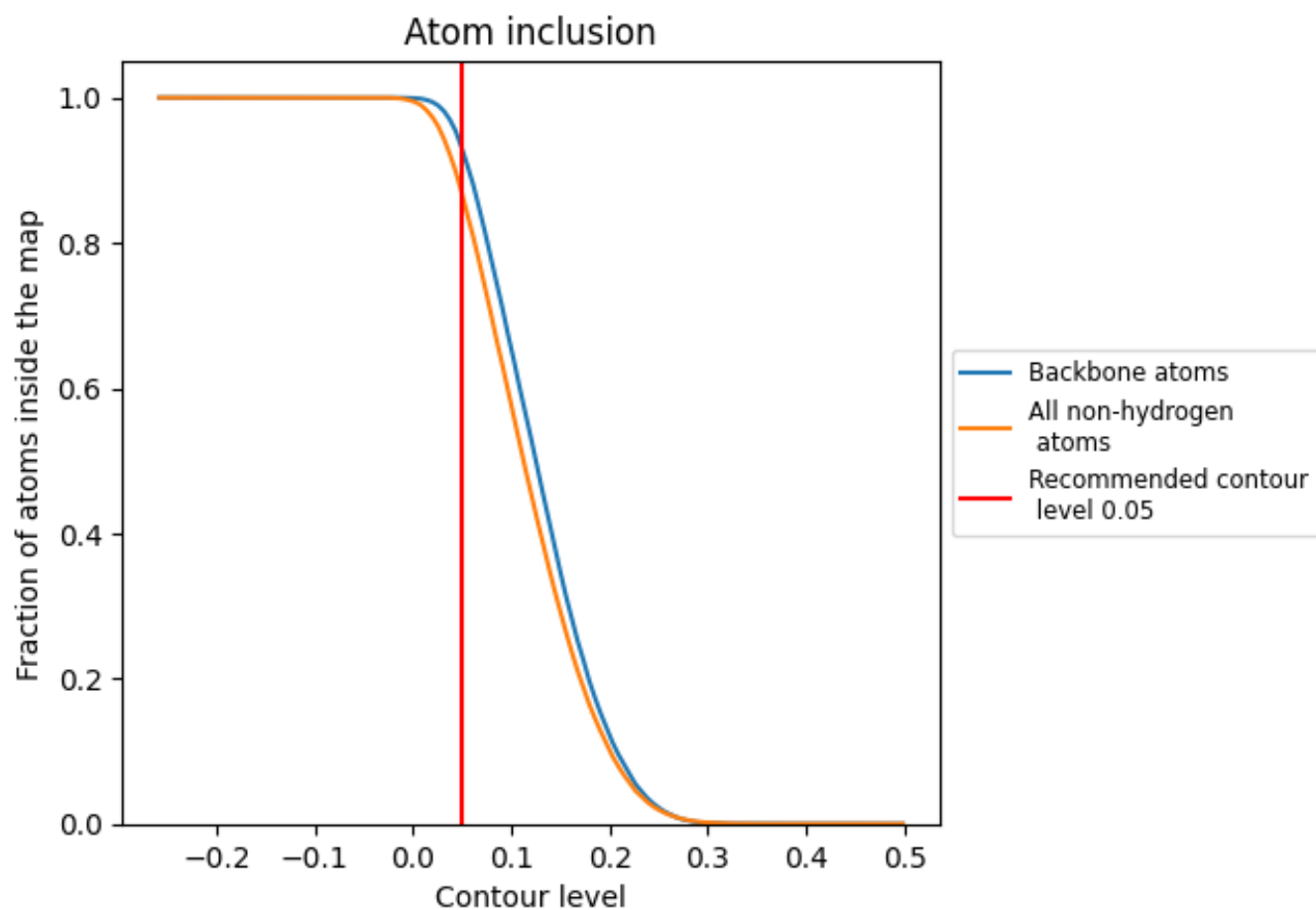
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8680 |  0.5670 |
| 1 |  0.8535 |  0.5660 |
| 2 |  0.5378 |  0.3290 |
| 3 |  0.8919 |  0.5820 |
| 4 |  0.8488 |  0.5440 |
| 5 |  0.8524 |  0.5470 |
| 6 |  0.8489 |  0.5510 |
| 7 |  0.8849 |  0.5860 |
| 8 |  0.8913 |  0.5830 |
| 9 |  0.6952 |  0.4490 |
| A |  0.9281 |  0.6080 |
| B |  0.9225 |  0.6090 |
| C |  0.9551 |  0.6010 |
| D |  0.9036 |  0.5730 |
| E |  0.8908 |  0.5830 |
| F |  0.8658 |  0.5660 |
| G |  0.8299 |  0.5500 |
| I |  0.8683 |  0.5680 |
| J |  0.9136 |  0.6010 |
| K |  0.7804 |  0.5270 |
| L |  0.8366 |  0.5420 |
| Z |  0.7812 |  0.5190 |

