# Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:52 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 7ZQD / pdb_00007zqd |
| EMDB ID | : | EMD-14871 |
| Title | : | Dimeric PSI of Chlamydomonas reinhardtii at 2.97 A resolution |
| Authors | : | Naschberger, A.; Amunts, A. |
| Deposited on | : | 2022-04-29 |
| Resolution | : | 2.97 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.

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

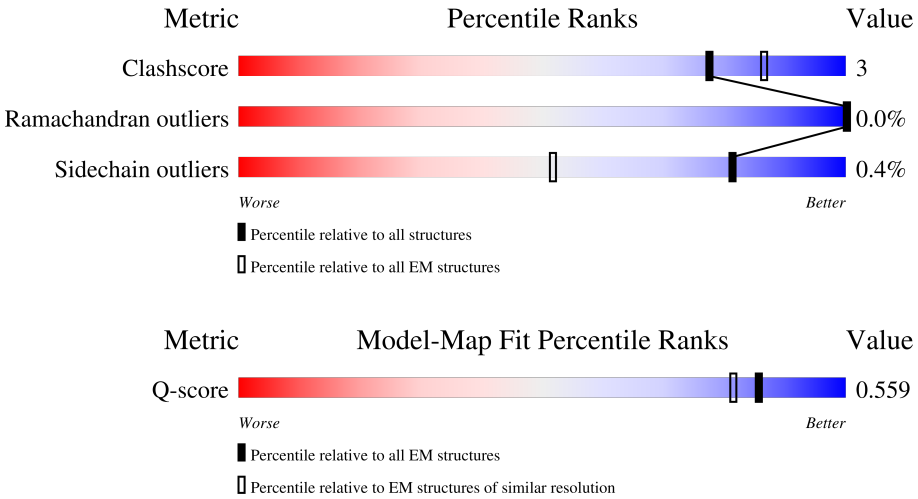
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 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.







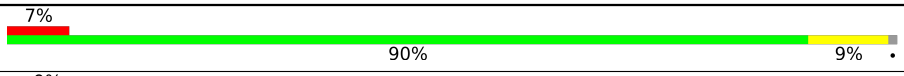
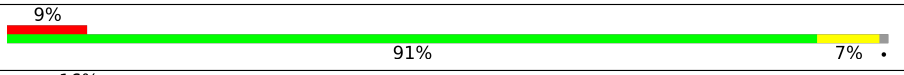
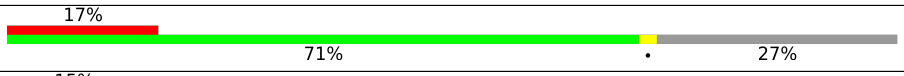
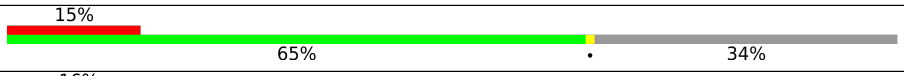
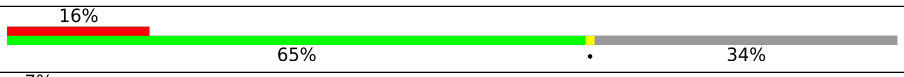
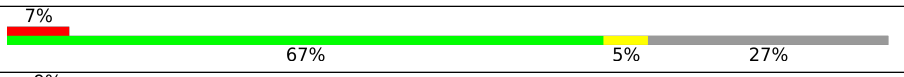
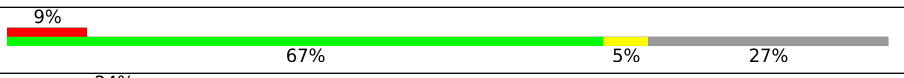
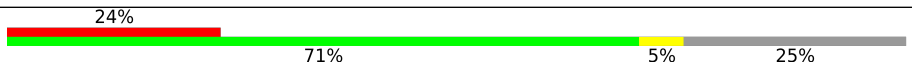
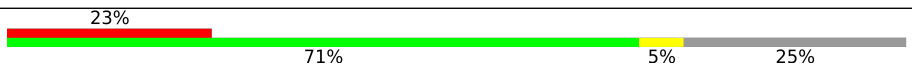
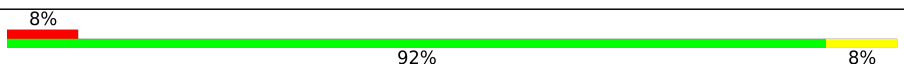
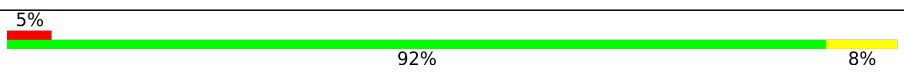
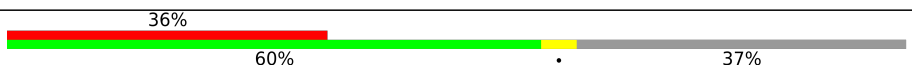
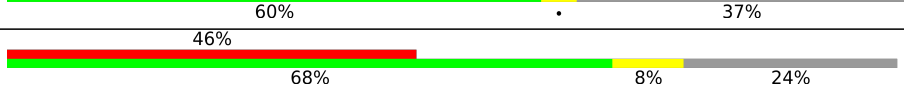
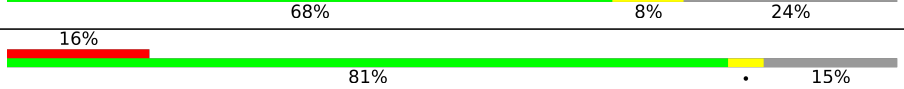
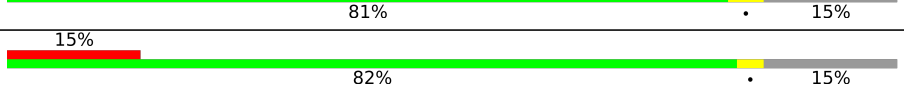
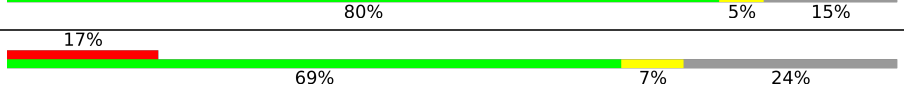
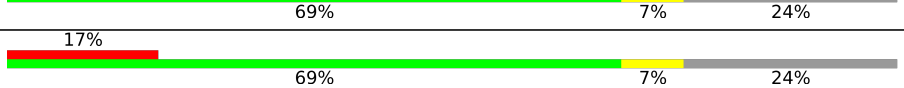
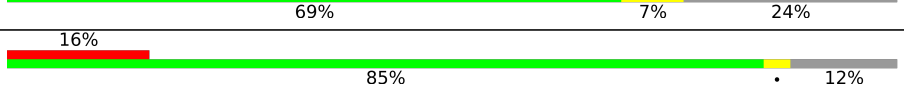
| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 13205 ( 2.47 - 3.47 ) |

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 <=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 | 93% 5% |
| 1 | A2 | 751 | 94% 5% |
| 2 | B | 735 | 94% 5% |
| 2 | B2 | 735 | 93% 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | C | 81 |   |
| 3 | C2 | 81 |   |
| 4 | D | 196 |   |
| 4 | D2 | 196 |   |
| 5 | E | 97 |   |
| 5 | E2 | 97 |   |
| 6 | F | 227 |   |
| 6 | F2 | 227 |   |
| 7 | G | 126 |   |
| 7 | G2 | 126 |   |
| 8 | I | 106 |   |
| 8 | I2 | 106 |   |
| 9 | J | 40 |   |
| 9 | J2 | 40 |   |
| 10 | L | 196 |   |
| 10 | L2 | 196 |   |
| 11 | K | 113 |   |
| 11 | K2 | 113 |   |
| 12 | 1 | 228 |   |
| 12 | 12 | 228 |   |
| 12 | Z | 228 |   |
| 12 | Z2 | 228 |   |
| 13 | 3 | 298 |   |
| 13 | 32 | 298 |   |
| 14 | 7 | 241 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 14 | 72 | 241 | 17% 85% 12% |
| 15 | 8 | 243 | 13% 86% 11% |
| 15 | 82 | 243 | 12% 87% 11% |
| 16 | 4 | 264 | 69% 77% 20% |
| 16 | 42 | 264 | 69% 77% 20% |
| 17 | 5 | 257 | 68% 83% 5% 12% |
| 17 | 52 | 257 | 70% 83% 5% 12% |
| 18 | 6 | 257 | 77% 86% 11% |
| 18 | 62 | 257 | 75% 86% 11% |
| 19 | 9 | 213 | 23% 83% 5% 13% |
| 19 | 92 | 213 | 23% 83% 5% 13% |

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 |
|---|---|---|---|---|---|---|---|
| 20 | CL0 | A | 801 | X | - | - | - |
| 20 | CL0 | A2 | 801 | X | - | - | - |
| 21 | CLA | 1 | 602 | X | - | - | - |
| 21 | CLA | 1 | 603 | X | - | - | - |
| 21 | CLA | 1 | 604 | X | - | - | - |
| 21 | CLA | 1 | 608 | X | - | - | - |
| 21 | CLA | 1 | 609 | X | - | - | - |
| 21 | CLA | 1 | 610 | X | - | - | - |
| 21 | CLA | 1 | 611 | X | - | - | - |
| 21 | CLA | 1 | 612 | X | - | - | - |
| 21 | CLA | 1 | 613 | X | - | - | - |
| 21 | CLA | 1 | 614 | X | - | - | - |
| 21 | CLA | 1 | 616 | X | - | - | - |
| 21 | CLA | 12 | 602 | X | - | - | - |
| 21 | CLA | 12 | 603 | X | - | - | - |
| 21 | CLA | 12 | 604 | X | - | - | - |
| 21 | CLA | 12 | 608 | X | - | - | - |
| 21 | CLA | 12 | 609 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 12 | 610 | X | - | - | - |
| 21 | CLA | 12 | 611 | X | - | - | - |
| 21 | CLA | 12 | 612 | X | - | - | - |
| 21 | CLA | 12 | 613 | X | - | - | - |
| 21 | CLA | 12 | 614 | X | - | - | - |
| 21 | CLA | 12 | 616 | X | - | - | - |
| 21 | CLA | 3 | 602 | X | - | - | - |
| 21 | CLA | 3 | 603 | X | - | - | - |
| 21 | CLA | 3 | 604 | X | - | - | - |
| 21 | CLA | 3 | 606 | X | - | - | - |
| 21 | CLA | 3 | 607 | X | - | - | - |
| 21 | CLA | 3 | 609 | X | - | - | - |
| 21 | CLA | 3 | 610 | X | - | - | - |
| 21 | CLA | 3 | 611 | X | - | - | - |
| 21 | CLA | 3 | 612 | X | - | - | - |
| 21 | CLA | 3 | 613 | X | - | - | - |
| 21 | CLA | 3 | 614 | X | - | - | - |
| 21 | CLA | 3 | 615 | X | - | - | - |
| 21 | CLA | 3 | 617 | X | - | - | - |
| 21 | CLA | 32 | 602 | X | - | - | - |
| 21 | CLA | 32 | 603 | X | - | - | - |
| 21 | CLA | 32 | 604 | X | - | - | - |
| 21 | CLA | 32 | 606 | X | - | - | - |
| 21 | CLA | 32 | 607 | X | - | - | - |
| 21 | CLA | 32 | 609 | X | - | - | - |
| 21 | CLA | 32 | 610 | X | - | - | - |
| 21 | CLA | 32 | 611 | X | - | - | - |
| 21 | CLA | 32 | 612 | X | - | - | - |
| 21 | CLA | 32 | 613 | X | - | - | - |
| 21 | CLA | 32 | 614 | X | - | - | - |
| 21 | CLA | 32 | 615 | X | - | - | - |
| 21 | CLA | 32 | 617 | X | - | - | - |
| 21 | CLA | 4 | 602 | X | - | - | - |
| 21 | CLA | 4 | 603 | X | - | - | - |
| 21 | CLA | 4 | 604 | X | - | - | - |
| 21 | CLA | 4 | 609 | X | - | - | - |
| 21 | CLA | 4 | 610 | X | - | - | - |
| 21 | CLA | 4 | 611 | X | - | - | - |
| 21 | CLA | 4 | 612 | X | - | - | - |
| 21 | CLA | 4 | 613 | X | - | - | - |
| 21 | CLA | 4 | 614 | X | - | - | - |
| 21 | CLA | 4 | 616 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 42 | 602 | X | - | - | - |
| 21 | CLA | 42 | 603 | X | - | - | - |
| 21 | CLA | 42 | 604 | X | - | - | - |
| 21 | CLA | 42 | 609 | X | - | - | - |
| 21 | CLA | 42 | 610 | X | - | - | - |
| 21 | CLA | 42 | 611 | X | - | - | - |
| 21 | CLA | 42 | 612 | X | - | - | - |
| 21 | CLA | 42 | 613 | X | - | - | - |
| 21 | CLA | 42 | 614 | X | - | - | - |
| 21 | CLA | 42 | 616 | X | - | - | - |
| 21 | CLA | 5 | 601 | X | - | - | - |
| 21 | CLA | 5 | 602 | X | - | - | - |
| 21 | CLA | 5 | 603 | X | - | - | - |
| 21 | CLA | 5 | 604 | X | - | - | - |
| 21 | CLA | 5 | 609 | X | - | - | - |
| 21 | CLA | 5 | 610 | X | - | - | - |
| 21 | CLA | 5 | 611 | X | - | - | - |
| 21 | CLA | 5 | 612 | X | - | - | - |
| 21 | CLA | 5 | 613 | X | - | - | - |
| 21 | CLA | 5 | 614 | X | - | - | - |
| 21 | CLA | 5 | 616 | X | - | - | - |
| 21 | CLA | 5 | 617 | X | - | - | - |
| 21 | CLA | 5 | 621 | X | - | - | - |
| 21 | CLA | 52 | 601 | X | - | - | - |
| 21 | CLA | 52 | 602 | X | - | - | - |
| 21 | CLA | 52 | 603 | X | - | - | - |
| 21 | CLA | 52 | 604 | X | - | - | - |
| 21 | CLA | 52 | 609 | X | - | - | - |
| 21 | CLA | 52 | 610 | X | - | - | - |
| 21 | CLA | 52 | 611 | X | - | - | - |
| 21 | CLA | 52 | 612 | X | - | - | - |
| 21 | CLA | 52 | 613 | X | - | - | - |
| 21 | CLA | 52 | 614 | X | - | - | - |
| 21 | CLA | 52 | 616 | X | - | - | - |
| 21 | CLA | 52 | 617 | X | - | - | - |
| 21 | CLA | 52 | 621 | X | - | - | - |
| 21 | CLA | 6 | 602 | X | - | - | - |
| 21 | CLA | 6 | 603 | X | - | - | - |
| 21 | CLA | 6 | 604 | X | - | - | - |
| 21 | CLA | 6 | 609 | X | - | - | - |
| 21 | CLA | 6 | 610 | X | - | - | - |
| 21 | CLA | 6 | 611 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 6 | 612 | X | - | - | - |
| 21 | CLA | 6 | 613 | X | - | - | - |
| 21 | CLA | 6 | 614 | X | - | - | - |
| 21 | CLA | 6 | 617 | X | - | - | - |
| 21 | CLA | 6 | 622 | X | - | - | - |
| 21 | CLA | 62 | 602 | X | - | - | - |
| 21 | CLA | 62 | 603 | X | - | - | - |
| 21 | CLA | 62 | 604 | X | - | - | - |
| 21 | CLA | 62 | 609 | X | - | - | - |
| 21 | CLA | 62 | 610 | X | - | - | - |
| 21 | CLA | 62 | 611 | X | - | - | - |
| 21 | CLA | 62 | 612 | X | - | - | - |
| 21 | CLA | 62 | 613 | X | - | - | - |
| 21 | CLA | 62 | 614 | X | - | - | - |
| 21 | CLA | 62 | 617 | X | - | - | - |
| 21 | CLA | 62 | 622 | X | - | - | - |
| 21 | CLA | 7 | 602 | X | - | - | - |
| 21 | CLA | 7 | 603 | X | - | - | - |
| 21 | CLA | 7 | 604 | X | - | - | - |
| 21 | CLA | 7 | 608 | X | - | - | - |
| 21 | CLA | 7 | 609 | X | - | - | - |
| 21 | CLA | 7 | 610 | X | - | - | - |
| 21 | CLA | 7 | 611 | X | - | - | - |
| 21 | CLA | 7 | 612 | X | - | - | - |
| 21 | CLA | 7 | 613 | X | - | - | - |
| 21 | CLA | 7 | 614 | X | - | - | - |
| 21 | CLA | 7 | 616 | X | - | - | - |
| 21 | CLA | 7 | 620 | X | - | - | - |
| 21 | CLA | 72 | 602 | X | - | - | - |
| 21 | CLA | 72 | 603 | X | - | - | - |
| 21 | CLA | 72 | 604 | X | - | - | - |
| 21 | CLA | 72 | 608 | X | - | - | - |
| 21 | CLA | 72 | 609 | X | - | - | - |
| 21 | CLA | 72 | 610 | X | - | - | - |
| 21 | CLA | 72 | 611 | X | - | - | - |
| 21 | CLA | 72 | 612 | X | - | - | - |
| 21 | CLA | 72 | 613 | X | - | - | - |
| 21 | CLA | 72 | 614 | X | - | - | - |
| 21 | CLA | 72 | 616 | X | - | - | - |
| 21 | CLA | 72 | 620 | X | - | - | - |
| 21 | CLA | 8 | 602 | X | - | - | - |
| 21 | CLA | 8 | 603 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 8 | 604 | X | - | - | - |
| 21 | CLA | 8 | 608 | X | - | - | - |
| 21 | CLA | 8 | 609 | X | - | - | - |
| 21 | CLA | 8 | 610 | X | - | - | - |
| 21 | CLA | 8 | 611 | X | - | - | - |
| 21 | CLA | 8 | 612 | X | - | - | - |
| 21 | CLA | 8 | 613 | X | - | - | - |
| 21 | CLA | 8 | 614 | X | - | - | - |
| 21 | CLA | 8 | 616 | X | - | - | - |
| 21 | CLA | 82 | 602 | X | - | - | - |
| 21 | CLA | 82 | 603 | X | - | - | - |
| 21 | CLA | 82 | 604 | X | - | - | - |
| 21 | CLA | 82 | 608 | X | - | - | - |
| 21 | CLA | 82 | 609 | X | - | - | - |
| 21 | CLA | 82 | 610 | X | - | - | - |
| 21 | CLA | 82 | 611 | X | - | - | - |
| 21 | CLA | 82 | 612 | X | - | - | - |
| 21 | CLA | 82 | 613 | X | - | - | - |
| 21 | CLA | 82 | 614 | X | - | - | - |
| 21 | CLA | 82 | 616 | X | - | - | - |
| 21 | CLA | 9 | 601 | X | - | - | - |
| 21 | CLA | 9 | 602 | X | - | - | - |
| 21 | CLA | 9 | 603 | X | - | - | - |
| 21 | CLA | 9 | 604 | X | - | - | - |
| 21 | CLA | 9 | 609 | X | - | - | - |
| 21 | CLA | 9 | 610 | X | - | - | - |
| 21 | CLA | 9 | 611 | X | - | - | - |
| 21 | CLA | 9 | 612 | X | - | - | - |
| 21 | CLA | 9 | 613 | X | - | - | - |
| 21 | CLA | 9 | 614 | X | - | - | - |
| 21 | CLA | 92 | 601 | X | - | - | - |
| 21 | CLA | 92 | 602 | X | - | - | - |
| 21 | CLA | 92 | 603 | X | - | - | - |
| 21 | CLA | 92 | 604 | X | - | - | - |
| 21 | CLA | 92 | 609 | X | - | - | - |
| 21 | CLA | 92 | 610 | X | - | - | - |
| 21 | CLA | 92 | 611 | X | - | - | - |
| 21 | CLA | 92 | 612 | X | - | - | - |
| 21 | CLA | 92 | 613 | X | - | - | - |
| 21 | CLA | 92 | 614 | X | - | - | - |
| 21 | CLA | A | 802 | X | - | - | - |
| 21 | CLA | A | 803 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | A | 804 | X | - | - | - |
| 21 | CLA | A | 805 | X | - | - | - |
| 21 | CLA | A | 806 | X | - | - | - |
| 21 | CLA | A | 807 | X | - | - | - |
| 21 | CLA | A | 808 | X | - | - | - |
| 21 | CLA | A | 809 | X | - | - | - |
| 21 | CLA | A | 810 | X | - | - | - |
| 21 | CLA | A | 811 | X | - | - | - |
| 21 | CLA | A | 812 | X | - | - | - |
| 21 | CLA | A | 813 | X | - | - | - |
| 21 | CLA | A | 814 | X | - | - | - |
| 21 | CLA | A | 815 | X | - | - | - |
| 21 | CLA | A | 816 | X | - | - | - |
| 21 | CLA | A | 817 | X | - | - | - |
| 21 | CLA | A | 818 | X | - | - | - |
| 21 | CLA | A | 819 | X | - | - | - |
| 21 | CLA | A | 820 | X | - | - | - |
| 21 | CLA | A | 821 | X | - | - | - |
| 21 | CLA | A | 822 | X | - | - | - |
| 21 | CLA | A | 823 | X | - | - | - |
| 21 | CLA | A | 824 | X | - | - | - |
| 21 | CLA | A | 825 | X | - | - | - |
| 21 | CLA | A | 826 | X | - | - | - |
| 21 | CLA | A | 827 | X | - | - | - |
| 21 | CLA | A | 828 | X | - | - | - |
| 21 | CLA | A | 829 | X | - | - | - |
| 21 | CLA | A | 830 | X | - | - | - |
| 21 | CLA | A | 831 | X | - | - | - |
| 21 | CLA | A | 832 | X | - | - | - |
| 21 | CLA | A | 833 | X | - | - | - |
| 21 | CLA | A | 834 | X | - | - | - |
| 21 | CLA | A | 835 | X | - | - | - |
| 21 | CLA | A | 836 | X | - | - | - |
| 21 | CLA | A | 837 | X | - | - | - |
| 21 | CLA | A | 838 | X | - | - | - |
| 21 | CLA | A | 839 | X | - | - | - |
| 21 | CLA | A | 840 | X | - | - | - |
| 21 | CLA | A | 841 | X | - | - | - |
| 21 | CLA | A | 842 | X | - | - | - |
| 21 | CLA | A | 843 | X | - | - | - |
| 21 | CLA | A | 845 | X | - | - | - |
| 21 | CLA | A | 854 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | A2 | 802 | X | - | - | - |
| 21 | CLA | A2 | 803 | X | - | - | - |
| 21 | CLA | A2 | 804 | X | - | - | - |
| 21 | CLA | A2 | 805 | X | - | - | - |
| 21 | CLA | A2 | 806 | X | - | - | - |
| 21 | CLA | A2 | 807 | X | - | - | - |
| 21 | CLA | A2 | 808 | X | - | - | - |
| 21 | CLA | A2 | 809 | X | - | - | - |
| 21 | CLA | A2 | 810 | X | - | - | - |
| 21 | CLA | A2 | 811 | X | - | - | - |
| 21 | CLA | A2 | 812 | X | - | - | - |
| 21 | CLA | A2 | 813 | X | - | - | - |
| 21 | CLA | A2 | 814 | X | - | - | - |
| 21 | CLA | A2 | 815 | X | - | - | - |
| 21 | CLA | A2 | 816 | X | - | - | - |
| 21 | CLA | A2 | 817 | X | - | - | - |
| 21 | CLA | A2 | 818 | X | - | - | - |
| 21 | CLA | A2 | 819 | X | - | - | - |
| 21 | CLA | A2 | 820 | X | - | - | - |
| 21 | CLA | A2 | 821 | X | - | - | - |
| 21 | CLA | A2 | 822 | X | - | - | - |
| 21 | CLA | A2 | 823 | X | - | - | - |
| 21 | CLA | A2 | 824 | X | - | - | - |
| 21 | CLA | A2 | 825 | X | - | - | - |
| 21 | CLA | A2 | 826 | X | - | - | - |
| 21 | CLA | A2 | 827 | X | - | - | - |
| 21 | CLA | A2 | 828 | X | - | - | - |
| 21 | CLA | A2 | 829 | X | - | - | - |
| 21 | CLA | A2 | 830 | X | - | - | - |
| 21 | CLA | A2 | 831 | X | - | - | - |
| 21 | CLA | A2 | 832 | X | - | - | - |
| 21 | CLA | A2 | 833 | X | - | - | - |
| 21 | CLA | A2 | 834 | X | - | - | - |
| 21 | CLA | A2 | 835 | X | - | - | - |
| 21 | CLA | A2 | 836 | X | - | - | - |
| 21 | CLA | A2 | 837 | X | - | - | - |
| 21 | CLA | A2 | 838 | X | - | - | - |
| 21 | CLA | A2 | 839 | X | - | - | - |
| 21 | CLA | A2 | 840 | X | - | - | - |
| 21 | CLA | A2 | 841 | X | - | - | - |
| 21 | CLA | A2 | 842 | X | - | - | - |
| 21 | CLA | A2 | 843 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | A2 | 845 | X | - | - | - |
| 21 | CLA | A2 | 854 | X | - | - | - |
| 21 | CLA | B | 802 | X | - | - | - |
| 21 | CLA | B | 803 | X | - | - | - |
| 21 | CLA | B | 804 | X | - | - | - |
| 21 | CLA | B | 805 | X | - | - | - |
| 21 | CLA | B | 806 | X | - | - | - |
| 21 | CLA | B | 807 | X | - | - | - |
| 21 | CLA | B | 808 | X | - | - | - |
| 21 | CLA | B | 809 | X | - | - | - |
| 21 | CLA | B | 810 | X | - | - | - |
| 21 | CLA | B | 811 | X | - | - | - |
| 21 | CLA | B | 812 | X | - | - | - |
| 21 | CLA | B | 813 | X | - | - | - |
| 21 | CLA | B | 814 | X | - | - | - |
| 21 | CLA | B | 815 | X | - | - | - |
| 21 | CLA | B | 816 | X | - | - | - |
| 21 | CLA | B | 817 | X | - | - | - |
| 21 | CLA | B | 818 | X | - | - | - |
| 21 | CLA | B | 819 | X | - | - | - |
| 21 | CLA | B | 820 | X | - | - | - |
| 21 | CLA | B | 821 | X | - | - | - |
| 21 | CLA | B | 822 | X | - | - | - |
| 21 | CLA | B | 823 | X | - | - | - |
| 21 | CLA | B | 824 | X | - | - | - |
| 21 | CLA | B | 825 | X | - | - | - |
| 21 | CLA | B | 826 | X | - | - | - |
| 21 | CLA | B | 827 | X | - | - | - |
| 21 | CLA | B | 828 | X | - | - | - |
| 21 | CLA | B | 829 | X | - | - | - |
| 21 | CLA | B | 830 | X | - | - | - |
| 21 | CLA | B | 831 | X | - | - | - |
| 21 | CLA | B | 832 | X | - | - | - |
| 21 | CLA | B | 833 | X | - | - | - |
| 21 | CLA | B | 834 | X | - | - | - |
| 21 | CLA | B | 835 | X | - | - | - |
| 21 | CLA | B | 836 | X | - | - | - |
| 21 | CLA | B | 837 | X | - | - | - |
| 21 | CLA | B | 838 | X | - | - | - |
| 21 | CLA | B | 839 | X | - | - | - |
| 21 | CLA | B | 840 | X | - | - | - |
| 21 | CLA | B | 841 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | B2 | 802 | X | - | - | - |
| 21 | CLA | B2 | 803 | X | - | - | - |
| 21 | CLA | B2 | 804 | X | - | - | - |
| 21 | CLA | B2 | 805 | X | - | - | - |
| 21 | CLA | B2 | 806 | X | - | - | - |
| 21 | CLA | B2 | 807 | X | - | - | - |
| 21 | CLA | B2 | 808 | X | - | - | - |
| 21 | CLA | B2 | 809 | X | - | - | - |
| 21 | CLA | B2 | 810 | X | - | - | - |
| 21 | CLA | B2 | 811 | X | - | - | - |
| 21 | CLA | B2 | 812 | X | - | - | - |
| 21 | CLA | B2 | 813 | X | - | - | - |
| 21 | CLA | B2 | 814 | X | - | - | - |
| 21 | CLA | B2 | 815 | X | - | - | - |
| 21 | CLA | B2 | 816 | X | - | - | - |
| 21 | CLA | B2 | 817 | X | - | - | - |
| 21 | CLA | B2 | 818 | X | - | - | - |
| 21 | CLA | B2 | 819 | X | - | - | - |
| 21 | CLA | B2 | 820 | X | - | - | - |
| 21 | CLA | B2 | 821 | X | - | - | - |
| 21 | CLA | B2 | 822 | X | - | - | - |
| 21 | CLA | B2 | 823 | X | - | - | - |
| 21 | CLA | B2 | 824 | X | - | - | - |
| 21 | CLA | B2 | 825 | X | - | - | - |
| 21 | CLA | B2 | 826 | X | - | - | - |
| 21 | CLA | B2 | 827 | X | - | - | - |
| 21 | CLA | B2 | 828 | X | - | - | - |
| 21 | CLA | B2 | 829 | X | - | - | - |
| 21 | CLA | B2 | 830 | X | - | - | - |
| 21 | CLA | B2 | 831 | X | - | - | - |
| 21 | CLA | B2 | 832 | X | - | - | - |
| 21 | CLA | B2 | 833 | X | - | - | - |
| 21 | CLA | B2 | 834 | X | - | - | - |
| 21 | CLA | B2 | 835 | X | - | - | - |
| 21 | CLA | B2 | 836 | X | - | - | - |
| 21 | CLA | B2 | 837 | X | - | - | - |
| 21 | CLA | B2 | 838 | X | - | - | - |
| 21 | CLA | B2 | 839 | X | - | - | - |
| 21 | CLA | B2 | 840 | X | - | - | - |
| 21 | CLA | B2 | 841 | X | - | - | - |
| 21 | CLA | F | 301 | X | - | - | - |
| 21 | CLA | F | 303 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | F | 304 | X | - | - | - |
| 21 | CLA | F2 | 301 | X | - | - | - |
| 21 | CLA | F2 | 303 | X | - | - | - |
| 21 | CLA | F2 | 304 | X | - | - | - |
| 21 | CLA | G | 203 | X | - | - | - |
| 21 | CLA | G | 204 | X | - | - | - |
| 21 | CLA | G2 | 203 | X | - | - | - |
| 21 | CLA | G2 | 204 | X | - | - | - |
| 21 | CLA | J | 101 | X | - | - | - |
| 21 | CLA | J2 | 101 | X | - | - | - |
| 21 | CLA | K | 201 | X | - | - | - |
| 21 | CLA | K | 203 | X | - | - | - |
| 21 | CLA | K | 204 | X | - | - | - |
| 21 | CLA | K | 206 | X | - | - | - |
| 21 | CLA | K2 | 201 | X | - | - | - |
| 21 | CLA | K2 | 203 | X | - | - | - |
| 21 | CLA | K2 | 204 | X | - | - | - |
| 21 | CLA | K2 | 206 | X | - | - | - |
| 21 | CLA | L | 203 | X | - | - | - |
| 21 | CLA | L | 204 | X | - | - | - |
| 21 | CLA | L2 | 203 | X | - | - | - |
| 21 | CLA | L2 | 204 | X | - | - | - |
| 21 | CLA | Z | 602 | X | - | - | - |
| 21 | CLA | Z | 603 | X | - | - | - |
| 21 | CLA | Z | 604 | X | - | - | - |
| 21 | CLA | Z | 608 | X | - | - | - |
| 21 | CLA | Z | 609 | X | - | - | - |
| 21 | CLA | Z | 610 | X | - | - | - |
| 21 | CLA | Z | 611 | X | - | - | - |
| 21 | CLA | Z | 612 | X | - | - | - |
| 21 | CLA | Z | 613 | X | - | - | - |
| 21 | CLA | Z | 614 | X | - | - | - |
| 21 | CLA | Z | 616 | X | - | - | - |
| 21 | CLA | Z2 | 602 | X | - | - | - |
| 21 | CLA | Z2 | 603 | X | - | - | - |
| 21 | CLA | Z2 | 604 | X | - | - | - |
| 21 | CLA | Z2 | 608 | X | - | - | - |
| 21 | CLA | Z2 | 609 | X | - | - | - |
| 21 | CLA | Z2 | 610 | X | - | - | - |
| 21 | CLA | Z2 | 611 | X | - | - | - |
| 21 | CLA | Z2 | 612 | X | - | - | - |
| 21 | CLA | Z2 | 613 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 21 | CLA | Z2 | 614 | X | - | - | - |
| 21 | CLA | Z2 | 616 | X | - | - | - |
| 30 | CHL | 1 | 601 | X | - | - | - |
| 30 | CHL | 1 | 606 | X | - | - | - |
| 30 | CHL | 1 | 607 | X | - | - | - |
| 30 | CHL | 12 | 601 | X | - | - | - |
| 30 | CHL | 12 | 606 | X | - | - | - |
| 30 | CHL | 12 | 607 | X | - | - | - |
| 30 | CHL | 3 | 608 | X | - | - | - |
| 30 | CHL | 32 | 608 | X | - | - | - |
| 30 | CHL | 4 | 601 | X | - | - | - |
| 30 | CHL | 4 | 606 | X | - | - | - |
| 30 | CHL | 4 | 607 | X | - | - | - |
| 30 | CHL | 4 | 608 | X | - | - | - |
| 30 | CHL | 4 | 618 | X | - | - | - |
| 30 | CHL | 42 | 601 | X | - | - | - |
| 30 | CHL | 42 | 606 | X | - | - | - |
| 30 | CHL | 42 | 607 | X | - | - | - |
| 30 | CHL | 42 | 608 | X | - | - | - |
| 30 | CHL | 42 | 618 | X | - | - | - |
| 30 | CHL | 5 | 606 | X | - | - | - |
| 30 | CHL | 5 | 607 | X | - | - | - |
| 30 | CHL | 5 | 608 | X | - | - | - |
| 30 | CHL | 5 | 618 | X | - | - | - |
| 30 | CHL | 52 | 606 | X | - | - | - |
| 30 | CHL | 52 | 607 | X | - | - | - |
| 30 | CHL | 52 | 608 | X | - | - | - |
| 30 | CHL | 52 | 618 | X | - | - | - |
| 30 | CHL | 6 | 601 | X | - | - | - |
| 30 | CHL | 6 | 606 | X | - | - | - |
| 30 | CHL | 6 | 607 | X | - | - | - |
| 30 | CHL | 6 | 608 | X | - | - | - |
| 30 | CHL | 6 | 616 | X | - | - | - |
| 30 | CHL | 6 | 618 | X | - | - | - |
| 30 | CHL | 62 | 601 | X | - | - | - |
| 30 | CHL | 62 | 606 | X | - | - | - |
| 30 | CHL | 62 | 607 | X | - | - | - |
| 30 | CHL | 62 | 608 | X | - | - | - |
| 30 | CHL | 62 | 616 | X | - | - | - |
| 30 | CHL | 62 | 618 | X | - | - | - |
| 30 | CHL | 7 | 601 | X | - | - | - |
| 30 | CHL | 7 | 606 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 30 | CHL | 7 | 607 | X | - | - | - |
| 30 | CHL | 72 | 601 | X | - | - | - |
| 30 | CHL | 72 | 606 | X | - | - | - |
| 30 | CHL | 72 | 607 | X | - | - | - |
| 30 | CHL | 8 | 601 | X | - | - | - |
| 30 | CHL | 8 | 606 | X | - | - | - |
| 30 | CHL | 8 | 607 | X | - | - | - |
| 30 | CHL | 82 | 601 | X | - | - | - |
| 30 | CHL | 82 | 606 | X | - | - | - |
| 30 | CHL | 82 | 607 | X | - | - | - |
| 30 | CHL | 9 | 606 | X | - | - | - |
| 30 | CHL | 9 | 607 | X | - | - | - |
| 30 | CHL | 92 | 606 | X | - | - | - |
| 30 | CHL | 92 | 607 | X | - | - | - |
| 30 | CHL | Z | 601 | X | - | - | - |
| 30 | CHL | Z | 606 | X | - | - | - |
| 30 | CHL | Z | 607 | X | - | - | - |
| 30 | CHL | Z2 | 601 | X | - | - | - |
| 30 | CHL | Z2 | 606 | X | - | - | - |
| 30 | CHL | Z2 | 607 | X | - | - | - |
| 31 | XAT | 5 | 624 | X | - | - | - |
| 31 | XAT | 52 | 624 | X | - | - | - |

# 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 202818 atoms, of which 101988 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 742 | Total | C | H | N | O | S | 0 | 0 |
| | | | 11500 | 3808 | 5675 | 994 | 1001 | 22 | | |
| 1 | A2 | 742 | Total | C | H | N | O | S | 0 | 0 |
| | | | 11500 | 3808 | 5675 | 994 | 1001 | 22 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 733 | Total | C | H | N | O | S | 0 | 0 |
| | | | 11400 | 3824 | 5576 | 977 | 1005 | 18 | | |
| 2 | B2 | 733 | Total | C | H | N | O | S | 0 | 0 |
| | | | 11400 | 3824 | 5576 | 977 | 1005 | 18 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 80 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1183 | 369 | 582 | 103 | 117 | 12 | | |
| 3 | C2 | 80 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1183 | 369 | 582 | 103 | 117 | 12 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 144 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2284 | 725 | 1151 | 200 | 201 | 7 | | |
| 4 | D2 | 144 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2284 | 725 | 1151 | 200 | 201 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 64 | Total | C | H | N | O | 0 | 0 |
| | | | 1011 | 322 | 505 | 89 | 95 | | |
| 5 | E2 | 64 | Total | C | H | N | O | 0 | 0 |
| | | | 1011 | 322 | 505 | 89 | 95 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 165 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2568 | 817 | 1302 | 213 | 233 | 3 | | |
| 6 | F2 | 165 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2568 | 817 | 1302 | 213 | 233 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 95 | Total | C | H | N | O | 0 | 0 |
| | | | 1393 | 452 | 687 | 119 | 135 | | |
| 7 | G2 | 95 | Total | C | H | N | O | 0 | 0 |
| | | | 1393 | 452 | 687 | 119 | 135 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | I | 37 | Total | C | H | N | O | S | 0 | 0 |
| | | | 573 | 195 | 292 | 39 | 46 | 1 | | |
| 8 | I2 | 37 | Total | C | H | N | O | S | 0 | 0 |
| | | | 573 | 195 | 292 | 39 | 46 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | J | 40 | Total | C | H | N | O | S | 0 | 0 |
| | | | 657 | 224 | 328 | 46 | 58 | 1 | | |
| 9 | J2 | 40 | Total | C | H | N | O | S | 0 | 0 |
| | | | 657 | 224 | 328 | 46 | 58 | 1 | | |

- Molecule 10 is a protein called PSI subunit V.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | L | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1806 | 586 | 907 | 146 | 164 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | L2 | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1806 | 586 | 907 | 146 | 164 | 3 | | |

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 86 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1203 | 370 | 620 | 100 | 111 | 2 | | |
| 11 | K2 | 86 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1203 | 370 | 620 | 100 | 111 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | 1 | 194 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2842 | 941 | 1397 | 240 | 261 | 3 | | |
| 12 | Z | 194 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2842 | 941 | 1397 | 240 | 261 | 3 | | |
| 12 | 12 | 194 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2842 | 941 | 1397 | 240 | 261 | 3 | | |
| 12 | Z2 | 194 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2842 | 941 | 1397 | 240 | 261 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | 3 | 227 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3431 | 1128 | 1695 | 283 | 317 | 8 | | |
| 13 | 32 | 227 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3431 | 1128 | 1695 | 283 | 317 | 8 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | 7 | 213 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3240 | 1072 | 1590 | 274 | 298 | 6 | | |
| 14 | 72 | 213 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3240 | 1072 | 1590 | 274 | 298 | 6 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | 8 | 217 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3280 | 1073 | 1630 | 280 | 293 | 4 | | |
| 15 | 82 | 217 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3280 | 1073 | 1630 | 280 | 293 | 4 | | |

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | 4 | 212 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3251 | 1080 | 1603 | 268 | 295 | 5 | | |
| 16 | 42 | 212 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3251 | 1080 | 1603 | 268 | 295 | 5 | | |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | 5 | 227 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3522 | 1154 | 1747 | 297 | 316 | 8 | | |
| 17 | 52 | 227 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3522 | 1154 | 1747 | 297 | 316 | 8 | | |

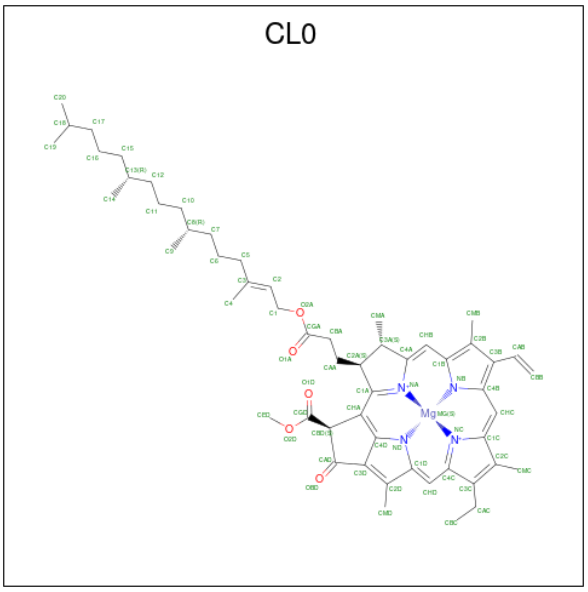
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | 6 | 230 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3542 | 1167 | 1770 | 293 | 306 | 6 | | |
| 18 | 62 | 230 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3542 | 1167 | 1770 | 293 | 306 | 6 | | |

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

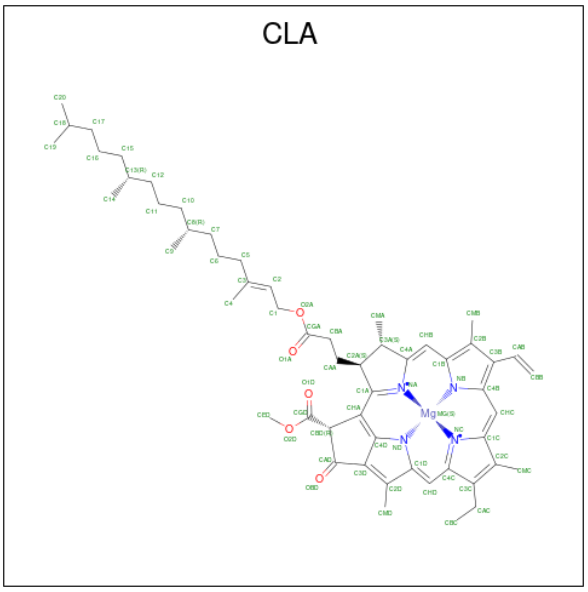
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | 9 | 186 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2820 | 918 | 1400 | 238 | 257 | 7 | | |
| 19 | 92 | 186 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2820 | 918 | 1400 | 238 | 257 | 7 | | |

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 20 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 20 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 92 | 41 | 41 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | A | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 107 | 46 | 51 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 117 | 49 | 58 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 113 | 48 | 55 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | F | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | F | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | F | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | G | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | G | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | J | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | L | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | L | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | K | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | K | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | K | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | K | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 122 | 51 | 61 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 73 | 34 | 31 | 1 | 4 | 3 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 122 | 51 | 61 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 95 | 42 | 43 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 92 | 41 | 41 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 95 | 42 | 43 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 76 | 35 | 33 | 1 | 4 | 3 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 98 | 43 | 45 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 125 | 52 | 63 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 107 | 46 | 51 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 98 | 43 | 45 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 113 | 48 | 55 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 98 | 43 | 45 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 92 | 41 | 41 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 92 | 41 | 41 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | A2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 107 | 46 | 51 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 117 | 49 | 58 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 113 | 48 | 55 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | B2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | F2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | F2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | F2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | G2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | G2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | J2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | L2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | L2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | K2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | K2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | K2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | K2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 122 | 51 | 61 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 73 | 34 | 31 | 1 | 4 | 3 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 122 | 51 | 61 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 95 | 42 | 43 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 92 | 41 | 41 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 95 | 42 | 43 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 76 | 35 | 33 | 1 | 4 | 3 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 98 | 43 | 45 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 125 | 52 | 63 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 110 | 47 | 53 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |

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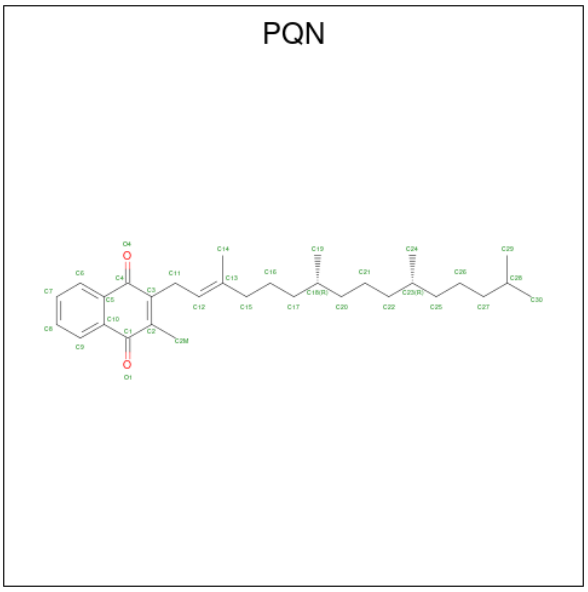
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 107 | 46 | 51 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 98 | 43 | 45 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |

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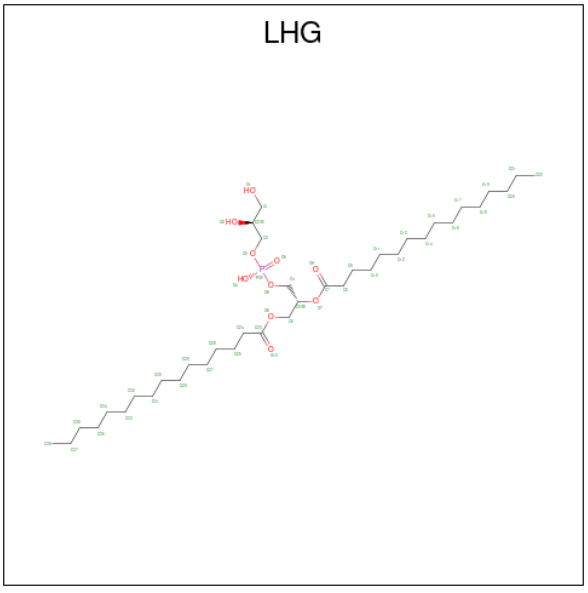
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 113 | 48 | 55 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 89 | 40 | 39 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |
| 21 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 79 | 36 | 33 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 104 | 45 | 49 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 98 | 43 | 45 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 92 | 41 | 41 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 119 | 50 | 59 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 137 | 55 | 72 | 1 | 4 | 5 | |
| 21 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 78 | 35 | 33 | 1 | 4 | 5 | |

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 22 | A | 1 | Total | C | H | O | 0 |
| | | | 79 | 31 | 46 | 2 | |
| 22 | B | 1 | Total | C | H | O | 0 |
| | | | 79 | 31 | 46 | 2 | |
| 22 | A2 | 1 | Total | C | H | O | 0 |
| | | | 79 | 31 | 46 | 2 | |
| 22 | B2 | 1 | Total | C | H | O | 0 |
| | | | 79 | 31 | 46 | 2 | |

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



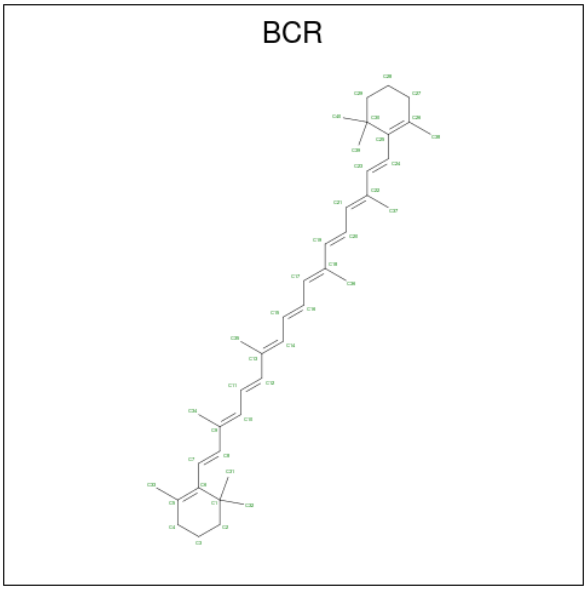
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 23 | A | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | A | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 27 | 49 | 10 | 1 | |
| 23 | B | 1 | Total | C | H | O | P | 0 |
| | | | 108 | 34 | 63 | 10 | 1 | |
| 23 | 1 | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 28 | 48 | 10 | 1 | |
| 23 | 3 | 1 | Total | C | H | O | P | 0 |
| | | | 63 | 20 | 32 | 10 | 1 | |
| 23 | 3 | 1 | Total | C | H | O | P | 0 |
| | | | 114 | 36 | 67 | 10 | 1 | |
| 23 | 7 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | 8 | 1 | Total | C | H | O | P | 0 |
| | | | 105 | 33 | 61 | 10 | 1 | |
| 23 | Z | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 28 | 48 | 10 | 1 | |
| 23 | 4 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | 4 | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 27 | 49 | 10 | 1 | |
| 23 | 5 | 1 | Total | C | H | O | P | 0 |
| | | | 81 | 26 | 44 | 10 | 1 | |
| 23 | 6 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | 6 | 1 | Total | C | H | O | P | 0 |
| | | | 78 | 25 | 42 | 10 | 1 | |
| 23 | 9 | 1 | Total | C | H | O | P | 0 |
| | | | 96 | 30 | 55 | 10 | 1 | |
| 23 | A2 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | A2 | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 27 | 49 | 10 | 1 | |
| 23 | B2 | 1 | Total | C | H | O | P | 0 |
| | | | 108 | 34 | 63 | 10 | 1 | |
| 23 | 12 | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 28 | 48 | 10 | 1 | |
| 23 | 32 | 1 | Total | C | H | O | P | 0 |
| | | | 63 | 20 | 32 | 10 | 1 | |
| 23 | 32 | 1 | Total | C | H | O | P | 0 |
| | | | 114 | 36 | 67 | 10 | 1 | |
| 23 | 72 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 23 | 82 | 1 | Total | C | H | O | P | 0 |
| | | | 105 | 33 | 61 | 10 | 1 | |
| 23 | Z2 | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 28 | 48 | 10 | 1 | |
| 23 | 42 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | 42 | 1 | Total | C | H | O | P | 0 |
| | | | 87 | 27 | 49 | 10 | 1 | |
| 23 | 52 | 1 | Total | C | H | O | P | 0 |
| | | | 81 | 26 | 44 | 10 | 1 | |
| 23 | 62 | 1 | Total | C | H | O | P | 0 |
| | | | 123 | 38 | 74 | 10 | 1 | |
| 23 | 62 | 1 | Total | C | H | O | P | 0 |
| | | | 78 | 25 | 42 | 10 | 1 | |
| 23 | 92 | 1 | Total | C | H | O | P | 0 |
| | | | 96 | 30 | 55 | 10 | 1 | |

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 24 | A | 1 | Total | C | H | 0 |
| | | | 96 | 40 | 56 | |
| 24 | A | 1 | Total | C | H | 0 |
| | | | 96 | 40 | 56 | |
| 24 | A | 1 | Total | C | H | 0 |
| | | | 96 | 40 | 56 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 24 | A | 1 | Total C H<br>96 40 56 | 0 |
| 24 | A | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B | 1 | Total C H<br>96 40 56 | 0 |
| 24 | G | 1 | Total C H<br>96 40 56 | 0 |
| 24 | I | 1 | Total C H<br>96 40 56 | 0 |
| 24 | J | 1 | Total C H<br>96 40 56 | 0 |
| 24 | L | 1 | Total C H<br>96 40 56 | 0 |
| 24 | L | 1 | Total C H<br>96 40 56 | 0 |
| 24 | K | 1 | Total C H<br>96 40 56 | 0 |
| 24 | K | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 3 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 3 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 3 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 7 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 8 | 1 | Total C H<br>96 40 56 | 0 |

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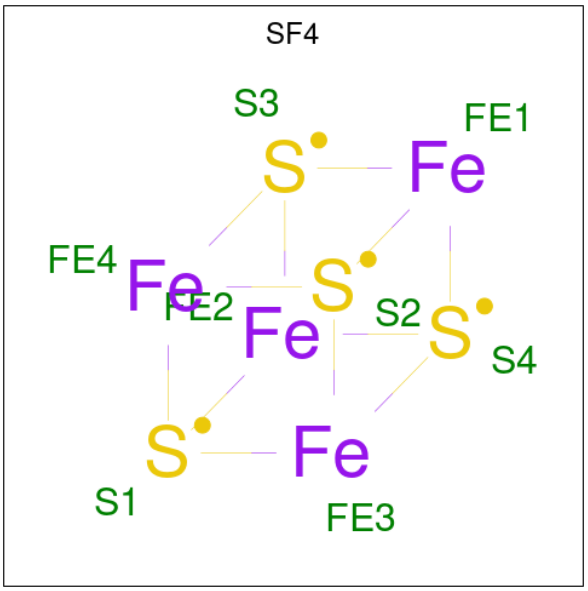
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 24 | 4 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 5 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 6 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 9 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | A2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | A2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | A2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | A2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | A2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | B2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | G2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | I2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | J2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | L2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | L2 | 1 | Total C H<br>96 40 56 | 0 |

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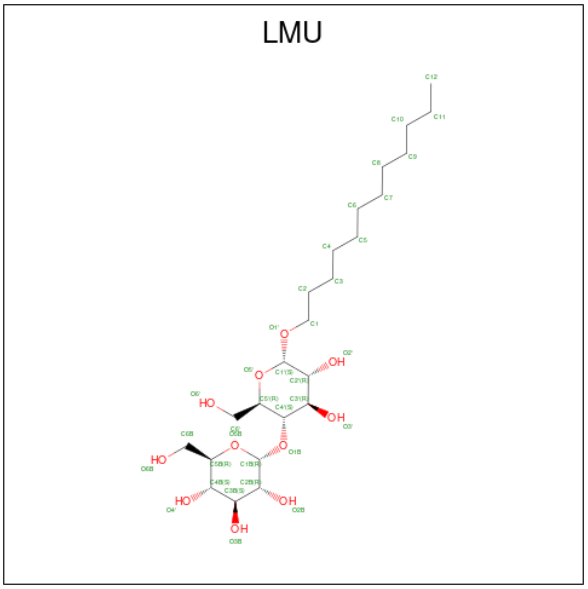
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 24 | K2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | K2 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 32 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 32 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 32 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 72 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 82 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 42 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 52 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 62 | 1 | Total C H<br>96 40 56 | 0 |
| 24 | 92 | 1 | Total C H<br>96 40 56 | 0 |

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



| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 25 | A | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | C | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | C | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | A2 | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | C2 | 1 | Total Fe S<br>8 4 4 | 0 |
| 25 | C2 | 1 | Total Fe S<br>8 4 4 | 0 |

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 26 | A | 1 | Total C H O<br>75 23 41 11 | 0 |
| 26 | A | 1 | Total C H O<br>81 24 46 11 | 0 |
| 26 | A | 1 | Total C H O<br>44 14 24 6 | 0 |
| 26 | A | 1 | Total C H O<br>59 18 35 6 | 0 |
| 26 | A | 1 | Total C H O<br>81 24 46 11 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 26 | A | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | A | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | B | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | G | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | K | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 1 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | 1 | 1 | Total | C | H | O | 0 |
| | | | 41 | 13 | 22 | 6 | |
| 26 | 1 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 1 | 1 | Total | C | H | O | 0 |
| | | | 50 | 16 | 28 | 6 | |
| 26 | 1 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 1 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 7 | 1 | Total | C | H | O | 0 |
| | | | 69 | 21 | 37 | 11 | |
| 26 | 7 | 1 | Total | C | H | O | 0 |
| | | | 50 | 16 | 28 | 6 | |
| 26 | 7 | 1 | Total | C | H | O | 0 |
| | | | 54 | 16 | 27 | 11 | |
| 26 | 8 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 8 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 8 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | 8 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | Z | 1 | Total | C | H | O | 0 |
| | | | 66 | 20 | 35 | 11 | |
| 26 | Z | 1 | Total | C | H | O | 0 |
| | | | 50 | 16 | 28 | 6 | |
| 26 | 4 | 1 | Total | C | H | O | 0 |
| | | | 72 | 22 | 39 | 11 | |

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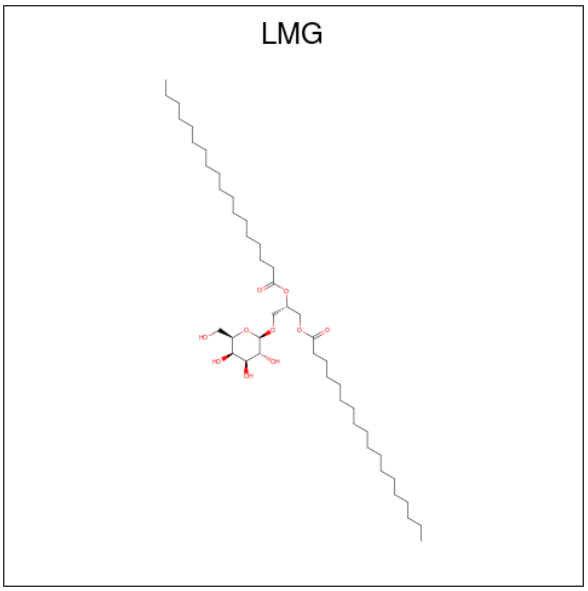
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 26 | 4 | 1 | Total | C | H | O | 0 |
| | | | 44 | 14 | 24 | 6 | |
| 26 | 5 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 6 | 1 | Total | C | H | O | 0 |
| | | | 44 | 14 | 24 | 6 | |
| 26 | 6 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 6 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 6 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 9 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 75 | 23 | 41 | 11 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 44 | 14 | 24 | 6 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | A2 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | B2 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | G2 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | K2 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 12 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | 12 | 1 | Total | C | H | O | 0 |
| | | | 41 | 13 | 22 | 6 | |
| 26 | 12 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 12 | 1 | Total | C | H | O | 0 |
| | | | 50 | 16 | 28 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 26 | 12 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 12 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 72 | 1 | Total | C | H | O | 0 |
| | | | 69 | 21 | 37 | 11 | |
| 26 | 72 | 1 | Total | C | H | O | 0 |
| | | | 50 | 16 | 28 | 6 | |
| 26 | 72 | 1 | Total | C | H | O | 0 |
| | | | 54 | 16 | 27 | 11 | |
| 26 | 82 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 82 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 82 | 1 | Total | C | H | O | 0 |
| | | | 81 | 24 | 46 | 11 | |
| 26 | 82 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | Z2 | 1 | Total | C | H | O | 0 |
| | | | 66 | 20 | 35 | 11 | |
| 26 | Z2 | 1 | Total | C | H | O | 0 |
| | | | 50 | 16 | 28 | 6 | |
| 26 | 42 | 1 | Total | C | H | O | 0 |
| | | | 72 | 22 | 39 | 11 | |
| 26 | 42 | 1 | Total | C | H | O | 0 |
| | | | 44 | 14 | 24 | 6 | |
| 26 | 52 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 62 | 1 | Total | C | H | O | 0 |
| | | | 44 | 14 | 24 | 6 | |
| 26 | 62 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 62 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 62 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |
| 26 | 92 | 1 | Total | C | H | O | 0 |
| | | | 59 | 18 | 35 | 6 | |

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



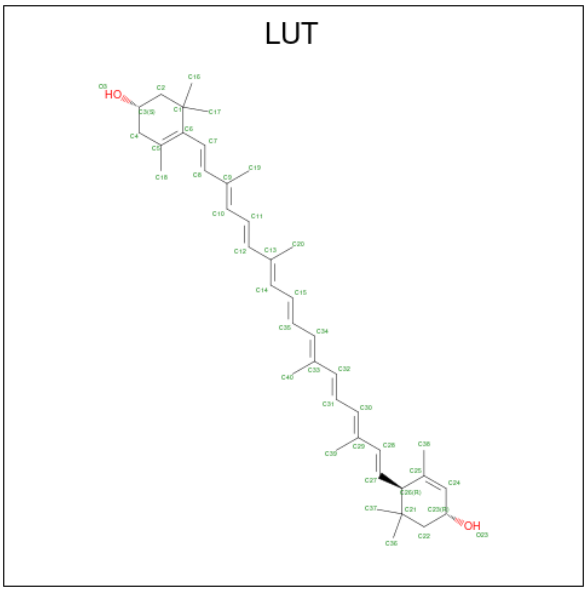

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 27 | A | 1 | Total<br>117 | C<br>38 | H<br>69 | O<br>10 | 0 |
| 27 | A | 1 | Total<br>78 | C<br>26 | H<br>42 | O<br>10 | 0 |
| 27 | B | 1 | Total<br>99 | C<br>33 | H<br>56 | O<br>10 | 0 |
| 27 | B | 1 | Total<br>78 | C<br>26 | H<br>42 | O<br>10 | 0 |
| 27 | J | 1 | Total<br>99 | C<br>32 | H<br>57 | O<br>10 | 0 |
| 27 | J | 1 | Total<br>75 | C<br>25 | H<br>40 | O<br>10 | 0 |
| 27 | 1 | 1 | Total<br>78 | C<br>26 | H<br>42 | O<br>10 | 0 |
| 27 | 1 | 1 | Total<br>96 | C<br>32 | H<br>54 | O<br>10 | 0 |
| 27 | 3 | 1 | Total<br>120 | C<br>40 | H<br>75 | O<br>5 | 0 |
| 27 | 7 | 1 | Total<br>81 | C<br>27 | H<br>44 | O<br>10 | 0 |
| 27 | 8 | 1 | Total<br>66 | C<br>22 | H<br>34 | O<br>10 | 0 |
| 27 | 8 | 1 | Total<br>99 | C<br>32 | H<br>57 | O<br>10 | 0 |
| 27 | 4 | 1 | Total<br>96 | C<br>31 | H<br>55 | O<br>10 | 0 |
| 27 | 6 | 1 | Total<br>55 | C<br>18 | H<br>35 | O<br>2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 27 | 9 | 1 | Total | C | H | O | 0 |
| | | | 105 | 34 | 61 | 10 | |
| 27 | A2 | 1 | Total | C | H | O | 0 |
| | | | 117 | 38 | 69 | 10 | |
| 27 | A2 | 1 | Total | C | H | O | 0 |
| | | | 78 | 26 | 42 | 10 | |
| 27 | B2 | 1 | Total | C | H | O | 0 |
| | | | 99 | 33 | 56 | 10 | |
| 27 | B2 | 1 | Total | C | H | O | 0 |
| | | | 78 | 26 | 42 | 10 | |
| 27 | J2 | 1 | Total | C | H | O | 0 |
| | | | 99 | 32 | 57 | 10 | |
| 27 | J2 | 1 | Total | C | H | O | 0 |
| | | | 75 | 25 | 40 | 10 | |
| 27 | 12 | 1 | Total | C | H | O | 0 |
| | | | 78 | 26 | 42 | 10 | |
| 27 | 12 | 1 | Total | C | H | O | 0 |
| | | | 96 | 32 | 54 | 10 | |
| 27 | 32 | 1 | Total | C | H | O | 0 |
| | | | 120 | 40 | 75 | 5 | |
| 27 | 72 | 1 | Total | C | H | O | 0 |
| | | | 81 | 27 | 44 | 10 | |
| 27 | 82 | 1 | Total | C | H | O | 0 |
| | | | 66 | 22 | 34 | 10 | |
| 27 | 82 | 1 | Total | C | H | O | 0 |
| | | | 99 | 32 | 57 | 10 | |
| 27 | 42 | 1 | Total | C | H | O | 0 |
| | | | 96 | 31 | 55 | 10 | |
| 27 | 62 | 1 | Total | C | H | O | 0 |
| | | | 55 | 18 | 35 | 2 | |
| 27 | 92 | 1 | Total | C | H | O | 0 |
| | | | 105 | 34 | 61 | 10 | |

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 28 | A | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | F | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 1 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 1 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 3 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 3 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 3 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 7 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 7 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 8 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | Z | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | Z | 1 | Total | C | H | O | 0 |
| | | | 59 | 25 | 33 | 1 | |
| 28 | 4 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 5 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |

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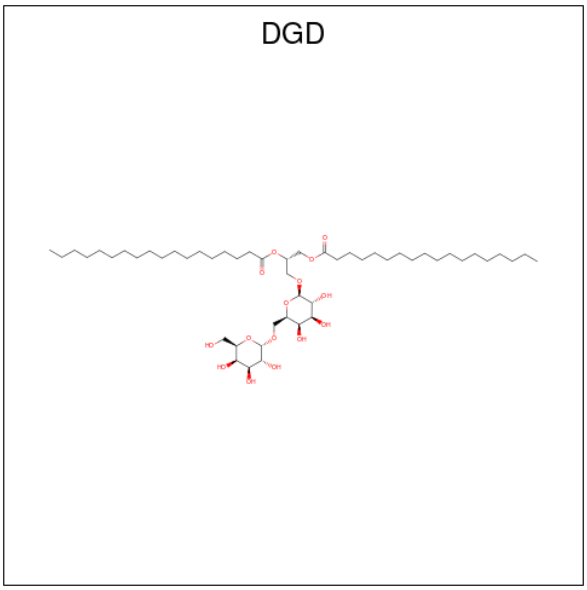
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 28 | 5 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 6 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 9 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 9 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | A2 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | F2 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 12 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 12 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 32 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 32 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 32 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 72 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 72 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 82 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | Z2 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | Z2 | 1 | Total | C | H | O | 0 |
| | | | 59 | 25 | 33 | 1 | |
| 28 | 42 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 52 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 52 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 62 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |
| 28 | 92 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |

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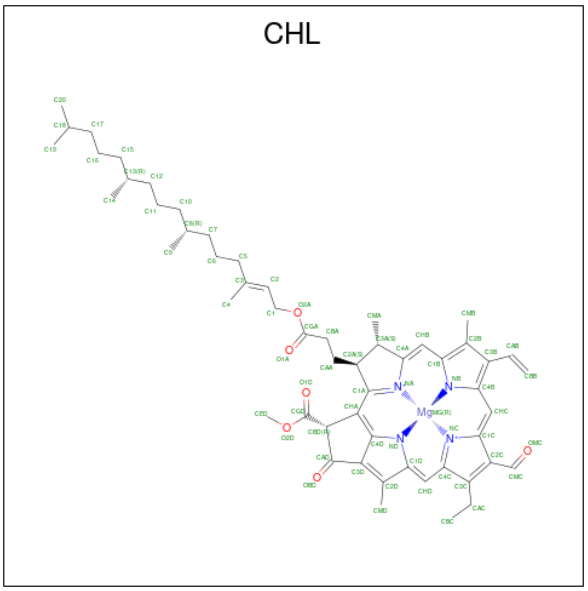
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 28 | 92 | 1 | Total | C | H | O | 0 |
| | | | 98 | 40 | 56 | 2 | |

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 29 | B | 1 | Total | C | H | O | 0 |
| | | | 138 | 44 | 79 | 15 | |
| 29 | B2 | 1 | Total | C | H | O | 0 |
| | | | 138 | 44 | 79 | 15 | |

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 1 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 3 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 7 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 8 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | Z | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 103 | 45 | 47 | 1 | 4 | 6 | |
| 30 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 4 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 88 | 40 | 37 | 1 | 4 | 6 | |
| 30 | 5 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 72 | 34 | 29 | 1 | 4 | 4 | |
| 30 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 109 | 47 | 51 | 1 | 4 | 6 | |
| 30 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 88 | 40 | 37 | 1 | 4 | 6 | |
| 30 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 6 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 72 | 34 | 29 | 1 | 4 | 4 | |
| 30 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 69 | 33 | 27 | 1 | 4 | 4 | |
| 30 | 9 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 88 | 40 | 37 | 1 | 4 | 6 | |
| 30 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 12 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 32 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |

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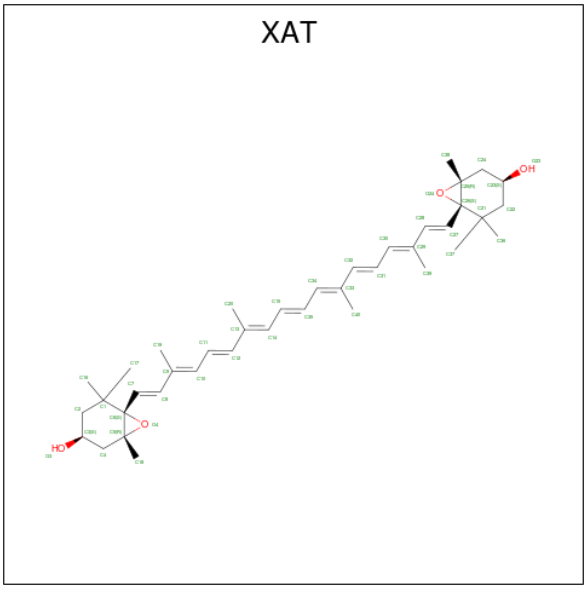
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 72 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 82 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | Z2 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 103 | 45 | 47 | 1 | 4 | 6 | |
| 30 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 42 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 77 | 35 | 31 | 1 | 4 | 6 | |
| 30 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 88 | 40 | 37 | 1 | 4 | 6 | |
| 30 | 52 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 72 | 34 | 29 | 1 | 4 | 4 | |
| 30 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 109 | 47 | 51 | 1 | 4 | 6 | |
| 30 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 88 | 40 | 37 | 1 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 30 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 136 | 55 | 70 | 1 | 4 | 6 | |
| 30 | 62 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 72 | 34 | 29 | 1 | 4 | 4 | |
| 30 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 69 | 33 | 27 | 1 | 4 | 4 | |
| 30 | 92 | 1 | Total | C | H | Mg | N | O | 0 |
| | | | 88 | 40 | 37 | 1 | 4 | 6 | |

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



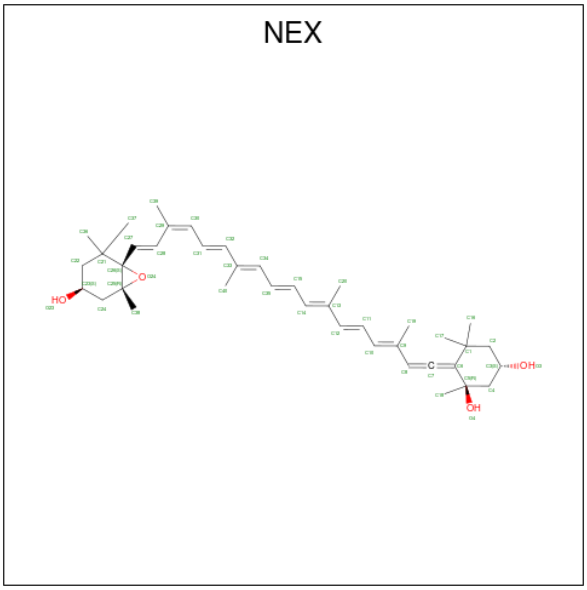

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 31 | 1 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 7 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 8 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | Z | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 4 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 5 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 31 | 6 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 12 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 72 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 82 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | Z2 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 42 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 52 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 31 | 62 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |

- Molecule 32 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 32 | 5 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 32 | 6 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 32 | 52 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |
| 32 | 62 | 1 | Total | C | H | O | 0 |
| | | | 100 | 40 | 56 | 4 | |

- Molecule 33 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 33 | H | 10 | Total | O | 0 |
| | | | 10 | 10 | |
| 33 | H | 19 | Total | O | 0 |
| | | | 19 | 19 | |
| 33 | H | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 33 | H | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 33 | H | 4 | Total | O | 0 |
| | | | 4 | 4 | |
| 33 | H | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 33 | H | 1 | Total | O | 0 |
| | | | 1 | 1 | |
| 33 | H | 7 | Total | O | 0 |
| | | | 7 | 7 | |
| 33 | H | 6 | Total | O | 0 |
| | | | 6 | 6 | |
| 33 | H | 6 | Total | O | 0 |
| | | | 6 | 6 | |
| 33 | H | 6 | Total | O | 0 |
| | | | 6 | 6 | |
| 33 | H | 5 | Total | O | 0 |
| | | | 5 | 5 | |
| 33 | H | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 33 | H | 5 | Total | O | 0 |
| | | | 5 | 5 | |
| 33 | H | 5 | Total | O | 0 |
| | | | 5 | 5 | |
| 33 | H | 1 | Total | O | 0 |
| | | | 1 | 1 | |

*Continued on next page...*

*Continued from previous page...*

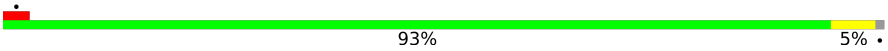
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 33 | H | 11 | Total O<br>11 11 | 0 |
| 33 | H | 18 | Total O<br>18 18 | 0 |
| 33 | H | 1 | Total O<br>1 1 | 0 |
| 33 | H | 1 | Total O<br>1 1 | 0 |
| 33 | H | 4 | Total O<br>4 4 | 0 |
| 33 | H | 1 | Total O<br>1 1 | 0 |
| 33 | H | 1 | Total O<br>1 1 | 0 |
| 33 | H | 7 | Total O<br>7 7 | 0 |
| 33 | H | 5 | Total O<br>5 5 | 0 |
| 33 | H | 6 | Total O<br>6 6 | 0 |
| 33 | H | 5 | Total O<br>5 5 | 0 |
| 33 | H | 5 | Total O<br>5 5 | 0 |
| 33 | H | 3 | Total O<br>3 3 | 0 |
| 33 | H | 5 | Total O<br>5 5 | 0 |
| 33 | H | 5 | Total O<br>5 5 | 0 |
| 33 | H | 1 | Total O<br>1 1 | 0 |

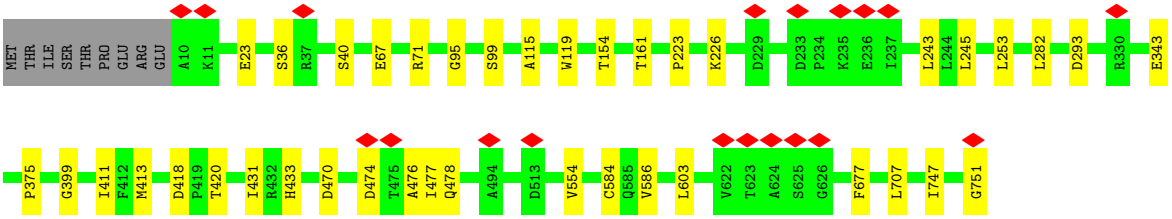
# 3 Residue-property plots (i)

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

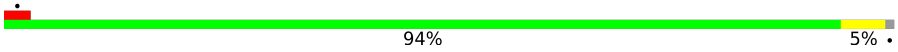
Chain A:

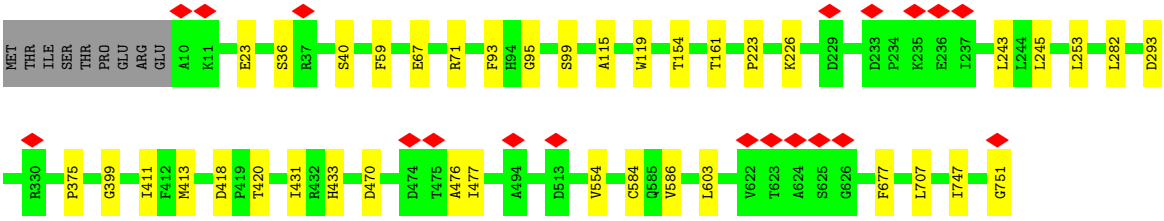



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

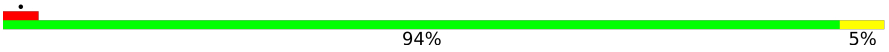
Chain A2:

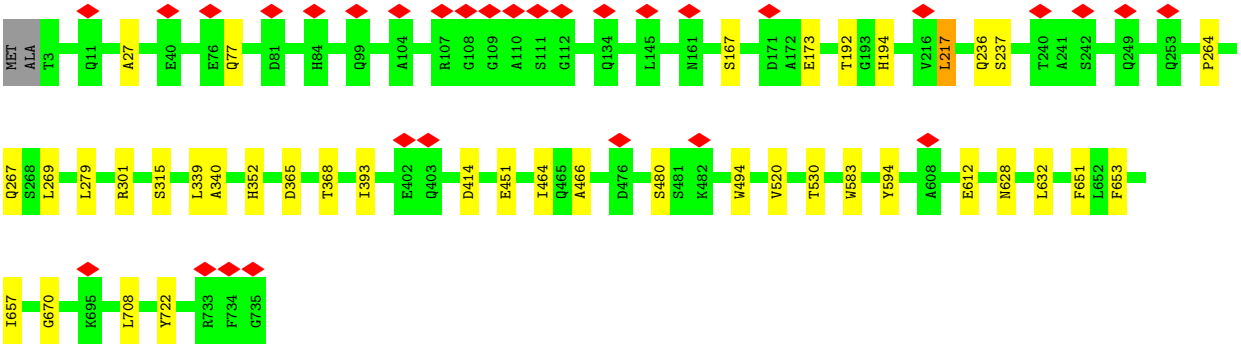



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

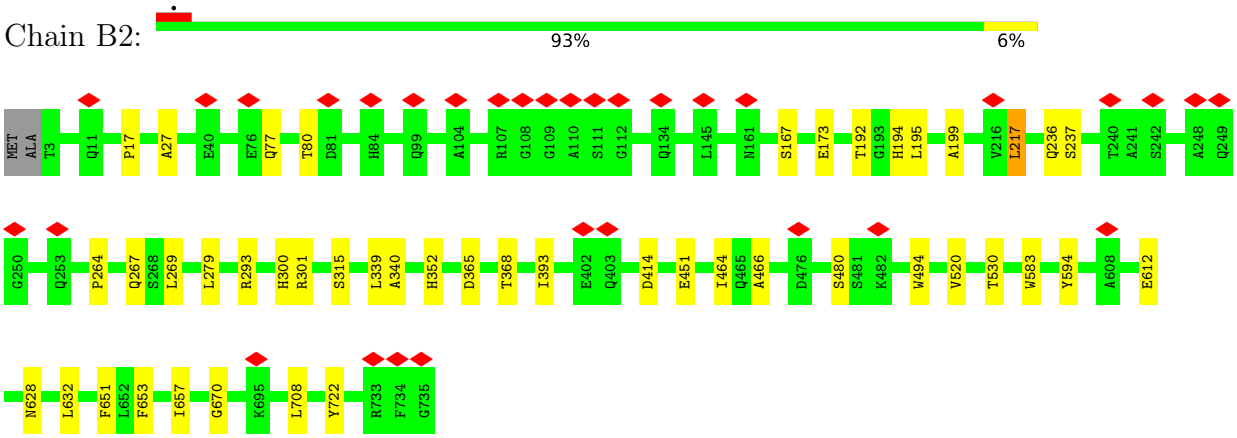
Chain B:



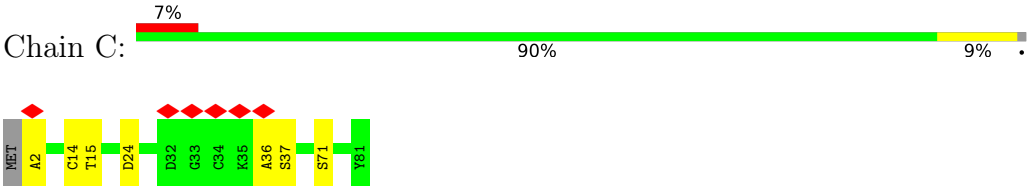
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B2:



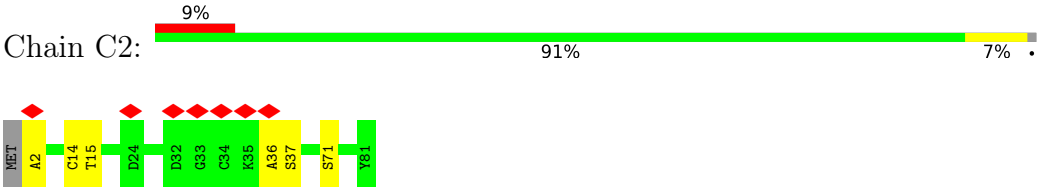

• Molecule 3: Photosystem I iron-sulfur center

Chain C:



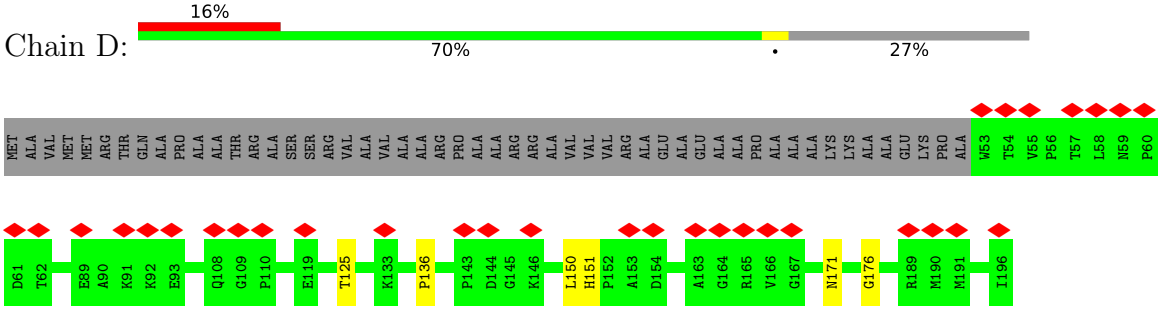

• Molecule 3: Photosystem I iron-sulfur center

Chain C2:



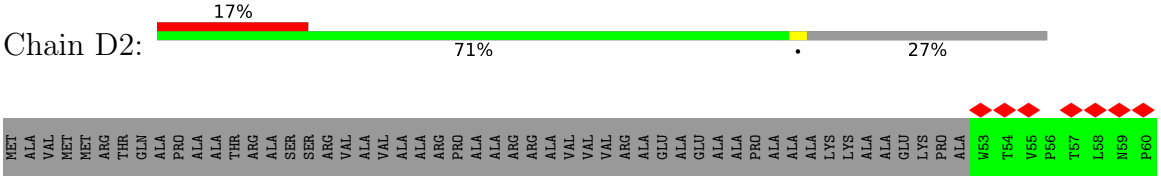

• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

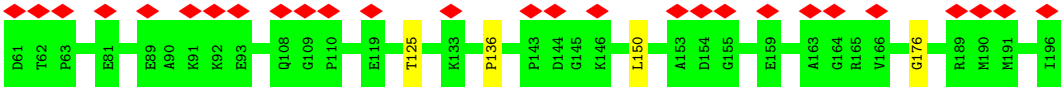
Chain D:




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

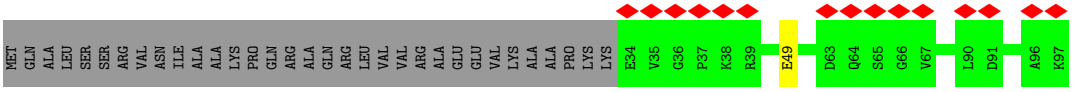
Chain D2:





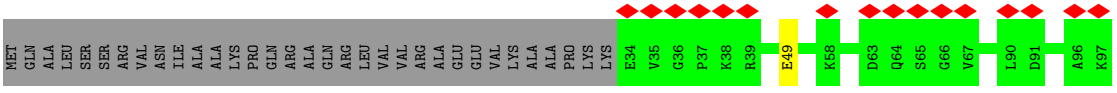

• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



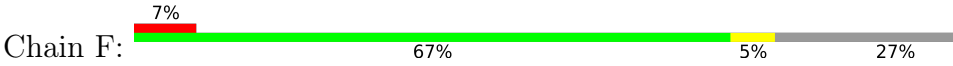



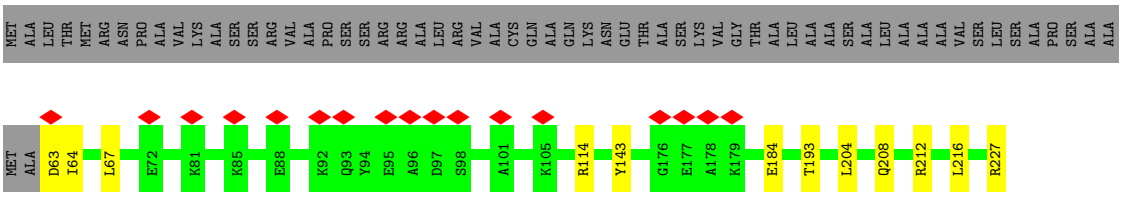

• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



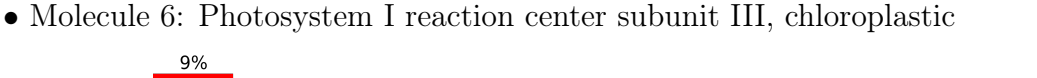



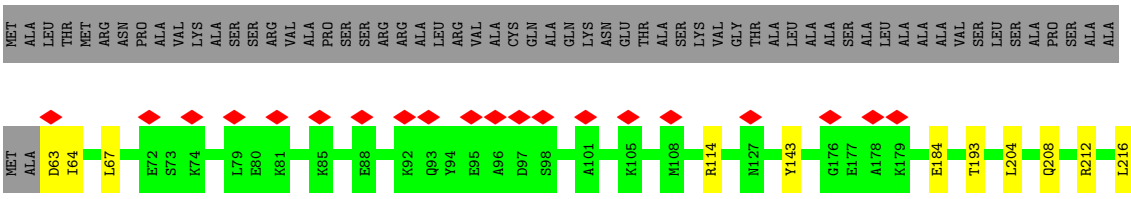

• Molecule 6: Photosystem I reaction center subunit III, chloroplastic



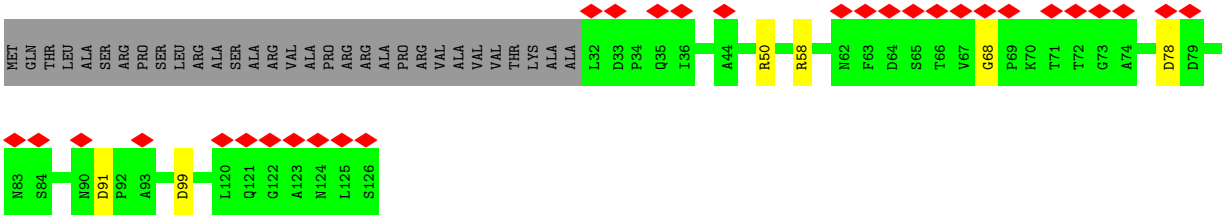

• Molecule 6: Photosystem I reaction center subunit III, chloroplastic



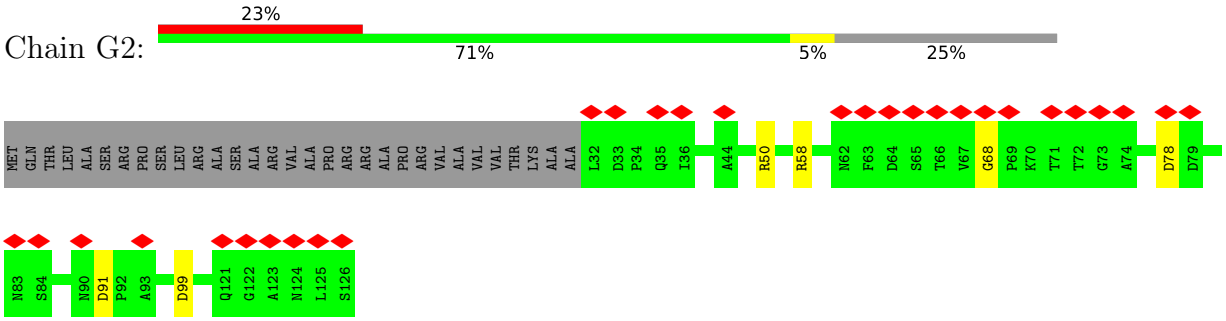

• Molecule 7: Photosystem I reaction center subunit V, chloroplastic



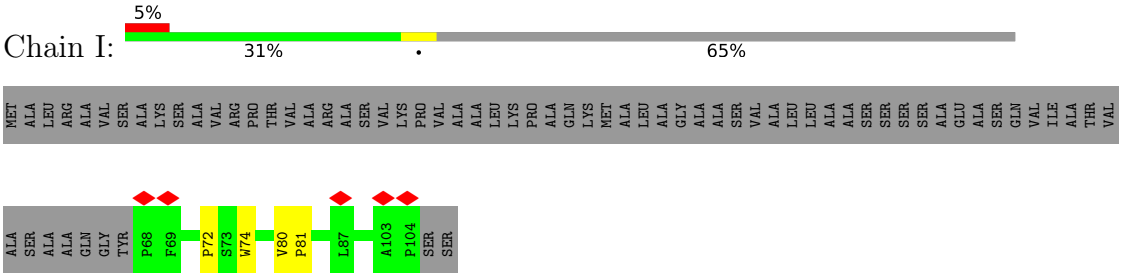
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G2:



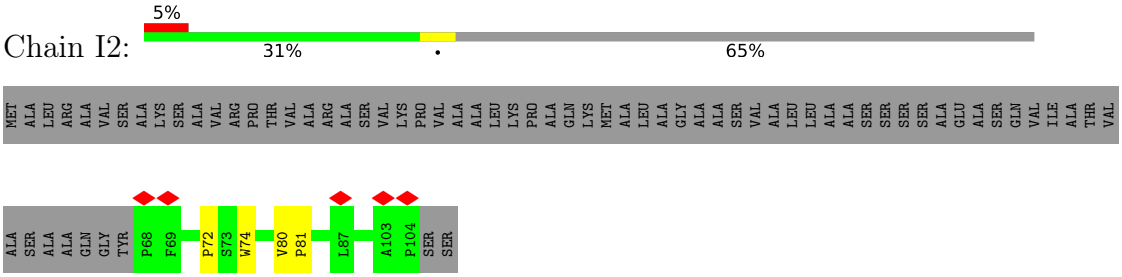

• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



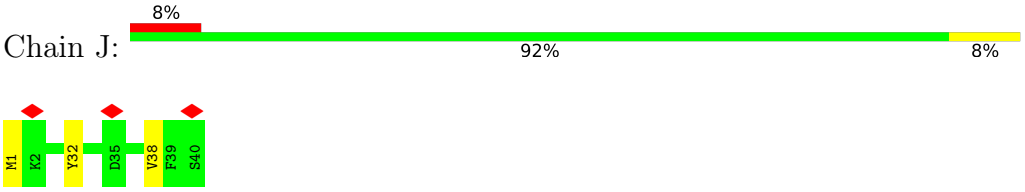

• Molecule 8: Photosystem I reaction center subunit VIII

Chain I2:



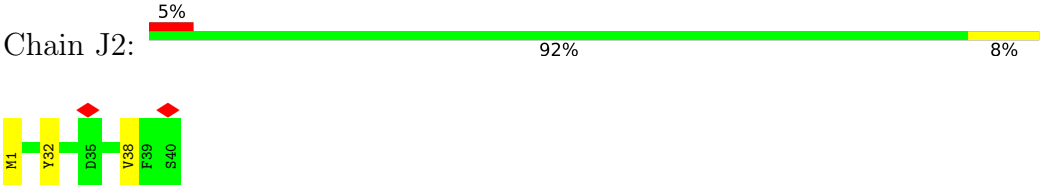

• Molecule 9: Photosystem I reaction center subunit IX

Chain J:




• Molecule 9: Photosystem I reaction center subunit IX

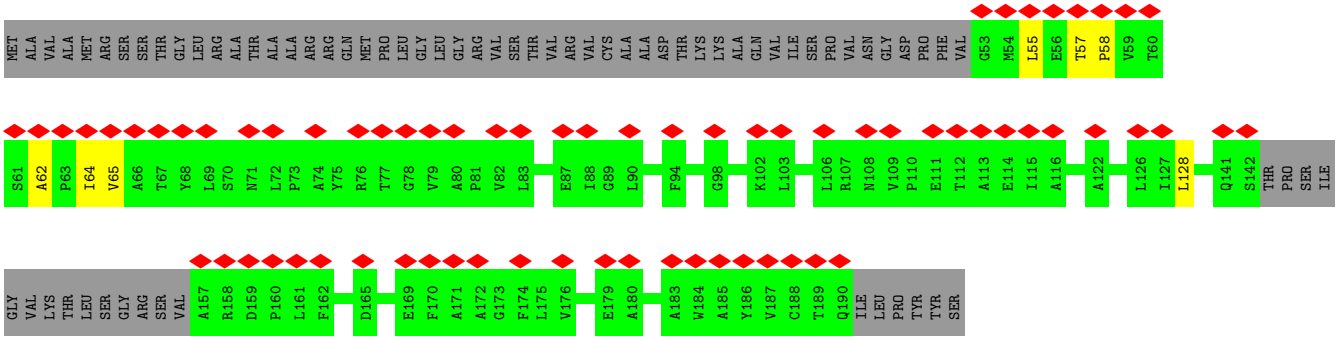
Chain J2:




• Molecule 10: PSI subunit V

Chain L:

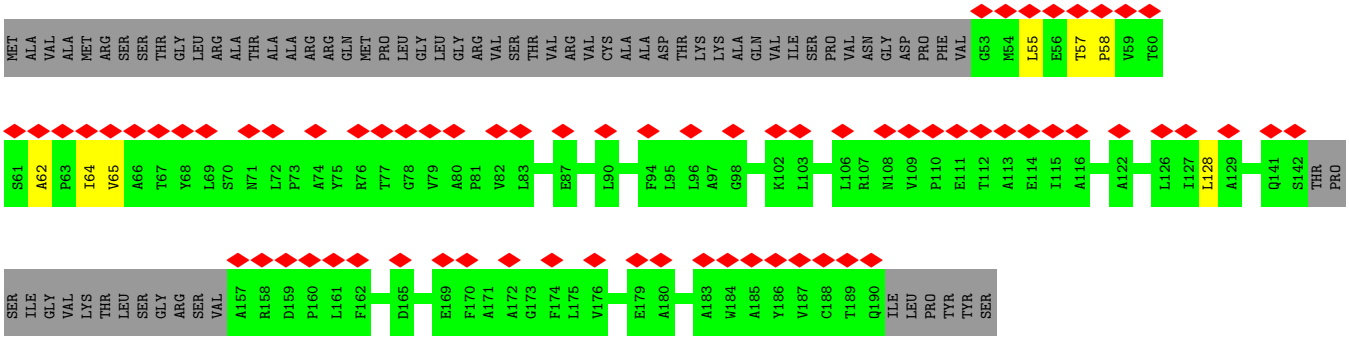





• Molecule 10: PSI subunit V

Chain L2:

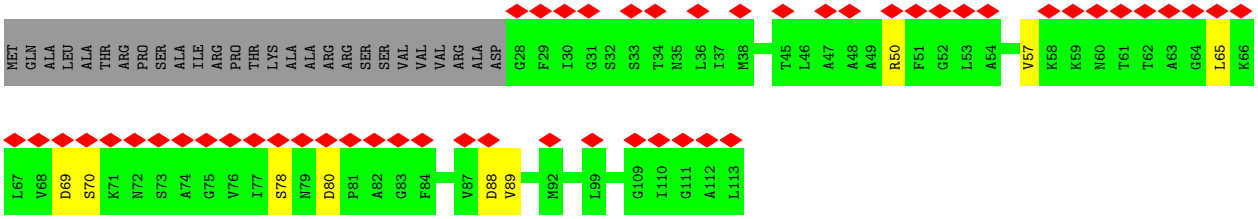



• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:

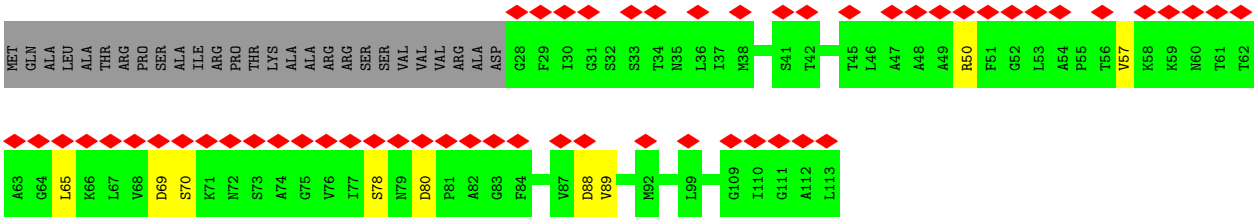



• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K2:

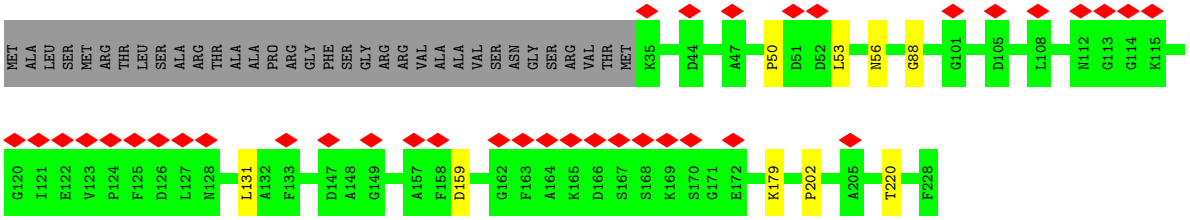



• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

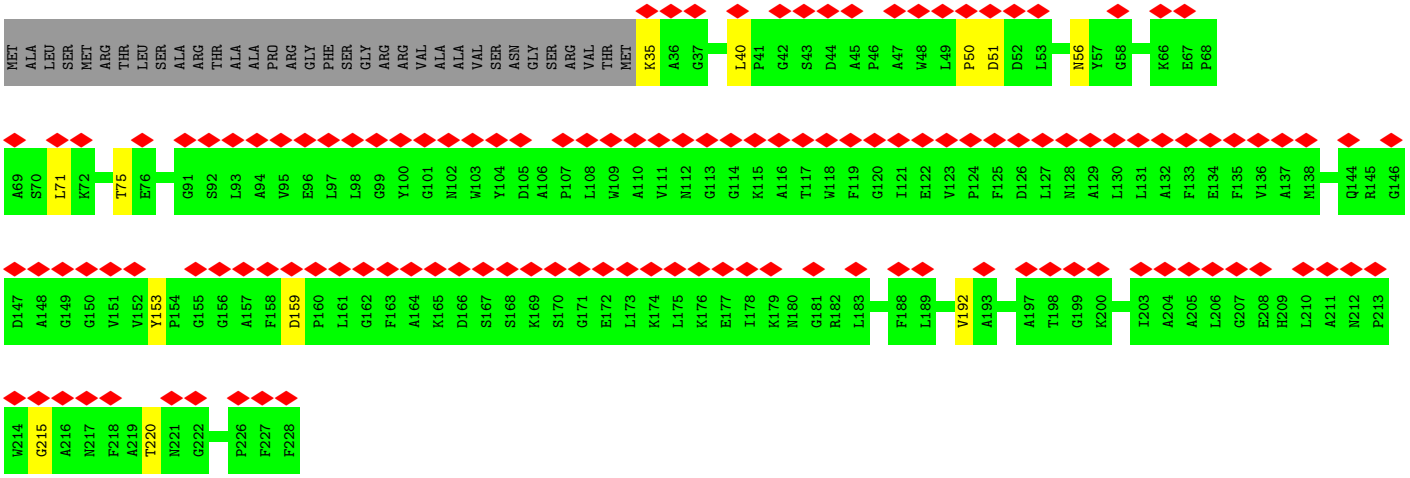



• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:

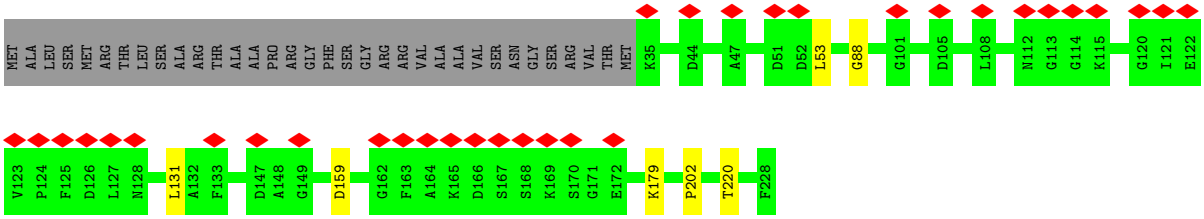



• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 12:

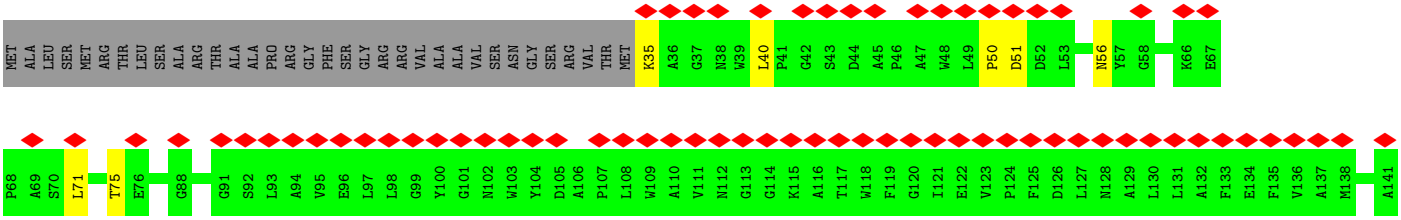



• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z2:



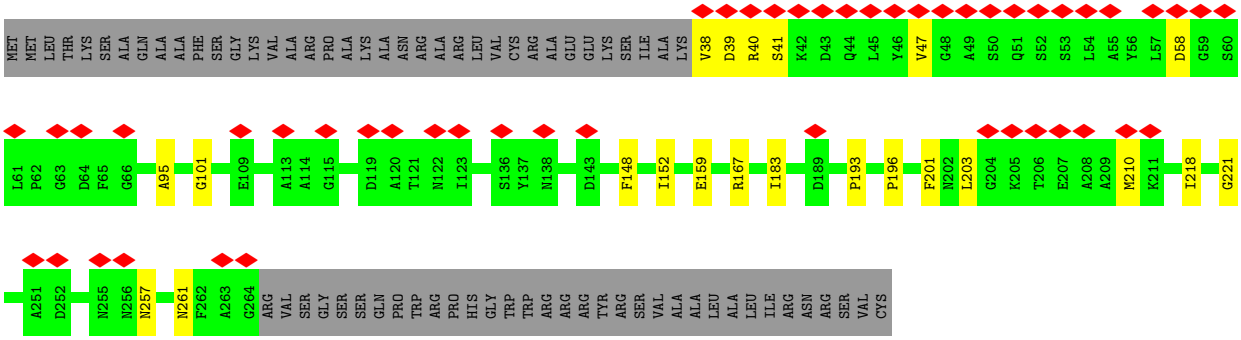






• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

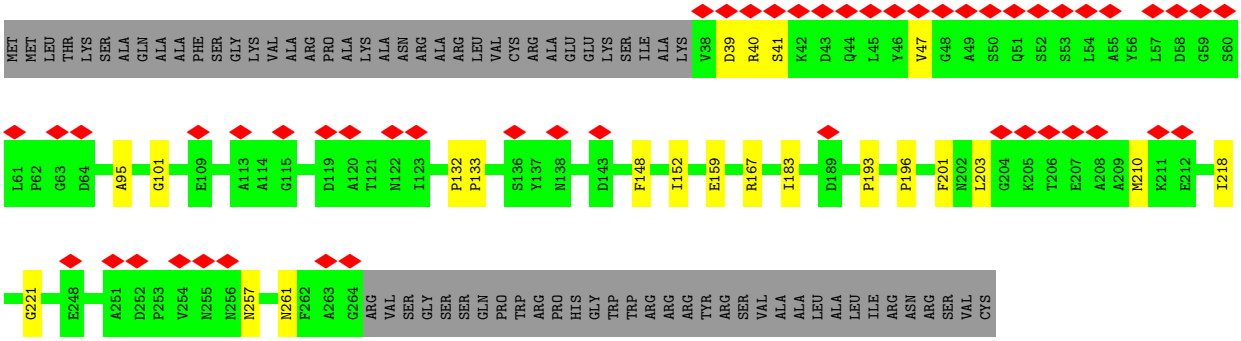



• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 32:

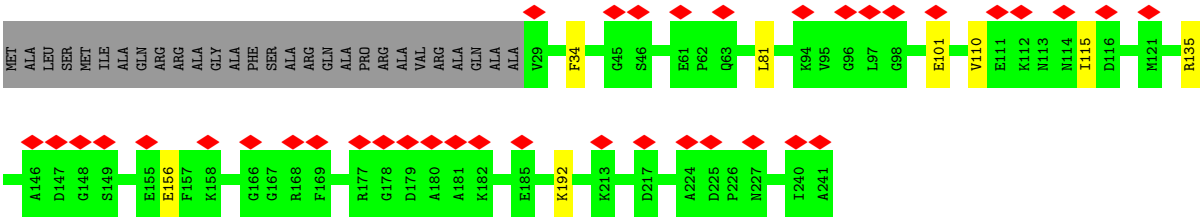



• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

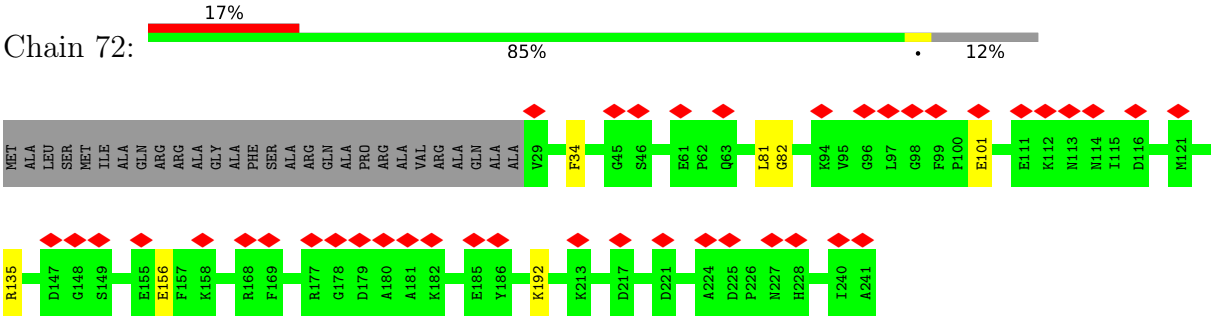
Chain 7:



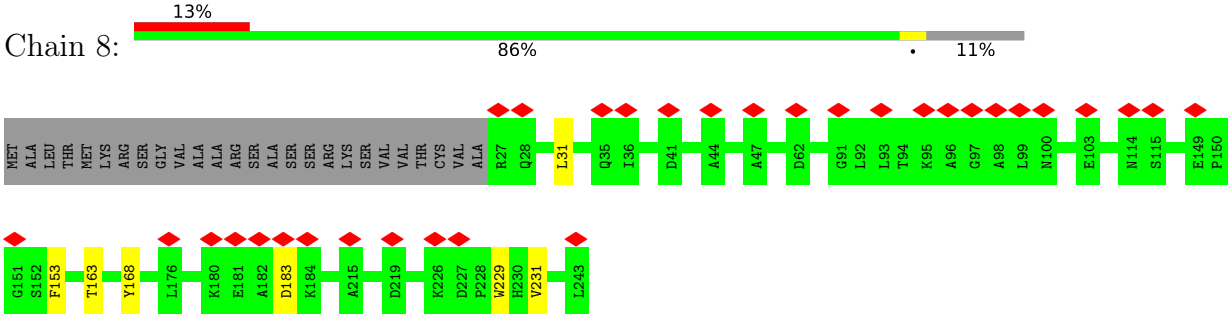

• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 72:



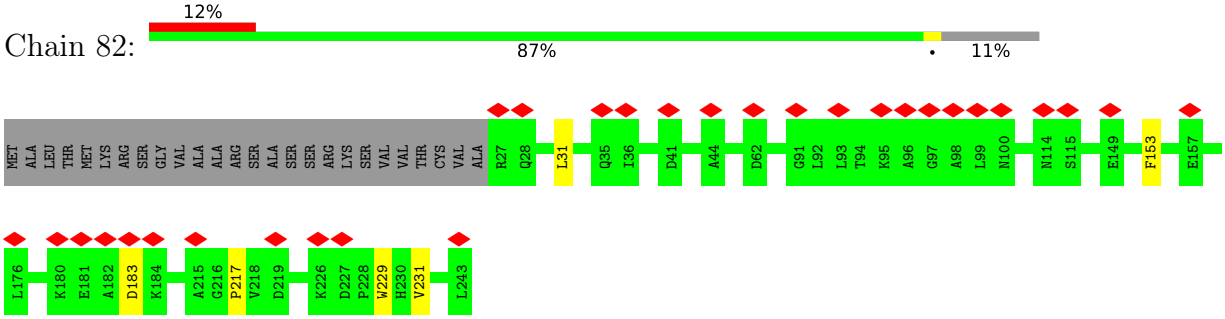

• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



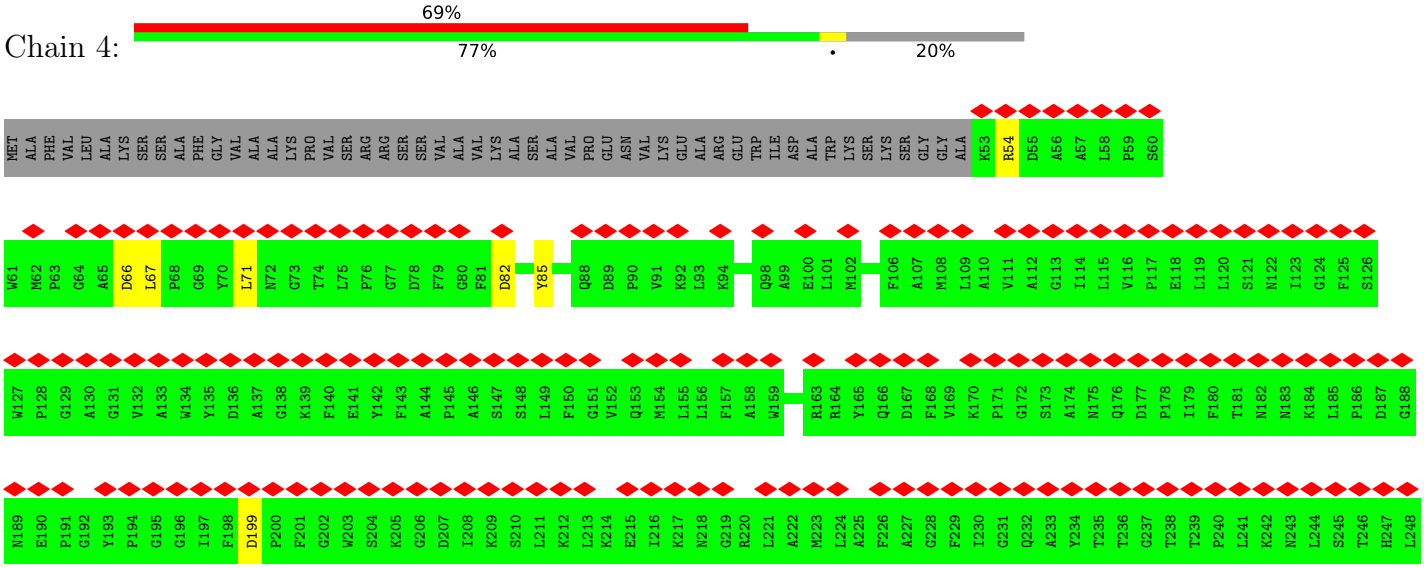

• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

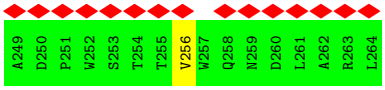
Chain 82:




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)

Chain 4:

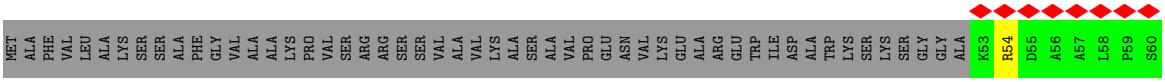


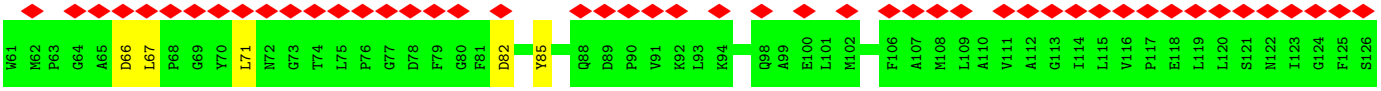


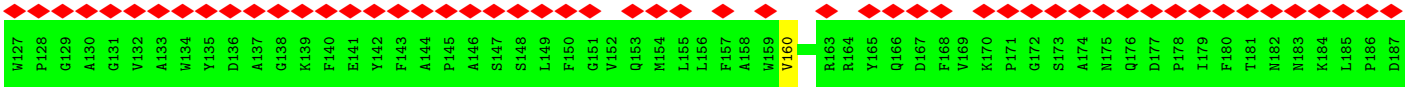

• Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)

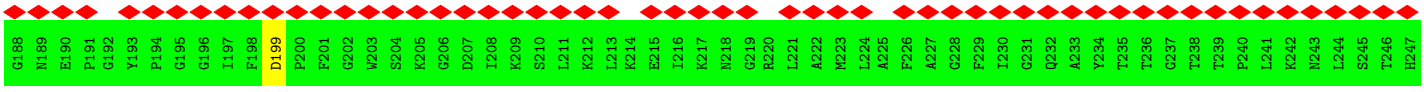
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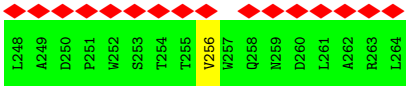


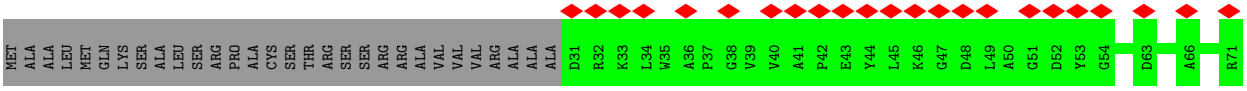



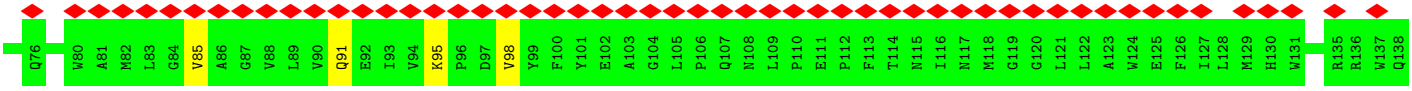



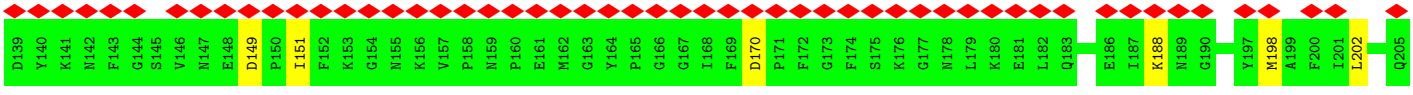

• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

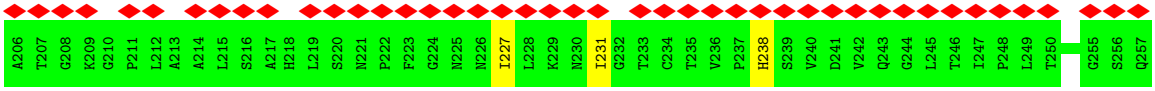
Chain 5:



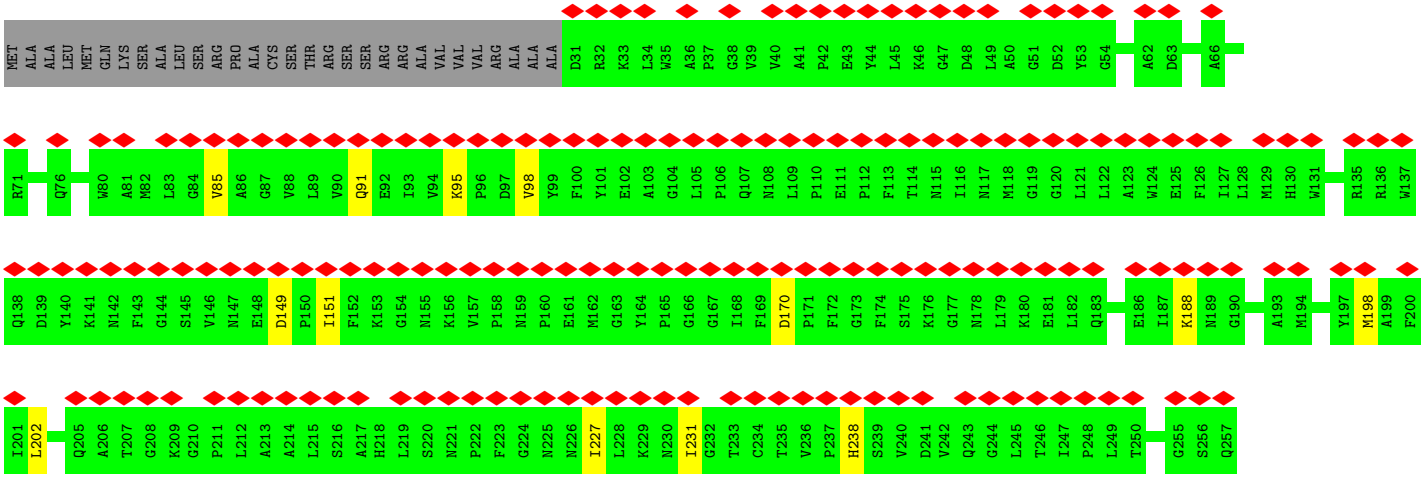




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 52:

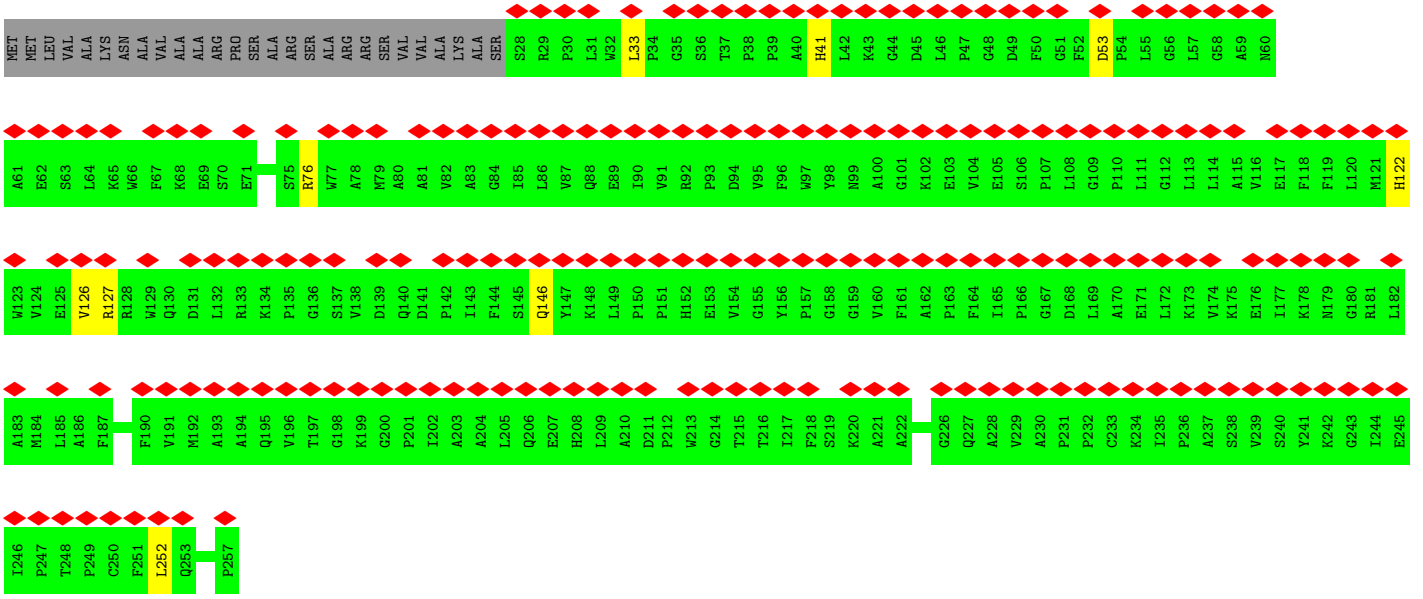





• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

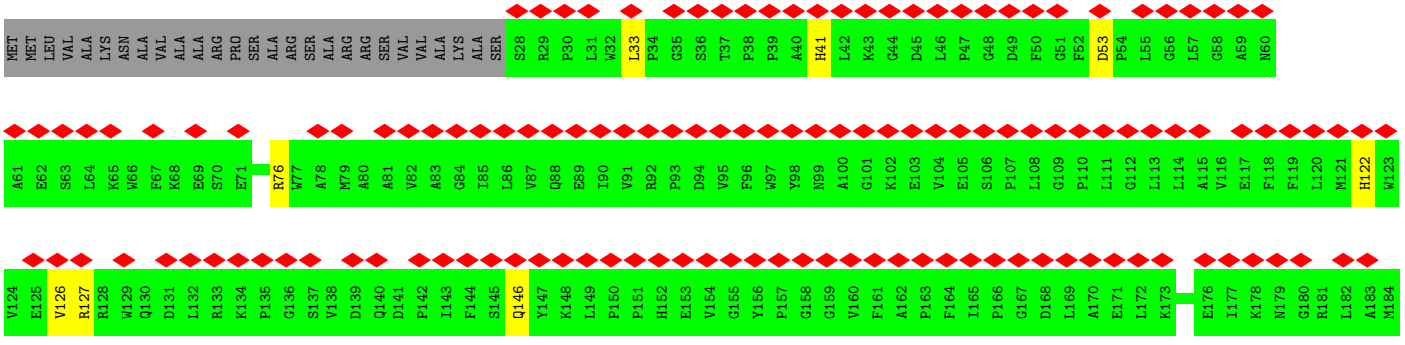



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 62:



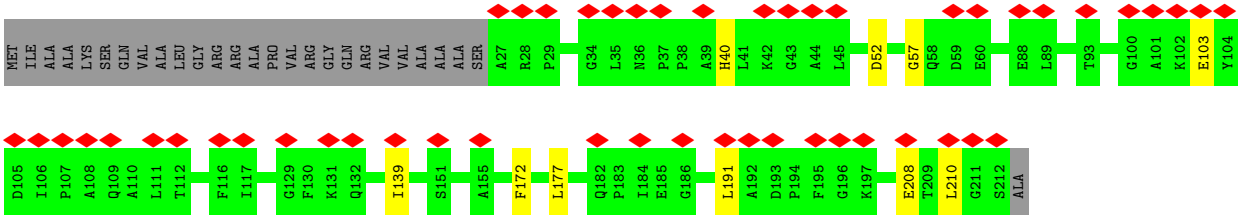






• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 9:

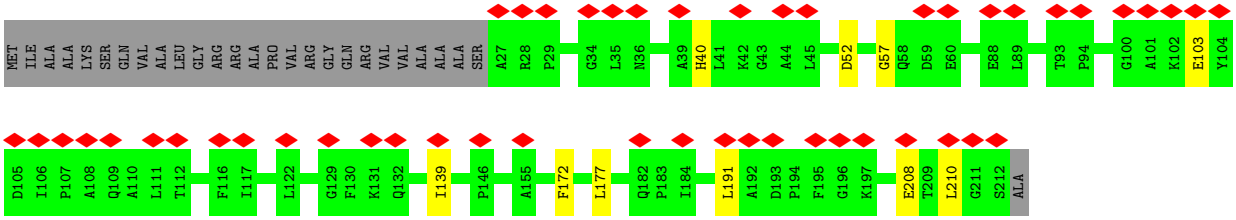



• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 92:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 17439 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 45.8 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 5000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.183 | Depositor |
| Minimum map value | -0.090 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.036 | Depositor |
| Map size (Å) | 588.0, 588.0, 588.0 | wwPDB |
| Map dimensions | 700, 700, 700 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.84, 0.84, 0.84 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, CLA, SF4, LMU, DGD, PQN, NEX, LMG, AME, LUT, XAT, BCR, CHL, LHG

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 | 0.14 | 0/6021 | 0.22 | 0/8208 |
| 1 | A2 | 0.15 | 0/6021 | 0.23 | 0/8208 |
| 2 | B | 0.15 | 0/6036 | 0.23 | 0/8240 |
| 2 | B2 | 0.15 | 0/6036 | 0.22 | 0/8240 |
| 3 | C | 0.14 | 0/611 | 0.28 | 0/826 |
| 3 | C2 | 0.14 | 0/611 | 0.27 | 0/826 |
| 4 | D | 0.13 | 0/1161 | 0.24 | 0/1567 |
| 4 | D2 | 0.13 | 0/1161 | 0.24 | 0/1567 |
| 5 | E | 0.13 | 0/516 | 0.18 | 0/700 |
| 5 | E2 | 0.13 | 0/516 | 0.18 | 0/700 |
| 6 | F | 0.13 | 0/1292 | 0.21 | 0/1747 |
| 6 | F2 | 0.13 | 0/1292 | 0.21 | 0/1747 |
| 7 | G | 0.12 | 0/721 | 0.19 | 0/980 |
| 7 | G2 | 0.12 | 0/721 | 0.19 | 0/980 |
| 8 | I | 0.13 | 0/293 | 0.26 | 0/406 |
| 8 | I2 | 0.13 | 0/293 | 0.26 | 0/406 |
| 9 | J | 0.14 | 0/329 | 0.22 | 0/452 |
| 9 | J2 | 0.14 | 0/329 | 0.22 | 0/452 |
| 10 | L | 0.12 | 0/920 | 0.19 | 0/1257 |
| 10 | L2 | 0.12 | 0/920 | 0.19 | 0/1257 |
| 11 | K | 0.13 | 0/588 | 0.17 | 0/795 |
| 11 | K2 | 0.13 | 0/588 | 0.17 | 0/795 |
| 12 | 1 | 0.12 | 0/1491 | 0.20 | 0/2028 |
| 12 | 12 | 0.12 | 0/1491 | 0.20 | 0/2028 |
| 12 | Z | 0.09 | 0/1491 | 0.18 | 0/2028 |
| 12 | Z2 | 0.10 | 0/1491 | 0.18 | 0/2028 |
| 13 | 3 | 0.12 | 0/1784 | 0.23 | 0/2420 |
| 13 | 32 | 0.12 | 0/1784 | 0.23 | 0/2420 |
| 14 | 7 | 0.12 | 0/1702 | 0.20 | 0/2310 |
| 14 | 72 | 0.12 | 0/1702 | 0.20 | 0/2310 |
| 15 | 8 | 0.12 | 0/1701 | 0.21 | 0/2315 |
| 15 | 82 | 0.12 | 0/1701 | 0.20 | 0/2315 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 16 | 4 | 0.09 | 0/1703 | 0.19 | 0/2321 |
| 16 | 42 | 0.09 | 0/1703 | 0.19 | 0/2321 |
| 17 | 5 | 0.09 | 0/1830 | 0.21 | 0/2492 |
| 17 | 52 | 0.09 | 0/1830 | 0.21 | 0/2492 |
| 18 | 6 | 0.09 | 0/1834 | 0.20 | 0/2505 |
| 18 | 62 | 0.09 | 0/1834 | 0.20 | 0/2505 |
| 19 | 9 | 0.12 | 0/1461 | 0.20 | 0/1987 |
| 19 | 92 | 0.12 | 0/1461 | 0.21 | 0/1987 |
| All | All | 0.13 | 0/66970 | 0.21 | 0/91168 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5825 | 5675 | 5675 | 27 | 0 |
| 1 | A2 | 5825 | 5675 | 5675 | 25 | 0 |
| 2 | B | 5824 | 5576 | 5577 | 35 | 0 |
| 2 | B2 | 5824 | 5576 | 5577 | 38 | 0 |
| 3 | C | 601 | 582 | 581 | 4 | 0 |
| 3 | C2 | 601 | 582 | 581 | 3 | 0 |
| 4 | D | 1133 | 1151 | 1150 | 4 | 0 |
| 4 | D2 | 1133 | 1151 | 1150 | 2 | 0 |
| 5 | E | 506 | 505 | 504 | 1 | 0 |
| 5 | E2 | 506 | 505 | 504 | 1 | 0 |
| 6 | F | 1266 | 1302 | 1301 | 10 | 0 |
| 6 | F2 | 1266 | 1302 | 1301 | 9 | 0 |
| 7 | G | 706 | 687 | 686 | 4 | 0 |
| 7 | G2 | 706 | 687 | 686 | 4 | 0 |
| 8 | I | 281 | 292 | 292 | 3 | 0 |
| 8 | I2 | 281 | 292 | 292 | 3 | 0 |
| 9 | J | 329 | 328 | 328 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 9 | J2 | 329 | 328 | 328 | 1 | 0 |
| 10 | L | 899 | 907 | 905 | 7 | 0 |
| 10 | L2 | 899 | 907 | 905 | 8 | 0 |
| 11 | K | 583 | 620 | 620 | 6 | 0 |
| 11 | K2 | 583 | 620 | 620 | 6 | 0 |
| 12 | 1 | 1445 | 1397 | 1396 | 8 | 0 |
| 12 | 12 | 1445 | 1397 | 1396 | 7 | 0 |
| 12 | Z | 1445 | 1397 | 1396 | 9 | 0 |
| 12 | Z2 | 1445 | 1397 | 1396 | 9 | 0 |
| 13 | 3 | 1736 | 1695 | 1694 | 15 | 0 |
| 13 | 32 | 1736 | 1695 | 1694 | 15 | 0 |
| 14 | 7 | 1650 | 1590 | 1589 | 8 | 0 |
| 14 | 72 | 1650 | 1590 | 1589 | 8 | 0 |
| 15 | 8 | 1650 | 1630 | 1629 | 6 | 0 |
| 15 | 82 | 1650 | 1630 | 1629 | 6 | 0 |
| 16 | 4 | 1648 | 1603 | 1602 | 6 | 0 |
| 16 | 42 | 1648 | 1603 | 1602 | 7 | 0 |
| 17 | 5 | 1775 | 1747 | 1746 | 11 | 0 |
| 17 | 52 | 1775 | 1747 | 1746 | 11 | 0 |
| 18 | 6 | 1772 | 1770 | 1770 | 9 | 0 |
| 18 | 62 | 1772 | 1770 | 1770 | 9 | 0 |
| 19 | 9 | 1420 | 1400 | 1399 | 9 | 0 |
| 19 | 92 | 1420 | 1400 | 1399 | 9 | 0 |
| 20 | A | 65 | 72 | 72 | 0 | 0 |
| 20 | A2 | 65 | 72 | 72 | 0 | 0 |
| 21 | 1 | 639 | 625 | 625 | 5 | 0 |
| 21 | 12 | 639 | 625 | 625 | 5 | 0 |
| 21 | 3 | 740 | 718 | 718 | 12 | 0 |
| 21 | 32 | 740 | 718 | 718 | 14 | 0 |
| 21 | 4 | 565 | 534 | 534 | 3 | 0 |
| 21 | 42 | 565 | 534 | 534 | 4 | 0 |
| 21 | 5 | 740 | 712 | 712 | 9 | 0 |
| 21 | 52 | 740 | 712 | 712 | 9 | 0 |
| 21 | 6 | 628 | 605 | 605 | 2 | 0 |
| 21 | 62 | 628 | 605 | 605 | 2 | 0 |
| 21 | 7 | 652 | 598 | 598 | 5 | 0 |
| 21 | 72 | 652 | 598 | 598 | 5 | 0 |
| 21 | 8 | 614 | 578 | 578 | 4 | 0 |
| 21 | 82 | 614 | 578 | 578 | 3 | 0 |
| 21 | 9 | 565 | 535 | 535 | 1 | 0 |
| 21 | 92 | 565 | 535 | 535 | 1 | 0 |
| 21 | A | 2718 | 2856 | 2856 | 26 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 21 | A2 | 2718 | 2856 | 2856 | 26 | 0 |
| 21 | B | 2463 | 2580 | 2580 | 28 | 0 |
| 21 | B2 | 2463 | 2580 | 2580 | 29 | 0 |
| 21 | F | 175 | 177 | 177 | 1 | 0 |
| 21 | F2 | 175 | 177 | 177 | 1 | 0 |
| 21 | G | 106 | 92 | 92 | 0 | 0 |
| 21 | G2 | 106 | 92 | 92 | 0 | 0 |
| 21 | J | 55 | 49 | 49 | 1 | 0 |
| 21 | J2 | 55 | 49 | 49 | 1 | 0 |
| 21 | K | 196 | 158 | 158 | 2 | 0 |
| 21 | K2 | 196 | 158 | 158 | 2 | 0 |
| 21 | L | 110 | 105 | 105 | 1 | 0 |
| 21 | L2 | 110 | 105 | 105 | 0 | 0 |
| 21 | Z | 627 | 593 | 593 | 7 | 0 |
| 21 | Z2 | 627 | 593 | 593 | 9 | 0 |
| 22 | A | 33 | 46 | 46 | 0 | 0 |
| 22 | A2 | 33 | 46 | 46 | 0 | 0 |
| 22 | B | 33 | 46 | 46 | 0 | 0 |
| 22 | B2 | 33 | 46 | 46 | 0 | 0 |
| 23 | 1 | 39 | 48 | 48 | 1 | 0 |
| 23 | 12 | 39 | 48 | 48 | 1 | 0 |
| 23 | 3 | 78 | 99 | 99 | 1 | 0 |
| 23 | 32 | 78 | 99 | 99 | 1 | 0 |
| 23 | 4 | 87 | 123 | 123 | 1 | 0 |
| 23 | 42 | 87 | 123 | 123 | 1 | 0 |
| 23 | 5 | 37 | 44 | 44 | 1 | 0 |
| 23 | 52 | 37 | 44 | 44 | 1 | 0 |
| 23 | 6 | 85 | 116 | 116 | 0 | 0 |
| 23 | 62 | 85 | 116 | 116 | 0 | 0 |
| 23 | 7 | 49 | 74 | 74 | 1 | 0 |
| 23 | 72 | 49 | 74 | 74 | 1 | 0 |
| 23 | 8 | 44 | 61 | 61 | 0 | 0 |
| 23 | 82 | 44 | 61 | 61 | 0 | 0 |
| 23 | 9 | 41 | 55 | 55 | 0 | 0 |
| 23 | 92 | 41 | 55 | 55 | 0 | 0 |
| 23 | A | 87 | 123 | 123 | 0 | 0 |
| 23 | A2 | 87 | 123 | 123 | 0 | 0 |
| 23 | B | 45 | 63 | 63 | 0 | 0 |
| 23 | B2 | 45 | 63 | 63 | 0 | 0 |
| 23 | Z | 39 | 48 | 48 | 0 | 0 |
| 23 | Z2 | 39 | 48 | 48 | 1 | 0 |
| 24 | 3 | 120 | 168 | 168 | 7 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 24 | 32 | 120 | 168 | 168 | 4 | 0 |
| 24 | 4 | 40 | 56 | 56 | 0 | 0 |
| 24 | 42 | 40 | 56 | 56 | 1 | 0 |
| 24 | 5 | 40 | 56 | 56 | 0 | 0 |
| 24 | 52 | 40 | 56 | 56 | 0 | 0 |
| 24 | 6 | 40 | 56 | 56 | 2 | 0 |
| 24 | 62 | 40 | 56 | 56 | 1 | 0 |
| 24 | 7 | 40 | 56 | 56 | 0 | 0 |
| 24 | 72 | 40 | 56 | 56 | 0 | 0 |
| 24 | 8 | 40 | 56 | 56 | 2 | 0 |
| 24 | 82 | 40 | 56 | 56 | 2 | 0 |
| 24 | 9 | 40 | 56 | 56 | 1 | 0 |
| 24 | 92 | 40 | 56 | 56 | 2 | 0 |
| 24 | A | 200 | 280 | 280 | 12 | 0 |
| 24 | A2 | 200 | 280 | 280 | 9 | 0 |
| 24 | B | 280 | 392 | 392 | 11 | 0 |
| 24 | B2 | 280 | 392 | 392 | 11 | 0 |
| 24 | G | 40 | 56 | 56 | 0 | 0 |
| 24 | G2 | 40 | 56 | 56 | 2 | 0 |
| 24 | I | 40 | 56 | 56 | 1 | 0 |
| 24 | I2 | 40 | 56 | 56 | 1 | 0 |
| 24 | J | 40 | 56 | 56 | 1 | 0 |
| 24 | J2 | 40 | 56 | 56 | 1 | 0 |
| 24 | K | 80 | 112 | 112 | 5 | 0 |
| 24 | K2 | 80 | 112 | 112 | 6 | 0 |
| 24 | L | 80 | 112 | 112 | 5 | 0 |
| 24 | L2 | 80 | 112 | 112 | 5 | 0 |
| 25 | A | 8 | 0 | 0 | 0 | 0 |
| 25 | A2 | 8 | 0 | 0 | 0 | 0 |
| 25 | C | 16 | 0 | 0 | 0 | 0 |
| 25 | C2 | 16 | 0 | 0 | 0 | 0 |
| 26 | 1 | 148 | 201 | 201 | 0 | 0 |
| 26 | 12 | 148 | 201 | 201 | 0 | 0 |
| 26 | 4 | 53 | 63 | 63 | 1 | 0 |
| 26 | 42 | 53 | 63 | 63 | 1 | 0 |
| 26 | 5 | 24 | 35 | 35 | 0 | 0 |
| 26 | 52 | 24 | 35 | 35 | 0 | 0 |
| 26 | 6 | 92 | 129 | 129 | 0 | 0 |
| 26 | 62 | 92 | 129 | 129 | 0 | 0 |
| 26 | 7 | 81 | 92 | 92 | 1 | 0 |
| 26 | 72 | 81 | 92 | 92 | 1 | 0 |
| 26 | 8 | 107 | 151 | 151 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 26 | 82 | 107 | 151 | 151 | 0 | 0 |
| 26 | 9 | 24 | 35 | 35 | 1 | 0 |
| 26 | 92 | 24 | 35 | 35 | 1 | 0 |
| 26 | A | 196 | 262 | 262 | 5 | 0 |
| 26 | A2 | 196 | 262 | 262 | 2 | 0 |
| 26 | B | 35 | 46 | 46 | 3 | 0 |
| 26 | B2 | 35 | 46 | 46 | 2 | 0 |
| 26 | G | 24 | 35 | 35 | 0 | 0 |
| 26 | G2 | 24 | 35 | 35 | 0 | 0 |
| 26 | K | 24 | 35 | 35 | 0 | 0 |
| 26 | K2 | 24 | 35 | 35 | 0 | 0 |
| 26 | Z | 53 | 63 | 63 | 1 | 0 |
| 26 | Z2 | 53 | 63 | 63 | 1 | 0 |
| 27 | 1 | 78 | 96 | 96 | 0 | 0 |
| 27 | 12 | 78 | 96 | 96 | 0 | 0 |
| 27 | 3 | 45 | 75 | 75 | 1 | 0 |
| 27 | 32 | 45 | 75 | 75 | 1 | 0 |
| 27 | 4 | 41 | 55 | 55 | 0 | 0 |
| 27 | 42 | 41 | 55 | 55 | 0 | 0 |
| 27 | 6 | 20 | 35 | 35 | 0 | 0 |
| 27 | 62 | 20 | 35 | 35 | 0 | 0 |
| 27 | 7 | 37 | 44 | 44 | 0 | 0 |
| 27 | 72 | 37 | 44 | 44 | 0 | 0 |
| 27 | 8 | 74 | 91 | 91 | 1 | 0 |
| 27 | 82 | 74 | 91 | 91 | 0 | 0 |
| 27 | 9 | 44 | 61 | 61 | 1 | 0 |
| 27 | 92 | 44 | 61 | 61 | 1 | 0 |
| 27 | A | 84 | 111 | 111 | 1 | 0 |
| 27 | A2 | 84 | 111 | 111 | 1 | 0 |
| 27 | B | 79 | 98 | 98 | 1 | 0 |
| 27 | B2 | 79 | 98 | 98 | 1 | 0 |
| 27 | J | 77 | 97 | 97 | 2 | 0 |
| 27 | J2 | 77 | 97 | 97 | 2 | 0 |
| 28 | 1 | 84 | 112 | 112 | 2 | 0 |
| 28 | 12 | 84 | 112 | 112 | 2 | 0 |
| 28 | 3 | 126 | 168 | 168 | 2 | 0 |
| 28 | 32 | 126 | 168 | 168 | 2 | 0 |
| 28 | 4 | 42 | 56 | 56 | 1 | 0 |
| 28 | 42 | 42 | 56 | 56 | 1 | 0 |
| 28 | 5 | 84 | 112 | 112 | 3 | 0 |
| 28 | 52 | 84 | 112 | 112 | 3 | 0 |
| 28 | 6 | 42 | 56 | 56 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 28 | 62 | 42 | 56 | 56 | 1 | 0 |
| 28 | 7 | 84 | 112 | 112 | 4 | 0 |
| 28 | 72 | 84 | 112 | 112 | 4 | 0 |
| 28 | 8 | 42 | 56 | 56 | 0 | 0 |
| 28 | 82 | 42 | 56 | 56 | 1 | 0 |
| 28 | 9 | 84 | 112 | 112 | 3 | 0 |
| 28 | 92 | 84 | 112 | 112 | 3 | 0 |
| 28 | A | 42 | 56 | 56 | 1 | 0 |
| 28 | A2 | 42 | 56 | 56 | 2 | 0 |
| 28 | F | 42 | 56 | 56 | 3 | 0 |
| 28 | F2 | 42 | 56 | 56 | 2 | 0 |
| 28 | Z | 68 | 89 | 89 | 2 | 0 |
| 28 | Z2 | 68 | 89 | 89 | 2 | 0 |
| 29 | B | 59 | 79 | 79 | 1 | 0 |
| 29 | B2 | 59 | 79 | 79 | 1 | 0 |
| 30 | 1 | 158 | 132 | 132 | 1 | 0 |
| 30 | 12 | 158 | 132 | 132 | 0 | 0 |
| 30 | 3 | 66 | 70 | 70 | 2 | 0 |
| 30 | 32 | 66 | 70 | 70 | 3 | 0 |
| 30 | 4 | 300 | 288 | 288 | 4 | 0 |
| 30 | 42 | 300 | 288 | 288 | 2 | 0 |
| 30 | 5 | 206 | 167 | 167 | 1 | 0 |
| 30 | 52 | 206 | 167 | 167 | 1 | 0 |
| 30 | 6 | 350 | 327 | 327 | 7 | 0 |
| 30 | 62 | 350 | 327 | 327 | 7 | 0 |
| 30 | 7 | 158 | 132 | 132 | 3 | 0 |
| 30 | 72 | 158 | 132 | 132 | 2 | 0 |
| 30 | 8 | 198 | 210 | 210 | 2 | 0 |
| 30 | 82 | 198 | 210 | 210 | 2 | 0 |
| 30 | 9 | 93 | 64 | 64 | 0 | 0 |
| 30 | 92 | 93 | 64 | 64 | 0 | 0 |
| 30 | Z | 178 | 171 | 171 | 1 | 0 |
| 30 | Z2 | 178 | 171 | 171 | 1 | 0 |
| 31 | 1 | 44 | 56 | 56 | 1 | 0 |
| 31 | 12 | 44 | 56 | 56 | 1 | 0 |
| 31 | 4 | 44 | 56 | 56 | 0 | 0 |
| 31 | 42 | 44 | 56 | 56 | 0 | 0 |
| 31 | 5 | 44 | 56 | 56 | 0 | 0 |
| 31 | 52 | 44 | 56 | 56 | 0 | 0 |
| 31 | 6 | 44 | 56 | 56 | 1 | 0 |
| 31 | 62 | 44 | 56 | 56 | 1 | 0 |
| 31 | 7 | 44 | 56 | 56 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 31 | 72 | 44 | 56 | 56 | 1 | 0 |
| 31 | 8 | 44 | 56 | 56 | 0 | 0 |
| 31 | 82 | 44 | 56 | 56 | 0 | 0 |
| 31 | Z | 44 | 56 | 56 | 0 | 0 |
| 31 | Z2 | 44 | 56 | 56 | 0 | 0 |
| 32 | 5 | 44 | 56 | 56 | 0 | 0 |
| 32 | 52 | 44 | 56 | 56 | 0 | 0 |
| 32 | 6 | 44 | 56 | 56 | 1 | 0 |
| 32 | 62 | 44 | 56 | 56 | 1 | 0 |
| 33 | H | 160 | 0 | 0 | 17 | 0 |
| All | All | 100830 | 101988 | 101960 | 579 | 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 3.

All (579) 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) |
|---|---|---|---|
| 28:7:624:LUT:H381 | 28:7:624:LUT:H28 | 1.51 | 0.93 |
| 28:72:624:LUT:H381 | 28:72:624:LUT:H28 | 1.51 | 0.91 |
| 1:A2:95:GLY:O | 1:A2:99:SER:OG | 1.95 | 0.83 |
| 17:5:170:ASP:OD1 | 28:5:620:LUT:O23 | 1.96 | 0.82 |
| 1:A:95:GLY:O | 1:A:99:SER:OG | 1.96 | 0.82 |
| 26:B:853:LMU:H2O1 | 26:B:853:LMU:H6' | 1.22 | 0.82 |
| 17:52:170:ASP:OD1 | 28:52:620:LUT:O23 | 1.96 | 0.82 |
| 2:B2:301:ARG:NH1 | 7:G2:68:GLY:O | 2.14 | 0.80 |
| 4:D:171:ASN:OD1 | 33:H:41:HOH:O | 2.00 | 0.80 |
| 2:B:301:ARG:NH1 | 7:G:68:GLY:O | 2.15 | 0.79 |
| 2:B:167:SER:OG | 7:G:78:ASP:OD1 | 2.00 | 0.78 |
| 2:B2:167:SER:OG | 7:G2:78:ASP:OD1 | 2.00 | 0.78 |
| 2:B:628:ASN:O | 33:H:14:HOH:O | 2.02 | 0.77 |
| 26:A:862:LMU:H2O2 | 26:A:863:LMU:H6B | 1.21 | 0.77 |
| 6:F2:184:GLU:OE1 | 33:H:176:HOH:O | 2.03 | 0.76 |
| 2:B2:628:ASN:O | 33:H:111:HOH:O | 2.03 | 0.76 |
| 7:G2:58:ARG:NH2 | 7:G2:99:ASP:OD2 | 2.19 | 0.76 |
| 7:G:58:ARG:NH2 | 7:G:99:ASP:OD2 | 2.19 | 0.75 |
| 6:F:184:GLU:OE1 | 33:H:88:HOH:O | 2.04 | 0.75 |
| 12:1:179:LYS:NZ | 23:1:620:LHG:O5 | 2.20 | 0.73 |
| 2:B2:269:LEU:O | 33:H:109:HOH:O | 2.05 | 0.73 |
| 1:A:226:LYS:NZ | 1:A:253:LEU:O | 2.21 | 0.73 |
| 1:A2:226:LYS:NZ | 1:A2:253:LEU:O | 2.22 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:12:179:LYS:NZ | 23:12:620:LHG:O5 | 2.21 | 0.72 |
| 30:42:601:CHL:OBD | 18:62:127:ARG:NH1 | 2.23 | 0.72 |
| 28:72:624:LUT:H381 | 28:72:624:LUT:C28 | 2.19 | 0.72 |
| 2:B:269:LEU:O | 33:H:12:HOH:O | 2.05 | 0.72 |
| 13:32:40:ARG:O | 13:32:41:SER:OG | 2.07 | 0.72 |
| 30:4:601:CHL:OBD | 18:6:127:ARG:NH1 | 2.22 | 0.72 |
| 26:72:628:LMU:O6' | 33:H:169:HOH:O | 2.08 | 0.71 |
| 26:7:628:LMU:O6' | 33:H:81:HOH:O | 2.08 | 0.70 |
| 26:B2:853:LMU:O6' | 26:B2:853:LMU:O2B | 1.99 | 0.69 |
| 13:3:40:ARG:O | 13:3:41:SER:OG | 2.06 | 0.69 |
| 28:7:624:LUT:H381 | 28:7:624:LUT:C28 | 2.19 | 0.69 |
| 13:32:159:GLU:OE2 | 33:H:131:HOH:O | 2.12 | 0.68 |
| 2:B:27:ALA:HA | 21:B:829:CLA:H43 | 1.76 | 0.68 |
| 1:A2:23:GLU:OE2 | 27:A2:860:LMG:O5 | 2.06 | 0.67 |
| 1:A:23:GLU:OE2 | 27:A:860:LMG:O5 | 2.07 | 0.66 |
| 2:B2:27:ALA:HA | 21:B2:829:CLA:H43 | 1.77 | 0.66 |
| 13:3:159:GLU:OE2 | 33:H:37:HOH:O | 2.13 | 0.66 |
| 21:A2:803:CLA:HBB1 | 21:A2:803:CLA:HMB1 | 1.78 | 0.66 |
| 21:A2:854:CLA:HMB3 | 21:B2:802:CLA:H193 | 1.78 | 0.65 |
| 30:62:606:CHL:OMC | 33:H:162:HOH:O | 2.15 | 0.65 |
| 13:32:148:PHE:CE2 | 13:32:152:ILE:HD11 | 2.32 | 0.65 |
| 30:8:606:CHL:OMC | 33:H:55:HOH:O | 2.15 | 0.65 |
| 30:6:606:CHL:OMC | 33:H:73:HOH:O | 2.15 | 0.65 |
| 21:A:803:CLA:HMB1 | 21:A:803:CLA:HBB1 | 1.78 | 0.64 |
| 21:A:854:CLA:HMB3 | 21:B:802:CLA:H193 | 1.79 | 0.64 |
| 6:F:63:ASP:N | 6:F:67:LEU:O | 2.30 | 0.64 |
| 2:B2:315:SER:OG | 21:B2:841:CLA:O1A | 2.08 | 0.64 |
| 6:F2:63:ASP:N | 6:F2:67:LEU:O | 2.30 | 0.64 |
| 2:B:315:SER:OG | 21:B:841:CLA:O1A | 2.08 | 0.64 |
| 21:Z2:603:CLA:HED2 | 21:Z2:603:CLA:H43 | 1.80 | 0.64 |
| 13:3:148:PHE:CE2 | 13:3:152:ILE:HD11 | 2.32 | 0.64 |
| 30:82:606:CHL:OMC | 33:H:144:HOH:O | 2.15 | 0.64 |
| 21:Z:616:CLA:H72 | 21:Z:616:CLA:H41 | 1.79 | 0.63 |
| 21:Z:603:CLA:HED2 | 21:Z:603:CLA:H43 | 1.80 | 0.63 |
| 2:B:217:LEU:CD1 | 19:9:210:LEU:HD23 | 2.29 | 0.63 |
| 21:A:811:CLA:H11 | 21:A:813:CLA:H42 | 1.80 | 0.63 |
| 19:9:208:GLU:N | 19:9:208:GLU:OE1 | 2.31 | 0.63 |
| 2:B2:217:LEU:CD1 | 19:92:210:LEU:HD23 | 2.29 | 0.63 |
| 21:Z2:616:CLA:H41 | 21:Z2:616:CLA:C7 | 2.29 | 0.63 |
| 21:Z2:616:CLA:H41 | 21:Z2:616:CLA:H72 | 1.79 | 0.63 |
| 19:92:208:GLU:N | 19:92:208:GLU:OE1 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Z:50:PRO:O | 12:Z:56:ASN:ND2 | 2.32 | 0.62 |
| 21:Z:616:CLA:H41 | 21:Z:616:CLA:C7 | 2.29 | 0.62 |
| 11:K:78:SER:OG | 21:K:201:CLA:O1D | 2.17 | 0.62 |
| 21:A2:811:CLA:H11 | 21:A2:813:CLA:H42 | 1.81 | 0.61 |
| 11:K2:78:SER:OG | 21:K2:201:CLA:O1D | 2.18 | 0.61 |
| 14:7:192:LYS:NZ | 23:7:625:LHG:O5 | 2.34 | 0.60 |
| 21:3:607:CLA:H93 | 24:3:719:BCR:H392 | 1.83 | 0.60 |
| 21:32:607:CLA:H93 | 24:32:719:BCR:H392 | 1.83 | 0.60 |
| 18:6:146:GLN:OE1 | 18:6:146:GLN:N | 2.33 | 0.60 |
| 26:A:862:LMU:O2' | 26:A:863:LMU:O6B | 2.03 | 0.60 |
| 18:62:146:GLN:OE1 | 18:62:146:GLN:N | 2.33 | 0.60 |
| 12:Z:40:LEU:HD13 | 30:Z:601:CHL:HMA3 | 1.83 | 0.59 |
| 18:62:41:HIS:NE2 | 18:62:53:ASP:OD2 | 2.32 | 0.59 |
| 14:72:192:LYS:NZ | 23:72:625:LHG:O5 | 2.34 | 0.59 |
| 12:Z2:50:PRO:O | 12:Z2:56:ASN:ND2 | 2.31 | 0.59 |
| 13:3:257:ASN:O | 13:3:261:ASN:ND2 | 2.36 | 0.59 |
| 21:5:602:CLA:H41 | 21:5:603:CLA:O1A | 2.02 | 0.59 |
| 13:32:167:ARG:NH1 | 27:32:722:LMG:O1 | 2.36 | 0.59 |
| 21:52:602:CLA:H41 | 21:52:603:CLA:O1A | 2.02 | 0.59 |
| 12:Z2:40:LEU:HD13 | 30:Z2:601:CHL:HMA3 | 1.83 | 0.59 |
| 13:3:167:ARG:NH1 | 27:3:722:LMG:O1 | 2.36 | 0.58 |
| 2:B2:708:LEU:HD23 | 29:B2:850:DGD:HA22 | 1.86 | 0.58 |
| 16:4:54:ARG:NH1 | 16:4:71:LEU:O | 2.36 | 0.58 |
| 2:B2:339:LEU:HD21 | 21:B2:829:CLA:HAB | 1.86 | 0.58 |
| 13:32:257:ASN:O | 13:32:261:ASN:ND2 | 2.36 | 0.58 |
| 21:B2:816:CLA:H142 | 21:B2:816:CLA:H101 | 1.86 | 0.58 |
| 16:42:54:ARG:NH1 | 16:42:71:LEU:O | 2.36 | 0.58 |
| 21:12:603:CLA:HED2 | 21:12:603:CLA:H43 | 1.85 | 0.58 |
| 2:B:339:LEU:HD21 | 21:B:829:CLA:HAB | 1.86 | 0.58 |
| 1:A:161:THR:HG21 | 21:A:817:CLA:HBA1 | 1.85 | 0.57 |
| 18:6:41:HIS:NE2 | 18:6:53:ASP:OD2 | 2.32 | 0.57 |
| 21:B:816:CLA:H101 | 21:B:816:CLA:H142 | 1.86 | 0.57 |
| 21:1:603:CLA:HED2 | 21:1:603:CLA:H43 | 1.84 | 0.57 |
| 21:7:620:CLA:O1A | 18:6:252:LEU:N | 2.38 | 0.57 |
| 21:A2:840:CLA:O1A | 21:A2:840:CLA:H42 | 2.04 | 0.57 |
| 12:12:159:ASP:OD1 | 28:12:617:LUT:O23 | 2.23 | 0.57 |
| 26:B:853:LMU:O2B | 26:B:853:LMU:O6' | 1.99 | 0.57 |
| 14:72:156:GLU:N | 14:72:156:GLU:OE1 | 2.38 | 0.57 |
| 12:1:220:THR:O | 12:1:220:THR:HG22 | 2.05 | 0.57 |
| 21:5:621:CLA:HED2 | 21:5:621:CLA:O1A | 2.05 | 0.57 |
| 21:A:840:CLA:H42 | 21:A:840:CLA:O1A | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A2:161:THR:HG21 | 21:A2:817:CLA:HBA1 | 1.85 | 0.56 |
| 21:Z2:603:CLA:H43 | 21:Z2:603:CLA:CED | 2.36 | 0.56 |
| 21:72:620:CLA:O1A | 18:62:252:LEU:N | 2.38 | 0.56 |
| 21:A2:829:CLA:HMB1 | 21:A2:829:CLA:HBB1 | 1.87 | 0.56 |
| 12:12:220:THR:HG22 | 12:12:220:THR:O | 2.05 | 0.56 |
| 21:12:613:CLA:H143 | 21:12:613:CLA:H102 | 1.87 | 0.56 |
| 21:52:621:CLA:HED2 | 21:52:621:CLA:O1A | 2.05 | 0.56 |
| 24:A:851:BCR:H23C | 24:A:851:BCR:H403 | 1.88 | 0.56 |
| 12:1:53:LEU:HD23 | 21:1:602:CLA:HED2 | 1.87 | 0.56 |
| 14:7:156:GLU:N | 14:7:156:GLU:OE1 | 2.38 | 0.56 |
| 24:A2:851:BCR:H403 | 24:A2:851:BCR:H23C | 1.88 | 0.56 |
| 11:K:89:VAL:HG22 | 21:K:201:CLA:HMD2 | 1.88 | 0.55 |
| 21:1:613:CLA:H102 | 21:1:613:CLA:H143 | 1.86 | 0.55 |
| 14:7:101:GLU:N | 14:7:101:GLU:OE1 | 2.39 | 0.55 |
| 21:A:829:CLA:HBB1 | 21:A:829:CLA:HMB1 | 1.87 | 0.55 |
| 11:K2:89:VAL:HG22 | 21:K2:201:CLA:HMD2 | 1.88 | 0.55 |
| 2:B:393:ILE:HD13 | 21:B:829:CLA:HED1 | 1.89 | 0.55 |
| 21:Z:603:CLA:H43 | 21:Z:603:CLA:CED | 2.35 | 0.55 |
| 14:72:101:GLU:OE1 | 14:72:101:GLU:N | 2.39 | 0.55 |
| 26:9:624:LMU:O5' | 8:I2:74:TRP:CZ2 | 2.60 | 0.55 |
| 12:12:53:LEU:HD23 | 21:12:602:CLA:HED2 | 1.87 | 0.55 |
| 16:4:256:VAL:N | 21:4:613:CLA:O1A | 2.39 | 0.55 |
| 21:A2:833:CLA:OBD | 10:L2:57:THR:HG21 | 2.07 | 0.55 |
| 6:F2:204:LEU:HA | 21:82:603:CLA:H42 | 1.89 | 0.55 |
| 4:D:125:THR:HG23 | 4:D:136:PRO:HG2 | 1.89 | 0.55 |
| 13:3:95:ALA:HB1 | 13:3:221:GLY:HA3 | 1.89 | 0.55 |
| 18:62:76:ARG:NH1 | 30:62:608:CHL:OBD | 2.37 | 0.55 |
| 28:7:624:LUT:H383 | 15:8:229:TRP:CE2 | 2.42 | 0.54 |
| 2:B2:393:ILE:HD13 | 21:B2:829:CLA:HED1 | 1.89 | 0.54 |
| 8:I:74:TRP:CZ2 | 26:92:624:LMU:O5' | 2.60 | 0.54 |
| 21:1:603:CLA:H43 | 21:1:603:CLA:CED | 2.38 | 0.54 |
| 28:72:624:LUT:H383 | 15:82:229:TRP:CE2 | 2.42 | 0.54 |
| 16:42:256:VAL:N | 21:42:613:CLA:O1A | 2.39 | 0.54 |
| 12:1:159:ASP:OD1 | 28:1:617:LUT:O23 | 2.23 | 0.54 |
| 21:3:615:CLA:H193 | 17:5:227:ILE:HG21 | 1.89 | 0.54 |
| 24:L2:205:BCR:C23 | 24:L2:205:BCR:H403 | 2.38 | 0.54 |
| 6:F:204:LEU:HA | 21:8:603:CLA:H42 | 1.89 | 0.54 |
| 21:A:833:CLA:OBD | 10:L:57:THR:HG21 | 2.07 | 0.54 |
| 2:B2:653:PHE:CZ | 2:B2:657:ILE:HD11 | 2.43 | 0.54 |
| 13:32:95:ALA:HB1 | 13:32:221:GLY:HA3 | 1.89 | 0.54 |
| 24:L:205:BCR:C23 | 24:L:205:BCR:H403 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:208:GLN:OE1 | 6:F:212:ARG:NH2 | 2.42 | 0.53 |
| 4:D2:125:THR:HG23 | 4:D2:136:PRO:HG2 | 1.89 | 0.53 |
| 2:B:464:ILE:HD11 | 21:B:836:CLA:H12 | 1.90 | 0.53 |
| 21:32:615:CLA:H193 | 17:52:227:ILE:HG21 | 1.89 | 0.53 |
| 2:B2:464:ILE:HD11 | 21:B2:836:CLA:H12 | 1.90 | 0.53 |
| 26:A:858:LMU:H2O1 | 26:A:858:LMU:H3O2 | 1.57 | 0.53 |
| 7:G2:50:ARG:NH2 | 7:G2:91:ASP:OD1 | 2.42 | 0.53 |
| 21:Z2:608:CLA:H12 | 28:Z2:617:LUT:H383 | 1.90 | 0.53 |
| 26:A2:858:LMU:O3' | 26:A2:858:LMU:O2B | 2.26 | 0.53 |
| 21:12:603:CLA:H43 | 21:12:603:CLA:CED | 2.38 | 0.53 |
| 21:B2:834:CLA:H141 | 27:B2:854:LMG:C34 | 2.38 | 0.53 |
| 21:Z:608:CLA:H12 | 28:Z:617:LUT:H383 | 1.90 | 0.53 |
| 6:F2:208:GLN:OE1 | 6:F2:212:ARG:NH2 | 2.42 | 0.53 |
| 2:B:217:LEU:HD13 | 19:9:210:LEU:HD23 | 1.91 | 0.52 |
| 21:F2:304:CLA:O1A | 21:F2:304:CLA:C2 | 2.58 | 0.52 |
| 2:B:653:PHE:CZ | 2:B:657:ILE:HD11 | 2.44 | 0.52 |
| 2:B:722:TYR:HB2 | 21:B:802:CLA:HED2 | 1.92 | 0.52 |
| 21:B:834:CLA:H141 | 27:B:854:LMG:C34 | 2.39 | 0.52 |
| 7:G:50:ARG:NH2 | 7:G:91:ASP:OD1 | 2.42 | 0.52 |
| 2:B2:393:ILE:HG21 | 21:B2:829:CLA:HED1 | 1.91 | 0.52 |
| 2:B2:722:TYR:HB2 | 21:B2:802:CLA:HED2 | 1.91 | 0.52 |
| 6:F:64:ILE:HD11 | 6:F:143:TYR:CD2 | 2.45 | 0.52 |
| 21:F:304:CLA:O1A | 21:F:304:CLA:C2 | 2.58 | 0.52 |
| 21:A2:843:CLA:H93 | 21:A2:843:CLA:H121 | 1.91 | 0.52 |
| 18:62:33:LEU:HD13 | 30:62:601:CHL:HMA3 | 1.92 | 0.52 |
| 13:3:210:MET:CE | 21:3:610:CLA:HED3 | 2.40 | 0.52 |
| 13:32:210:MET:CE | 21:32:610:CLA:HED3 | 2.40 | 0.52 |
| 24:A:848:BCR:H362 | 24:A:849:BCR:H21C | 1.92 | 0.52 |
| 30:6:608:CHL:H11 | 28:6:621:LUT:H383 | 1.92 | 0.52 |
| 24:B:801:BCR:H331 | 24:B:801:BCR:C8 | 2.40 | 0.52 |
| 6:F2:64:ILE:HD11 | 6:F2:143:TYR:CD2 | 2.45 | 0.52 |
| 24:A2:848:BCR:H362 | 24:A2:849:BCR:H21C | 1.92 | 0.51 |
| 8:I2:72:PRO:HG3 | 8:I2:74:TRP:CZ2 | 2.46 | 0.51 |
| 21:A:802:CLA:H141 | 21:A:804:CLA:H191 | 1.92 | 0.51 |
| 24:B:843:BCR:H331 | 24:B:843:BCR:C8 | 2.40 | 0.51 |
| 2:B2:217:LEU:HD13 | 19:92:210:LEU:HD23 | 1.91 | 0.51 |
| 21:42:613:CLA:H43 | 21:42:614:CLA:OBD | 2.11 | 0.51 |
| 30:62:608:CHL:H11 | 28:62:621:LUT:H383 | 1.92 | 0.51 |
| 21:A:843:CLA:H93 | 21:A:843:CLA:H121 | 1.91 | 0.51 |
| 24:J:102:BCR:H331 | 24:J:102:BCR:C8 | 2.40 | 0.51 |
| 12:Z2:71:LEU:O | 12:Z2:75:THR:HG23 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I:72:PRO:HG3 | 8:I:74:TRP:CZ2 | 2.46 | 0.51 |
| 21:32:615:CLA:H42 | 17:52:231:ILE:CG1 | 2.41 | 0.51 |
| 30:4:606:CHL:C4A | 33:H:64:HOH:O | 2.28 | 0.51 |
| 18:6:76:ARG:NH1 | 30:6:608:CHL:OBD | 2.37 | 0.51 |
| 2:B:708:LEU:HD23 | 29:B:850:DGD:HA22 | 1.93 | 0.51 |
| 21:4:613:CLA:H43 | 21:4:614:CLA:OBD | 2.11 | 0.51 |
| 2:B:393:ILE:HG21 | 21:B:829:CLA:HED1 | 1.92 | 0.50 |
| 21:3:615:CLA:H42 | 17:5:231:ILE:CG1 | 2.41 | 0.50 |
| 24:B2:843:BCR:H331 | 24:B2:843:BCR:C8 | 2.40 | 0.50 |
| 24:J2:102:BCR:H331 | 24:J2:102:BCR:C8 | 2.40 | 0.50 |
| 12:Z:71:LEU:O | 12:Z:75:THR:HG23 | 2.11 | 0.50 |
| 21:A2:802:CLA:H141 | 21:A2:804:CLA:H191 | 1.92 | 0.50 |
| 24:A2:852:BCR:H331 | 24:A2:852:BCR:C8 | 2.42 | 0.50 |
| 24:B2:801:BCR:H331 | 24:B2:801:BCR:C8 | 2.40 | 0.50 |
| 21:A:818:CLA:H91 | 24:K:207:BCR:HC21 | 1.94 | 0.50 |
| 1:A:67:GLU:OE2 | 1:A:71:ARG:NH2 | 2.45 | 0.50 |
| 24:A:852:BCR:H331 | 24:A:852:BCR:C8 | 2.41 | 0.50 |
| 18:6:33:LEU:HD13 | 30:6:601:CHL:HMA3 | 1.92 | 0.49 |
| 21:32:611:CLA:H41 | 21:32:611:CLA:H71 | 1.94 | 0.49 |
| 21:32:602:CLA:HBA1 | 28:32:622:LUT:H182 | 1.94 | 0.49 |
| 15:82:31:LEU:HD13 | 30:82:601:CHL:HMA3 | 1.93 | 0.49 |
| 1:A2:67:GLU:OE2 | 1:A2:71:ARG:NH2 | 2.45 | 0.49 |
| 15:8:31:LEU:HD13 | 30:8:601:CHL:HMA3 | 1.94 | 0.49 |
| 16:42:199:ASP:OD1 | 28:42:619:LUT:O23 | 2.29 | 0.49 |
| 21:A2:818:CLA:H91 | 24:K2:207:BCR:HC21 | 1.94 | 0.49 |
| 24:B2:844:BCR:H382 | 24:B2:844:BCR:H23C | 1.94 | 0.49 |
| 2:B:520:VAL:HG11 | 2:B:594:TYR:CG | 2.47 | 0.49 |
| 2:B2:340:ALA:HB2 | 24:B2:847:BCR:H372 | 1.95 | 0.49 |
| 19:9:40:HIS:ND1 | 19:9:57:GLY:O | 2.46 | 0.49 |
| 24:L2:205:BCR:C8 | 24:L2:205:BCR:H331 | 2.43 | 0.49 |
| 19:92:40:HIS:ND1 | 19:92:57:GLY:O | 2.46 | 0.49 |
| 2:B2:77:GLN:OE1 | 2:B2:77:GLN:N | 2.46 | 0.49 |
| 13:32:39:ASP:HB2 | 13:32:47:VAL:HG23 | 1.95 | 0.49 |
| 21:82:604:CLA:H43 | 24:82:619:BCR:H272 | 1.95 | 0.49 |
| 13:3:39:ASP:HB2 | 13:3:47:VAL:HG23 | 1.95 | 0.49 |
| 14:7:135:ARG:NH1 | 21:7:609:CLA:O1D | 2.44 | 0.48 |
| 2:B2:520:VAL:HG11 | 2:B2:594:TYR:CG | 2.47 | 0.48 |
| 17:52:85:VAL:HG11 | 28:52:620:LUT:H12 | 1.95 | 0.48 |
| 1:A:418:ASP:OD2 | 1:A:420:THR:OG1 | 2.31 | 0.48 |
| 21:3:602:CLA:HBA1 | 28:3:622:LUT:H182 | 1.94 | 0.48 |
| 2:B:340:ALA:HB2 | 24:B:847:BCR:H372 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:3:611:CLA:H41 | 21:3:611:CLA:H71 | 1.94 | 0.48 |
| 30:4:606:CHL:C1A | 33:H:64:HOH:O | 2.36 | 0.48 |
| 19:9:103:GLU:N | 19:9:103:GLU:OE1 | 2.46 | 0.48 |
| 1:A2:399:GLY:HA3 | 1:A2:603:LEU:HD11 | 1.95 | 0.48 |
| 21:A2:854:CLA:HBB1 | 21:A2:854:CLA:HMB1 | 1.95 | 0.48 |
| 21:A:854:CLA:HBB1 | 21:A:854:CLA:HMB1 | 1.95 | 0.48 |
| 2:B:466:ALA:O | 2:B:480:SER:OG | 2.28 | 0.48 |
| 24:B:844:BCR:H382 | 24:B:844:BCR:H23C | 1.95 | 0.48 |
| 19:9:52:ASP:OD1 | 28:9:617:LUT:O23 | 2.31 | 0.48 |
| 28:F:305:LUT:C28 | 28:F:305:LUT:H381 | 2.40 | 0.48 |
| 21:B:839:CLA:H93 | 24:I:172:BCR:H333 | 1.96 | 0.48 |
| 17:5:85:VAL:HG11 | 28:5:620:LUT:H12 | 1.95 | 0.48 |
| 10:L2:58:PRO:O | 10:L2:62:ALA:HB2 | 2.14 | 0.48 |
| 11:K2:57:VAL:HG23 | 11:K2:88:ASP:OD1 | 2.14 | 0.48 |
| 24:L:205:BCR:H331 | 24:L:205:BCR:C8 | 2.43 | 0.47 |
| 21:8:604:CLA:H43 | 24:8:619:BCR:H272 | 1.95 | 0.47 |
| 21:B2:829:CLA:HMB1 | 21:B2:829:CLA:HBB1 | 1.96 | 0.47 |
| 19:92:103:GLU:N | 19:92:103:GLU:OE1 | 2.47 | 0.47 |
| 13:3:193:PRO:CG | 30:3:608:CHL:HMD1 | 2.45 | 0.47 |
| 13:32:193:PRO:CG | 30:32:608:CHL:HMD1 | 2.44 | 0.47 |
| 10:L:128:LEU:HD22 | 24:L:205:BCR:H401 | 1.96 | 0.47 |
| 2:B:192:THR:HG21 | 2:B:279:LEU:HB2 | 1.96 | 0.47 |
| 21:B2:839:CLA:H93 | 24:I2:172:BCR:H333 | 1.96 | 0.47 |
| 16:4:199:ASP:OD1 | 28:4:619:LUT:O23 | 2.29 | 0.47 |
| 1:A:223:PRO:HB2 | 1:A:243:LEU:HD13 | 1.96 | 0.47 |
| 1:A:399:GLY:HA3 | 1:A:603:LEU:HD11 | 1.95 | 0.47 |
| 13:3:201:PHE:O | 13:3:203:LEU:N | 2.47 | 0.47 |
| 15:8:183:ASP:N | 15:8:183:ASP:OD1 | 2.46 | 0.47 |
| 30:4:607:CHL:O1A | 26:4:625:LMU:O6' | 2.33 | 0.47 |
| 27:9:620:LMG:O2 | 27:9:620:LMG:O9 | 2.33 | 0.47 |
| 1:A2:433:HIS:HB3 | 10:L2:55:LEU:HD22 | 1.96 | 0.47 |
| 10:L2:128:LEU:HD22 | 24:L2:205:BCR:H401 | 1.96 | 0.47 |
| 10:L:58:PRO:O | 10:L:62:ALA:HB2 | 2.14 | 0.47 |
| 11:K:57:VAL:HG23 | 11:K:88:ASP:OD1 | 2.14 | 0.47 |
| 1:A:433:HIS:HB3 | 10:L:55:LEU:HD22 | 1.96 | 0.47 |
| 1:A2:413:MET:CE | 1:A2:431:ILE:HD11 | 2.45 | 0.47 |
| 21:B2:841:CLA:HBC1 | 26:B2:853:LMU:H2' | 1.96 | 0.47 |
| 15:82:183:ASP:OD1 | 15:82:183:ASP:N | 2.46 | 0.46 |
| 1:A2:223:PRO:HB2 | 1:A2:243:LEU:HD13 | 1.96 | 0.46 |
| 2:B2:192:THR:HG21 | 2:B2:279:LEU:HB2 | 1.96 | 0.46 |
| 24:B2:845:BCR:H342 | 19:92:177:LEU:HD21 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:I2:80:VAL:HB | 8:I2:81:PRO:HD3 | 1.97 | 0.46 |
| 21:B:821:CLA:H191 | 12:1:131:LEU:HD22 | 1.98 | 0.46 |
| 4:D2:176:GLY:N | 5:E2:49:GLU:OE1 | 2.49 | 0.46 |
| 13:32:201:PHE:O | 13:32:203:LEU:N | 2.47 | 0.46 |
| 27:92:620:LMG:O2 | 27:92:620:LMG:O9 | 2.33 | 0.46 |
| 16:4:82:ASP:OD1 | 16:4:85:TYR:N | 2.49 | 0.46 |
| 21:B:841:CLA:HBC1 | 26:B:853:LMU:H2' | 1.97 | 0.46 |
| 12:1:88:GLY:HA2 | 31:1:618:XAT:H181 | 1.98 | 0.46 |
| 21:7:608:CLA:O1A | 21:7:610:CLA:HMD2 | 2.16 | 0.46 |
| 28:F2:305:LUT:C28 | 28:F2:305:LUT:H381 | 2.40 | 0.46 |
| 8:I:80:VAL:HB | 8:I:81:PRO:HD3 | 1.97 | 0.46 |
| 21:3:603:CLA:HMD1 | 24:3:719:BCR:H403 | 1.98 | 0.46 |
| 12:12:88:GLY:HA2 | 31:12:618:XAT:H181 | 1.98 | 0.46 |
| 21:72:608:CLA:O1A | 21:72:610:CLA:HMD2 | 2.15 | 0.46 |
| 30:42:607:CHL:O1A | 26:42:625:LMU:O6' | 2.32 | 0.46 |
| 17:52:188:LYS:NZ | 23:52:623:LHG:O5 | 2.49 | 0.46 |
| 21:A:811:CLA:HBA1 | 21:A:813:CLA:HMD2 | 1.98 | 0.46 |
| 24:B:845:BCR:H342 | 19:9:177:LEU:HD21 | 1.98 | 0.46 |
| 21:32:615:CLA:H42 | 17:52:231:ILE:HG13 | 1.98 | 0.46 |
| 30:62:607:CHL:H42 | 32:62:625:NEX:H403 | 1.97 | 0.46 |
| 21:B:829:CLA:HBB1 | 21:B:829:CLA:HMB1 | 1.96 | 0.46 |
| 4:D:176:GLY:N | 5:E:49:GLU:OE1 | 2.49 | 0.46 |
| 30:6:607:CHL:H42 | 32:6:625:NEX:H403 | 1.97 | 0.46 |
| 21:A:833:CLA:H42 | 10:L:65:VAL:HG13 | 1.97 | 0.46 |
| 1:A2:677:PHE:CG | 24:A2:852:BCR:H363 | 2.51 | 0.46 |
| 1:A:677:PHE:CG | 24:A:852:BCR:H363 | 2.51 | 0.46 |
| 10:L:57:THR:HG22 | 10:L:58:PRO:HD2 | 1.98 | 0.46 |
| 1:A:245:LEU:O | 26:A:857:LMU:O2B | 2.34 | 0.45 |
| 2:B:269:LEU:HD13 | 21:B:817:CLA:HMA2 | 1.98 | 0.45 |
| 2:B:365:ASP:OD2 | 2:B:368:THR:OG1 | 2.29 | 0.45 |
| 17:5:188:LYS:NZ | 23:5:623:LHG:O5 | 2.49 | 0.45 |
| 18:62:122:HIS:O | 18:62:126:VAL:HG23 | 2.16 | 0.45 |
| 17:5:149:ASP:OD1 | 17:5:151:ILE:N | 2.49 | 0.45 |
| 21:B2:821:CLA:H191 | 12:12:131:LEU:HD22 | 1.98 | 0.45 |
| 16:42:82:ASP:OD1 | 16:42:85:TYR:N | 2.49 | 0.45 |
| 21:A:809:CLA:H91 | 21:A:812:CLA:H201 | 1.98 | 0.45 |
| 2:B:77:GLN:OE1 | 2:B:77:GLN:N | 2.46 | 0.45 |
| 24:9:623:BCR:H20C | 24:9:623:BCR:H361 | 1.83 | 0.45 |
| 1:A2:59:PHE:CD2 | 21:A2:806:CLA:HMC2 | 2.51 | 0.45 |
| 1:A:411:ILE:HD13 | 21:A:831:CLA:CED | 2.47 | 0.45 |
| 2:B:236:GLN:O | 2:B:237:SER:OG | 2.33 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:1:603:CLA:H61 | 21:1:603:CLA:H41 | 1.87 | 0.45 |
| 2:B2:269:LEU:HD13 | 21:B2:817:CLA:HMA2 | 1.98 | 0.45 |
| 10:L2:57:THR:HG22 | 10:L2:58:PRO:HD2 | 1.98 | 0.45 |
| 1:A:36:SER:O | 1:A:40:SER:OG | 2.32 | 0.45 |
| 1:A:413:MET:CE | 1:A:431:ILE:HD11 | 2.46 | 0.45 |
| 2:B:451:GLU:OE2 | 6:F:114:ARG:NH1 | 2.49 | 0.45 |
| 24:B:845:BCR:H331 | 24:B:845:BCR:C8 | 2.47 | 0.45 |
| 21:A2:811:CLA:HBA1 | 21:A2:813:CLA:HMD2 | 1.98 | 0.45 |
| 21:32:603:CLA:HMD1 | 24:32:719:BCR:H403 | 1.98 | 0.45 |
| 12:12:202:PRO:O | 28:12:617:LUT:O3 | 2.33 | 0.45 |
| 2:B2:466:ALA:O | 2:B2:480:SER:OG | 2.28 | 0.45 |
| 24:K2:202:BCR:C23 | 24:K2:202:BCR:H392 | 2.47 | 0.45 |
| 17:52:149:ASP:OD1 | 17:52:151:ILE:N | 2.49 | 0.45 |
| 24:K:202:BCR:H392 | 24:K:202:BCR:C23 | 2.47 | 0.45 |
| 12:Z:35:LYS:N | 12:Z:51:ASP:OD1 | 2.50 | 0.45 |
| 18:6:33:LEU:HD13 | 30:6:601:CHL:CMA | 2.47 | 0.45 |
| 17:52:95:LYS:HB3 | 17:52:98:VAL:HG13 | 1.99 | 0.45 |
| 24:62:623:BCR:H331 | 24:62:623:BCR:C8 | 2.46 | 0.45 |
| 19:92:172:PHE:CE1 | 28:92:616:LUT:H182 | 2.52 | 0.45 |
| 21:3:615:CLA:H42 | 17:5:231:ILE:HG13 | 1.98 | 0.44 |
| 18:6:122:HIS:O | 18:6:126:VAL:HG23 | 2.16 | 0.44 |
| 19:9:172:PHE:CE1 | 28:9:616:LUT:H182 | 2.52 | 0.44 |
| 1:A2:411:ILE:HD13 | 21:A2:831:CLA:CED | 2.47 | 0.44 |
| 2:B2:264:PRO:O | 2:B2:267:GLN:NE2 | 2.50 | 0.44 |
| 2:B:414:ASP:O | 6:F:227:ARG:NH1 | 2.50 | 0.44 |
| 1:A2:245:LEU:O | 26:A2:857:LMU:O2B | 2.34 | 0.44 |
| 24:A2:850:BCR:H24C | 24:A2:850:BCR:H371 | 1.86 | 0.44 |
| 18:62:33:LEU:HD12 | 30:62:601:CHL:HED2 | 1.99 | 0.44 |
| 1:A:119:TRP:CD2 | 21:A:810:CLA:HED3 | 2.52 | 0.44 |
| 21:A2:833:CLA:H42 | 10:L2:65:VAL:HG13 | 1.97 | 0.44 |
| 24:6:623:BCR:H331 | 24:6:623:BCR:C8 | 2.46 | 0.44 |
| 12:Z2:35:LYS:N | 12:Z2:51:ASP:OD1 | 2.50 | 0.44 |
| 12:1:202:PRO:O | 28:1:617:LUT:O3 | 2.32 | 0.44 |
| 14:7:81:LEU:HD22 | 21:7:610:CLA:H201 | 1.99 | 0.44 |
| 21:A2:809:CLA:H91 | 21:A2:812:CLA:H201 | 1.98 | 0.44 |
| 13:32:101:GLY:HA2 | 28:32:622:LUT:H381 | 2.00 | 0.44 |
| 14:72:34:PHE:CE1 | 30:72:601:CHL:HED2 | 2.53 | 0.44 |
| 21:Z:613:CLA:CGA | 21:Z:613:CLA:C1A | 2.96 | 0.44 |
| 2:B2:414:ASP:O | 6:F2:227:ARG:NH1 | 2.51 | 0.44 |
| 2:B2:451:GLU:OE2 | 6:F2:114:ARG:NH1 | 2.50 | 0.44 |
| 24:32:719:BCR:C8 | 24:32:719:BCR:H331 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:B:844:BCR:C8 | 24:B:844:BCR:H331 | 2.47 | 0.44 |
| 14:7:34:PHE:HE1 | 30:7:601:CHL:HED2 | 1.83 | 0.44 |
| 24:B2:845:BCR:H331 | 24:B2:845:BCR:C8 | 2.47 | 0.44 |
| 17:52:198:MET:HE3 | 21:52:603:CLA:CAB | 2.48 | 0.44 |
| 17:5:198:MET:HE3 | 21:5:603:CLA:CAB | 2.48 | 0.44 |
| 1:A2:470:ASP:HB3 | 21:A2:835:CLA:HED3 | 1.99 | 0.44 |
| 21:Z2:603:CLA:H61 | 21:Z2:603:CLA:H41 | 1.83 | 0.44 |
| 21:Z2:611:CLA:C1B | 23:Z2:620:LHG:O4 | 2.59 | 0.44 |
| 16:42:54:ARG:HD3 | 16:42:67:LEU:HD12 | 1.99 | 0.44 |
| 17:52:198:MET:HE3 | 21:52:603:CLA:HAB | 2.00 | 0.44 |
| 21:52:617:CLA:H61 | 21:52:617:CLA:H41 | 1.90 | 0.44 |
| 17:5:95:LYS:HB3 | 17:5:98:VAL:HG13 | 1.99 | 0.44 |
| 1:A2:418:ASP:OD2 | 1:A2:420:THR:OG1 | 2.31 | 0.44 |
| 14:72:135:ARG:NH1 | 21:72:609:CLA:O1D | 2.44 | 0.44 |
| 21:42:613:CLA:H62 | 21:42:613:CLA:H41 | 1.93 | 0.44 |
| 13:3:210:MET:HE2 | 21:3:610:CLA:HED3 | 2.00 | 0.43 |
| 16:4:54:ARG:HD3 | 16:4:67:LEU:HD12 | 1.99 | 0.43 |
| 18:6:33:LEU:HD12 | 30:6:601:CHL:HED2 | 1.99 | 0.43 |
| 1:A2:586:VAL:HG13 | 2:B2:670:GLY:HA3 | 1.99 | 0.43 |
| 14:72:34:PHE:HE1 | 30:72:601:CHL:HED2 | 1.83 | 0.43 |
| 1:A:282:LEU:HD21 | 1:A:375:PRO:HD2 | 1.99 | 0.43 |
| 24:K:202:BCR:H331 | 24:K:202:BCR:C8 | 2.48 | 0.43 |
| 28:7:624:LUT:H383 | 15:8:229:TRP:CZ2 | 2.53 | 0.43 |
| 24:K2:202:BCR:H403 | 24:K2:202:BCR:H23C | 1.99 | 0.43 |
| 21:B:816:CLA:H142 | 21:B:816:CLA:C10 | 2.49 | 0.43 |
| 24:B2:844:BCR:C8 | 24:B2:844:BCR:H331 | 2.47 | 0.43 |
| 21:12:603:CLA:H61 | 21:12:603:CLA:H41 | 1.87 | 0.43 |
| 21:32:603:CLA:HBC1 | 21:32:609:CLA:CBC | 2.48 | 0.43 |
| 21:72:610:CLA:H13 | 21:62:603:CLA:H142 | 2.00 | 0.43 |
| 21:42:610:CLA:H62 | 21:42:610:CLA:H41 | 1.94 | 0.43 |
| 21:52:621:CLA:HAA2 | 21:52:621:CLA:CBD | 2.49 | 0.43 |
| 21:B:806:CLA:H2 | 21:B:806:CLA:HED3 | 2.00 | 0.43 |
| 21:3:603:CLA:HBC1 | 21:3:609:CLA:CBC | 2.48 | 0.43 |
| 1:A:586:VAL:HG13 | 2:B:670:GLY:HA3 | 1.99 | 0.43 |
| 2:B:264:PRO:O | 2:B:267:GLN:NE2 | 2.51 | 0.43 |
| 2:B:632:LEU:HD21 | 2:B:651:PHE:CD1 | 2.54 | 0.43 |
| 14:7:34:PHE:CE1 | 30:7:601:CHL:HED2 | 2.53 | 0.43 |
| 28:72:624:LUT:H383 | 15:82:229:TRP:CZ2 | 2.53 | 0.43 |
| 21:Z2:613:CLA:C1A | 21:Z2:613:CLA:CGA | 2.96 | 0.43 |
| 24:K:202:BCR:H23C | 24:K:202:BCR:H403 | 1.99 | 0.43 |
| 24:K:207:BCR:H24C | 24:K:207:BCR:H371 | 1.88 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:5:621:CLA:CBD | 21:5:621:CLA:HAA2 | 2.49 | 0.43 |
| 1:A2:119:TRP:CD2 | 21:A2:810:CLA:HED3 | 2.53 | 0.43 |
| 6:F2:193:THR:HG21 | 27:J2:104:LMG:H142 | 2.00 | 0.43 |
| 26:A:858:LMU:O3' | 26:A:858:LMU:O2B | 2.26 | 0.43 |
| 24:L:201:BCR:H24C | 24:L:201:BCR:H371 | 1.91 | 0.43 |
| 11:K:50:ARG:NH1 | 11:K:80:ASP:OD2 | 2.51 | 0.43 |
| 1:A2:282:LEU:HD21 | 1:A2:375:PRO:HD2 | 1.99 | 0.43 |
| 24:A2:849:BCR:C8 | 24:A2:849:BCR:H331 | 2.49 | 0.43 |
| 18:62:33:LEU:HD13 | 30:62:601:CHL:CMA | 2.47 | 0.43 |
| 2:B:173:GLU:OE1 | 2:B:173:GLU:N | 2.50 | 0.43 |
| 21:B:808:CLA:CGA | 21:B:808:CLA:C1A | 2.97 | 0.43 |
| 17:5:198:MET:HE3 | 21:5:603:CLA:HAB | 2.00 | 0.43 |
| 14:72:81:LEU:HD22 | 21:72:610:CLA:H201 | 1.99 | 0.43 |
| 30:1:601:CHL:H62 | 30:1:601:CHL:H41 | 1.77 | 0.43 |
| 24:B:848:BCR:H24C | 24:B:848:BCR:H371 | 1.91 | 0.43 |
| 24:L:205:BCR:H403 | 24:L:205:BCR:H23C | 2.01 | 0.43 |
| 24:3:719:BCR:C8 | 24:3:719:BCR:H331 | 2.47 | 0.43 |
| 28:92:617:LUT:C28 | 28:92:617:LUT:H381 | 2.47 | 0.43 |
| 1:A:470:ASP:HB3 | 21:A:835:CLA:HED3 | 1.99 | 0.42 |
| 1:A:584:CYS:O | 2:B:670:GLY:N | 2.51 | 0.42 |
| 24:A:849:BCR:C8 | 24:A:849:BCR:H331 | 2.49 | 0.42 |
| 13:3:101:GLY:HA2 | 28:3:622:LUT:H381 | 2.00 | 0.42 |
| 21:A2:854:CLA:HMB3 | 21:B2:802:CLA:C19 | 2.48 | 0.42 |
| 2:B2:365:ASP:OD2 | 2:B2:368:THR:OG1 | 2.29 | 0.42 |
| 2:B2:530:THR:HG21 | 2:B2:583:TRP:CE2 | 2.54 | 0.42 |
| 21:B2:806:CLA:H2 | 21:B2:806:CLA:HED3 | 2.00 | 0.42 |
| 24:B2:848:BCR:H20C | 24:B2:848:BCR:H361 | 1.91 | 0.42 |
| 3:C2:36:ALA:O | 3:C2:37:SER:OG | 2.30 | 0.42 |
| 21:32:615:CLA:C19 | 17:52:227:ILE:HG21 | 2.49 | 0.42 |
| 19:92:52:ASP:OD1 | 28:92:617:LUT:O23 | 2.31 | 0.42 |
| 6:F:193:THR:HG21 | 27:J:104:LMG:H142 | 2.00 | 0.42 |
| 28:9:617:LUT:C28 | 28:9:617:LUT:H381 | 2.48 | 0.42 |
| 11:K2:50:ARG:NH1 | 11:K2:80:ASP:OD2 | 2.51 | 0.42 |
| 24:K2:202:BCR:H331 | 24:K2:202:BCR:C8 | 2.48 | 0.42 |
| 1:A:554:VAL:HG11 | 21:A:822:CLA:H203 | 2.01 | 0.42 |
| 24:A:850:BCR:C8 | 24:A:850:BCR:H331 | 2.49 | 0.42 |
| 21:3:615:CLA:C19 | 17:5:227:ILE:HG21 | 2.49 | 0.42 |
| 21:7:610:CLA:H13 | 21:6:603:CLA:H142 | 2.00 | 0.42 |
| 21:A2:829:CLA:H72 | 21:A2:829:CLA:C12 | 2.50 | 0.42 |
| 21:B2:808:CLA:CGA | 21:B2:808:CLA:C1A | 2.97 | 0.42 |
| 24:G2:205:BCR:H20C | 24:G2:205:BCR:H361 | 1.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:J2:103:LMG:O1 | 27:J2:103:LMG:HC61 | 2.20 | 0.42 |
| 24:92:623:BCR:H361 | 24:92:623:BCR:H20C | 1.83 | 0.42 |
| 21:6:602:CLA:HMC2 | 31:6:624:XAT:C11 | 2.49 | 0.42 |
| 24:K2:207:BCR:H20C | 24:K2:207:BCR:H361 | 1.90 | 0.42 |
| 3:C:2:ALA:N | 3:C:71:SER:O | 2.53 | 0.42 |
| 21:5:616:CLA:H62 | 21:5:616:CLA:H41 | 1.93 | 0.42 |
| 2:B2:494:TRP:CH2 | 21:B2:835:CLA:HED3 | 2.55 | 0.42 |
| 1:A:115:ALA:HB3 | 21:A:809:CLA:HED3 | 2.01 | 0.42 |
| 21:A:802:CLA:CGA | 21:A:802:CLA:H3A | 2.50 | 0.42 |
| 2:B:194:HIS:CE1 | 21:B:814:CLA:NA | 2.87 | 0.42 |
| 21:B:837:CLA:H41 | 28:F:305:LUT:C37 | 2.49 | 0.42 |
| 24:B:843:BCR:H24C | 24:B:843:BCR:H371 | 1.91 | 0.42 |
| 27:J:103:LMG:O1 | 27:J:103:LMG:HC61 | 2.20 | 0.42 |
| 24:3:719:BCR:H24C | 24:3:719:BCR:H371 | 1.85 | 0.42 |
| 1:A2:584:CYS:O | 2:B2:670:GLY:N | 2.51 | 0.42 |
| 24:A2:850:BCR:C8 | 24:A2:850:BCR:H331 | 2.49 | 0.42 |
| 21:B2:837:CLA:H41 | 28:F2:305:LUT:C37 | 2.50 | 0.42 |
| 23:32:623:LHG:H111 | 21:52:616:CLA:HMC2 | 2.02 | 0.42 |
| 24:3:718:BCR:H24C | 24:3:718:BCR:H371 | 1.90 | 0.42 |
| 12:Z:220:THR:HG22 | 12:Z:220:THR:O | 2.20 | 0.42 |
| 1:A2:36:SER:O | 1:A2:40:SER:OG | 2.31 | 0.42 |
| 1:A2:115:ALA:HB3 | 21:A2:809:CLA:HED3 | 2.01 | 0.42 |
| 2:B2:236:GLN:O | 2:B2:237:SER:OG | 2.33 | 0.42 |
| 24:B2:843:BCR:H24C | 24:B2:843:BCR:H371 | 1.91 | 0.42 |
| 13:32:210:MET:HE2 | 21:32:610:CLA:HED3 | 2.00 | 0.42 |
| 2:B:494:TRP:CH2 | 21:B:835:CLA:HED3 | 2.55 | 0.42 |
| 21:B:840:CLA:H122 | 21:B:840:CLA:H91 | 2.02 | 0.42 |
| 1:A2:747:ILE:O | 1:A2:751:GLY:N | 2.51 | 0.42 |
| 21:62:602:CLA:HMC2 | 31:62:624:XAT:C11 | 2.49 | 0.42 |
| 12:1:50:PRO:O | 12:1:56:ASN:ND2 | 2.52 | 0.42 |
| 21:3:615:CLA:HAA2 | 21:5:616:CLA:HED2 | 2.02 | 0.42 |
| 2:B2:632:LEU:HD21 | 2:B2:651:PHE:CD1 | 2.54 | 0.42 |
| 21:A:829:CLA:H62 | 21:A:829:CLA:H41 | 1.83 | 0.42 |
| 24:A:848:BCR:H24C | 24:A:848:BCR:H371 | 1.87 | 0.42 |
| 13:3:183:ILE:HG22 | 13:3:196:PRO:HG2 | 2.02 | 0.42 |
| 21:B2:816:CLA:H142 | 21:B2:816:CLA:C10 | 2.48 | 0.42 |
| 21:52:610:CLA:H62 | 21:52:610:CLA:H41 | 1.83 | 0.42 |
| 1:A:707:LEU:HD23 | 6:F:216:LEU:HD23 | 2.02 | 0.41 |
| 13:3:58:ASP:OD1 | 13:3:58:ASP:N | 2.53 | 0.41 |
| 1:A2:554:VAL:HG11 | 21:A2:822:CLA:H203 | 2.01 | 0.41 |
| 2:B2:194:HIS:CE1 | 21:B2:814:CLA:NA | 2.87 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:L2:205:BCR:H403 | 24:L2:205:BCR:H23C | 2.01 | 0.41 |
| 24:K2:202:BCR:H24C | 24:K2:202:BCR:H371 | 1.92 | 0.41 |
| 21:32:615:CLA:HAA2 | 21:52:616:CLA:HED2 | 2.02 | 0.41 |
| 12:Z2:220:THR:HG22 | 12:Z2:220:THR:O | 2.20 | 0.41 |
| 24:A:851:BCR:H371 | 24:A:851:BCR:H24C | 1.89 | 0.41 |
| 11:K:69:ASP:OD1 | 11:K:70:SER:N | 2.54 | 0.41 |
| 24:3:719:BCR:H20C | 24:3:719:BCR:H361 | 1.91 | 0.41 |
| 16:4:66:ASP:O | 23:4:623:LHG:O4 | 2.39 | 0.41 |
| 13:32:183:ILE:HG22 | 13:32:196:PRO:HG2 | 2.02 | 0.41 |
| 12:Z2:192:VAL:HG13 | 26:Z2:622:LMU:O2' | 2.20 | 0.41 |
| 1:A:747:ILE:O | 1:A:751:GLY:N | 2.51 | 0.41 |
| 2:B:632:LEU:HD21 | 2:B:651:PHE:CG | 2.55 | 0.41 |
| 12:Z:215:GLY:O | 12:Z:220:THR:HG21 | 2.20 | 0.41 |
| 24:A2:848:BCR:H361 | 24:A2:848:BCR:H20C | 1.85 | 0.41 |
| 3:C2:2:ALA:N | 3:C2:71:SER:O | 2.53 | 0.41 |
| 1:A:343:GLU:OE1 | 1:A:343:GLU:N | 2.48 | 0.41 |
| 21:A:829:CLA:H72 | 21:A:829:CLA:C12 | 2.50 | 0.41 |
| 21:A2:802:CLA:CGA | 21:A2:802:CLA:H3A | 2.50 | 0.41 |
| 2:B2:195:LEU:HA | 2:B2:199:ALA:HB3 | 2.02 | 0.41 |
| 21:B2:827:CLA:H141 | 21:B2:829:CLA:H143 | 2.03 | 0.41 |
| 30:52:608:CHL:H12 | 28:52:620:LUT:H383 | 2.02 | 0.41 |
| 9:J:32:TYR:OH | 21:J:101:CLA:HED3 | 2.21 | 0.41 |
| 21:L:203:CLA:H62 | 21:L:203:CLA:H41 | 1.90 | 0.41 |
| 19:9:191:LEU:HD21 | 21:9:614:CLA:HMC2 | 2.03 | 0.41 |
| 2:B2:352:HIS:CE1 | 21:B2:826:CLA:NB | 2.89 | 0.41 |
| 12:Z2:159:ASP:OD1 | 28:Z2:617:LUT:O23 | 2.38 | 0.41 |
| 15:8:231:VAL:HG12 | 21:8:613:CLA:HED1 | 2.02 | 0.41 |
| 24:6:623:BCR:H20C | 24:6:623:BCR:H361 | 1.96 | 0.41 |
| 1:A2:707:LEU:HD23 | 6:F2:216:LEU:HD23 | 2.02 | 0.41 |
| 24:A2:850:BCR:H20C | 24:A2:850:BCR:H361 | 1.89 | 0.41 |
| 2:B2:632:LEU:HD21 | 2:B2:651:PHE:CG | 2.56 | 0.41 |
| 21:B2:822:CLA:HMC1 | 21:B2:823:CLA:O1A | 2.21 | 0.41 |
| 24:B2:801:BCR:H24C | 24:B2:801:BCR:H371 | 1.92 | 0.41 |
| 3:C2:14:CYS:O | 3:C2:15:THR:OG1 | 2.26 | 0.41 |
| 24:G2:205:BCR:H24C | 24:G2:205:BCR:H371 | 1.87 | 0.41 |
| 13:32:193:PRO:HG3 | 30:32:608:CHL:HMD1 | 2.02 | 0.41 |
| 15:82:231:VAL:HG12 | 21:82:613:CLA:HED1 | 2.03 | 0.41 |
| 21:B:827:CLA:H141 | 21:B:829:CLA:H143 | 2.02 | 0.41 |
| 6:F:212:ARG:NH2 | 27:8:626:LMG:O3 | 2.47 | 0.41 |
| 30:5:608:CHL:H12 | 28:5:620:LUT:H383 | 2.02 | 0.41 |
| 24:32:719:BCR:H24C | 24:32:719:BCR:H371 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:3:620:BCR:H24C | 24:3:620:BCR:H371 | 1.92 | 0.41 |
| 12:Z:192:VAL:HG13 | 26:Z:622:LMU:O2' | 2.20 | 0.41 |
| 21:A2:820:CLA:CAD | 21:A2:830:CLA:H41 | 2.51 | 0.41 |
| 21:A2:833:CLA:C4 | 10:L2:65:VAL:HG13 | 2.51 | 0.41 |
| 12:Z2:153:TYR:HB3 | 21:Z2:610:CLA:HED2 | 2.03 | 0.41 |
| 16:42:66:ASP:O | 23:42:623:LHG:O4 | 2.39 | 0.41 |
| 24:92:623:BCR:H24C | 24:92:623:BCR:H371 | 1.89 | 0.41 |
| 1:A:474:ASP:O | 1:A:478:GLN:NE2 | 2.54 | 0.41 |
| 21:A:833:CLA:C4 | 10:L:65:VAL:HG13 | 2.51 | 0.41 |
| 24:A:848:BCR:H20C | 24:A:848:BCR:H361 | 1.86 | 0.41 |
| 24:A:851:BCR:H20C | 24:A:851:BCR:H361 | 1.94 | 0.41 |
| 28:A:856:LUT:H8 | 28:A:856:LUT:H171 | 2.03 | 0.41 |
| 2:B:352:HIS:CE1 | 21:B:826:CLA:NB | 2.88 | 0.41 |
| 21:B:837:CLA:H41 | 28:F:305:LUT:H371 | 2.03 | 0.41 |
| 21:B:840:CLA:H91 | 21:B:840:CLA:C12 | 2.51 | 0.41 |
| 3:C:36:ALA:O | 3:C:37:SER:OG | 2.31 | 0.41 |
| 23:3:623:LHG:H111 | 21:5:616:CLA:HMC2 | 2.02 | 0.41 |
| 30:7:601:CHL:H61 | 30:7:601:CHL:H41 | 1.84 | 0.41 |
| 21:B2:840:CLA:C12 | 21:B2:840:CLA:H91 | 2.51 | 0.41 |
| 30:32:608:CHL:H191 | 21:32:610:CLA:H142 | 2.03 | 0.41 |
| 12:Z2:215:GLY:O | 12:Z2:220:THR:HG21 | 2.20 | 0.41 |
| 21:A:811:CLA:C1 | 21:A:813:CLA:H42 | 2.50 | 0.41 |
| 24:A:852:BCR:H24C | 24:A:852:BCR:H371 | 1.91 | 0.41 |
| 21:B:822:CLA:HMC1 | 21:B:823:CLA:O1A | 2.21 | 0.41 |
| 3:C:24:ASP:OD2 | 4:D:151:HIS:ND1 | 2.50 | 0.41 |
| 15:8:163:THR:OG1 | 15:8:168:TYR:O | 2.37 | 0.41 |
| 12:Z:159:ASP:OD1 | 28:Z:617:LUT:O23 | 2.38 | 0.41 |
| 2:B2:293:ARG:N | 2:B2:300:HIS:O | 2.53 | 0.41 |
| 11:K2:69:ASP:OD1 | 11:K2:70:SER:N | 2.54 | 0.41 |
| 21:32:615:CLA:H61 | 21:32:615:CLA:H41 | 1.94 | 0.41 |
| 15:82:217:PRO:O | 28:82:617:LUT:O3 | 2.39 | 0.41 |
| 24:82:619:BCR:HC8 | 24:82:619:BCR:H311 | 2.02 | 0.41 |
| 21:A:810:CLA:HAB | 21:B:833:CLA:HMD2 | 2.04 | 0.40 |
| 2:B:530:THR:HG21 | 2:B:583:TRP:CE2 | 2.55 | 0.40 |
| 24:B:845:BCR:H24C | 24:B:845:BCR:H371 | 1.84 | 0.40 |
| 26:8:627:LMU:H2' | 26:8:627:LMU:H6D | 2.03 | 0.40 |
| 21:5:621:CLA:HAA2 | 21:5:621:CLA:HBD | 2.03 | 0.40 |
| 21:B2:832:CLA:HBB1 | 24:B2:801:BCR:H323 | 2.03 | 0.40 |
| 11:K2:65:LEU:HD12 | 11:K2:65:LEU:N | 2.37 | 0.40 |
| 1:A:476:ALA:O | 1:A:477:ILE:C | 2.65 | 0.40 |
| 11:K:65:LEU:N | 11:K:65:LEU:HD12 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:3:193:PRO:HG3 | 30:3:608:CHL:HMD1 | 2.02 | 0.40 |
| 21:A2:832:CLA:HED2 | 10:L2:55:LEU:HD21 | 2.02 | 0.40 |
| 21:B2:840:CLA:H62 | 21:B2:840:CLA:H41 | 1.85 | 0.40 |
| 13:32:132:PRO:N | 13:32:133:PRO:CD | 2.84 | 0.40 |
| 16:42:160:VAL:HG11 | 24:42:621:BCR:H362 | 2.03 | 0.40 |
| 3:C:14:CYS:O | 3:C:15:THR:OG1 | 2.26 | 0.40 |
| 28:A2:856:LUT:C28 | 28:A2:856:LUT:H381 | 2.51 | 0.40 |
| 21:B2:840:CLA:H91 | 21:B2:840:CLA:H122 | 2.02 | 0.40 |
| 24:L2:201:BCR:H24C | 24:L2:201:BCR:H371 | 1.91 | 0.40 |
| 1:A:411:ILE:HD13 | 21:A:831:CLA:HED1 | 2.04 | 0.40 |
| 24:A:852:BCR:H20C | 24:A:852:BCR:H361 | 1.88 | 0.40 |
| 24:B:844:BCR:H24C | 24:B:844:BCR:H371 | 1.97 | 0.40 |
| 24:8:619:BCR:HC8 | 24:8:619:BCR:H311 | 2.02 | 0.40 |
| 12:Z:153:TYR:HB3 | 21:Z:610:CLA:HED2 | 2.03 | 0.40 |
| 1:A2:476:ALA:O | 1:A2:477:ILE:C | 2.65 | 0.40 |
| 28:A2:856:LUT:H171 | 28:A2:856:LUT:H8 | 2.03 | 0.40 |
| 2:B2:173:GLU:OE1 | 2:B2:173:GLU:N | 2.50 | 0.40 |
| 9:J2:32:TYR:OH | 21:J2:101:CLA:HED3 | 2.21 | 0.40 |
| 14:7:110:VAL:HG13 | 14:7:115:ILE:O | 2.22 | 0.40 |
| 21:8:612:CLA:H43 | 21:4:609:CLA:H11 | 2.04 | 0.40 |
| 2:B2:77:GLN:O | 2:B2:80:THR:OG1 | 2.36 | 0.40 |
| 14:72:82:GLY:HA2 | 31:72:622:XAT:H381 | 2.03 | 0.40 |
| 19:92:191:LEU:HD21 | 21:92:614:CLA:HMC2 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 740/751 (98%) | 727 (98%) | 13 (2%) | 0 | 100 | 100 |
| 1 | A2 | 740/751 (98%) | 727 (98%) | 13 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | B | 731/735 (100%) | 718 (98%) | 13 (2%) | 0 | 100 | 100 |
| 2 | B2 | 731/735 (100%) | 718 (98%) | 13 (2%) | 0 | 100 | 100 |
| 3 | C | 78/81 (96%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 3 | C2 | 78/81 (96%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | D | 142/196 (72%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 4 | D2 | 142/196 (72%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | E | 62/97 (64%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 5 | E2 | 62/97 (64%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 163/227 (72%) | 163 (100%) | 0 | 0 | 100 | 100 |
| 6 | F2 | 163/227 (72%) | 162 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | G | 93/126 (74%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | G2 | 93/126 (74%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |
| 8 | I | 35/106 (33%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 8 | I2 | 35/106 (33%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 9 | J | 38/40 (95%) | 37 (97%) | 1 (3%) | 0 | 100 | 100 |
| 9 | J2 | 38/40 (95%) | 37 (97%) | 1 (3%) | 0 | 100 | 100 |
| 10 | L | 120/196 (61%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 10 | L2 | 120/196 (61%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 11 | K | 84/113 (74%) | 82 (98%) | 2 (2%) | 0 | 100 | 100 |
| 11 | K2 | 84/113 (74%) | 82 (98%) | 2 (2%) | 0 | 100 | 100 |
| 12 | 1 | 192/228 (84%) | 192 (100%) | 0 | 0 | 100 | 100 |
| 12 | 12 | 192/228 (84%) | 192 (100%) | 0 | 0 | 100 | 100 |
| 12 | Z | 192/228 (84%) | 190 (99%) | 2 (1%) | 0 | 100 | 100 |
| 12 | Z2 | 192/228 (84%) | 190 (99%) | 2 (1%) | 0 | 100 | 100 |
| 13 | 3 | 225/298 (76%) | 218 (97%) | 7 (3%) | 0 | 100 | 100 |
| 13 | 32 | 225/298 (76%) | 218 (97%) | 7 (3%) | 0 | 100 | 100 |
| 14 | 7 | 211/241 (88%) | 210 (100%) | 1 (0%) | 0 | 100 | 100 |
| 14 | 72 | 211/241 (88%) | 210 (100%) | 1 (0%) | 0 | 100 | 100 |
| 15 | 8 | 215/243 (88%) | 212 (99%) | 3 (1%) | 0 | 100 | 100 |
| 15 | 82 | 215/243 (88%) | 212 (99%) | 3 (1%) | 0 | 100 | 100 |
| 16 | 4 | 210/264 (80%) | 207 (99%) | 3 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 16 | 42 | 210/264 (80%) | 207 (99%) | 3 (1%) | 0 | 100 | 100 |
| 17 | 5 | 225/257 (88%) | 220 (98%) | 5 (2%) | 0 | 100 | 100 |
| 17 | 52 | 225/257 (88%) | 220 (98%) | 5 (2%) | 0 | 100 | 100 |
| 18 | 6 | 228/257 (89%) | 225 (99%) | 3 (1%) | 0 | 100 | 100 |
| 18 | 62 | 228/257 (89%) | 225 (99%) | 3 (1%) | 0 | 100 | 100 |
| 19 | 9 | 184/213 (86%) | 179 (97%) | 4 (2%) | 1 (0%) | 24 | 58 |
| 19 | 92 | 184/213 (86%) | 179 (97%) | 4 (2%) | 1 (0%) | 24 | 58 |
| All | All | 8336/9794 (85%) | 8203 (98%) | 131 (2%) | 2 (0%) | 100 | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | 9 | 139 | ILE |
| 19 | 92 | 139 | ILE |

### 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 | 601/610 (98%) | 599 (100%) | 2 (0%) | 86 | 91 |
| 1 | A2 | 601/610 (98%) | 598 (100%) | 3 (0%) | 81 | 89 |
| 2 | B | 596/597 (100%) | 594 (100%) | 2 (0%) | 86 | 91 |
| 2 | B2 | 596/597 (100%) | 593 (100%) | 3 (0%) | 81 | 89 |
| 3 | C | 69/70 (99%) | 69 (100%) | 0 | 100 | 100 |
| 3 | C2 | 69/70 (99%) | 69 (100%) | 0 | 100 | 100 |
| 4 | D | 121/152 (80%) | 120 (99%) | 1 (1%) | 73 | 86 |
| 4 | D2 | 121/152 (80%) | 120 (99%) | 1 (1%) | 73 | 86 |
| 5 | E | 55/81 (68%) | 55 (100%) | 0 | 100 | 100 |
| 5 | E2 | 55/81 (68%) | 55 (100%) | 0 | 100 | 100 |
| 6 | F | 127/169 (75%) | 127 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | F2 | 127/169 (75%) | 127 (100%) | 0 | 100 | 100 |
| 7 | G | 71/94 (76%) | 71 (100%) | 0 | 100 | 100 |
| 7 | G2 | 71/94 (76%) | 71 (100%) | 0 | 100 | 100 |
| 8 | I | 31/76 (41%) | 31 (100%) | 0 | 100 | 100 |
| 8 | I2 | 31/76 (41%) | 31 (100%) | 0 | 100 | 100 |
| 9 | J | 35/35 (100%) | 34 (97%) | 1 (3%) | 37 | 68 |
| 9 | J2 | 35/35 (100%) | 34 (97%) | 1 (3%) | 37 | 68 |
| 10 | L | 90/148 (61%) | 89 (99%) | 1 (1%) | 65 | 82 |
| 10 | L2 | 90/148 (61%) | 89 (99%) | 1 (1%) | 65 | 82 |
| 11 | K | 59/80 (74%) | 59 (100%) | 0 | 100 | 100 |
| 11 | K2 | 59/80 (74%) | 59 (100%) | 0 | 100 | 100 |
| 12 | 1 | 137/162 (85%) | 137 (100%) | 0 | 100 | 100 |
| 12 | 12 | 137/162 (85%) | 137 (100%) | 0 | 100 | 100 |
| 12 | Z | 137/162 (85%) | 137 (100%) | 0 | 100 | 100 |
| 12 | Z2 | 137/162 (85%) | 137 (100%) | 0 | 100 | 100 |
| 13 | 3 | 174/230 (76%) | 172 (99%) | 2 (1%) | 65 | 82 |
| 13 | 32 | 174/230 (76%) | 173 (99%) | 1 (1%) | 78 | 88 |
| 14 | 7 | 164/181 (91%) | 164 (100%) | 0 | 100 | 100 |
| 14 | 72 | 164/181 (91%) | 164 (100%) | 0 | 100 | 100 |
| 15 | 8 | 163/183 (89%) | 162 (99%) | 1 (1%) | 78 | 88 |
| 15 | 82 | 163/183 (89%) | 162 (99%) | 1 (1%) | 78 | 88 |
| 16 | 4 | 166/205 (81%) | 166 (100%) | 0 | 100 | 100 |
| 16 | 42 | 166/205 (81%) | 166 (100%) | 0 | 100 | 100 |
| 17 | 5 | 184/206 (89%) | 181 (98%) | 3 (2%) | 55 | 78 |
| 17 | 52 | 184/206 (89%) | 181 (98%) | 3 (2%) | 55 | 78 |
| 18 | 6 | 184/203 (91%) | 184 (100%) | 0 | 100 | 100 |
| 18 | 62 | 184/203 (91%) | 184 (100%) | 0 | 100 | 100 |
| 19 | 9 | 142/159 (89%) | 142 (100%) | 0 | 100 | 100 |
| 19 | 92 | 142/159 (89%) | 142 (100%) | 0 | 100 | 100 |
| All | All | 6612/7606 (87%) | 6585 (100%) | 27 (0%) | 81 | 90 |

All (27) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 154 | THR |
| 1 | A | 293 | ASP |
| 2 | B | 217 | LEU |
| 2 | B | 612 | GLU |
| 4 | D | 150 | LEU |
| 9 | J | 38 | VAL |
| 10 | L | 64 | ILE |
| 13 | 3 | 38 | VAL |
| 13 | 3 | 218 | ILE |
| 15 | 8 | 153 | PHE |
| 17 | 5 | 91 | GLN |
| 17 | 5 | 202 | LEU |
| 17 | 5 | 238 | HIS |
| 1 | A2 | 93 | PHE |
| 1 | A2 | 154 | THR |
| 1 | A2 | 293 | ASP |
| 2 | B2 | 17 | PRO |
| 2 | B2 | 217 | LEU |
| 2 | B2 | 612 | GLU |
| 4 | D2 | 150 | LEU |
| 9 | J2 | 38 | VAL |
| 10 | L2 | 64 | ILE |
| 13 | 32 | 218 | ILE |
| 15 | 82 | 153 | PHE |
| 17 | 52 | 91 | GLN |
| 17 | 52 | 202 | LEU |
| 17 | 52 | 238 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 488 | GLN |
| 1 | A | 659 | GLN |
| 2 | B | 157 | HIS |
| 2 | B | 369 | GLN |
| 2 | B | 606 | ASN |
| 2 | B | 609 | GLN |
| 2 | B | 631 | GLN |
| 10 | L | 108 | ASN |
| 12 | 1 | 180 | ASN |
| 12 | 1 | 195 | HIS |
| 15 | 8 | 220 | ASN |
| 12 | Z | 194 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | 4 | 166 | GLN |
| 17 | 5 | 72 | GLN |
| 17 | 5 | 91 | GLN |
| 17 | 5 | 257 | GLN |
| 18 | 6 | 88 | GLN |
| 19 | 9 | 109 | GLN |
| 1 | A2 | 44 | ASN |
| 1 | A2 | 488 | GLN |
| 1 | A2 | 659 | GLN |
| 2 | B2 | 157 | HIS |
| 2 | B2 | 369 | GLN |
| 2 | B2 | 609 | GLN |
| 2 | B2 | 631 | GLN |
| 4 | D2 | 127 | GLN |
| 6 | F2 | 93 | GLN |
| 10 | L2 | 108 | ASN |
| 12 | 12 | 195 | HIS |
| 15 | 82 | 220 | ASN |
| 12 | Z2 | 194 | GLN |
| 16 | 42 | 166 | GLN |
| 17 | 52 | 72 | GLN |
| 17 | 52 | 91 | GLN |
| 19 | 92 | 109 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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 | $\#\|Z\|>2$ |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 9 | AME | J2 | 1 | 9 | 9,10,11 | 0.54 | 0 | 9,11,13 | 0.88 | 1 (11%) |
| 9 | AME | J | 1 | 9 | 9,10,11 | 0.54 | 0 | 9,11,13 | 0.87 | 1 (11%) |

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 |
|---|---|---|---|---|---|---|---|
| 9 | AME | J2 | 1 | 9 | - | 3/9/10/12 | - |
| 9 | AME | J | 1 | 9 | - | 3/9/10/12 | - |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | J2 | 1 | AME | O-C-CA | -2.56 | 118.17 | 124.77 |
| 9 | J | 1 | AME | O-C-CA | -2.55 | 118.20 | 124.77 |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 9 | J | 1 | AME | C-CA-CB-CG |
| 9 | J | 1 | AME | N-CA-CB-CG |
| 9 | J2 | 1 | AME | C-CA-CB-CG |
| 9 | J2 | 1 | AME | N-CA-CB-CG |
| 9 | J | 1 | AME | CB-CA-N-CT1 |
| 9 | J2 | 1 | AME | CB-CA-N-CT1 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

706 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 | $\#\|Z\| > 2$ |
| 20 | CL0 | A2 | 801 | - | 58,73,73 | 1.48 | 6 (10%) | 60,113,113 | 1.57 | 3 (5%) |
| 21 | CLA | 9 | 603 | 19,27 | 59,63,73 | 1.26 | 5 (8%) | 70,101,113 | 0.89 | 4 (5%) |
| 24 | BCR | L | 201 | - | 41,41,41 | 0.17 | 0 | 56,56,56 | 0.35 | 0 |
| 21 | CLA | B | 802 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | B2 | 828 | - | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.80 | 3 (3%) |
| 21 | CLA | 72 | 603 | - | 56,60,73 | 1.30 | 5 (8%) | 65,97,113 | 0.93 | 3 (4%) |
| 23 | LHG | 42 | 623 | - | 37,37,48 | 0.24 | 0 | 40,43,54 | 0.29 | 0 |
| 27 | LMG | A | 860 | - | 36,36,55 | 0.19 | 0 | 44,44,63 | 0.25 | 0 |
| 26 | LMU | Z | 621 | - | 22,22,36 | 0.14 | 0 | 27,27,47 | 0.26 | 0 |
| 30 | CHL | 72 | 601 | 14 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.04 | 5 (8%) |
| 21 | CLA | Z | 616 | 12 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 27 | LMG | 12 | 624 | - | 36,36,55 | 0.19 | 0 | 44,44,63 | 0.18 | 0 |
| 21 | CLA | A | 845 | 23 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.95 | 2 (3%) |
| 21 | CLA | K2 | 204 | - | 50,54,73 | 1.37 | 4 (8%) | 59,90,113 | 0.98 | 3 (5%) |
| 30 | CHL | 6 | 606 | 33 | 52,66,74 | 2.10 | 10 (19%) | 48,104,114 | 1.18 | 5 (10%) |
| 21 | CLA | 1 | 613 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | B | 823 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.85 | 3 (3%) |
| 28 | LUT | F | 305 | - | 42,43,43 | 0.38 | 0 | 51,60,60 | 0.89 | 2 (3%) |
| 21 | CLA | A2 | 809 | 1 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.89 | 4 (4%) |
| 21 | CLA | A2 | 834 | - | 69,73,73 | 1.20 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | Z2 | 612 | 12 | 49,53,73 | 1.35 | 4 (8%) | 58,89,113 | 0.95 | 2 (3%) |
| 25 | SF4 | C2 | 102 | 3 | 0,12,12 | - | - | - | | |
| 21 | CLA | A | 831 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.82 | 2 (2%) |
| 26 | LMU | 72 | 629 | - | 28,28,36 | 0.10 | 0 | 39,39,47 | 0.28 | 0 |
| 21 | CLA | B | 821 | - | 69,73,73 | 1.20 | 5 (7%) | 82,113,113 | 0.83 | 2 (2%) |
| 30 | CHL | 82 | 601 | 15 | 60,74,74 | 1.93 | 10 (16%) | 58,114,114 | 1.09 | 4 (6%) |
| 23 | LHG | A2 | 847 | 21 | 37,37,48 | 0.26 | 0 | 40,43,54 | 0.30 | 0 |
| 23 | LHG | 8 | 620 | 21 | 43,43,48 | 0.24 | 0 | 46,49,54 | 0.27 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 52 | 617 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 21 | CLA | 5 | 609 | 17 | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 30 | CHL | 5 | 606 | 33 | 40,54,74 | 2.38 | 10 (25%) | 34,90,114 | 1.41 | 5 (14%) |
| 24 | BCR | B | 845 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.36 | 0 |
| 21 | CLA | A | 820 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 62 | 614 | - | 54,58,73 | 1.32 | 4 (7%) | 64,95,113 | 0.94 | 3 (4%) |
| 21 | CLA | 6 | 611 | 23 | 62,66,73 | 1.25 | 4 (6%) | 73,104,113 | 0.87 | 3 (4%) |
| 21 | CLA | K2 | 201 | 11 | 49,53,73 | 1.41 | 4 (8%) | 58,89,113 | 0.97 | 1 (1%) |
| 24 | BCR | 3 | 620 | - | 41,41,41 | 0.19 | 0 | 56,56,56 | 0.36 | 0 |
| 26 | LMU | 8 | 628 | - | 24,24,36 | 0.15 | 0 | 29,29,47 | 0.32 | 0 |
| 21 | CLA | A | 819 | - | 64,68,73 | 1.26 | 4 (6%) | 76,107,113 | 0.87 | 2 (2%) |
| 21 | CLA | A2 | 811 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.81 | 3 (3%) |
| 26 | LMU | A2 | 861 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.30 | 0 |
| 21 | CLA | B2 | 834 | - | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 30 | CHL | 5 | 618 | 17 | 37,51,74 | 2.45 | 10 (27%) | 30,86,114 | 1.48 | 5 (16%) |
| 24 | BCR | A | 849 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.31 | 0 |
| 21 | CLA | B | 841 | 23 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.85 | 4 (4%) |
| 31 | XAT | 72 | 622 | - | 41,47,47 | 0.13 | 0 | 54,74,74 | 0.59 | 0 |
| 21 | CLA | 82 | 613 | 15 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | B | 809 | 2 | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 24 | BCR | B2 | 847 | - | 41,41,41 | 0.19 | 0 | 56,56,56 | 0.41 | 0 |
| 21 | CLA | K | 203 | 33 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.86 | 2 (2%) |
| 26 | LMU | A2 | 858 | - | 36,36,36 | 0.08 | 0 | 47,47,47 | 0.19 | 0 |
| 30 | CHL | 42 | 608 | - | 60,74,74 | 1.96 | 10 (16%) | 58,114,114 | 1.05 | 5 (8%) |
| 21 | CLA | 6 | 613 | 33 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | A2 | 841 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | 5 | 614 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | 4 | 609 | 16 | 64,68,73 | 1.25 | 4 (6%) | 76,107,113 | 0.87 | 2 (2%) |
| 24 | BCR | B | 844 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.46 | 0 |
| 21 | CLA | B | 833 | - | 62,66,73 | 1.21 | 5 (8%) | 73,104,113 | 0.89 | 3 (4%) |
| 30 | CHL | Z | 601 | 12 | 60,74,74 | 1.93 | 10 (16%) | 58,114,114 | 1.11 | 5 (8%) |
| 24 | BCR | B | 843 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.31 | 0 |
| 28 | LUT | 52 | 626 | - | 42,43,43 | 0.24 | 0 | 51,60,60 | 0.40 | 0 |
| 28 | LUT | 7 | 624 | - | 42,43,43 | 0.22 | 0 | 51,60,60 | 0.44 | 0 |
| 26 | LMU | K | 208 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.30 | 0 |
| 21 | CLA | 1 | 612 | 12 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.96 | 3 (5%) |
| 21 | CLA | 32 | 602 | 13 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 25 | SF4 | A2 | 853 | 1,2 | 0,12,12 | - | - | - | | |
| 21 | CLA | 3 | 609 | 13 | 65,69,73 | 1.23 | 4 (6%) | 77,108,113 | 0.84 | 2 (2%) |
| 21 | CLA | 52 | 602 | 17 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 21 | CLA | 5 | 604 | 33 | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.88 | 3 (4%) |
| 21 | CLA | A2 | 816 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 23 | LHG | B2 | 851 | 21 | 44,44,48 | 0.25 | 0 | 47,50,54 | 0.32 | 0 |
| 24 | BCR | 5 | 622 | - | 41,41,41 | 0.17 | 0 | 56,56,56 | 0.33 | 0 |
| 26 | LMU | 42 | 626 | - | 20,20,36 | 0.15 | 0 | 25,25,47 | 0.28 | 0 |
| 30 | CHL | 8 | 607 | 33 | 60,74,74 | 1.91 | 10 (16%) | 58,114,114 | 1.10 | 5 (8%) |
| 21 | CLA | 72 | 613 | 14 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 23 | LHG | 5 | 623 | 21 | 36,36,48 | 0.25 | 0 | 39,42,54 | 0.28 | 0 |
| 22 | PQN | B2 | 842 | - | 34,34,34 | 0.31 | 0 | 43,45,45 | 0.43 | 0 |
| 30 | CHL | 9 | 606 | - | 36,50,74 | 2.54 | 10 (27%) | 29,85,114 | 1.40 | 4 (13%) |
| 21 | CLA | 52 | 614 | - | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 28 | LUT | Z | 617 | - | 42,43,43 | 0.26 | 0 | 51,60,60 | 0.44 | 0 |
| 21 | CLA | B2 | 814 | - | 64,68,73 | 1.20 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 21 | CLA | 42 | 616 | 16 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 22 | PQN | A | 844 | - | 34,34,34 | 0.32 | 0 | 43,45,45 | 0.43 | 0 |
| 21 | CLA | 1 | 609 | 12 | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | B | 811 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | A2 | 813 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.85 | 3 (3%) |
| 26 | LMU | 72 | 628 | - | 22,22,36 | 0.14 | 0 | 27,27,47 | 0.33 | 0 |
| 21 | CLA | B | 837 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 8 | 612 | 15 | 59,63,73 | 1.24 | 4 (6%) | 70,101,113 | 0.87 | 3 (4%) |
| 21 | CLA | 4 | 616 | 16 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | 4 | 612 | 16 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.96 | 3 (5%) |
| 24 | BCR | 9 | 623 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.34 | 0 |
| 21 | CLA | 4 | 604 | 33 | 54,58,73 | 1.32 | 4 (7%) | 64,95,113 | 0.93 | 3 (4%) |
| 28 | LUT | 32 | 622 | - | 42,43,43 | 0.32 | 0 | 51,60,60 | 0.47 | 0 |
| 26 | LMU | Z2 | 622 | - | 32,32,36 | 0.10 | 0 | 43,43,47 | 0.18 | 0 |
| 21 | CLA | B2 | 804 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.94 | 2 (3%) |
| 21 | CLA | 72 | 608 | 33 | 54,58,73 | 1.34 | 4 (7%) | 64,95,113 | 0.91 | 3 (4%) |
| 30 | CHL | 62 | 601 | 18 | 60,74,74 | 1.97 | 10 (16%) | 58,114,114 | 0.99 | 4 (6%) |
| 21 | CLA | A | 824 | - | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.99 | 3 (5%) |
| 21 | CLA | 8 | 610 | 15 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | B2 | 832 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.83 | 2 (2%) |
| 23 | LHG | A2 | 846 | - | 48,48,48 | 0.24 | 0 | 51,54,54 | 0.29 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 24 | BCR | 8 | 619 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.32 | 0 |
| 30 | CHL | 8 | 606 | 33 | 60,74,74 | 1.97 | 10 (16%) | 58,114,114 | 1.09 | 5 (8%) |
| 21 | CLA | Z2 | 614 | - | 54,58,73 | 1.31 | 4 (7%) | 64,95,113 | 0.93 | 3 (4%) |
| 28 | LUT | 6 | 621 | - | 42,43,43 | 0.24 | 0 | 51,60,60 | 0.40 | 0 |
| 24 | BCR | A | 852 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.38 | 0 |
| 30 | CHL | 7 | 607 | 33 | 40,54,74 | 2.39 | 10 (25%) | 34,90,114 | 1.43 | 5 (14%) |
| 21 | CLA | 6 | 610 | 18 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 21 | CLA | 8 | 614 | - | 61,65,73 | 1.25 | 4 (6%) | 72,103,113 | 0.85 | 2 (2%) |
| 27 | LMG | 6 | 633 | - | 19,19,55 | 0.30 | 0 | 19,19,63 | 0.29 | 0 |
| 21 | CLA | B2 | 824 | 33 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.84 | 2 (2%) |
| 23 | LHG | 3 | 721 | - | 30,30,48 | 0.27 | 0 | 33,36,54 | 0.36 | 0 |
| 26 | LMU | 8 | 625 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.27 | 0 |
| 24 | BCR | A2 | 852 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.37 | 0 |
| 21 | CLA | 8 | 608 | 33 | 54,58,73 | 1.35 | 4 (7%) | 64,95,113 | 0.92 | 2 (3%) |
| 21 | CLA | F2 | 301 | 33 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 26 | LMU | A2 | 863 | - | 36,36,36 | 0.09 | 0 | 47,47,47 | 0.27 | 0 |
| 21 | CLA | A | 805 | - | 59,63,73 | 1.28 | 5 (8%) | 70,101,113 | 0.85 | 2 (2%) |
| 26 | LMU | 6 | 632 | - | 20,20,36 | 0.15 | 0 | 25,25,47 | 0.26 | 0 |
| 27 | LMG | 8 | 626 | - | 32,32,55 | 0.19 | 0 | 40,40,63 | 0.19 | 0 |
| 27 | LMG | 4 | 624 | - | 41,41,55 | 0.18 | 0 | 49,49,63 | 0.26 | 0 |
| 21 | CLA | Z | 602 | 12 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 21 | CLA | B2 | 823 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.85 | 3 (3%) |
| 21 | CLA | 5 | 611 | 23 | 59,63,73 | 1.27 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 21 | CLA | 72 | 609 | 14 | 49,53,73 | 1.42 | 4 (8%) | 58,89,113 | 0.96 | 3 (5%) |
| 21 | CLA | 82 | 602 | 15 | 66,70,73 | 1.23 | 5 (7%) | 78,109,113 | 0.84 | 2 (2%) |
| 30 | CHL | 62 | 608 | 33 | 45,59,74 | 2.27 | 10 (22%) | 40,96,114 | 1.28 | 5 (12%) |
| 23 | LHG | 12 | 620 | 21 | 38,38,48 | 0.25 | 0 | 41,44,54 | 0.30 | 0 |
| 21 | CLA | 8 | 611 | 23 | 49,53,73 | 1.40 | 5 (10%) | 58,89,113 | 1.01 | 3 (5%) |
| 21 | CLA | L | 204 | - | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.98 | 3 (5%) |
| 21 | CLA | Z | 609 | 12 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 21 | CLA | A | 822 | 33 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | B2 | 838 | - | 54,58,73 | 1.36 | 4 (7%) | 64,95,113 | 0.91 | 2 (3%) |
| 21 | CLA | A | 838 | - | 55,59,73 | 1.30 | 4 (7%) | 64,96,113 | 0.93 | 2 (3%) |
| 24 | BCR | 32 | 620 | - | 41,41,41 | 0.19 | 0 | 56,56,56 | 0.37 | 0 |
| 21 | CLA | B | 820 | - | 60,64,73 | 1.28 | 4 (6%) | 71,102,113 | 0.87 | 2 (2%) |
| 21 | CLA | 5 | 621 | 33 | 50,54,73 | 1.41 | 4 (8%) | 59,90,113 | 1.07 | 5 (8%) |
| 24 | BCR | 42 | 621 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.36 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | A | 803 | 33 | 69,73,73 | 1.23 | 5 (7%) | 82,113,113 | 0.83 | 4 (4%) |
| 21 | CLA | 3 | 604 | 33 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | B2 | 825 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.79 | 3 (3%) |
| 21 | CLA | 82 | 604 | 33 | 64,68,73 | 1.23 | 5 (7%) | 76,107,113 | 0.87 | 3 (3%) |
| 27 | LMG | J2 | 104 | - | 35,35,55 | 0.19 | 0 | 43,43,63 | 0.20 | 0 |
| 27 | LMG | 1 | 624 | - | 36,36,55 | 0.19 | 0 | 44,44,63 | 0.19 | 0 |
| 21 | CLA | B | 817 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 24 | BCR | A | 848 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.30 | 0 |
| 21 | CLA | B2 | 809 | 2 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 26 | LMU | 7 | 628 | - | 22,22,36 | 0.14 | 0 | 27,27,47 | 0.33 | 0 |
| 23 | LHG | 62 | 619 | 21 | 48,48,48 | 0.22 | 0 | 51,54,54 | 0.24 | 0 |
| 24 | BCR | K2 | 207 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.28 | 0 |
| 21 | CLA | A | 834 | - | 69,73,73 | 1.20 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 28 | LUT | 92 | 616 | - | 42,43,43 | 0.26 | 0 | 51,60,60 | 0.40 | 0 |
| 21 | CLA | B2 | 833 | - | 62,66,73 | 1.21 | 5 (8%) | 73,104,113 | 0.89 | 3 (4%) |
| 21 | CLA | 7 | 608 | 33 | 54,58,73 | 1.33 | 4 (7%) | 64,95,113 | 0.92 | 3 (4%) |
| 30 | CHL | 72 | 607 | 33 | 40,54,74 | 2.39 | 10 (25%) | 34,90,114 | 1.44 | 5 (14%) |
| 29 | DGD | B2 | 850 | - | 60,60,67 | 0.16 | 0 | 74,74,81 | 0.33 | 0 |
| 24 | BCR | 82 | 619 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.32 | 0 |
| 26 | LMU | 6 | 631 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.27 | 0 |
| 21 | CLA | B | 810 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 30 | CHL | Z2 | 607 | 33 | 60,74,74 | 1.96 | 10 (16%) | 58,114,114 | 1.09 | 6 (10%) |
| 21 | CLA | B | 834 | - | 64,68,73 | 1.23 | 5 (7%) | 76,107,113 | 0.86 | 3 (3%) |
| 23 | LHG | 52 | 623 | 21 | 36,36,48 | 0.25 | 0 | 39,42,54 | 0.28 | 0 |
| 30 | CHL | 42 | 607 | 33 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.03 | 4 (6%) |
| 21 | CLA | A2 | 804 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.80 | 3 (3%) |
| 21 | CLA | Z2 | 611 | 23 | 64,68,73 | 1.20 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 24 | BCR | 32 | 719 | - | 41,41,41 | 0.11 | 0 | 56,56,56 | 0.41 | 0 |
| 21 | CLA | F | 304 | 6 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.90 | 3 (3%) |
| 26 | LMU | A | 863 | - | 36,36,36 | 0.09 | 0 | 47,47,47 | 0.27 | 0 |
| 21 | CLA | B | 818 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 26 | LMU | Z | 622 | - | 32,32,36 | 0.10 | 0 | 43,43,47 | 0.17 | 0 |
| 21 | CLA | 9 | 610 | 19 | 64,68,73 | 1.22 | 5 (7%) | 76,107,113 | 0.88 | 3 (3%) |
| 30 | CHL | 42 | 606 | 33 | 50,64,74 | 2.13 | 10 (20%) | 46,102,114 | 1.26 | 6 (13%) |
| 21 | CLA | A | 839 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.83 | 4 (4%) |
| 21 | CLA | B2 | 817 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 7 | 609 | 14 | 49,53,73 | 1.43 | 4 (8%) | 58,89,113 | 0.95 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | B | 831 | - | 59,63,73 | 1.26 | 5 (8%) | 70,101,113 | 0.88 | 3 (4%) |
| 23 | LHG | A | 847 | 21 | 37,37,48 | 0.26 | 0 | 40,43,54 | 0.30 | 0 |
| 21 | CLA | 3 | 611 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 24 | BCR | B2 | 844 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.46 | 0 |
| 31 | XAT | 5 | 624 | - | 41,47,47 | 0.12 | 0 | 54,74,74 | 0.64 | 0 |
| 21 | CLA | B | 838 | - | 54,58,73 | 1.36 | 4 (7%) | 64,95,113 | 0.91 | 2 (3%) |
| 21 | CLA | A | 832 | - | 59,63,73 | 1.26 | 5 (8%) | 70,101,113 | 0.90 | 3 (4%) |
| 24 | BCR | 62 | 623 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.35 | 0 |
| 24 | BCR | 72 | 623 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.38 | 0 |
| 21 | CLA | 42 | 610 | 16 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.83 | 3 (3%) |
| 27 | LMG | 42 | 624 | - | 41,41,55 | 0.18 | 0 | 49,49,63 | 0.26 | 0 |
| 21 | CLA | 92 | 601 | 19 | 50,54,73 | 1.40 | 4 (8%) | 59,90,113 | 0.98 | 3 (5%) |
| 28 | LUT | 12 | 619 | - | 42,43,43 | 0.21 | 0 | 51,60,60 | 0.42 | 0 |
| 30 | CHL | 4 | 606 | 33 | 50,64,74 | 2.13 | 10 (20%) | 46,102,114 | 1.27 | 6 (13%) |
| 26 | LMU | 9 | 624 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.37 | 0 |
| 21 | CLA | F | 301 | 33 | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 26 | LMU | Z2 | 621 | - | 22,22,36 | 0.14 | 0 | 27,27,47 | 0.27 | 0 |
| 27 | LMG | 8 | 629 | - | 42,42,55 | 0.18 | 0 | 50,50,63 | 0.15 | 0 |
| 30 | CHL | 4 | 607 | 33 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.03 | 4 (6%) |
| 26 | LMU | 1 | 623 | - | 24,24,36 | 0.13 | 0 | 29,29,47 | 0.27 | 0 |
| 21 | CLA | 52 | 610 | 17 | 64,68,73 | 1.21 | 4 (6%) | 76,107,113 | 0.83 | 3 (3%) |
| 21 | CLA | B | 812 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.84 | 2 (2%) |
| 21 | CLA | B2 | 826 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 24 | BCR | 3 | 718 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.34 | 0 |
| 21 | CLA | 7 | 611 | 23 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 24 | BCR | 6 | 623 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.35 | 0 |
| 21 | CLA | A2 | 835 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 26 | LMU | 4 | 626 | - | 20,20,36 | 0.15 | 0 | 25,25,47 | 0.28 | 0 |
| 21 | CLA | A | 840 | - | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 28 | LUT | 1 | 617 | - | 42,43,43 | 0.26 | 0 | 51,60,60 | 0.42 | 0 |
| 26 | LMU | 52 | 627 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.26 | 0 |
| 21 | CLA | 6 | 602 | 18 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 1 | 614 | - | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 21 | CLA | 12 | 612 | 12 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.96 | 2 (3%) |
| 21 | CLA | 3 | 602 | 13 | 64,68,73 | 1.23 | 5 (7%) | 76,107,113 | 0.85 | 3 (3%) |
| 30 | CHL | 62 | 606 | 33 | 52,66,74 | 2.10 | 10 (19%) | 48,104,114 | 1.18 | 5 (10%) |
| 24 | BCR | L | 205 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.39 | 0 |
| 21 | CLA | 6 | 604 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 27 | LMG | A2 | 860 | - | 36,36,55 | 0.19 | 0 | 44,44,63 | 0.26 | 0 |
| 21 | CLA | B | 816 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | 72 | 620 | 33 | 57,61,73 | 1.29 | 4 (7%) | 67,98,113 | 0.89 | 2 (2%) |
| 21 | CLA | G2 | 204 | 7 | 50,54,73 | 1.38 | 4 (8%) | 59,90,113 | 0.96 | 3 (5%) |
| 30 | CHL | 3 | 608 | 33 | 60,74,74 | 1.99 | 10 (16%) | 58,114,114 | 1.10 | 5 (8%) |
| 23 | LHG | 62 | 629 | - | 35,35,48 | 0.26 | 0 | 38,41,54 | 0.29 | 0 |
| 28 | LUT | F2 | 305 | - | 42,43,43 | 0.37 | 0 | 51,60,60 | 0.89 | 2 (3%) |
| 31 | XAT | 82 | 618 | - | 41,47,47 | 0.15 | 0 | 54,74,74 | 0.61 | 0 |
| 23 | LHG | 72 | 625 | 21 | 48,48,48 | 0.23 | 0 | 51,54,54 | 0.23 | 0 |
| 21 | CLA | 1 | 604 | 33 | 54,58,73 | 1.32 | 4 (7%) | 64,95,113 | 0.94 | 3 (4%) |
| 26 | LMU | K2 | 208 | - | 24,24,36 | 0.10 | 0 | 29,29,47 | 0.30 | 0 |
| 30 | CHL | 6 | 608 | 33 | 45,59,74 | 2.25 | 10 (22%) | 40,96,114 | 1.28 | 5 (12%) |
| 21 | CLA | B | 835 | 33 | 49,53,73 | 1.41 | 4 (8%) | 58,89,113 | 0.97 | 2 (3%) |
| 21 | CLA | 4 | 614 | - | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.88 | 3 (4%) |
| 21 | CLA | 82 | 610 | 15 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 24 | BCR | I | 172 | - | 41,41,41 | 0.20 | 0 | 56,56,56 | 0.37 | 0 |
| 21 | CLA | A | 813 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.85 | 3 (3%) |
| 26 | LMU | 12 | 627 | - | 22,22,36 | 0.13 | 0 | 27,27,47 | 0.30 | 0 |
| 23 | LHG | 6 | 629 | - | 35,35,48 | 0.26 | 0 | 38,41,54 | 0.29 | 0 |
| 26 | LMU | 5 | 627 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.26 | 0 |
| 26 | LMU | 7 | 627 | - | 33,33,36 | 0.10 | 0 | 44,44,47 | 0.17 | 0 |
| 21 | CLA | 82 | 614 | - | 61,65,73 | 1.26 | 4 (6%) | 72,103,113 | 0.86 | 2 (2%) |
| 21 | CLA | Z2 | 603 | - | 59,63,73 | 1.28 | 5 (8%) | 70,101,113 | 0.87 | 2 (2%) |
| 21 | CLA | 72 | 616 | 14 | 50,54,73 | 1.37 | 4 (8%) | 59,90,113 | 0.95 | 3 (5%) |
| 21 | CLA | 7 | 603 | - | 56,60,73 | 1.31 | 5 (8%) | 65,97,113 | 0.93 | 3 (4%) |
| 32 | NEX | 52 | 625 | - | 40,46,46 | 0.45 | 1 (2%) | 50,70,70 | 0.80 | 3 (6%) |
| 21 | CLA | 9 | 614 | - | 49,53,73 | 1.43 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | F2 | 304 | 6 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.90 | 3 (3%) |
| 27 | LMG | 82 | 626 | - | 32,32,55 | 0.20 | 0 | 40,40,63 | 0.19 | 0 |
| 21 | CLA | 9 | 609 | 19 | 55,59,73 | 1.31 | 4 (7%) | 64,96,113 | 0.92 | 3 (4%) |
| 21 | CLA | A2 | 812 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.80 | 4 (4%) |
| 21 | CLA | Z | 612 | 12 | 49,53,73 | 1.36 | 4 (8%) | 58,89,113 | 0.95 | 2 (3%) |
| 25 | SF4 | C2 | 101 | 3 | 0,12,12 | - | - | - | | |
| 21 | CLA | 7 | 602 | 14 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | 72 | 610 | 14 | 69,73,73 | 1.21 | 4 (5%) | 82,113,113 | 0.86 | 3 (3%) |
| 21 | CLA | B | 805 | - | 69,73,73 | 1.14 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 5 | 603 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | A | 815 | - | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.87 | 2 (2%) |
| 21 | CLA | B2 | 806 | 2 | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.77 | 2 (2%) |
| 21 | CLA | 12 | 603 | - | 61,65,73 | 1.25 | 4 (6%) | 72,103,113 | 0.86 | 2 (2%) |
| 28 | LUT | Z2 | 619 | - | 26,26,43 | 0.38 | 0 | 33,35,60 | 0.37 | 0 |
| 23 | LHG | 32 | 721 | - | 30,30,48 | 0.26 | 0 | 33,36,54 | 0.36 | 0 |
| 25 | SF4 | C | 102 | 3 | 0,12,12 | - | - | - | | |
| 21 | CLA | Z | 610 | 12 | 64,68,73 | 1.20 | 4 (6%) | 76,107,113 | 0.84 | 3 (3%) |
| 21 | CLA | L2 | 204 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.98 | 3 (5%) |
| 21 | CLA | 62 | 609 | 18 | 59,63,73 | 1.26 | 4 (6%) | 70,101,113 | 0.93 | 4 (5%) |
| 24 | BCR | L2 | 205 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.39 | 0 |
| 24 | BCR | A2 | 850 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.24 | 0 |
| 32 | NEX | 62 | 625 | - | 40,46,46 | 0.28 | 0 | 50,70,70 | 0.88 | 3 (6%) |
| 21 | CLA | 32 | 604 | 33 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | 82 | 603 | - | 69,73,73 | 1.20 | 5 (7%) | 82,113,113 | 0.81 | 3 (3%) |
| 21 | CLA | B2 | 812 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.84 | 2 (2%) |
| 21 | CLA | 82 | 616 | 15 | 49,53,73 | 1.38 | 5 (10%) | 58,89,113 | 0.99 | 3 (5%) |
| 26 | LMU | A | 865 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.46 | 0 |
| 21 | CLA | 52 | 604 | 33 | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 30 | CHL | 62 | 607 | 33 | 60,74,74 | 1.94 | 10 (16%) | 58,114,114 | 1.12 | 6 (10%) |
| 21 | CLA | 32 | 613 | 13 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 23 | LHG | 32 | 623 | - | 46,46,48 | 0.22 | 0 | 49,52,54 | 0.27 | 0 |
| 28 | LUT | 42 | 619 | - | 42,43,43 | 0.24 | 0 | 51,60,60 | 0.49 | 0 |
| 21 | CLA | 32 | 603 | - | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 26 | LMU | G2 | 206 | - | 24,24,36 | 0.13 | 0 | 29,29,47 | 0.24 | 0 |
| 21 | CLA | A | 808 | - | 54,58,73 | 1.33 | 5 (9%) | 64,95,113 | 0.91 | 2 (3%) |
| 21 | CLA | B2 | 829 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.84 | 2 (2%) |
| 21 | CLA | A | 804 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.81 | 3 (3%) |
| 21 | CLA | 7 | 620 | 33 | 57,61,73 | 1.29 | 4 (7%) | 67,98,113 | 0.89 | 2 (2%) |
| 21 | CLA | 62 | 604 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 21 | CLA | 9 | 604 | 19 | 57,61,73 | 1.27 | 5 (8%) | 67,98,113 | 0.91 | 3 (4%) |
| 21 | CLA | B2 | 830 | - | 49,53,73 | 1.36 | 5 (10%) | 58,89,113 | 0.99 | 3 (5%) |
| 30 | CHL | 82 | 606 | 33 | 60,74,74 | 1.96 | 10 (16%) | 58,114,114 | 1.08 | 5 (8%) |
| 30 | CHL | 7 | 601 | 14 | 60,74,74 | 1.94 | 10 (16%) | 58,114,114 | 1.05 | 5 (8%) |
| 30 | CHL | 52 | 618 | 17 | 37,51,74 | 2.45 | 10 (27%) | 30,86,114 | 1.48 | 5 (16%) |
| 24 | BCR | K | 207 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.27 | 0 |
| 24 | BCR | B2 | 801 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.38 | 0 |
| 21 | CLA | 32 | 609 | 13 | 65,69,73 | 1.22 | 4 (6%) | 77,108,113 | 0.84 | 2 (2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 28 | LUT | 9 | 616 | - | 42,43,43 | 0.26 | 0 | 51,60,60 | 0.39 | 0 |
| 26 | LMU | A | 858 | - | 36,36,36 | 0.08 | 0 | 47,47,47 | 0.19 | 0 |
| 21 | CLA | 62 | 611 | 23 | 62,66,73 | 1.24 | 4 (6%) | 73,104,113 | 0.87 | 3 (4%) |
| 21 | CLA | A2 | 815 | - | 59,63,73 | 1.29 | 4 (6%) | 70,101,113 | 0.86 | 2 (2%) |
| 21 | CLA | 52 | 609 | 17 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 30 | CHL | 5 | 607 | 33 | 60,74,74 | 1.99 | 10 (16%) | 58,114,114 | 0.98 | 4 (6%) |
| 28 | LUT | 3 | 720 | - | 42,43,43 | 0.23 | 0 | 51,60,60 | 0.34 | 0 |
| 21 | CLA | F2 | 303 | 33 | 49,53,73 | 1.38 | 4 (8%) | 58,89,113 | 0.96 | 3 (5%) |
| 21 | CLA | Z2 | 616 | 12 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 21 | CLA | A | 826 | 33 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | A | 842 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.83 | 2 (2%) |
| 21 | CLA | 8 | 603 | - | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 21 | CLA | 62 | 613 | 33 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | 42 | 602 | 16 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 31 | XAT | 8 | 618 | - | 41,47,47 | 0.16 | 0 | 54,74,74 | 0.60 | 0 |
| 28 | LUT | 62 | 621 | - | 42,43,43 | 0.23 | 0 | 51,60,60 | 0.40 | 0 |
| 21 | CLA | B2 | 841 | 23 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.84 | 4 (4%) |
| 21 | CLA | 42 | 612 | 16 | 49,53,73 | 1.38 | 4 (8%) | 58,89,113 | 0.95 | 2 (3%) |
| 23 | LHG | 4 | 622 | 21 | 48,48,48 | 0.23 | 0 | 51,54,54 | 0.27 | 0 |
| 21 | CLA | B2 | 822 | - | 63,67,73 | 1.22 | 4 (6%) | 74,105,113 | 0.87 | 3 (4%) |
| 30 | CHL | Z2 | 606 | 33 | 40,54,74 | 2.35 | 10 (25%) | 34,90,114 | 1.43 | 5 (14%) |
| 21 | CLA | 32 | 614 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | B2 | 820 | - | 60,64,73 | 1.28 | 4 (6%) | 71,102,113 | 0.87 | 2 (2%) |
| 27 | LMG | 62 | 633 | - | 19,19,55 | 0.30 | 0 | 19,19,63 | 0.29 | 0 |
| 21 | CLA | B2 | 819 | 33 | 64,68,73 | 1.24 | 5 (7%) | 76,107,113 | 0.84 | 3 (3%) |
| 26 | LMU | 12 | 623 | - | 24,24,36 | 0.13 | 0 | 29,29,47 | 0.27 | 0 |
| 21 | CLA | Z | 608 | 33 | 54,58,73 | 1.34 | 4 (7%) | 64,95,113 | 0.95 | 3 (4%) |
| 26 | LMU | 62 | 632 | - | 20,20,36 | 0.15 | 0 | 25,25,47 | 0.25 | 0 |
| 24 | BCR | 52 | 622 | - | 41,41,41 | 0.17 | 0 | 56,56,56 | 0.32 | 0 |
| 28 | LUT | 3 | 621 | - | 42,43,43 | 0.29 | 0 | 51,60,60 | 0.40 | 0 |
| 21 | CLA | 5 | 613 | 17 | 60,64,73 | 1.24 | 4 (6%) | 71,102,113 | 0.88 | 3 (4%) |
| 31 | XAT | 7 | 622 | - | 41,47,47 | 0.13 | 0 | 54,74,74 | 0.59 | 0 |
| 21 | CLA | 7 | 610 | 14 | 69,73,73 | 1.21 | 4 (5%) | 82,113,113 | 0.86 | 3 (3%) |
| 21 | CLA | B2 | 836 | - | 64,68,73 | 1.21 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 26 | LMU | 1 | 626 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.27 | 0 |
| 21 | CLA | B2 | 802 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | 32 | 611 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 92 | 604 | 19 | 57,61,73 | 1.27 | 5 (8%) | 67,98,113 | 0.91 | 3 (4%) |
| 21 | CLA | 5 | 617 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 26 | LMU | A2 | 862 | - | 20,20,36 | 0.12 | 0 | 25,25,47 | 0.28 | 0 |
| 21 | CLA | A2 | 838 | - | 55,59,73 | 1.30 | 4 (7%) | 64,96,113 | 0.93 | 2 (3%) |
| 21 | CLA | 12 | 609 | 12 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 30 | CHL | 12 | 606 | 33 | 40,54,74 | 2.40 | 10 (25%) | 34,90,114 | 1.38 | 5 (14%) |
| 21 | CLA | B2 | 803 | - | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.78 | 2 (2%) |
| 21 | CLA | 52 | 601 | 17 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 2 (2%) |
| 30 | CHL | 52 | 606 | 33 | 40,54,74 | 2.39 | 10 (25%) | 34,90,114 | 1.41 | 5 (14%) |
| 21 | CLA | K | 201 | 11 | 49,53,73 | 1.41 | 4 (8%) | 58,89,113 | 0.97 | 2 (3%) |
| 30 | CHL | 7 | 606 | 33 | 40,54,74 | 2.38 | 10 (25%) | 34,90,114 | 1.40 | 5 (14%) |
| 21 | CLA | B | 813 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 6 | 617 | - | 49,53,73 | 1.41 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | A2 | 840 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 21 | CLA | 3 | 617 | 13 | 50,54,73 | 1.38 | 4 (8%) | 59,90,113 | 0.98 | 2 (3%) |
| 21 | CLA | B2 | 821 | - | 69,73,73 | 1.21 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | B2 | 805 | - | 69,73,73 | 1.14 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 24 | BCR | A2 | 848 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.30 | 0 |
| 30 | CHL | 1 | 606 | 33 | 40,54,74 | 2.40 | 10 (25%) | 34,90,114 | 1.39 | 5 (14%) |
| 31 | XAT | 6 | 624 | - | 41,47,47 | 0.13 | 0 | 54,74,74 | 0.64 | 0 |
| 24 | BCR | B | 846 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.34 | 0 |
| 28 | LUT | 9 | 617 | - | 42,43,43 | 0.21 | 0 | 51,60,60 | 0.40 | 0 |
| 28 | LUT | 92 | 617 | - | 42,43,43 | 0.21 | 0 | 51,60,60 | 0.40 | 0 |
| 31 | XAT | 1 | 618 | - | 41,47,47 | 0.13 | 0 | 54,74,74 | 0.70 | 1 (1%) |
| 21 | CLA | 7 | 613 | 14 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.84 | 2 (2%) |
| 28 | LUT | 72 | 621 | - | 42,43,43 | 0.25 | 0 | 51,60,60 | 0.39 | 0 |
| 21 | CLA | A2 | 825 | - | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 21 | CLA | 62 | 603 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 21 | CLA | 32 | 617 | 13 | 50,54,73 | 1.38 | 4 (8%) | 59,90,113 | 0.98 | 2 (3%) |
| 21 | CLA | 12 | 614 | - | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.88 | 3 (3%) |
| 21 | CLA | A2 | 808 | - | 54,58,73 | 1.33 | 4 (7%) | 64,95,113 | 0.91 | 2 (3%) |
| 21 | CLA | B2 | 827 | - | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.83 | 2 (2%) |
| 21 | CLA | A2 | 805 | - | 59,63,73 | 1.28 | 5 (8%) | 70,101,113 | 0.85 | 2 (2%) |
| 21 | CLA | A2 | 826 | 33 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | B | 839 | 33 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.85 | 3 (3%) |
| 26 | LMU | 1 | 621 | - | 36,36,36 | 0.09 | 0 | 47,47,47 | 0.29 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 8 | 604 | 33 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 21 | CLA | A2 | 824 | - | 49,53,73 | 1.39 | 5 (10%) | 58,89,113 | 0.99 | 3 (5%) |
| 28 | LUT | 1 | 619 | - | 42,43,43 | 0.21 | 0 | 51,60,60 | 0.42 | 0 |
| 21 | CLA | 3 | 603 | - | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | 12 | 613 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | A | 830 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 27 | LMG | A2 | 859 | - | 48,48,55 | 0.18 | 0 | 56,56,63 | 0.17 | 0 |
| 21 | CLA | B | 807 | - | 59,63,73 | 1.29 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 21 | CLA | 92 | 614 | - | 49,53,73 | 1.43 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 30 | CHL | 1 | 601 | 12 | 60,74,74 | 1.94 | 10 (16%) | 58,114,114 | 1.05 | 4 (6%) |
| 21 | CLA | Z2 | 609 | 12 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 24 | BCR | K2 | 202 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.37 | 0 |
| 27 | LMG | 92 | 620 | 21 | 44,44,55 | 0.17 | 0 | 52,52,63 | 0.36 | 0 |
| 21 | CLA | B2 | 835 | 33 | 49,53,73 | 1.40 | 5 (10%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | 52 | 603 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | 52 | 612 | 17 | 49,53,73 | 1.37 | 4 (8%) | 58,89,113 | 0.96 | 2 (3%) |
| 26 | LMU | 62 | 631 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.28 | 0 |
| 24 | BCR | B | 847 | - | 41,41,41 | 0.19 | 0 | 56,56,56 | 0.41 | 0 |
| 27 | LMG | B | 852 | - | 43,43,55 | 0.17 | 0 | 51,51,63 | 0.23 | 0 |
| 21 | CLA | 9 | 601 | 19 | 50,54,73 | 1.39 | 4 (8%) | 59,90,113 | 0.98 | 3 (5%) |
| 21 | CLA | K | 206 | 11 | 49,53,73 | 1.39 | 4 (8%) | 58,89,113 | 0.97 | 2 (3%) |
| 26 | LMU | 62 | 630 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.28 | 0 |
| 21 | CLA | Z | 611 | 23 | 64,68,73 | 1.20 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 21 | CLA | 5 | 610 | 17 | 64,68,73 | 1.21 | 4 (6%) | 76,107,113 | 0.84 | 3 (3%) |
| 21 | CLA | 92 | 611 | 23 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | 82 | 612 | 15 | 59,63,73 | 1.25 | 4 (6%) | 70,101,113 | 0.87 | 2 (2%) |
| 31 | XAT | 42 | 620 | - | 41,47,47 | 0.12 | 0 | 54,74,74 | 0.68 | 0 |
| 21 | CLA | A | 825 | - | 59,63,73 | 1.28 | 5 (8%) | 70,101,113 | 0.89 | 3 (4%) |
| 24 | BCR | B2 | 846 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.35 | 0 |
| 21 | CLA | A | 829 | - | 69,73,73 | 1.23 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 9 | 612 | 19 | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | 32 | 607 | 13 | 59,63,73 | 1.27 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 24 | BCR | 7 | 623 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.38 | 0 |
| 21 | CLA | 12 | 608 | 33 | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 4 | 603 | 16 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.80 | 2 (2%) |
| 21 | CLA | A | 814 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 28 | LUT | 32 | 621 | - | 42,43,43 | 0.28 | 0 | 51,60,60 | 0.40 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 3 | 615 | 33 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | Z2 | 608 | 33 | 54,58,73 | 1.34 | 4 (7%) | 64,95,113 | 0.94 | 3 (4%) |
| 23 | LHG | 82 | 620 | 21 | 43,43,48 | 0.24 | 0 | 46,49,54 | 0.27 | 0 |
| 31 | XAT | 52 | 624 | - | 41,47,47 | 0.11 | 0 | 54,74,74 | 0.64 | 0 |
| 21 | CLA | B2 | 811 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.83 | 2 (2%) |
| 21 | CLA | A2 | 820 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | A2 | 836 | - | 69,73,73 | 1.20 | 5 (7%) | 82,113,113 | 0.82 | 2 (2%) |
| 21 | CLA | A2 | 837 | 1 | 61,65,73 | 1.31 | 4 (6%) | 72,103,113 | 0.91 | 3 (4%) |
| 23 | LHG | B | 851 | 21 | 44,44,48 | 0.25 | 0 | 47,50,54 | 0.32 | 0 |
| 21 | CLA | 5 | 616 | 17 | 57,61,73 | 1.29 | 4 (7%) | 67,98,113 | 0.91 | 2 (2%) |
| 21 | CLA | 72 | 602 | 14 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 7 | 604 | 33 | 55,59,73 | 1.30 | 4 (7%) | 64,96,113 | 0.93 | 3 (4%) |
| 21 | CLA | 4 | 602 | 16 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 21 | CLA | Z | 614 | - | 54,58,73 | 1.31 | 4 (7%) | 64,95,113 | 0.93 | 3 (4%) |
| 21 | CLA | Z2 | 604 | 33 | 61,65,73 | 1.24 | 4 (6%) | 72,103,113 | 0.87 | 3 (4%) |
| 30 | CHL | 6 | 616 | 18 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.09 | 6 (10%) |
| 21 | CLA | 42 | 604 | 33 | 54,58,73 | 1.32 | 4 (7%) | 64,95,113 | 0.94 | 3 (4%) |
| 30 | CHL | 5 | 608 | 33 | 45,59,74 | 2.26 | 10 (22%) | 40,96,114 | 1.33 | 5 (12%) |
| 21 | CLA | A2 | 823 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.81 | 3 (3%) |
| 27 | LMG | 12 | 628 | - | 42,42,55 | 0.18 | 0 | 50,50,63 | 0.28 | 0 |
| 21 | CLA | 42 | 613 | 16 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.83 | 2 (2%) |
| 26 | LMU | 82 | 625 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.28 | 0 |
| 21 | CLA | F | 303 | 33 | 49,53,73 | 1.38 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 23 | LHG | 9 | 622 | 21 | 40,40,48 | 0.24 | 0 | 43,46,54 | 0.29 | 0 |
| 26 | LMU | 82 | 624 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.26 | 0 |
| 24 | BCR | 92 | 623 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.35 | 0 |
| 21 | CLA | 12 | 611 | 23 | 65,69,73 | 1.21 | 4 (6%) | 77,108,113 | 0.83 | 3 (3%) |
| 31 | XAT | 4 | 620 | - | 41,47,47 | 0.11 | 0 | 54,74,74 | 0.68 | 0 |
| 27 | LMG | 7 | 626 | - | 37,37,55 | 0.19 | 0 | 45,45,63 | 0.27 | 0 |
| 21 | CLA | B | 808 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 3 | 613 | 13 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.86 | 3 (3%) |
| 21 | CLA | 12 | 610 | 12 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.81 | 3 (3%) |
| 21 | CLA | B | 815 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | A2 | 827 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | K2 | 206 | 11 | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.98 | 3 (5%) |
| 21 | CLA | B | 832 | - | 69,73,73 | 1.14 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | A | 854 | 33 | 69,73,73 | 1.24 | 5 (7%) | 82,113,113 | 0.79 | 2 (2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | A2 | 839 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.84 | 4 (4%) |
| 23 | LHG | Z | 620 | 21 | 38,38,48 | 0.25 | 0 | 41,44,54 | 0.29 | 0 |
| 21 | CLA | A2 | 806 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 24 | BCR | J2 | 102 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.30 | 0 |
| 30 | CHL | 52 | 608 | 33 | 45,59,74 | 2.27 | 10 (22%) | 40,96,114 | 1.33 | 5 (12%) |
| 21 | CLA | A2 | 819 | - | 64,68,73 | 1.25 | 4 (6%) | 76,107,113 | 0.86 | 2 (2%) |
| 21 | CLA | 8 | 616 | 15 | 49,53,73 | 1.38 | 5 (10%) | 58,89,113 | 0.99 | 3 (5%) |
| 24 | BCR | A2 | 849 | - | 41,41,41 | 0.17 | 0 | 56,56,56 | 0.31 | 0 |
| 24 | BCR | A2 | 851 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.34 | 0 |
| 21 | CLA | J | 101 | 9 | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.88 | 2 (2%) |
| 26 | LMU | 42 | 625 | - | 34,34,36 | 0.10 | 0 | 45,45,47 | 0.20 | 0 |
| 23 | LHG | 42 | 622 | 21 | 48,48,48 | 0.23 | 0 | 51,54,54 | 0.27 | 0 |
| 30 | CHL | 12 | 607 | 33 | 40,54,74 | 2.41 | 10 (25%) | 34,90,114 | 1.27 | 4 (11%) |
| 21 | CLA | 1 | 608 | 33 | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.83 | 2 (2%) |
| 21 | CLA | 4 | 613 | 16 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.84 | 2 (2%) |
| 26 | LMU | G | 206 | - | 24,24,36 | 0.13 | 0 | 29,29,47 | 0.25 | 0 |
| 21 | CLA | A2 | 828 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.78 | 2 (2%) |
| 21 | CLA | B2 | 831 | - | 59,63,73 | 1.26 | 5 (8%) | 70,101,113 | 0.88 | 3 (4%) |
| 21 | CLA | 8 | 602 | 15 | 66,70,73 | 1.23 | 5 (7%) | 78,109,113 | 0.84 | 2 (2%) |
| 21 | CLA | A2 | 832 | - | 59,63,73 | 1.26 | 5 (8%) | 70,101,113 | 0.90 | 2 (2%) |
| 26 | LMU | 4 | 625 | - | 34,34,36 | 0.11 | 0 | 45,45,47 | 0.20 | 0 |
| 28 | LUT | 5 | 626 | - | 42,43,43 | 0.25 | 0 | 51,60,60 | 0.40 | 0 |
| 26 | LMU | A | 857 | - | 35,35,36 | 0.09 | 0 | 46,46,47 | 0.18 | 0 |
| 21 | CLA | 92 | 609 | 19 | 55,59,73 | 1.32 | 5 (9%) | 64,96,113 | 0.93 | 3 (4%) |
| 30 | CHL | 92 | 606 | - | 36,50,74 | 2.53 | 10 (27%) | 29,85,114 | 1.39 | 4 (13%) |
| 27 | LMG | 3 | 722 | - | 44,44,55 | 0.20 | 0 | 46,46,63 | 0.25 | 0 |
| 27 | LMG | J2 | 103 | - | 42,42,55 | 0.17 | 0 | 50,50,63 | 0.39 | 0 |
| 21 | CLA | 42 | 611 | 23 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 26 | LMU | 12 | 626 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.27 | 0 |
| 21 | CLA | B | 814 | - | 64,68,73 | 1.21 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 30 | CHL | 92 | 607 | 33 | 45,59,74 | 2.20 | 10 (22%) | 40,96,114 | 1.24 | 7 (17%) |
| 21 | CLA | A | 817 | 33 | 59,63,73 | 1.30 | 4 (6%) | 70,101,113 | 0.88 | 2 (2%) |
| 21 | CLA | A | 835 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 25 | SF4 | A | 853 | 1,2 | 0,12,12 | - | - | - | | |
| 27 | LMG | J | 103 | - | 42,42,55 | 0.17 | 0 | 50,50,63 | 0.38 | 0 |
| 21 | CLA | A | 833 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 26 | LMU | 6 | 628 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.29 | 0 |
| 21 | CLA | A2 | 818 | - | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 30 | CHL | 1 | 607 | 33 | 40,54,74 | 2.42 | 10 (25%) | 34,90,114 | 1.28 | 4 (11%) |
| 21 | CLA | B | 804 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.94 | 2 (3%) |
| 27 | LMG | B2 | 854 | - | 36,36,55 | 0.20 | 0 | 44,44,63 | 0.17 | 0 |
| 21 | CLA | 72 | 612 | 14 | 56,60,73 | 1.28 | 4 (7%) | 65,97,113 | 0.89 | 2 (3%) |
| 21 | CLA | 6 | 614 | - | 54,58,73 | 1.32 | 4 (7%) | 64,95,113 | 0.93 | 3 (4%) |
| 32 | NEX | 6 | 625 | - | 40,46,46 | 0.20 | 0 | 50,70,70 | 0.84 | 3 (6%) |
| 28 | LUT | A | 856 | - | 42,43,43 | 0.27 | 0 | 51,60,60 | 0.41 | 0 |
| 24 | BCR | 32 | 718 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.34 | 0 |
| 21 | CLA | B | 803 | - | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.78 | 2 (2%) |
| 21 | CLA | A | 828 | - | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.78 | 2 (2%) |
| 21 | CLA | 62 | 602 | 18 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | A2 | 830 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 24 | BCR | G | 205 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.32 | 0 |
| 21 | CLA | 92 | 613 | 19 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.85 | 4 (4%) |
| 21 | CLA | A2 | 803 | 33 | 69,73,73 | 1.23 | 5 (7%) | 82,113,113 | 0.83 | 4 (4%) |
| 31 | XAT | Z | 618 | - | 41,47,47 | 0.14 | 0 | 54,74,74 | 0.61 | 0 |
| 26 | LMU | 1 | 622 | - | 19,19,36 | 0.13 | 0 | 24,24,47 | 0.31 | 0 |
| 21 | CLA | B | 824 | 33 | 69,73,73 | 1.21 | 4 (5%) | 82,113,113 | 0.83 | 2 (2%) |
| 26 | LMU | 12 | 621 | - | 36,36,36 | 0.09 | 0 | 47,47,47 | 0.29 | 0 |
| 21 | CLA | B2 | 818 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | A2 | 810 | 1 | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.85 | 2 (2%) |
| 30 | CHL | 8 | 601 | 15 | 60,74,74 | 1.93 | 10 (16%) | 58,114,114 | 1.09 | 4 (6%) |
| 26 | LMU | 72 | 627 | - | 33,33,36 | 0.10 | 0 | 44,44,47 | 0.17 | 0 |
| 21 | CLA | 6 | 622 | 33 | 59,63,73 | 1.29 | 4 (6%) | 70,101,113 | 0.87 | 2 (2%) |
| 30 | CHL | 82 | 607 | 33 | 60,74,74 | 1.92 | 10 (16%) | 58,114,114 | 1.11 | 5 (8%) |
| 23 | LHG | 4 | 623 | - | 37,37,48 | 0.24 | 0 | 40,43,54 | 0.29 | 0 |
| 26 | LMU | 8 | 627 | - | 36,36,36 | 0.10 | 0 | 47,47,47 | 0.37 | 0 |
| 21 | CLA | 5 | 602 | 17 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 30 | CHL | 42 | 618 | 16 | 40,54,74 | 2.36 | 10 (25%) | 34,90,114 | 1.37 | 5 (14%) |
| 26 | LMU | A | 864 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.28 | 0 |
| 21 | CLA | 32 | 606 | 33 | 46,50,73 | 1.46 | 4 (8%) | 53,85,113 | 1.00 | 2 (3%) |
| 30 | CHL | 6 | 607 | 33 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.11 | 6 (10%) |
| 21 | CLA | A | 827 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 30 | CHL | 9 | 607 | 33 | 45,59,74 | 2.25 | 10 (22%) | 40,96,114 | 1.20 | 6 (15%) |
| 24 | BCR | G2 | 205 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.32 | 0 |
| 21 | CLA | 5 | 612 | 17 | 49,53,73 | 1.38 | 4 (8%) | 58,89,113 | 0.96 | 2 (3%) |
| 24 | BCR | L2 | 201 | - | 41,41,41 | 0.17 | 0 | 56,56,56 | 0.35 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | A2 | 829 | - | 69,73,73 | 1.23 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 28 | LUT | Z | 619 | - | 26,26,43 | 0.38 | 0 | 33,35,60 | 0.37 | 0 |
| 21 | CLA | B | 840 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 30 | CHL | Z | 606 | 33 | 40,54,74 | 2.34 | 10 (25%) | 34,90,114 | 1.43 | 5 (14%) |
| 30 | CHL | 4 | 618 | 16 | 40,54,74 | 2.36 | 10 (25%) | 34,90,114 | 1.37 | 5 (14%) |
| 26 | LMU | 1 | 625 | - | 24,24,36 | 0.10 | 0 | 29,29,47 | 0.30 | 0 |
| 21 | CLA | K2 | 203 | 33 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.86 | 2 (2%) |
| 21 | CLA | B2 | 810 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 24 | BCR | B | 848 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.47 | 0 |
| 23 | LHG | 7 | 625 | 21 | 48,48,48 | 0.23 | 0 | 51,54,54 | 0.23 | 0 |
| 21 | CLA | B | 825 | 33 | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.80 | 3 (3%) |
| 21 | CLA | 52 | 613 | 17 | 60,64,73 | 1.24 | 4 (6%) | 71,102,113 | 0.88 | 3 (4%) |
| 21 | CLA | A | 841 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 24 | BCR | I2 | 172 | - | 41,41,41 | 0.19 | 0 | 56,56,56 | 0.37 | 0 |
| 24 | BCR | B2 | 848 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.47 | 0 |
| 21 | CLA | 1 | 611 | 23 | 65,69,73 | 1.21 | 4 (6%) | 77,108,113 | 0.83 | 3 (3%) |
| 21 | CLA | A | 836 | - | 69,73,73 | 1.20 | 5 (7%) | 82,113,113 | 0.82 | 2 (2%) |
| 21 | CLA | A2 | 842 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.84 | 2 (2%) |
| 27 | LMG | B2 | 852 | - | 43,43,55 | 0.17 | 0 | 51,51,63 | 0.23 | 0 |
| 21 | CLA | 3 | 607 | 13 | 59,63,73 | 1.27 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 21 | CLA | 9 | 613 | 19 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.85 | 3 (3%) |
| 24 | BCR | J | 102 | - | 41,41,41 | 0.14 | 0 | 56,56,56 | 0.31 | 0 |
| 21 | CLA | A2 | 814 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 21 | CLA | 9 | 611 | 23 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 30 | CHL | 12 | 601 | 12 | 60,74,74 | 1.94 | 10 (16%) | 58,114,114 | 1.05 | 4 (6%) |
| 21 | CLA | 92 | 603 | 19,27 | 59,63,73 | 1.26 | 5 (8%) | 70,101,113 | 0.90 | 4 (5%) |
| 21 | CLA | 92 | 612 | 19 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | A | 823 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.81 | 3 (3%) |
| 28 | LUT | 52 | 620 | - | 42,43,43 | 0.24 | 0 | 51,60,60 | 0.48 | 0 |
| 29 | DGD | B | 850 | - | 60,60,67 | 0.17 | 0 | 74,74,81 | 0.50 | 0 |
| 21 | CLA | A | 811 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 30 | CHL | Z2 | 601 | 12 | 60,74,74 | 1.93 | 10 (16%) | 58,114,114 | 1.10 | 5 (8%) |
| 30 | CHL | 42 | 601 | 16 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.11 | 5 (8%) |
| 21 | CLA | A | 821 | - | 59,63,73 | 1.27 | 5 (8%) | 70,101,113 | 0.86 | 2 (2%) |
| 21 | CLA | B | 826 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.82 | 3 (3%) |
| 28 | LUT | 7 | 621 | - | 42,43,43 | 0.25 | 0 | 51,60,60 | 0.39 | 0 |
| 21 | CLA | 92 | 610 | 19 | 64,68,73 | 1.22 | 5 (7%) | 76,107,113 | 0.89 | 3 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 26 | LMU | 6 | 630 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.28 | 0 |
| 28 | LUT | 72 | 624 | - | 42,43,43 | 0.22 | 0 | 51,60,60 | 0.44 | 0 |
| 21 | CLA | 4 | 611 | 23 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 21 | CLA | G | 203 | - | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.81 | 2 (2%) |
| 21 | CLA | 5 | 601 | 17 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 2 (2%) |
| 21 | CLA | Z2 | 610 | 12 | 64,68,73 | 1.21 | 4 (6%) | 76,107,113 | 0.84 | 3 (3%) |
| 21 | CLA | B2 | 816 | - | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | 62 | 617 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.96 | 3 (5%) |
| 27 | LMG | 32 | 722 | - | 44,44,55 | 0.21 | 0 | 46,46,63 | 0.25 | 0 |
| 21 | CLA | 12 | 604 | 33 | 54,58,73 | 1.33 | 4 (7%) | 64,95,113 | 0.94 | 3 (4%) |
| 21 | CLA | B2 | 815 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | 1 | 610 | 12 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | B | 822 | - | 63,67,73 | 1.21 | 4 (6%) | 74,105,113 | 0.87 | 3 (4%) |
| 21 | CLA | 7 | 614 | - | 47,51,73 | 1.44 | 4 (8%) | 55,86,113 | 1.01 | 3 (5%) |
| 31 | XAT | 12 | 618 | - | 41,47,47 | 0.13 | 0 | 54,74,74 | 0.71 | 2 (3%) |
| 21 | CLA | B2 | 839 | 33 | 69,73,73 | 1.18 | 4 (5%) | 82,113,113 | 0.85 | 3 (3%) |
| 28 | LUT | Z2 | 617 | - | 42,43,43 | 0.26 | 0 | 51,60,60 | 0.44 | 0 |
| 26 | LMU | A | 862 | - | 20,20,36 | 0.13 | 0 | 25,25,47 | 0.28 | 0 |
| 28 | LUT | 82 | 617 | - | 42,43,43 | 0.28 | 0 | 51,60,60 | 0.45 | 0 |
| 26 | LMU | 92 | 624 | - | 24,24,36 | 0.14 | 0 | 29,29,47 | 0.36 | 0 |
| 24 | BCR | A | 851 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.34 | 0 |
| 24 | BCR | K | 202 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.37 | 0 |
| 21 | CLA | 1 | 616 | 12 | 50,54,73 | 1.39 | 4 (8%) | 59,90,113 | 0.98 | 3 (5%) |
| 27 | LMG | J | 104 | - | 35,35,55 | 0.19 | 0 | 43,43,63 | 0.20 | 0 |
| 21 | CLA | 6 | 609 | 18 | 59,63,73 | 1.26 | 4 (6%) | 70,101,113 | 0.93 | 4 (5%) |
| 26 | LMU | 82 | 628 | - | 24,24,36 | 0.15 | 0 | 29,29,47 | 0.31 | 0 |
| 21 | CLA | A | 802 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.77 | 2 (2%) |
| 26 | LMU | A2 | 865 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.46 | 0 |
| 21 | CLA | A | 818 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | Z | 603 | - | 59,63,73 | 1.29 | 5 (8%) | 70,101,113 | 0.87 | 2 (2%) |
| 21 | CLA | 72 | 604 | 33 | 55,59,73 | 1.31 | 4 (7%) | 64,96,113 | 0.93 | 3 (4%) |
| 28 | LUT | 4 | 619 | - | 42,43,43 | 0.24 | 0 | 51,60,60 | 0.49 | 0 |
| 21 | CLA | 82 | 608 | 33 | 54,58,73 | 1.35 | 4 (7%) | 64,95,113 | 0.94 | 2 (3%) |
| 30 | CHL | 72 | 606 | 33 | 40,54,74 | 2.40 | 10 (25%) | 34,90,114 | 1.40 | 5 (14%) |
| 21 | CLA | 3 | 606 | 33 | 46,50,73 | 1.47 | 4 (8%) | 53,85,113 | 1.00 | 2 (3%) |
| 21 | CLA | A2 | 833 | - | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 24 | BCR | B | 801 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.38 | 0 |
| 24 | BCR | B2 | 845 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.36 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 26 | LMU | 12 | 625 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.31 | 0 |
| 21 | CLA | 12 | 602 | 12 | 64,68,73 | 1.23 | 5 (7%) | 76,107,113 | 0.86 | 3 (3%) |
| 21 | CLA | Z2 | 613 | 33 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 42 | 603 | 16 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.81 | 2 (2%) |
| 21 | CLA | G2 | 203 | - | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.81 | 2 (2%) |
| 21 | CLA | 62 | 612 | 18 | 49,53,73 | 1.37 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | A | 812 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.80 | 4 (4%) |
| 28 | LUT | A2 | 856 | - | 42,43,43 | 0.27 | 0 | 51,60,60 | 0.41 | 0 |
| 21 | CLA | B | 827 | - | 69,73,73 | 1.20 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 21 | CLA | 8 | 613 | 15 | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | A | 806 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | J2 | 101 | 9 | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.89 | 2 (2%) |
| 21 | CLA | A | 810 | 1 | 69,73,73 | 1.21 | 4 (5%) | 82,113,113 | 0.85 | 2 (2%) |
| 31 | XAT | 62 | 624 | - | 41,47,47 | 0.13 | 0 | 54,74,74 | 0.64 | 0 |
| 21 | CLA | B2 | 840 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 30 | CHL | 52 | 607 | 33 | 60,74,74 | 1.99 | 10 (16%) | 58,114,114 | 0.98 | 4 (6%) |
| 28 | LUT | 12 | 617 | - | 42,43,43 | 0.26 | 0 | 51,60,60 | 0.42 | 0 |
| 26 | LMU | B | 853 | - | 36,36,36 | 0.12 | 0 | 47,47,47 | 0.68 | 2 (4%) |
| 21 | CLA | 72 | 614 | - | 47,51,73 | 1.43 | 4 (8%) | 55,86,113 | 1.01 | 4 (7%) |
| 21 | CLA | 6 | 612 | 18 | 49,53,73 | 1.37 | 4 (8%) | 58,89,113 | 0.97 | 3 (5%) |
| 21 | CLA | 62 | 610 | 18 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 24 | BCR | B2 | 843 | - | 41,41,41 | 0.16 | 0 | 56,56,56 | 0.31 | 0 |
| 26 | LMU | A2 | 864 | - | 24,24,36 | 0.11 | 0 | 29,29,47 | 0.28 | 0 |
| 21 | CLA | 82 | 609 | 15 | 49,53,73 | 1.41 | 4 (8%) | 58,89,113 | 0.95 | 2 (3%) |
| 21 | CLA | A | 809 | 1 | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.89 | 4 (4%) |
| 26 | LMU | 12 | 622 | - | 19,19,36 | 0.13 | 0 | 24,24,47 | 0.31 | 0 |
| 30 | CHL | Z | 607 | 33 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.09 | 6 (10%) |
| 25 | SF4 | C | 101 | 3 | 0,12,12 | - | - | - | | |
| 21 | CLA | 32 | 612 | 13 | 50,54,73 | 1.36 | 4 (8%) | 59,90,113 | 0.94 | 3 (5%) |
| 30 | CHL | 4 | 608 | - | 60,74,74 | 1.96 | 10 (16%) | 58,114,114 | 1.06 | 5 (8%) |
| 23 | LHG | Z2 | 620 | 21 | 38,38,48 | 0.25 | 0 | 41,44,54 | 0.29 | 0 |
| 21 | CLA | B | 828 | - | 69,73,73 | 1.15 | 4 (5%) | 82,113,113 | 0.80 | 3 (3%) |
| 30 | CHL | 62 | 616 | 18 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.10 | 6 (10%) |
| 21 | CLA | 52 | 611 | 23 | 59,63,73 | 1.26 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 21 | CLA | 52 | 621 | 33 | 50,54,73 | 1.41 | 4 (8%) | 59,90,113 | 1.07 | 5 (8%) |
| 21 | CLA | 3 | 610 | 13 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 27 | LMG | 82 | 629 | - | 42,42,55 | 0.18 | 0 | 50,50,63 | 0.16 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 30 | CHL | 32 | 608 | 33 | 60,74,74 | 1.99 | 10 (16%) | 58,114,114 | 1.10 | 5 (8%) |
| 27 | LMG | B | 854 | - | 36,36,55 | 0.19 | 0 | 44,44,63 | 0.17 | 0 |
| 24 | BCR | A | 850 | - | 41,41,41 | 0.15 | 0 | 56,56,56 | 0.24 | 0 |
| 21 | CLA | Z | 604 | 33 | 61,65,73 | 1.24 | 4 (6%) | 72,103,113 | 0.87 | 3 (4%) |
| 30 | CHL | 6 | 601 | 18 | 60,74,74 | 1.96 | 10 (16%) | 58,114,114 | 0.98 | 4 (6%) |
| 23 | LHG | 6 | 619 | 21 | 48,48,48 | 0.22 | 0 | 51,54,54 | 0.24 | 0 |
| 21 | CLA | L2 | 203 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.80 | 3 (3%) |
| 21 | CLA | Z2 | 602 | 12 | 64,68,73 | 1.23 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 21 | CLA | 3 | 614 | - | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.98 | 3 (5%) |
| 24 | BCR | 4 | 621 | - | 41,41,41 | 0.13 | 0 | 56,56,56 | 0.36 | 0 |
| 21 | CLA | A2 | 843 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 31 | XAT | Z2 | 618 | - | 41,47,47 | 0.14 | 0 | 54,74,74 | 0.61 | 0 |
| 28 | LUT | 8 | 617 | - | 42,43,43 | 0.28 | 0 | 51,60,60 | 0.45 | 0 |
| 21 | CLA | 7 | 612 | 14 | 56,60,73 | 1.29 | 4 (7%) | 65,97,113 | 0.90 | 2 (3%) |
| 21 | CLA | Z | 613 | 33 | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 26 | LMU | 1 | 627 | - | 22,22,36 | 0.13 | 0 | 27,27,47 | 0.29 | 0 |
| 21 | CLA | 42 | 609 | 16 | 64,68,73 | 1.25 | 4 (6%) | 76,107,113 | 0.87 | 2 (2%) |
| 21 | CLA | 32 | 610 | 13 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | A | 816 | - | 69,73,73 | 1.16 | 4 (5%) | 82,113,113 | 0.83 | 3 (3%) |
| 26 | LMU | 82 | 627 | - | 36,36,36 | 0.10 | 0 | 47,47,47 | 0.37 | 0 |
| 21 | CLA | 82 | 611 | 23 | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 1.00 | 3 (5%) |
| 21 | CLA | A | 837 | 1 | 61,65,73 | 1.31 | 5 (8%) | 72,103,113 | 0.90 | 3 (4%) |
| 32 | NEX | 5 | 625 | - | 40,46,46 | 0.52 | 1 (2%) | 50,70,70 | 0.81 | 3 (6%) |
| 21 | CLA | B | 819 | 33 | 64,68,73 | 1.23 | 5 (7%) | 76,107,113 | 0.84 | 3 (3%) |
| 22 | PQN | A2 | 844 | - | 34,34,34 | 0.32 | 0 | 43,45,45 | 0.43 | 0 |
| 27 | LMG | 1 | 628 | - | 42,42,55 | 0.18 | 0 | 50,50,63 | 0.28 | 0 |
| 27 | LMG | 9 | 620 | 21 | 44,44,55 | 0.17 | 0 | 52,52,63 | 0.35 | 0 |
| 21 | CLA | 1 | 603 | - | 61,65,73 | 1.26 | 4 (6%) | 72,103,113 | 0.86 | 2 (2%) |
| 21 | CLA | B2 | 837 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 92 | 602 | 19 | 64,68,73 | 1.24 | 4 (6%) | 76,107,113 | 0.85 | 3 (3%) |
| 21 | CLA | 42 | 614 | - | 59,63,73 | 1.28 | 4 (6%) | 70,101,113 | 0.88 | 3 (4%) |
| 21 | CLA | A2 | 831 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.82 | 3 (3%) |
| 21 | CLA | 52 | 616 | 17 | 57,61,73 | 1.29 | 4 (7%) | 67,98,113 | 0.91 | 2 (2%) |
| 23 | LHG | A | 846 | - | 48,48,48 | 0.23 | 0 | 51,54,54 | 0.29 | 0 |
| 27 | LMG | A | 859 | - | 48,48,55 | 0.17 | 0 | 56,56,63 | 0.17 | 0 |
| 28 | LUT | 5 | 620 | - | 42,43,43 | 0.24 | 0 | 51,60,60 | 0.48 | 0 |
| 21 | CLA | K | 204 | - | 50,54,73 | 1.38 | 5 (10%) | 59,90,113 | 0.99 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 21 | CLA | 62 | 622 | 33 | 59,63,73 | 1.29 | 4 (6%) | 70,101,113 | 0.87 | 2 (2%) |
| 21 | CLA | L | 203 | - | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.80 | 3 (3%) |
| 21 | CLA | 72 | 611 | 23 | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.81 | 3 (3%) |
| 21 | CLA | B | 829 | - | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.84 | 2 (2%) |
| 21 | CLA | B2 | 808 | - | 69,73,73 | 1.15 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 1 | 602 | 12 | 64,68,73 | 1.23 | 5 (7%) | 76,107,113 | 0.87 | 3 (3%) |
| 22 | PQN | B | 842 | - | 34,34,34 | 0.32 | 0 | 43,45,45 | 0.43 | 0 |
| 28 | LUT | 32 | 720 | - | 42,43,43 | 0.22 | 0 | 51,60,60 | 0.33 | 0 |
| 21 | CLA | A | 807 | 1 | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.77 | 2 (2%) |
| 21 | CLA | A2 | 817 | 33 | 59,63,73 | 1.30 | 4 (6%) | 70,101,113 | 0.88 | 2 (2%) |
| 30 | CHL | 62 | 618 | 18 | 37,51,74 | 2.45 | 10 (27%) | 30,86,114 | 1.51 | 5 (16%) |
| 21 | CLA | B | 830 | - | 49,53,73 | 1.35 | 5 (10%) | 58,89,113 | 0.98 | 3 (5%) |
| 26 | LMU | 7 | 629 | - | 28,28,36 | 0.10 | 0 | 39,39,47 | 0.27 | 0 |
| 23 | LHG | 92 | 622 | 21 | 40,40,48 | 0.24 | 0 | 43,46,54 | 0.29 | 0 |
| 24 | BCR | 3 | 719 | - | 41,41,41 | 0.12 | 0 | 56,56,56 | 0.41 | 0 |
| 30 | CHL | 4 | 601 | 16 | 60,74,74 | 1.95 | 10 (16%) | 58,114,114 | 1.10 | 5 (8%) |
| 21 | CLA | A2 | 854 | 33 | 69,73,73 | 1.24 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 23 | LHG | 3 | 623 | - | 46,46,48 | 0.22 | 0 | 49,52,54 | 0.27 | 0 |
| 21 | CLA | G | 204 | 7 | 50,54,73 | 1.38 | 4 (8%) | 59,90,113 | 0.96 | 2 (3%) |
| 20 | CL0 | A | 801 | - | 58,73,73 | 1.48 | 6 (10%) | 60,113,113 | 1.57 | 3 (5%) |
| 21 | CLA | B2 | 807 | - | 59,63,73 | 1.29 | 4 (6%) | 70,101,113 | 0.89 | 3 (4%) |
| 21 | CLA | 7 | 616 | 14 | 50,54,73 | 1.37 | 5 (10%) | 59,90,113 | 0.95 | 3 (5%) |
| 21 | CLA | A2 | 802 | - | 69,73,73 | 1.16 | 5 (7%) | 82,113,113 | 0.77 | 2 (2%) |
| 21 | CLA | 32 | 615 | 33 | 69,73,73 | 1.19 | 4 (5%) | 82,113,113 | 0.84 | 2 (2%) |
| 27 | LMG | 72 | 626 | - | 37,37,55 | 0.18 | 0 | 45,45,63 | 0.27 | 0 |
| 21 | CLA | 6 | 603 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.80 | 2 (2%) |
| 26 | LMU | 62 | 628 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.29 | 0 |
| 28 | LUT | 3 | 622 | - | 42,43,43 | 0.31 | 0 | 51,60,60 | 0.47 | 0 |
| 21 | CLA | B | 806 | 2 | 69,73,73 | 1.19 | 5 (7%) | 82,113,113 | 0.76 | 2 (2%) |
| 21 | CLA | A2 | 845 | 23 | 49,53,73 | 1.40 | 4 (8%) | 58,89,113 | 0.95 | 2 (3%) |
| 21 | CLA | A2 | 821 | - | 59,63,73 | 1.27 | 5 (8%) | 70,101,113 | 0.86 | 2 (2%) |
| 26 | LMU | 8 | 624 | - | 24,24,36 | 0.13 | 0 | 29,29,47 | 0.26 | 0 |
| 30 | CHL | 6 | 618 | 18 | 37,51,74 | 2.44 | 10 (27%) | 30,86,114 | 1.51 | 5 (16%) |
| 21 | CLA | 9 | 602 | 19 | 64,68,73 | 1.24 | 5 (7%) | 76,107,113 | 0.85 | 3 (3%) |
| 21 | CLA | A2 | 807 | 1 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.78 | 2 (2%) |
| 21 | CLA | A2 | 822 | 33 | 69,73,73 | 1.18 | 5 (7%) | 82,113,113 | 0.83 | 3 (3%) |
| 21 | CLA | 12 | 616 | 12 | 50,54,73 | 1.39 | 4 (8%) | 59,90,113 | 0.97 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 26 | LMU | B2 | 853 | - | 36,36,36 | 0.12 | 0 | 47,47,47 | 0.68 | 2 (4%) |
| 21 | CLA | A | 843 | 33 | 69,73,73 | 1.17 | 5 (7%) | 82,113,113 | 0.84 | 3 (3%) |
| 21 | CLA | 8 | 609 | 15 | 49,53,73 | 1.41 | 4 (8%) | 58,89,113 | 0.95 | 3 (5%) |
| 23 | LHG | 1 | 620 | 21 | 38,38,48 | 0.25 | 0 | 41,44,54 | 0.30 | 0 |
| 21 | CLA | B2 | 813 | - | 69,73,73 | 1.17 | 4 (5%) | 82,113,113 | 0.82 | 2 (2%) |
| 26 | LMU | A | 861 | - | 24,24,36 | 0.12 | 0 | 29,29,47 | 0.30 | 0 |
| 26 | LMU | A2 | 857 | - | 35,35,36 | 0.09 | 0 | 46,46,47 | 0.18 | 0 |
| 21 | CLA | B | 836 | - | 64,68,73 | 1.20 | 4 (6%) | 76,107,113 | 0.87 | 3 (3%) |
| 21 | CLA | 4 | 610 | 16 | 64,68,73 | 1.22 | 4 (6%) | 76,107,113 | 0.83 | 3 (3%) |
| 21 | CLA | 3 | 612 | 13 | 50,54,73 | 1.37 | 4 (8%) | 59,90,113 | 0.94 | 3 (5%) |

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 |
|---|---|---|---|---|---|---|---|
| 20 | CL0 | A2 | 801 | - | 3/3/25/25 | 3/37/135/135 | - |
| 21 | CLA | 9 | 603 | 19,27 | 1/1/18/20 | 6/27/103/115 | - |
| 24 | BCR | L | 201 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | B | 802 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | B2 | 828 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 72 | 603 | - | 1/1/17/20 | 4/24/100/115 | - |
| 30 | CHL | 72 | 601 | 14 | 3/3/26/26 | 5/39/137/137 | - |
| 23 | LHG | 42 | 623 | - | - | 15/42/42/53 | - |
| 26 | LMU | Z | 621 | - | - | 2/13/33/61 | 0/1/1/2 |
| 27 | LMG | A | 860 | - | - | 6/31/51/70 | 0/1/1/1 |
| 21 | CLA | Z | 616 | 12 | 1/1/19/20 | 4/33/109/115 | - |
| 27 | LMG | 12 | 624 | - | - | 4/31/51/70 | 0/1/1/1 |
| 21 | CLA | A | 845 | 23 | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | K2 | 204 | - | 1/1/15/20 | 4/17/93/115 | - |
| 30 | CHL | 6 | 606 | 33 | 3/3/24/26 | 2/30/128/137 | - |
| 21 | CLA | 1 | 613 | 33 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | B | 823 | - | 1/1/20/20 | 4/39/115/115 | - |
| 28 | LUT | F | 305 | - | - | 5/29/67/67 | 0/2/2/2 |
| 21 | CLA | A2 | 809 | 1 | 1/1/20/20 | 7/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | A2 | 834 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | Z2 | 612 | 12 | 1/1/15/20 | 5/15/91/115 | - |
| 25 | SF4 | C2 | 102 | 3 | - | - | 0/6/5/5 |
| 21 | CLA | A | 831 | - | 1/1/20/20 | 2/39/115/115 | - |
| 26 | LMU | 72 | 629 | - | - | 4/13/53/61 | 0/2/2/2 |
| 21 | CLA | B | 821 | - | 1/1/20/20 | 5/39/115/115 | - |
| 30 | CHL | 82 | 601 | 15 | 3/3/26/26 | 7/39/137/137 | - |
| 23 | LHG | A2 | 847 | 21 | - | 4/42/42/53 | - |
| 23 | LHG | 8 | 620 | 21 | - | 15/48/48/53 | - |
| 21 | CLA | 52 | 617 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | 5 | 609 | 17 | 1/1/20/20 | 2/39/115/115 | - |
| 30 | CHL | 5 | 606 | 33 | 3/3/21/26 | 2/15/113/137 | - |
| 24 | BCR | B | 845 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 820 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | 62 | 614 | - | 1/1/17/20 | 2/21/97/115 | - |
| 21 | CLA | 6 | 611 | 23 | 1/1/18/20 | 4/31/107/115 | - |
| 21 | CLA | K2 | 201 | 11 | 1/1/15/20 | 2/15/91/115 | - |
| 24 | BCR | 3 | 620 | - | - | 4/29/63/63 | 0/2/2/2 |
| 26 | LMU | 8 | 628 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | A | 819 | - | 1/1/19/20 | 3/33/109/115 | - |
| 21 | CLA | A2 | 811 | - | 1/1/20/20 | 4/39/115/115 | - |
| 30 | CHL | 5 | 618 | 17 | 3/3/20/26 | 2/12/110/137 | - |
| 21 | CLA | B2 | 834 | - | 1/1/19/20 | 8/33/109/115 | - |
| 26 | LMU | A2 | 861 | - | - | 2/15/35/61 | 0/1/1/2 |
| 24 | BCR | A | 849 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | B | 841 | 23 | 1/1/20/20 | 8/39/115/115 | - |
| 31 | XAT | 72 | 622 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | 82 | 613 | 15 | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | B | 809 | 2 | 1/1/20/20 | 5/39/115/115 | - |
| 24 | BCR | B2 | 847 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | K | 203 | 33 | 1/1/19/20 | 1/33/109/115 | - |
| 30 | CHL | 42 | 608 | - | 3/3/26/26 | 5/39/137/137 | - |
| 26 | LMU | A2 | 858 | - | - | 6/21/61/61 | 0/2/2/2 |
| 21 | CLA | 6 | 613 | 33 | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | A2 | 841 | - | 1/1/20/20 | 7/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 5 | 614 | - | 1/1/15/20 | 4/15/91/115 | - |
| 21 | CLA | 4 | 609 | 16 | 1/1/19/20 | 6/33/109/115 | - |
| 30 | CHL | Z | 601 | 12 | 3/3/26/26 | 7/39/137/137 | - |
| 21 | CLA | B | 833 | - | 1/1/18/20 | 4/31/107/115 | - |
| 24 | BCR | B | 844 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | B | 843 | - | - | 0/29/63/63 | 0/2/2/2 |
| 28 | LUT | 52 | 626 | - | - | 4/29/67/67 | 0/2/2/2 |
| 28 | LUT | 7 | 624 | - | - | 4/29/67/67 | 0/2/2/2 |
| 26 | LMU | K | 208 | - | - | 3/15/35/61 | 0/1/1/2 |
| 21 | CLA | 1 | 612 | 12 | 1/1/15/20 | 7/15/91/115 | - |
| 21 | CLA | 32 | 602 | 13 | 1/1/19/20 | 2/33/109/115 | - |
| 25 | SF4 | A2 | 853 | 1,2 | - | - | 0/6/5/5 |
| 21 | CLA | 3 | 609 | 13 | 1/1/19/20 | 2/35/111/115 | - |
| 21 | CLA | 52 | 602 | 17 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 5 | 604 | 33 | 1/1/18/20 | 4/27/103/115 | - |
| 21 | CLA | A2 | 816 | - | 1/1/20/20 | 4/39/115/115 | - |
| 23 | LHG | B2 | 851 | 21 | - | 11/49/49/53 | - |
| 30 | CHL | 8 | 607 | 33 | 3/3/26/26 | 8/39/137/137 | - |
| 24 | BCR | 5 | 622 | - | - | 2/29/63/63 | 0/2/2/2 |
| 26 | LMU | 42 | 626 | - | - | 0/11/31/61 | 0/1/1/2 |
| 21 | CLA | 72 | 613 | 14 | 1/1/20/20 | 0/39/115/115 | - |
| 23 | LHG | 5 | 623 | 21 | - | 11/41/41/53 | - |
| 22 | PQN | B2 | 842 | - | - | 1/23/43/43 | 0/2/2/2 |
| 30 | CHL | 9 | 606 | - | 3/3/20/26 | 0/10/108/137 | - |
| 21 | CLA | 52 | 614 | - | 1/1/15/20 | 4/15/91/115 | - |
| 28 | LUT | Z | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | B2 | 814 | - | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | 42 | 616 | 16 | 1/1/15/20 | 0/15/91/115 | - |
| 22 | PQN | A | 844 | - | - | 3/23/43/43 | 0/2/2/2 |
| 21 | CLA | 1 | 609 | 12 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | B | 811 | - | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | A2 | 813 | - | 1/1/20/20 | 4/39/115/115 | - |
| 26 | LMU | 72 | 628 | - | - | 3/13/33/61 | 0/1/1/2 |
| 21 | CLA | B | 837 | - | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | 8 | 612 | 15 | 1/1/18/20 | 5/27/103/115 | - |
| 21 | CLA | 4 | 616 | 16 | 1/1/15/20 | 0/15/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 4 | 612 | 16 | 1/1/15/20 | 4/15/91/115 | - |
| 24 | BCR | 9 | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 4 | 604 | 33 | 1/1/17/20 | 1/21/97/115 | - |
| 28 | LUT | 32 | 622 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | LMU | Z2 | 622 | - | - | 3/17/57/61 | 0/2/2/2 |
| 21 | CLA | B2 | 804 | - | 1/1/15/20 | 4/15/91/115 | - |
| 21 | CLA | 72 | 608 | 33 | 1/1/17/20 | 0/21/97/115 | - |
| 30 | CHL | 62 | 601 | 18 | 3/3/26/26 | 5/39/137/137 | - |
| 21 | CLA | A | 824 | - | 1/1/15/20 | 4/15/91/115 | - |
| 21 | CLA | 8 | 610 | 15 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | B2 | 832 | - | 1/1/20/20 | 4/39/115/115 | - |
| 23 | LHG | A2 | 846 | - | - | 9/53/53/53 | - |
| 24 | BCR | 8 | 619 | - | - | 4/29/63/63 | 0/2/2/2 |
| 30 | CHL | 8 | 606 | 33 | 3/3/26/26 | 1/39/137/137 | - |
| 21 | CLA | Z2 | 614 | - | 1/1/17/20 | 0/21/97/115 | - |
| 28 | LUT | 6 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 24 | BCR | A | 852 | - | - | 4/29/63/63 | 0/2/2/2 |
| 30 | CHL | 7 | 607 | 33 | 3/3/21/26 | 1/15/113/137 | - |
| 21 | CLA | 6 | 610 | 18 | 1/1/19/20 | 0/33/109/115 | - |
| 21 | CLA | 8 | 614 | - | 1/1/18/20 | 6/30/106/115 | - |
| 27 | LMG | 6 | 633 | - | - | 1/17/17/70 | - |
| 21 | CLA | B2 | 824 | 33 | 1/1/20/20 | 3/39/115/115 | - |
| 23 | LHG | 3 | 721 | - | - | 12/35/35/53 | - |
| 26 | LMU | 8 | 625 | - | - | 2/15/35/61 | 0/1/1/2 |
| 24 | BCR | A2 | 852 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | 8 | 608 | 33 | 1/1/17/20 | 2/21/97/115 | - |
| 21 | CLA | F2 | 301 | 33 | 1/1/20/20 | 3/39/115/115 | - |
| 26 | LMU | A2 | 863 | - | - | 7/21/61/61 | 0/2/2/2 |
| 21 | CLA | A | 805 | - | 1/1/18/20 | 1/27/103/115 | - |
| 26 | LMU | 6 | 632 | - | - | 3/11/31/61 | 0/1/1/2 |
| 27 | LMG | 8 | 626 | - | - | 6/27/47/70 | 0/1/1/1 |
| 27 | LMG | 4 | 624 | - | - | 6/36/56/70 | 0/1/1/1 |
| 21 | CLA | Z | 602 | 12 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | B2 | 823 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 5 | 611 | 23 | 1/1/18/20 | 4/27/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 72 | 609 | 14 | 1/1/15/20 | 1/15/91/115 | - |
| 21 | CLA | 82 | 602 | 15 | 1/1/19/20 | 3/36/112/115 | - |
| 30 | CHL | 62 | 608 | 33 | 3/3/23/26 | 0/21/119/137 | - |
| 23 | LHG | 12 | 620 | 21 | - | 7/43/43/53 | - |
| 21 | CLA | 8 | 611 | 23 | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | L | 204 | - | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | Z | 609 | 12 | 1/1/20/20 | 9/39/115/115 | - |
| 21 | CLA | A | 822 | 33 | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | B2 | 838 | - | 1/1/17/20 | 1/21/97/115 | - |
| 21 | CLA | A | 838 | - | 1/1/17/20 | 0/23/99/115 | - |
| 24 | BCR | 32 | 620 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | B | 820 | - | 1/1/18/20 | 5/29/105/115 | - |
| 21 | CLA | 5 | 621 | 33 | 1/1/15/20 | 10/17/93/115 | - |
| 24 | BCR | 42 | 621 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 803 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 3 | 604 | 33 | 1/1/20/20 | 1/39/115/115 | - |
| 21 | CLA | B2 | 825 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 82 | 604 | 33 | 1/1/19/20 | 2/33/109/115 | - |
| 27 | LMG | J2 | 104 | - | - | 8/30/50/70 | 0/1/1/1 |
| 27 | LMG | 1 | 624 | - | - | 4/31/51/70 | 0/1/1/1 |
| 21 | CLA | B | 817 | - | 1/1/20/20 | 8/39/115/115 | - |
| 24 | BCR | A | 848 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | B2 | 809 | 2 | 1/1/20/20 | 5/39/115/115 | - |
| 26 | LMU | 7 | 628 | - | - | 3/13/33/61 | 0/1/1/2 |
| 23 | LHG | 62 | 619 | 21 | - | 3/53/53/53 | - |
| 24 | BCR | K2 | 207 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 834 | - | 1/1/20/20 | 6/39/115/115 | - |
| 28 | LUT | 92 | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | B2 | 833 | - | 1/1/18/20 | 4/31/107/115 | - |
| 21 | CLA | 7 | 608 | 33 | 1/1/17/20 | 0/21/97/115 | - |
| 30 | CHL | 72 | 607 | 33 | 3/3/21/26 | 1/15/113/137 | - |
| 29 | DGD | B2 | 850 | - | - | 10/48/88/95 | 0/2/2/2 |
| 24 | BCR | 82 | 619 | - | - | 4/29/63/63 | 0/2/2/2 |
| 26 | LMU | 6 | 631 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | B | 810 | - | 1/1/20/20 | 2/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 30 | CHL | Z2 | 607 | 33 | 3/3/26/26 | 4/39/137/137 | - |
| 21 | CLA | B | 834 | - | 1/1/19/20 | 8/33/109/115 | - |
| 23 | LHG | 52 | 623 | 21 | - | 11/41/41/53 | - |
| 30 | CHL | 42 | 607 | 33 | 3/3/26/26 | 1/39/137/137 | - |
| 21 | CLA | A2 | 804 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | Z2 | 611 | 23 | 1/1/19/20 | 6/33/109/115 | - |
| 24 | BCR | 32 | 719 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | F | 304 | 6 | 1/1/20/20 | 7/39/115/115 | - |
| 26 | LMU | A | 863 | - | - | 7/21/61/61 | 0/2/2/2 |
| 21 | CLA | B | 818 | - | 1/1/20/20 | 4/39/115/115 | - |
| 26 | LMU | Z | 622 | - | - | 3/17/57/61 | 0/2/2/2 |
| 21 | CLA | 9 | 610 | 19 | 1/1/19/20 | 0/33/109/115 | - |
| 30 | CHL | 42 | 606 | 33 | 3/3/24/26 | 1/27/125/137 | - |
| 21 | CLA | A | 839 | - | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | B2 | 817 | - | 1/1/20/20 | 8/39/115/115 | - |
| 21 | CLA | 7 | 609 | 14 | 1/1/15/20 | 1/15/91/115 | - |
| 21 | CLA | B | 831 | - | 1/1/18/20 | 1/27/103/115 | - |
| 23 | LHG | A | 847 | 21 | - | 4/42/42/53 | - |
| 21 | CLA | 3 | 611 | - | 1/1/20/20 | 6/39/115/115 | - |
| 24 | BCR | B2 | 844 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | XAT | 5 | 624 | - | 1/1/26/26 | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | B | 838 | - | 1/1/17/20 | 1/21/97/115 | - |
| 21 | CLA | A | 832 | - | 1/1/18/20 | 0/27/103/115 | - |
| 24 | BCR | 62 | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 24 | BCR | 72 | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 42 | 610 | 16 | 1/1/19/20 | 3/33/109/115 | - |
| 27 | LMG | 42 | 624 | - | - | 6/36/56/70 | 0/1/1/1 |
| 21 | CLA | 92 | 601 | 19 | 1/1/15/20 | 2/17/93/115 | - |
| 28 | LUT | 12 | 619 | - | - | 2/29/67/67 | 0/2/2/2 |
| 30 | CHL | 4 | 606 | 33 | 3/3/24/26 | 1/27/125/137 | - |
| 26 | LMU | 9 | 624 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | F | 301 | 33 | 1/1/20/20 | 3/39/115/115 | - |
| 26 | LMU | Z2 | 621 | - | - | 2/13/33/61 | 0/1/1/2 |
| 27 | LMG | 8 | 629 | - | - | 9/37/57/70 | 0/1/1/1 |
| 30 | CHL | 4 | 607 | 33 | 3/3/26/26 | 1/39/137/137 | - |
| 26 | LMU | 1 | 623 | - | - | 1/15/35/61 | 0/1/1/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 52 | 610 | 17 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | B | 812 | - | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | B2 | 826 | - | 1/1/20/20 | 4/39/115/115 | - |
| 24 | BCR | 3 | 718 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 7 | 611 | 23 | 1/1/20/20 | 7/39/115/115 | - |
| 24 | BCR | 6 | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | A2 | 835 | - | 1/1/20/20 | 6/39/115/115 | - |
| 26 | LMU | 4 | 626 | - | - | 0/11/31/61 | 0/1/1/2 |
| 21 | CLA | A | 840 | - | 1/1/20/20 | 7/39/115/115 | - |
| 28 | LUT | 1 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | LMU | 52 | 627 | - | - | 1/15/35/61 | 0/1/1/2 |
| 21 | CLA | 6 | 602 | 18 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 1 | 614 | - | 1/1/19/20 | 7/33/109/115 | - |
| 21 | CLA | 12 | 612 | 12 | 1/1/15/20 | 7/15/91/115 | - |
| 21 | CLA | 3 | 602 | 13 | 1/1/19/20 | 2/33/109/115 | - |
| 30 | CHL | 62 | 606 | 33 | 3/3/24/26 | 2/30/128/137 | - |
| 24 | BCR | L | 205 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 6 | 604 | - | 1/1/20/20 | 2/39/115/115 | - |
| 27 | LMG | A2 | 860 | - | - | 6/31/51/70 | 0/1/1/1 |
| 21 | CLA | B | 816 | - | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | 72 | 620 | 33 | 1/1/17/20 | 6/25/101/115 | - |
| 21 | CLA | G2 | 204 | 7 | 1/1/15/20 | 4/17/93/115 | - |
| 30 | CHL | 3 | 608 | 33 | 3/3/26/26 | 3/39/137/137 | - |
| 23 | LHG | 62 | 629 | - | - | 10/40/40/53 | - |
| 28 | LUT | F2 | 305 | - | - | 5/29/67/67 | 0/2/2/2 |
| 31 | XAT | 82 | 618 | - | - | 0/31/93/93 | 0/4/4/4 |
| 23 | LHG | 72 | 625 | 21 | - | 12/53/53/53 | - |
| 21 | CLA | 1 | 604 | 33 | 1/1/17/20 | 0/21/97/115 | - |
| 26 | LMU | K2 | 208 | - | - | 3/15/35/61 | 0/1/1/2 |
| 30 | CHL | 6 | 608 | 33 | 3/3/23/26 | 0/21/119/137 | - |
| 21 | CLA | B | 835 | 33 | 1/1/15/20 | 0/15/91/115 | - |
| 21 | CLA | 4 | 614 | - | 1/1/18/20 | 5/27/103/115 | - |
| 21 | CLA | 82 | 610 | 15 | 1/1/20/20 | 2/39/115/115 | - |
| 24 | BCR | I | 172 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 813 | - | 1/1/20/20 | 4/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 26 | LMU | 12 | 627 | - | - | 3/13/33/61 | 0/1/1/2 |
| 23 | LHG | 6 | 629 | - | - | 10/40/40/53 | - |
| 26 | LMU | 5 | 627 | - | - | 1/15/35/61 | 0/1/1/2 |
| 26 | LMU | 7 | 627 | - | - | 2/18/58/61 | 0/2/2/2 |
| 21 | CLA | 82 | 614 | - | 1/1/18/20 | 6/30/106/115 | - |
| 21 | CLA | Z2 | 603 | - | 1/1/18/20 | 6/27/103/115 | - |
| 21 | CLA | 72 | 616 | 14 | 1/1/15/20 | 3/17/93/115 | - |
| 21 | CLA | 7 | 603 | - | 1/1/17/20 | 4/24/100/115 | - |
| 32 | NEX | 52 | 625 | - | - | 2/27/83/83 | 1/3/3/3 |
| 21 | CLA | 9 | 614 | - | 1/1/15/20 | 4/15/91/115 | - |
| 21 | CLA | F2 | 304 | 6 | 1/1/20/20 | 7/39/115/115 | - |
| 27 | LMG | 82 | 626 | - | - | 6/27/47/70 | 0/1/1/1 |
| 21 | CLA | 9 | 609 | 19 | 1/1/17/20 | 4/23/99/115 | - |
| 21 | CLA | A2 | 812 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | Z | 612 | 12 | 1/1/15/20 | 5/15/91/115 | - |
| 25 | SF4 | C2 | 101 | 3 | - | - | 0/6/5/5 |
| 21 | CLA | 7 | 602 | 14 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 72 | 610 | 14 | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | B | 805 | - | 1/1/20/20 | 8/39/115/115 | - |
| 21 | CLA | 5 | 603 | - | 1/1/20/20 | 15/39/115/115 | - |
| 21 | CLA | A | 815 | - | 1/1/18/20 | 2/27/103/115 | - |
| 21 | CLA | B2 | 806 | 2 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 12 | 603 | - | 1/1/18/20 | 6/30/106/115 | - |
| 28 | LUT | Z2 | 619 | - | - | 2/18/37/67 | 0/1/1/2 |
| 23 | LHG | 32 | 721 | - | - | 12/35/35/53 | - |
| 25 | SF4 | C | 102 | 3 | - | - | 0/6/5/5 |
| 21 | CLA | Z | 610 | 12 | 1/1/19/20 | 0/33/109/115 | - |
| 21 | CLA | L2 | 204 | - | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | 62 | 609 | 18 | 1/1/18/20 | 4/27/103/115 | - |
| 24 | BCR | L2 | 205 | - | - | 2/29/63/63 | 0/2/2/2 |
| 24 | BCR | A2 | 850 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | NEX | 62 | 625 | - | - | 5/27/83/83 | 0/3/3/3 |
| 21 | CLA | 32 | 604 | 33 | 1/1/20/20 | 1/39/115/115 | - |
| 21 | CLA | 82 | 603 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | B2 | 812 | - | 1/1/20/20 | 2/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 82 | 616 | 15 | 1/1/15/20 | 0/15/91/115 | - |
| 26 | LMU | A | 865 | - | - | 3/15/35/61 | 0/1/1/2 |
| 21 | CLA | 52 | 604 | 33 | 1/1/18/20 | 4/27/103/115 | - |
| 30 | CHL | 62 | 607 | 33 | 3/3/26/26 | 10/39/137/137 | - |
| 21 | CLA | 32 | 613 | 13 | 1/1/19/20 | 5/33/109/115 | - |
| 23 | LHG | 32 | 623 | - | - | 13/51/51/53 | - |
| 28 | LUT | 42 | 619 | - | - | 1/29/67/67 | 0/2/2/2 |
| 21 | CLA | 32 | 603 | - | 1/1/20/20 | 5/39/115/115 | - |
| 26 | LMU | G2 | 206 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | A | 808 | - | 1/1/17/20 | 0/21/97/115 | - |
| 21 | CLA | B2 | 829 | - | 1/1/20/20 | 3/39/115/115 | - |
| 21 | CLA | A | 804 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 7 | 620 | 33 | 1/1/17/20 | 6/25/101/115 | - |
| 21 | CLA | 62 | 604 | - | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 9 | 604 | 19 | 1/1/17/20 | 0/25/101/115 | - |
| 21 | CLA | B2 | 830 | - | 1/1/15/20 | 0/15/91/115 | - |
| 30 | CHL | 82 | 606 | 33 | 3/3/26/26 | 1/39/137/137 | - |
| 30 | CHL | 7 | 601 | 14 | 3/3/26/26 | 4/39/137/137 | - |
| 30 | CHL | 52 | 618 | 17 | 3/3/20/26 | 2/12/110/137 | - |
| 24 | BCR | K | 207 | - | - | 4/29/63/63 | 0/2/2/2 |
| 24 | BCR | B2 | 801 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | 32 | 609 | 13 | 1/1/19/20 | 2/35/111/115 | - |
| 28 | LUT | 9 | 616 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | LMU | A | 858 | - | - | 6/21/61/61 | 0/2/2/2 |
| 21 | CLA | 62 | 611 | 23 | 1/1/18/20 | 4/31/107/115 | - |
| 21 | CLA | A2 | 815 | - | 1/1/18/20 | 2/27/103/115 | - |
| 21 | CLA | 52 | 609 | 17 | 1/1/20/20 | 2/39/115/115 | - |
| 30 | CHL | 5 | 607 | 33 | 3/3/26/26 | 11/39/137/137 | - |
| 28 | LUT | 3 | 720 | - | - | 0/29/67/67 | 0/2/2/2 |
| 21 | CLA | F2 | 303 | 33 | 1/1/15/20 | 1/15/91/115 | - |
| 21 | CLA | Z2 | 616 | 12 | 1/1/19/20 | 4/33/109/115 | - |
| 21 | CLA | A | 826 | 33 | 1/1/20/20 | 8/39/115/115 | - |
| 21 | CLA | A | 842 | - | 1/1/20/20 | 3/39/115/115 | - |
| 21 | CLA | 8 | 603 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 62 | 613 | 33 | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 42 | 602 | 16 | 1/1/19/20 | 2/33/109/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | XAT | 8 | 618 | - | - | 0/31/93/93 | 0/4/4/4 |
| 28 | LUT | 62 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | B2 | 841 | 23 | 1/1/20/20 | 8/39/115/115 | - |
| 21 | CLA | 42 | 612 | 16 | 1/1/15/20 | 4/15/91/115 | - |
| 23 | LHG | 4 | 622 | 21 | - | 14/53/53/53 | - |
| 21 | CLA | B2 | 822 | - | 1/1/18/20 | 3/32/108/115 | - |
| 30 | CHL | Z2 | 606 | 33 | 3/3/21/26 | 4/15/113/137 | - |
| 21 | CLA | 32 | 614 | - | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | B2 | 820 | - | 1/1/18/20 | 5/29/105/115 | - |
| 27 | LMG | 62 | 633 | - | - | 1/17/17/70 | - |
| 21 | CLA | B2 | 819 | 33 | 1/1/19/20 | 5/33/109/115 | - |
| 26 | LMU | 12 | 623 | - | - | 1/15/35/61 | 0/1/1/2 |
| 21 | CLA | Z | 608 | 33 | 1/1/17/20 | 2/21/97/115 | - |
| 26 | LMU | 62 | 632 | - | - | 3/11/31/61 | 0/1/1/2 |
| 24 | BCR | 52 | 622 | - | - | 2/29/63/63 | 0/2/2/2 |
| 28 | LUT | 3 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 5 | 613 | 17 | 1/1/18/20 | 4/29/105/115 | - |
| 31 | XAT | 7 | 622 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | 7 | 610 | 14 | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | B2 | 836 | - | 1/1/19/20 | 4/33/109/115 | - |
| 26 | LMU | 1 | 626 | - | - | 0/15/35/61 | 0/1/1/2 |
| 21 | CLA | B2 | 802 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | 32 | 611 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | 92 | 604 | 19 | 1/1/17/20 | 0/25/101/115 | - |
| 21 | CLA | 5 | 617 | - | 1/1/20/20 | 6/39/115/115 | - |
| 26 | LMU | A2 | 862 | - | - | 2/11/31/61 | 0/1/1/2 |
| 21 | CLA | A2 | 838 | - | 1/1/17/20 | 0/23/99/115 | - |
| 21 | CLA | 12 | 609 | 12 | 1/1/20/20 | 5/39/115/115 | - |
| 30 | CHL | 12 | 606 | 33 | 3/3/21/26 | 0/15/113/137 | - |
| 21 | CLA | B2 | 803 | - | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 52 | 601 | 17 | 1/1/20/20 | 5/39/115/115 | - |
| 30 | CHL | 52 | 606 | 33 | 3/3/21/26 | 2/15/113/137 | - |
| 21 | CLA | K | 201 | 11 | 1/1/15/20 | 2/15/91/115 | - |
| 30 | CHL | 7 | 606 | 33 | 3/3/21/26 | 2/15/113/137 | - |
| 21 | CLA | B | 813 | - | 1/1/20/20 | 3/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 6 | 617 | - | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | A2 | 840 | - | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | 3 | 617 | 13 | 1/1/15/20 | 2/17/93/115 | - |
| 21 | CLA | B2 | 821 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | B2 | 805 | - | 1/1/20/20 | 8/39/115/115 | - |
| 24 | BCR | A2 | 848 | - | - | 2/29/63/63 | 0/2/2/2 |
| 30 | CHL | 1 | 606 | 33 | 3/3/21/26 | 0/15/113/137 | - |
| 31 | XAT | 6 | 624 | - | - | 0/31/93/93 | 0/4/4/4 |
| 24 | BCR | B | 846 | - | - | 2/29/63/63 | 0/2/2/2 |
| 28 | LUT | 9 | 617 | - | - | 0/29/67/67 | 0/2/2/2 |
| 28 | LUT | 92 | 617 | - | - | 0/29/67/67 | 0/2/2/2 |
| 31 | XAT | 1 | 618 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | 7 | 613 | 14 | 1/1/20/20 | 1/39/115/115 | - |
| 28 | LUT | 72 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | A2 | 825 | - | 1/1/18/20 | 6/27/103/115 | - |
| 21 | CLA | 62 | 603 | - | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | 32 | 617 | 13 | 1/1/15/20 | 2/17/93/115 | - |
| 21 | CLA | 12 | 614 | - | 1/1/19/20 | 7/33/109/115 | - |
| 21 | CLA | A2 | 808 | - | 1/1/17/20 | 0/21/97/115 | - |
| 21 | CLA | B2 | 827 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | A2 | 805 | - | 1/1/18/20 | 1/27/103/115 | - |
| 21 | CLA | A2 | 826 | 33 | 1/1/20/20 | 8/39/115/115 | - |
| 21 | CLA | B | 839 | 33 | 1/1/20/20 | 6/39/115/115 | - |
| 26 | LMU | 1 | 621 | - | - | 6/21/61/61 | 0/2/2/2 |
| 21 | CLA | 8 | 604 | 33 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | A2 | 824 | - | 1/1/15/20 | 4/15/91/115 | - |
| 28 | LUT | 1 | 619 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 3 | 603 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | 12 | 613 | 33 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | A | 830 | - | 1/1/20/20 | 4/39/115/115 | - |
| 27 | LMG | A2 | 859 | - | - | 9/43/63/70 | 0/1/1/1 |
| 21 | CLA | B | 807 | - | 1/1/18/20 | 4/27/103/115 | - |
| 21 | CLA | 92 | 614 | - | 1/1/15/20 | 4/15/91/115 | - |
| 30 | CHL | 1 | 601 | 12 | 3/3/26/26 | 9/39/137/137 | - |
| 21 | CLA | Z2 | 609 | 12 | 1/1/20/20 | 9/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | BCR | K2 | 202 | - | - | 2/29/63/63 | 0/2/2/2 |
| 27 | LMG | 92 | 620 | 21 | - | 6/39/59/70 | 0/1/1/1 |
| 21 | CLA | B2 | 835 | 33 | 1/1/15/20 | 1/15/91/115 | - |
| 21 | CLA | 52 | 603 | - | 1/1/20/20 | 15/39/115/115 | - |
| 21 | CLA | 52 | 612 | 17 | 1/1/15/20 | 6/15/91/115 | - |
| 26 | LMU | 62 | 631 | - | - | 4/15/35/61 | 0/1/1/2 |
| 24 | BCR | B | 847 | - | - | 2/29/63/63 | 0/2/2/2 |
| 27 | LMG | B | 852 | - | - | 5/38/58/70 | 0/1/1/1 |
| 21 | CLA | 9 | 601 | 19 | 1/1/15/20 | 2/17/93/115 | - |
| 21 | CLA | K | 206 | 11 | 1/1/15/20 | 4/15/91/115 | - |
| 26 | LMU | 62 | 630 | - | - | 1/15/35/61 | 0/1/1/2 |
| 21 | CLA | Z | 611 | 23 | 1/1/19/20 | 6/33/109/115 | - |
| 21 | CLA | 5 | 610 | 17 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | 92 | 611 | 23 | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | 82 | 612 | 15 | 1/1/18/20 | 5/27/103/115 | - |
| 31 | XAT | 42 | 620 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | A | 825 | - | 1/1/18/20 | 6/27/103/115 | - |
| 24 | BCR | B2 | 846 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | A | 829 | - | 1/1/20/20 | 8/39/115/115 | - |
| 21 | CLA | 9 | 612 | 19 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | 32 | 607 | 13 | 1/1/18/20 | 5/27/103/115 | - |
| 24 | BCR | 7 | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 12 | 608 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 4 | 603 | 16 | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | A | 814 | - | 1/1/20/20 | 4/39/115/115 | - |
| 28 | LUT | 32 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 3 | 615 | 33 | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | Z2 | 608 | 33 | 1/1/17/20 | 2/21/97/115 | - |
| 31 | XAT | 52 | 624 | - | 1/1/26/26 | 0/31/93/93 | 0/4/4/4 |
| 23 | LHG | 82 | 620 | 21 | - | 15/48/48/53 | - |
| 21 | CLA | B2 | 811 | - | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | A2 | 820 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | A2 | 836 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | A2 | 837 | 1 | 1/1/18/20 | 0/30/106/115 | - |
| 23 | LHG | B | 851 | 21 | - | 11/49/49/53 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 5 | 616 | 17 | 1/1/17/20 | 7/25/101/115 | - |
| 21 | CLA | 72 | 602 | 14 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 7 | 604 | 33 | 1/1/17/20 | 1/23/99/115 | - |
| 21 | CLA | 4 | 602 | 16 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | Z | 614 | - | 1/1/17/20 | 0/21/97/115 | - |
| 21 | CLA | Z2 | 604 | 33 | 1/1/18/20 | 3/30/106/115 | - |
| 30 | CHL | 6 | 616 | 18 | 3/3/26/26 | 3/39/137/137 | - |
| 21 | CLA | 42 | 604 | 33 | 1/1/17/20 | 1/21/97/115 | - |
| 30 | CHL | 5 | 608 | 33 | 3/3/23/26 | 0/21/119/137 | - |
| 21 | CLA | A2 | 823 | - | 1/1/20/20 | 7/39/115/115 | - |
| 27 | LMG | 12 | 628 | - | - | 6/37/57/70 | 0/1/1/1 |
| 21 | CLA | 42 | 613 | 16 | 1/1/20/20 | 6/39/115/115 | - |
| 26 | LMU | 82 | 625 | - | - | 2/15/35/61 | 0/1/1/2 |
| 21 | CLA | F | 303 | 33 | 1/1/15/20 | 1/15/91/115 | - |
| 23 | LHG | 9 | 622 | 21 | - | 13/45/45/53 | - |
| 26 | LMU | 82 | 624 | - | - | 1/15/35/61 | 0/1/1/2 |
| 24 | BCR | 92 | 623 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 12 | 611 | 23 | 1/1/19/20 | 4/35/111/115 | - |
| 31 | XAT | 4 | 620 | - | - | 0/31/93/93 | 0/4/4/4 |
| 27 | LMG | 7 | 626 | - | - | 7/32/52/70 | 0/1/1/1 |
| 21 | CLA | B | 808 | - | 1/1/20/20 | 9/39/115/115 | - |
| 21 | CLA | 3 | 613 | 13 | 1/1/19/20 | 5/33/109/115 | - |
| 21 | CLA | 12 | 610 | 12 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | B | 815 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | A2 | 827 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | K2 | 206 | 11 | 1/1/15/20 | 4/15/91/115 | - |
| 21 | CLA | B | 832 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | A | 854 | 33 | 1/1/20/20 | 1/39/115/115 | - |
| 21 | CLA | A2 | 839 | - | 1/1/20/20 | 2/39/115/115 | - |
| 23 | LHG | Z | 620 | 21 | - | 6/43/43/53 | - |
| 21 | CLA | A2 | 806 | - | 1/1/20/20 | 10/39/115/115 | - |
| 24 | BCR | J2 | 102 | - | - | 2/29/63/63 | 0/2/2/2 |
| 30 | CHL | 52 | 608 | 33 | 3/3/23/26 | 0/21/119/137 | - |
| 21 | CLA | A2 | 819 | - | 1/1/19/20 | 3/33/109/115 | - |
| 21 | CLA | 8 | 616 | 15 | 1/1/15/20 | 0/15/91/115 | - |
| 24 | BCR | A2 | 849 | - | - | 0/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | BCR | A2 | 851 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | J | 101 | 9 | 1/1/18/20 | 3/27/103/115 | - |
| 26 | LMU | 42 | 625 | - | - | 3/19/59/61 | 0/2/2/2 |
| 23 | LHG | 42 | 622 | 21 | - | 14/53/53/53 | - |
| 30 | CHL | 12 | 607 | 33 | 3/3/21/26 | 2/15/113/137 | - |
| 21 | CLA | 1 | 608 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 4 | 613 | 16 | 1/1/20/20 | 6/39/115/115 | - |
| 26 | LMU | G | 206 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | A2 | 828 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | B2 | 831 | - | 1/1/18/20 | 1/27/103/115 | - |
| 21 | CLA | 8 | 602 | 15 | 1/1/19/20 | 3/36/112/115 | - |
| 21 | CLA | A2 | 832 | - | 1/1/18/20 | 0/27/103/115 | - |
| 26 | LMU | 4 | 625 | - | - | 3/19/59/61 | 0/2/2/2 |
| 28 | LUT | 5 | 626 | - | - | 4/29/67/67 | 0/2/2/2 |
| 26 | LMU | A | 857 | - | - | 3/20/60/61 | 0/2/2/2 |
| 21 | CLA | 92 | 609 | 19 | 1/1/17/20 | 4/23/99/115 | - |
| 30 | CHL | 92 | 606 | - | 3/3/20/26 | 0/10/108/137 | - |
| 27 | LMG | 3 | 722 | - | - | 5/46/46/70 | - |
| 27 | LMG | J2 | 103 | - | - | 3/37/57/70 | 0/1/1/1 |
| 21 | CLA | 42 | 611 | 23 | 1/1/19/20 | 5/33/109/115 | - |
| 26 | LMU | 12 | 626 | - | - | 0/15/35/61 | 0/1/1/2 |
| 21 | CLA | B | 814 | - | 1/1/19/20 | 2/33/109/115 | - |
| 30 | CHL | 92 | 607 | 33 | 3/3/23/26 | 9/21/119/137 | - |
| 21 | CLA | A | 817 | 33 | 1/1/18/20 | 4/27/103/115 | - |
| 21 | CLA | A | 835 | - | 1/1/20/20 | 6/39/115/115 | - |
| 25 | SF4 | A | 853 | 1,2 | - | - | 0/6/5/5 |
| 27 | LMG | J | 103 | - | - | 3/37/57/70 | 0/1/1/1 |
| 21 | CLA | A | 833 | - | 1/1/20/20 | 1/39/115/115 | - |
| 30 | CHL | 1 | 607 | 33 | 3/3/21/26 | 2/15/113/137 | - |
| 21 | CLA | A2 | 818 | - | 1/1/20/20 | 2/39/115/115 | - |
| 26 | LMU | 6 | 628 | - | - | 2/15/35/61 | 0/1/1/2 |
| 21 | CLA | B | 804 | - | 1/1/15/20 | 4/15/91/115 | - |
| 27 | LMG | B2 | 854 | - | - | 2/31/51/70 | 0/1/1/1 |
| 21 | CLA | 72 | 612 | 14 | 1/1/17/20 | 3/24/100/115 | - |
| 21 | CLA | 6 | 614 | - | 1/1/17/20 | 2/21/97/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 32 | NEX | 6 | 625 | - | - | 5/27/83/83 | 0/3/3/3 |
| 28 | LUT | A | 856 | - | - | 4/29/67/67 | 0/2/2/2 |
| 24 | BCR | 32 | 718 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | B | 803 | - | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | A | 828 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | 62 | 602 | 18 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | A2 | 830 | - | 1/1/20/20 | 5/39/115/115 | - |
| 24 | BCR | G | 205 | - | - | 1/29/63/63 | 0/2/2/2 |
| 21 | CLA | 92 | 613 | 19 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | A2 | 803 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 31 | XAT | Z | 618 | - | - | 0/31/93/93 | 0/4/4/4 |
| 26 | LMU | 1 | 622 | - | - | 4/10/30/61 | 0/1/1/2 |
| 21 | CLA | B | 824 | 33 | 1/1/20/20 | 3/39/115/115 | - |
| 26 | LMU | 12 | 621 | - | - | 6/21/61/61 | 0/2/2/2 |
| 21 | CLA | B2 | 818 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | A2 | 810 | 1 | 1/1/20/20 | 8/39/115/115 | - |
| 30 | CHL | 8 | 601 | 15 | 3/3/26/26 | 7/39/137/137 | - |
| 26 | LMU | 72 | 627 | - | - | 2/18/58/61 | 0/2/2/2 |
| 21 | CLA | 6 | 622 | 33 | 1/1/18/20 | 2/27/103/115 | - |
| 30 | CHL | 82 | 607 | 33 | 3/3/26/26 | 8/39/137/137 | - |
| 30 | CHL | 42 | 618 | 16 | 3/3/21/26 | 0/15/113/137 | - |
| 23 | LHG | 4 | 623 | - | - | 15/42/42/53 | - |
| 21 | CLA | 5 | 602 | 17 | 1/1/20/20 | 2/39/115/115 | - |
| 26 | LMU | 8 | 627 | - | - | 9/21/61/61 | 0/2/2/2 |
| 26 | LMU | A | 864 | - | - | 3/15/35/61 | 0/1/1/2 |
| 21 | CLA | 32 | 606 | 33 | 1/1/14/20 | 0/12/88/115 | - |
| 30 | CHL | 6 | 607 | 33 | 3/3/26/26 | 10/39/137/137 | - |
| 21 | CLA | A | 827 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 30 | CHL | 9 | 607 | 33 | 3/3/23/26 | 10/21/119/137 | - |
| 24 | BCR | G2 | 205 | - | - | 1/29/63/63 | 0/2/2/2 |
| 21 | CLA | 5 | 612 | 17 | 1/1/15/20 | 6/15/91/115 | - |
| 24 | BCR | L2 | 201 | - | - | 4/29/63/63 | 0/2/2/2 |
| 21 | CLA | A2 | 829 | - | 1/1/20/20 | 7/39/115/115 | - |
| 28 | LUT | Z | 619 | - | - | 2/18/37/67 | 0/1/1/2 |
| 21 | CLA | B | 840 | - | 1/1/20/20 | 7/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 30 | CHL | Z | 606 | 33 | 3/3/21/26 | 4/15/113/137 | - |
| 30 | CHL | 4 | 618 | 16 | 3/3/21/26 | 0/15/113/137 | - |
| 26 | LMU | 1 | 625 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | K2 | 203 | 33 | 1/1/19/20 | 1/33/109/115 | - |
| 21 | CLA | B2 | 810 | - | 1/1/20/20 | 2/39/115/115 | - |
| 24 | BCR | B | 848 | - | - | 2/29/63/63 | 0/2/2/2 |
| 23 | LHG | 7 | 625 | 21 | - | 12/53/53/53 | - |
| 21 | CLA | B | 825 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 52 | 613 | 17 | 1/1/18/20 | 4/29/105/115 | - |
| 21 | CLA | A | 841 | - | 1/1/20/20 | 7/39/115/115 | - |
| 24 | BCR | I2 | 172 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | B2 | 848 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 1 | 611 | 23 | 1/1/19/20 | 4/35/111/115 | - |
| 21 | CLA | A | 836 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | A2 | 842 | - | 1/1/20/20 | 3/39/115/115 | - |
| 27 | LMG | B2 | 852 | - | - | 5/38/58/70 | 0/1/1/1 |
| 21 | CLA | 3 | 607 | 13 | 1/1/18/20 | 4/27/103/115 | - |
| 21 | CLA | 9 | 613 | 19 | 1/1/20/20 | 5/39/115/115 | - |
| 24 | BCR | J | 102 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | A2 | 814 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 9 | 611 | 23 | 1/1/20/20 | 6/39/115/115 | - |
| 30 | CHL | 12 | 601 | 12 | 3/3/26/26 | 9/39/137/137 | - |
| 21 | CLA | 92 | 603 | 19,27 | 1/1/18/20 | 6/27/103/115 | - |
| 21 | CLA | 92 | 612 | 19 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | A | 823 | - | 1/1/20/20 | 7/39/115/115 | - |
| 28 | LUT | 52 | 620 | - | - | 2/29/67/67 | 0/2/2/2 |
| 29 | DGD | B | 850 | - | - | 14/48/88/95 | 0/2/2/2 |
| 21 | CLA | A | 811 | - | 1/1/20/20 | 4/39/115/115 | - |
| 30 | CHL | Z2 | 601 | 12 | 3/3/26/26 | 7/39/137/137 | - |
| 30 | CHL | 42 | 601 | 16 | 3/3/26/26 | 6/39/137/137 | - |
| 21 | CLA | A | 821 | - | 1/1/18/20 | 4/27/103/115 | - |
| 21 | CLA | B | 826 | - | 1/1/20/20 | 4/39/115/115 | - |
| 28 | LUT | 7 | 621 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 92 | 610 | 19 | 1/1/19/20 | 0/33/109/115 | - |
| 26 | LMU | 6 | 630 | - | - | 1/15/35/61 | 0/1/1/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 28 | LUT | 72 | 624 | - | - | 4/29/67/67 | 0/2/2/2 |
| 21 | CLA | 4 | 611 | 23 | 1/1/19/20 | 5/33/109/115 | - |
| 21 | CLA | G | 203 | - | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | 5 | 601 | 17 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | Z2 | 610 | 12 | 1/1/19/20 | 0/33/109/115 | - |
| 21 | CLA | B2 | 816 | - | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | 62 | 617 | - | 1/1/15/20 | 2/15/91/115 | - |
| 27 | LMG | 32 | 722 | - | - | 5/46/46/70 | - |
| 21 | CLA | 12 | 604 | 33 | 1/1/17/20 | 0/21/97/115 | - |
| 21 | CLA | B2 | 815 | - | 1/1/20/20 | 4/39/115/115 | - |
| 21 | CLA | 1 | 610 | 12 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | B | 822 | - | 1/1/18/20 | 3/32/108/115 | - |
| 21 | CLA | 7 | 614 | - | 1/1/14/20 | 5/13/89/115 | - |
| 31 | XAT | 12 | 618 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | B2 | 839 | 33 | 1/1/20/20 | 6/39/115/115 | - |
| 28 | LUT | Z2 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | LMU | A | 862 | - | - | 2/11/31/61 | 0/1/1/2 |
| 28 | LUT | 82 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | LMU | 92 | 624 | - | - | 4/15/35/61 | 0/1/1/2 |
| 24 | BCR | A | 851 | - | - | 2/29/63/63 | 0/2/2/2 |
| 24 | BCR | K | 202 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | 1 | 616 | 12 | 1/1/15/20 | 2/17/93/115 | - |
| 27 | LMG | J | 104 | - | - | 8/30/50/70 | 0/1/1/1 |
| 21 | CLA | 6 | 609 | 18 | 1/1/18/20 | 4/27/103/115 | - |
| 26 | LMU | 82 | 628 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | A | 802 | - | 1/1/20/20 | 0/39/115/115 | - |
| 26 | LMU | A2 | 865 | - | - | 3/15/35/61 | 0/1/1/2 |
| 21 | CLA | A | 818 | - | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | Z | 603 | - | 1/1/18/20 | 6/27/103/115 | - |
| 21 | CLA | 72 | 604 | 33 | 1/1/17/20 | 1/23/99/115 | - |
| 28 | LUT | 4 | 619 | - | - | 1/29/67/67 | 0/2/2/2 |
| 21 | CLA | 82 | 608 | 33 | 1/1/17/20 | 2/21/97/115 | - |
| 30 | CHL | 72 | 606 | 33 | 3/3/21/26 | 2/15/113/137 | - |
| 21 | CLA | 3 | 606 | 33 | 1/1/14/20 | 0/12/88/115 | - |
| 21 | CLA | A2 | 833 | - | 1/1/20/20 | 1/39/115/115 | - |
| 24 | BCR | B | 801 | - | - | 0/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | BCR | B2 | 845 | - | - | 4/29/63/63 | 0/2/2/2 |
| 26 | LMU | 12 | 625 | - | - | 4/15/35/61 | 0/1/1/2 |
| 21 | CLA | 12 | 602 | 12 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | Z2 | 613 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | 42 | 603 | 16 | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | G2 | 203 | - | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | 62 | 612 | 18 | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | A | 812 | - | 1/1/20/20 | 6/39/115/115 | - |
| 28 | LUT | A2 | 856 | - | - | 4/29/67/67 | 0/2/2/2 |
| 21 | CLA | B | 827 | - | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | 8 | 613 | 15 | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | A | 806 | - | 1/1/20/20 | 10/39/115/115 | - |
| 21 | CLA | J2 | 101 | 9 | 1/1/18/20 | 3/27/103/115 | - |
| 21 | CLA | A | 810 | 1 | 1/1/20/20 | 7/39/115/115 | - |
| 31 | XAT | 62 | 624 | - | - | 0/31/93/93 | 0/4/4/4 |
| 21 | CLA | B2 | 840 | - | 1/1/20/20 | 7/39/115/115 | - |
| 30 | CHL | 52 | 607 | 33 | 3/3/26/26 | 11/39/137/137 | - |
| 28 | LUT | 12 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 26 | LMU | B | 853 | - | - | 7/21/61/61 | 0/2/2/2 |
| 21 | CLA | 72 | 614 | - | 1/1/14/20 | 5/13/89/115 | - |
| 21 | CLA | 6 | 612 | 18 | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | 62 | 610 | 18 | 1/1/19/20 | 0/33/109/115 | - |
| 24 | BCR | B2 | 843 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | LMU | A2 | 864 | - | - | 2/15/35/61 | 0/1/1/2 |
| 21 | CLA | 82 | 609 | 15 | 1/1/15/20 | 0/15/91/115 | - |
| 21 | CLA | A | 809 | 1 | 1/1/20/20 | 7/39/115/115 | - |
| 30 | CHL | Z | 607 | 33 | 3/3/26/26 | 4/39/137/137 | - |
| 26 | LMU | 12 | 622 | - | - | 4/10/30/61 | 0/1/1/2 |
| 25 | SF4 | C | 101 | 3 | - | - | 0/6/5/5 |
| 21 | CLA | 32 | 612 | 13 | 1/1/15/20 | 2/17/93/115 | - |
| 30 | CHL | 4 | 608 | - | 3/3/26/26 | 5/39/137/137 | - |
| 30 | CHL | 62 | 616 | 18 | 3/3/26/26 | 3/39/137/137 | - |
| 21 | CLA | B | 828 | - | 1/1/20/20 | 4/39/115/115 | - |
| 23 | LHG | Z2 | 620 | 21 | - | 6/43/43/53 | - |
| 21 | CLA | 52 | 611 | 23 | 1/1/18/20 | 4/27/103/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 52 | 621 | 33 | 1/1/15/20 | 10/17/93/115 | - |
| 21 | CLA | 3 | 610 | 13 | 1/1/20/20 | 0/39/115/115 | - |
| 27 | LMG | 82 | 629 | - | - | 9/37/57/70 | 0/1/1/1 |
| 30 | CHL | 32 | 608 | 33 | 3/3/26/26 | 3/39/137/137 | - |
| 27 | LMG | B | 854 | - | - | 2/31/51/70 | 0/1/1/1 |
| 24 | BCR | A | 850 | - | - | 0/29/63/63 | 0/2/2/2 |
| 21 | CLA | Z | 604 | 33 | 1/1/18/20 | 3/30/106/115 | - |
| 30 | CHL | 6 | 601 | 18 | 3/3/26/26 | 5/39/137/137 | - |
| 23 | LHG | 6 | 619 | 21 | - | 4/53/53/53 | - |
| 21 | CLA | L2 | 203 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | Z2 | 602 | 12 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | 3 | 614 | - | 1/1/15/20 | 2/15/91/115 | - |
| 24 | BCR | 4 | 621 | - | - | 2/29/63/63 | 0/2/2/2 |
| 21 | CLA | A2 | 843 | 33 | 1/1/20/20 | 4/39/115/115 | - |
| 31 | XAT | Z2 | 618 | - | - | 0/31/93/93 | 0/4/4/4 |
| 28 | LUT | 8 | 617 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | 7 | 612 | 14 | 1/1/17/20 | 2/24/100/115 | - |
| 21 | CLA | Z | 613 | 33 | 1/1/20/20 | 2/39/115/115 | - |
| 26 | LMU | 1 | 627 | - | - | 3/13/33/61 | 0/1/1/2 |
| 21 | CLA | 42 | 609 | 16 | 1/1/19/20 | 6/33/109/115 | - |
| 21 | CLA | 32 | 610 | 13 | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | A | 816 | - | 1/1/20/20 | 4/39/115/115 | - |
| 26 | LMU | 82 | 627 | - | - | 9/21/61/61 | 0/2/2/2 |
| 21 | CLA | 82 | 611 | 23 | 1/1/15/20 | 2/15/91/115 | - |
| 21 | CLA | A | 837 | 1 | 1/1/18/20 | 0/30/106/115 | - |
| 32 | NEX | 5 | 625 | - | - | 2/27/83/83 | 1/3/3/3 |
| 21 | CLA | B | 819 | 33 | 1/1/19/20 | 5/33/109/115 | - |
| 22 | PQN | A2 | 844 | - | - | 3/23/43/43 | 0/2/2/2 |
| 27 | LMG | 1 | 628 | - | - | 6/37/57/70 | 0/1/1/1 |
| 27 | LMG | 9 | 620 | 21 | - | 6/39/59/70 | 0/1/1/1 |
| 21 | CLA | 1 | 603 | - | 1/1/18/20 | 6/30/106/115 | - |
| 21 | CLA | B2 | 837 | - | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | 92 | 602 | 19 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | 42 | 614 | - | 1/1/18/20 | 5/27/103/115 | - |
| 21 | CLA | A2 | 831 | - | 1/1/20/20 | 2/39/115/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | 52 | 616 | 17 | 1/1/17/20 | 7/25/101/115 | - |
| 23 | LHG | A | 846 | - | - | 9/53/53/53 | - |
| 27 | LMG | A | 859 | - | - | 9/43/63/70 | 0/1/1/1 |
| 28 | LUT | 5 | 620 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | K | 204 | - | 1/1/15/20 | 4/17/93/115 | - |
| 21 | CLA | 62 | 622 | 33 | 1/1/18/20 | 2/27/103/115 | - |
| 21 | CLA | L | 203 | - | 1/1/20/20 | 6/39/115/115 | - |
| 21 | CLA | 72 | 611 | 23 | 1/1/20/20 | 7/39/115/115 | - |
| 21 | CLA | B | 829 | - | 1/1/20/20 | 3/39/115/115 | - |
| 21 | CLA | B2 | 808 | - | 1/1/20/20 | 9/39/115/115 | - |
| 21 | CLA | 1 | 602 | 12 | 1/1/19/20 | 2/33/109/115 | - |
| 22 | PQN | B | 842 | - | - | 1/23/43/43 | 0/2/2/2 |
| 28 | LUT | 32 | 720 | - | - | 0/29/67/67 | 0/2/2/2 |
| 21 | CLA | A | 807 | 1 | 1/1/20/20 | 3/39/115/115 | - |
| 21 | CLA | A2 | 817 | 33 | 1/1/18/20 | 4/27/103/115 | - |
| 30 | CHL | 62 | 618 | 18 | 3/3/20/26 | 0/12/110/137 | - |
| 21 | CLA | B | 830 | - | 1/1/15/20 | 0/15/91/115 | - |
| 26 | LMU | 7 | 629 | - | - | 4/13/53/61 | 0/2/2/2 |
| 23 | LHG | 92 | 622 | 21 | - | 13/45/45/53 | - |
| 24 | BCR | 3 | 719 | - | - | 2/29/63/63 | 0/2/2/2 |
| 30 | CHL | 4 | 601 | 16 | 3/3/26/26 | 6/39/137/137 | - |
| 21 | CLA | A2 | 854 | 33 | 1/1/20/20 | 1/39/115/115 | - |
| 23 | LHG | 3 | 623 | - | - | 13/51/51/53 | - |
| 21 | CLA | G | 204 | 7 | 1/1/15/20 | 4/17/93/115 | - |
| 20 | CL0 | A | 801 | - | 3/3/25/25 | 3/37/135/135 | - |
| 21 | CLA | B2 | 807 | - | 1/1/18/20 | 4/27/103/115 | - |
| 21 | CLA | 7 | 616 | 14 | 1/1/15/20 | 3/17/93/115 | - |
| 21 | CLA | A2 | 802 | - | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | 32 | 615 | 33 | 1/1/20/20 | 6/39/115/115 | - |
| 27 | LMG | 72 | 626 | - | - | 7/32/52/70 | 0/1/1/1 |
| 21 | CLA | 6 | 603 | - | 1/1/20/20 | 7/39/115/115 | - |
| 26 | LMU | 62 | 628 | - | - | 2/15/35/61 | 0/1/1/2 |
| 28 | LUT | 3 | 622 | - | - | 2/29/67/67 | 0/2/2/2 |
| 21 | CLA | B | 806 | 2 | 1/1/20/20 | 2/39/115/115 | - |
| 21 | CLA | A2 | 845 | 23 | 1/1/15/20 | 2/15/91/115 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CLA | A2 | 821 | - | 1/1/18/20 | 4/27/103/115 | - |
| 30 | CHL | 6 | 618 | 18 | 3/3/20/26 | 0/12/110/137 | - |
| 26 | LMU | 8 | 624 | - | - | 1/15/35/61 | 0/1/1/2 |
| 21 | CLA | 9 | 602 | 19 | 1/1/19/20 | 2/33/109/115 | - |
| 21 | CLA | A2 | 807 | 1 | 1/1/20/20 | 3/39/115/115 | - |
| 21 | CLA | A2 | 822 | 33 | 1/1/20/20 | 0/39/115/115 | - |
| 21 | CLA | 12 | 616 | 12 | 1/1/15/20 | 2/17/93/115 | - |
| 26 | LMU | B2 | 853 | - | - | 7/21/61/61 | 0/2/2/2 |
| 21 | CLA | A | 843 | 33 | 1/1/20/20 | 5/39/115/115 | - |
| 21 | CLA | 8 | 609 | 15 | 1/1/15/20 | 0/15/91/115 | - |
| 23 | LHG | 1 | 620 | 21 | - | 7/43/43/53 | - |
| 21 | CLA | B2 | 813 | - | 1/1/20/20 | 3/39/115/115 | - |
| 26 | LMU | A | 861 | - | - | 2/15/35/61 | 0/1/1/2 |
| 26 | LMU | A2 | 857 | - | - | 3/20/60/61 | 0/2/2/2 |
| 21 | CLA | B | 836 | - | 1/1/19/20 | 4/33/109/115 | - |
| 21 | CLA | 4 | 610 | 16 | 1/1/19/20 | 3/33/109/115 | - |
| 21 | CLA | 3 | 612 | 13 | 1/1/15/20 | 2/17/93/115 | - |

All (2327) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 9 | 607 | CHL | C1B-C2B | 7.62 | 1.48 | 1.39 |
| 30 | 62 | 601 | CHL | MG-NB | -7.46 | 1.91 | 2.05 |
| 30 | 6 | 601 | CHL | MG-NB | -7.43 | 1.91 | 2.05 |
| 30 | Z | 601 | CHL | MG-NB | -7.41 | 1.91 | 2.05 |
| 30 | Z2 | 601 | CHL | MG-NB | -7.41 | 1.91 | 2.05 |
| 30 | 9 | 607 | CHL | MG-NB | -7.33 | 1.91 | 2.05 |
| 30 | 3 | 608 | CHL | MG-NB | -7.32 | 1.91 | 2.05 |
| 30 | Z | 606 | CHL | MG-NB | -7.32 | 1.91 | 2.05 |
| 30 | 4 | 601 | CHL | MG-NB | -7.32 | 1.91 | 2.05 |
| 30 | 32 | 608 | CHL | MG-NB | -7.31 | 1.91 | 2.05 |
| 30 | 1 | 607 | CHL | MG-NB | -7.30 | 1.91 | 2.05 |
| 30 | 12 | 607 | CHL | MG-NB | -7.30 | 1.91 | 2.05 |
| 30 | Z2 | 606 | CHL | MG-NB | -7.30 | 1.91 | 2.05 |
| 30 | 72 | 601 | CHL | MG-NB | -7.30 | 1.91 | 2.05 |
| 30 | Z | 607 | CHL | MG-NB | -7.30 | 1.91 | 2.05 |
| 30 | 7 | 601 | CHL | MG-NB | -7.30 | 1.91 | 2.05 |
| 30 | 8 | 601 | CHL | MG-NB | -7.29 | 1.91 | 2.05 |
| 30 | 92 | 607 | CHL | MG-NB | -7.29 | 1.91 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 52 | 606 | CHL | MG-NB | -7.28 | 1.91 | 2.05 |
| 30 | Z2 | 607 | CHL | MG-NB | -7.28 | 1.91 | 2.05 |
| 30 | 42 | 607 | CHL | MG-NB | -7.27 | 1.91 | 2.05 |
| 30 | 52 | 608 | CHL | MG-NB | -7.27 | 1.91 | 2.05 |
| 30 | 9 | 606 | CHL | MG-NB | -7.27 | 1.91 | 2.05 |
| 30 | 42 | 608 | CHL | MG-NB | -7.27 | 1.91 | 2.05 |
| 30 | 82 | 601 | CHL | MG-NB | -7.26 | 1.91 | 2.05 |
| 30 | 92 | 606 | CHL | MG-NB | -7.25 | 1.91 | 2.05 |
| 30 | 5 | 608 | CHL | MG-NB | -7.25 | 1.91 | 2.05 |
| 30 | 42 | 601 | CHL | MG-NB | -7.25 | 1.91 | 2.05 |
| 30 | 8 | 607 | CHL | MG-NB | -7.24 | 1.91 | 2.05 |
| 30 | 4 | 618 | CHL | MG-NB | -7.24 | 1.91 | 2.05 |
| 30 | 5 | 606 | CHL | MG-NB | -7.24 | 1.91 | 2.05 |
| 30 | 1 | 606 | CHL | MG-NB | -7.24 | 1.91 | 2.05 |
| 30 | 4 | 608 | CHL | MG-NB | -7.24 | 1.91 | 2.05 |
| 30 | 82 | 607 | CHL | MG-NB | -7.24 | 1.91 | 2.05 |
| 30 | 1 | 601 | CHL | MG-NB | -7.23 | 1.91 | 2.05 |
| 30 | 4 | 607 | CHL | MG-NB | -7.23 | 1.91 | 2.05 |
| 30 | 42 | 606 | CHL | MG-NB | -7.22 | 1.91 | 2.05 |
| 30 | 4 | 606 | CHL | MG-NB | -7.22 | 1.91 | 2.05 |
| 30 | 6 | 616 | CHL | MG-NB | -7.21 | 1.91 | 2.05 |
| 30 | 72 | 607 | CHL | MG-NB | -7.21 | 1.91 | 2.05 |
| 30 | 52 | 607 | CHL | MG-NB | -7.21 | 1.91 | 2.05 |
| 30 | 42 | 618 | CHL | MG-NB | -7.21 | 1.91 | 2.05 |
| 30 | 5 | 607 | CHL | MG-NB | -7.21 | 1.91 | 2.05 |
| 30 | 62 | 608 | CHL | MG-NB | -7.20 | 1.91 | 2.05 |
| 30 | 42 | 601 | CHL | C1B-C2B | 7.20 | 1.47 | 1.39 |
| 30 | 12 | 606 | CHL | MG-NB | -7.20 | 1.91 | 2.05 |
| 30 | 7 | 607 | CHL | MG-NB | -7.19 | 1.91 | 2.05 |
| 30 | 62 | 616 | CHL | MG-NB | -7.19 | 1.91 | 2.05 |
| 30 | 6 | 606 | CHL | MG-NB | -7.18 | 1.91 | 2.05 |
| 30 | 62 | 606 | CHL | MG-NB | -7.18 | 1.91 | 2.05 |
| 30 | 12 | 601 | CHL | MG-NB | -7.18 | 1.91 | 2.05 |
| 30 | 72 | 606 | CHL | MG-NB | -7.18 | 1.91 | 2.05 |
| 30 | 82 | 601 | CHL | C1B-C2B | 7.18 | 1.47 | 1.39 |
| 30 | 7 | 606 | CHL | MG-NB | -7.17 | 1.91 | 2.05 |
| 30 | 62 | 618 | CHL | MG-NB | -7.16 | 1.91 | 2.05 |
| 30 | 6 | 608 | CHL | MG-NB | -7.16 | 1.91 | 2.05 |
| 30 | 4 | 601 | CHL | C1B-C2B | 7.16 | 1.47 | 1.39 |
| 30 | 6 | 607 | CHL | MG-NB | -7.15 | 1.91 | 2.05 |
| 30 | 62 | 607 | CHL | MG-NB | -7.15 | 1.91 | 2.05 |
| 30 | 8 | 601 | CHL | C1B-C2B | 7.15 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 5 | 618 | CHL | MG-NB | -7.15 | 1.91 | 2.05 |
| 30 | 82 | 606 | CHL | MG-NB | -7.14 | 1.91 | 2.05 |
| 30 | 6 | 618 | CHL | MG-NB | -7.13 | 1.91 | 2.05 |
| 30 | 8 | 606 | CHL | MG-NB | -7.10 | 1.91 | 2.05 |
| 30 | 52 | 618 | CHL | MG-NB | -7.08 | 1.91 | 2.05 |
| 30 | 12 | 601 | CHL | C1B-C2B | 7.00 | 1.47 | 1.39 |
| 30 | 1 | 601 | CHL | C1B-C2B | 6.98 | 1.47 | 1.39 |
| 30 | 82 | 606 | CHL | C1B-C2B | 6.95 | 1.47 | 1.39 |
| 30 | 52 | 618 | CHL | C1B-C2B | 6.95 | 1.47 | 1.39 |
| 30 | 9 | 606 | CHL | C1B-C2B | 6.95 | 1.47 | 1.39 |
| 30 | 42 | 618 | CHL | C1B-C2B | 6.94 | 1.47 | 1.39 |
| 30 | Z2 | 606 | CHL | C1B-C2B | 6.93 | 1.47 | 1.39 |
| 30 | 92 | 606 | CHL | C1B-C2B | 6.92 | 1.47 | 1.39 |
| 30 | 4 | 618 | CHL | C1B-C2B | 6.92 | 1.47 | 1.39 |
| 30 | 8 | 606 | CHL | C1B-C2B | 6.91 | 1.47 | 1.39 |
| 30 | 5 | 618 | CHL | C1B-C2B | 6.90 | 1.47 | 1.39 |
| 30 | 6 | 606 | CHL | C1B-C2B | 6.86 | 1.47 | 1.39 |
| 30 | 62 | 606 | CHL | C1B-C2B | 6.86 | 1.47 | 1.39 |
| 30 | Z2 | 601 | CHL | C1B-C2B | 6.86 | 1.47 | 1.39 |
| 30 | Z | 601 | CHL | C1B-C2B | 6.84 | 1.47 | 1.39 |
| 30 | Z | 606 | CHL | C1B-C2B | 6.81 | 1.47 | 1.39 |
| 30 | 3 | 608 | CHL | C1B-C2B | 6.79 | 1.47 | 1.39 |
| 30 | 72 | 606 | CHL | C1B-C2B | 6.78 | 1.47 | 1.39 |
| 30 | 6 | 618 | CHL | C1B-C2B | 6.74 | 1.47 | 1.39 |
| 30 | 62 | 618 | CHL | C1B-C2B | 6.74 | 1.47 | 1.39 |
| 30 | 7 | 606 | CHL | C1B-C2B | 6.72 | 1.47 | 1.39 |
| 30 | 5 | 606 | CHL | C1B-C2B | 6.71 | 1.47 | 1.39 |
| 30 | 52 | 606 | CHL | C1B-C2B | 6.71 | 1.47 | 1.39 |
| 30 | 32 | 608 | CHL | C1B-C2B | 6.70 | 1.47 | 1.39 |
| 30 | Z2 | 607 | CHL | C1B-C2B | 6.69 | 1.47 | 1.39 |
| 30 | 4 | 607 | CHL | C1B-C2B | 6.69 | 1.47 | 1.39 |
| 30 | 4 | 608 | CHL | C1B-C2B | 6.68 | 1.47 | 1.39 |
| 30 | Z | 607 | CHL | C1B-C2B | 6.67 | 1.47 | 1.39 |
| 30 | 6 | 608 | CHL | C1B-C2B | 6.66 | 1.47 | 1.39 |
| 30 | 62 | 608 | CHL | C1B-C2B | 6.66 | 1.47 | 1.39 |
| 30 | 42 | 607 | CHL | C1B-C2B | 6.66 | 1.47 | 1.39 |
| 30 | 42 | 608 | CHL | C1B-C2B | 6.66 | 1.47 | 1.39 |
| 30 | 7 | 607 | CHL | C1B-C2B | 6.64 | 1.47 | 1.39 |
| 30 | 5 | 607 | CHL | C1B-C2B | 6.62 | 1.47 | 1.39 |
| 30 | 52 | 607 | CHL | C1B-C2B | 6.62 | 1.47 | 1.39 |
| 30 | 92 | 607 | CHL | C1B-C2B | 6.58 | 1.47 | 1.39 |
| 30 | 5 | 608 | CHL | C1B-C2B | 6.57 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 1 | 607 | CHL | C1B-C2B | 6.57 | 1.47 | 1.39 |
| 30 | 6 | 607 | CHL | C1B-C2B | 6.57 | 1.47 | 1.39 |
| 30 | 12 | 607 | CHL | C1B-C2B | 6.57 | 1.47 | 1.39 |
| 30 | 72 | 607 | CHL | C1B-C2B | 6.56 | 1.47 | 1.39 |
| 30 | 4 | 606 | CHL | C1B-C2B | 6.54 | 1.47 | 1.39 |
| 30 | 82 | 607 | CHL | C1B-C2B | 6.52 | 1.47 | 1.39 |
| 30 | 52 | 608 | CHL | C1B-C2B | 6.51 | 1.46 | 1.39 |
| 30 | 62 | 607 | CHL | C1B-C2B | 6.48 | 1.46 | 1.39 |
| 30 | 6 | 601 | CHL | C1B-C2B | 6.47 | 1.46 | 1.39 |
| 30 | 62 | 601 | CHL | C1B-C2B | 6.47 | 1.46 | 1.39 |
| 30 | 62 | 616 | CHL | C1B-C2B | 6.44 | 1.46 | 1.39 |
| 30 | 8 | 607 | CHL | C1B-C2B | 6.44 | 1.46 | 1.39 |
| 30 | 72 | 601 | CHL | C1B-C2B | 6.44 | 1.46 | 1.39 |
| 30 | 42 | 606 | CHL | C1B-C2B | 6.43 | 1.46 | 1.39 |
| 30 | 12 | 606 | CHL | C1B-C2B | 6.41 | 1.46 | 1.39 |
| 30 | 1 | 606 | CHL | C1B-C2B | 6.41 | 1.46 | 1.39 |
| 30 | 6 | 616 | CHL | C1B-C2B | 6.39 | 1.46 | 1.39 |
| 30 | 7 | 601 | CHL | C1B-C2B | 6.36 | 1.46 | 1.39 |
| 30 | 9 | 607 | CHL | MG-ND | -6.26 | 1.93 | 2.05 |
| 30 | 32 | 608 | CHL | MG-ND | -6.10 | 1.93 | 2.05 |
| 30 | 3 | 608 | CHL | MG-ND | -6.10 | 1.93 | 2.05 |
| 30 | 92 | 607 | CHL | MG-ND | -6.07 | 1.93 | 2.05 |
| 30 | Z2 | 601 | CHL | MG-ND | -6.05 | 1.93 | 2.05 |
| 30 | 1 | 607 | CHL | MG-ND | -6.05 | 1.93 | 2.05 |
| 30 | Z | 601 | CHL | MG-ND | -6.05 | 1.93 | 2.05 |
| 30 | 6 | 601 | CHL | MG-ND | -6.05 | 1.93 | 2.05 |
| 30 | 62 | 601 | CHL | MG-ND | -6.03 | 1.93 | 2.05 |
| 30 | Z | 607 | CHL | MG-ND | -6.01 | 1.93 | 2.05 |
| 30 | Z2 | 607 | CHL | MG-ND | -6.01 | 1.93 | 2.05 |
| 30 | 12 | 607 | CHL | MG-ND | -6.01 | 1.93 | 2.05 |
| 30 | 7 | 607 | CHL | MG-ND | -5.96 | 1.94 | 2.05 |
| 30 | 72 | 607 | CHL | MG-ND | -5.96 | 1.94 | 2.05 |
| 30 | 5 | 606 | CHL | MG-ND | -5.96 | 1.94 | 2.05 |
| 30 | 82 | 607 | CHL | MG-ND | -5.95 | 1.94 | 2.05 |
| 30 | 82 | 601 | CHL | MG-ND | -5.95 | 1.94 | 2.05 |
| 30 | 4 | 607 | CHL | MG-ND | -5.94 | 1.94 | 2.05 |
| 30 | 4 | 608 | CHL | MG-ND | -5.94 | 1.94 | 2.05 |
| 30 | 52 | 606 | CHL | MG-ND | -5.93 | 1.94 | 2.05 |
| 30 | 42 | 601 | CHL | MG-ND | -5.93 | 1.94 | 2.05 |
| 30 | 8 | 607 | CHL | MG-ND | -5.93 | 1.94 | 2.05 |
| 30 | 12 | 606 | CHL | MG-ND | -5.93 | 1.94 | 2.05 |
| 30 | 42 | 608 | CHL | MG-ND | -5.91 | 1.94 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 803 | CLA | MG-NB | -5.91 | 1.94 | 2.05 |
| 30 | 8 | 601 | CHL | MG-ND | -5.91 | 1.94 | 2.05 |
| 30 | 6 | 616 | CHL | MG-ND | -5.91 | 1.94 | 2.05 |
| 30 | 62 | 616 | CHL | MG-ND | -5.91 | 1.94 | 2.05 |
| 30 | 42 | 607 | CHL | MG-ND | -5.90 | 1.94 | 2.05 |
| 30 | 4 | 606 | CHL | MG-ND | -5.90 | 1.94 | 2.05 |
| 30 | 6 | 606 | CHL | MG-ND | -5.90 | 1.94 | 2.05 |
| 30 | 62 | 606 | CHL | MG-ND | -5.90 | 1.94 | 2.05 |
| 30 | 42 | 606 | CHL | MG-ND | -5.89 | 1.94 | 2.05 |
| 30 | 4 | 601 | CHL | MG-ND | -5.89 | 1.94 | 2.05 |
| 21 | A | 803 | CLA | MG-NB | -5.88 | 1.94 | 2.05 |
| 30 | 1 | 601 | CHL | MG-ND | -5.88 | 1.94 | 2.05 |
| 30 | 1 | 606 | CHL | MG-ND | -5.87 | 1.94 | 2.05 |
| 30 | 12 | 601 | CHL | MG-ND | -5.87 | 1.94 | 2.05 |
| 30 | 9 | 606 | CHL | MG-ND | -5.87 | 1.94 | 2.05 |
| 30 | 92 | 606 | CHL | MG-ND | -5.87 | 1.94 | 2.05 |
| 30 | 62 | 608 | CHL | MG-ND | -5.87 | 1.94 | 2.05 |
| 30 | 52 | 608 | CHL | MG-ND | -5.86 | 1.94 | 2.05 |
| 30 | 5 | 607 | CHL | MG-ND | -5.84 | 1.94 | 2.05 |
| 30 | 8 | 606 | CHL | MG-ND | -5.84 | 1.94 | 2.05 |
| 30 | 5 | 608 | CHL | MG-ND | -5.83 | 1.94 | 2.05 |
| 30 | 6 | 608 | CHL | MG-ND | -5.83 | 1.94 | 2.05 |
| 21 | A | 854 | CLA | MG-NB | -5.82 | 1.94 | 2.05 |
| 30 | 82 | 606 | CHL | MG-ND | -5.82 | 1.94 | 2.05 |
| 30 | 72 | 606 | CHL | MG-ND | -5.81 | 1.94 | 2.05 |
| 30 | 6 | 607 | CHL | MG-ND | -5.81 | 1.94 | 2.05 |
| 30 | 62 | 607 | CHL | MG-ND | -5.81 | 1.94 | 2.05 |
| 30 | 52 | 607 | CHL | MG-ND | -5.80 | 1.94 | 2.05 |
| 21 | A2 | 829 | CLA | MG-NB | -5.80 | 1.94 | 2.05 |
| 30 | 7 | 601 | CHL | MG-ND | -5.79 | 1.94 | 2.05 |
| 30 | 7 | 606 | CHL | MG-ND | -5.78 | 1.94 | 2.05 |
| 21 | A | 837 | CLA | MG-NB | -5.78 | 1.94 | 2.05 |
| 21 | A2 | 854 | CLA | MG-NB | -5.78 | 1.94 | 2.05 |
| 30 | 72 | 601 | CHL | MG-ND | -5.77 | 1.94 | 2.05 |
| 21 | A | 829 | CLA | MG-NB | -5.77 | 1.94 | 2.05 |
| 30 | 52 | 618 | CHL | MG-ND | -5.77 | 1.94 | 2.05 |
| 21 | A2 | 837 | CLA | MG-NB | -5.76 | 1.94 | 2.05 |
| 30 | 6 | 618 | CHL | MG-ND | -5.73 | 1.94 | 2.05 |
| 21 | 72 | 610 | CLA | MG-NB | -5.73 | 1.94 | 2.05 |
| 30 | Z2 | 606 | CHL | MG-ND | -5.72 | 1.94 | 2.05 |
| 21 | 7 | 610 | CLA | MG-NB | -5.70 | 1.94 | 2.05 |
| 30 | 62 | 618 | CHL | MG-ND | -5.70 | 1.94 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 5 | 618 | CHL | MG-ND | -5.70 | 1.94 | 2.05 |
| 30 | 42 | 618 | CHL | MG-ND | -5.69 | 1.94 | 2.05 |
| 21 | B2 | 821 | CLA | MG-NB | -5.68 | 1.94 | 2.05 |
| 30 | 4 | 618 | CHL | MG-ND | -5.67 | 1.94 | 2.05 |
| 30 | Z | 606 | CHL | MG-ND | -5.67 | 1.94 | 2.05 |
| 20 | A | 801 | CL0 | MG-NB | -5.63 | 1.94 | 2.05 |
| 20 | A2 | 801 | CL0 | MG-NB | -5.63 | 1.94 | 2.05 |
| 21 | B | 821 | CLA | MG-NB | -5.60 | 1.94 | 2.05 |
| 21 | 3 | 606 | CLA | MG-NB | -5.56 | 1.94 | 2.05 |
| 21 | A2 | 819 | CLA | MG-NB | -5.54 | 1.94 | 2.05 |
| 21 | A | 810 | CLA | MG-NB | -5.53 | 1.94 | 2.05 |
| 21 | B | 803 | CLA | MG-NB | -5.52 | 1.94 | 2.05 |
| 21 | B | 824 | CLA | MG-NB | -5.51 | 1.94 | 2.05 |
| 21 | 32 | 606 | CLA | MG-NB | -5.51 | 1.94 | 2.05 |
| 21 | B2 | 803 | CLA | MG-NB | -5.50 | 1.94 | 2.05 |
| 21 | 3 | 609 | CLA | MG-NB | -5.48 | 1.94 | 2.05 |
| 21 | A | 819 | CLA | MG-NB | -5.48 | 1.94 | 2.05 |
| 21 | B2 | 824 | CLA | MG-NB | -5.47 | 1.94 | 2.05 |
| 21 | 9 | 602 | CLA | MG-NB | -5.47 | 1.94 | 2.05 |
| 21 | A2 | 810 | CLA | MG-NB | -5.46 | 1.95 | 2.05 |
| 21 | 1 | 602 | CLA | MG-NB | -5.46 | 1.95 | 2.05 |
| 21 | 72 | 609 | CLA | MG-NB | -5.45 | 1.95 | 2.05 |
| 21 | 9 | 614 | CLA | MG-NB | -5.44 | 1.95 | 2.05 |
| 21 | 7 | 609 | CLA | MG-NB | -5.43 | 1.95 | 2.05 |
| 21 | 82 | 602 | CLA | MG-NB | -5.43 | 1.95 | 2.05 |
| 21 | 32 | 609 | CLA | MG-NB | -5.43 | 1.95 | 2.05 |
| 21 | 6 | 622 | CLA | MG-NB | -5.42 | 1.95 | 2.05 |
| 21 | 92 | 602 | CLA | MG-NB | -5.42 | 1.95 | 2.05 |
| 21 | B | 827 | CLA | MG-NB | -5.42 | 1.95 | 2.05 |
| 21 | 92 | 614 | CLA | MG-NB | -5.42 | 1.95 | 2.05 |
| 21 | 4 | 609 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | 42 | 609 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | 12 | 616 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | A2 | 805 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | 8 | 602 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | 62 | 622 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | 12 | 602 | CLA | MG-NB | -5.41 | 1.95 | 2.05 |
| 21 | Z | 602 | CLA | MG-NB | -5.40 | 1.95 | 2.05 |
| 21 | B2 | 841 | CLA | MG-NB | -5.40 | 1.95 | 2.05 |
| 21 | B2 | 819 | CLA | MG-NB | -5.39 | 1.95 | 2.05 |
| 21 | B | 819 | CLA | MG-NB | -5.39 | 1.95 | 2.05 |
| 21 | 32 | 603 | CLA | MG-NB | -5.39 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B2 | 809 | CLA | MG-NB | -5.38 | 1.95 | 2.05 |
| 21 | B | 820 | CLA | MG-NB | -5.37 | 1.95 | 2.05 |
| 21 | B2 | 827 | CLA | MG-NB | -5.37 | 1.95 | 2.05 |
| 21 | A | 834 | CLA | MG-NB | -5.37 | 1.95 | 2.05 |
| 21 | 42 | 602 | CLA | MG-NB | -5.37 | 1.95 | 2.05 |
| 21 | A2 | 834 | CLA | MG-NB | -5.37 | 1.95 | 2.05 |
| 21 | A | 805 | CLA | MG-NB | -5.37 | 1.95 | 2.05 |
| 21 | 4 | 612 | CLA | C1D-ND | 5.36 | 1.44 | 1.37 |
| 21 | 12 | 610 | CLA | MG-NB | -5.36 | 1.95 | 2.05 |
| 21 | 1 | 616 | CLA | MG-NB | -5.36 | 1.95 | 2.05 |
| 21 | 8 | 609 | CLA | MG-NB | -5.36 | 1.95 | 2.05 |
| 21 | Z2 | 602 | CLA | MG-NB | -5.36 | 1.95 | 2.05 |
| 21 | 3 | 603 | CLA | MG-NB | -5.35 | 1.95 | 2.05 |
| 21 | A2 | 833 | CLA | MG-NB | -5.35 | 1.95 | 2.05 |
| 21 | B2 | 812 | CLA | MG-NB | -5.35 | 1.95 | 2.05 |
| 21 | B | 809 | CLA | MG-NB | -5.35 | 1.95 | 2.05 |
| 21 | 4 | 602 | CLA | MG-NB | -5.35 | 1.95 | 2.05 |
| 21 | 7 | 602 | CLA | MG-NB | -5.34 | 1.95 | 2.05 |
| 21 | B2 | 820 | CLA | MG-NB | -5.34 | 1.95 | 2.05 |
| 21 | B | 841 | CLA | MG-NB | -5.34 | 1.95 | 2.05 |
| 21 | 82 | 603 | CLA | MG-NB | -5.34 | 1.95 | 2.05 |
| 21 | A | 817 | CLA | MG-NB | -5.33 | 1.95 | 2.05 |
| 21 | A2 | 817 | CLA | MG-NB | -5.33 | 1.95 | 2.05 |
| 21 | B2 | 807 | CLA | MG-NB | -5.33 | 1.95 | 2.05 |
| 21 | B | 807 | CLA | MG-NB | -5.33 | 1.95 | 2.05 |
| 21 | A2 | 825 | CLA | MG-NB | -5.33 | 1.95 | 2.05 |
| 21 | A | 807 | CLA | MG-NB | -5.33 | 1.95 | 2.05 |
| 21 | B2 | 829 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | 5 | 621 | CLA | C1D-ND | 5.32 | 1.44 | 1.37 |
| 21 | 82 | 609 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | 3 | 602 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | B | 829 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | B | 834 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | A2 | 836 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | 3 | 610 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | 32 | 610 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | 32 | 602 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | 9 | 611 | CLA | MG-NB | -5.32 | 1.95 | 2.05 |
| 21 | B | 838 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | B2 | 838 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | B | 818 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | B2 | 818 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | Z2 | 608 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | 1 | 610 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | B | 837 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | J | 101 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | A | 833 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | A | 825 | CLA | MG-NB | -5.31 | 1.95 | 2.05 |
| 21 | B2 | 802 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | 9 | 601 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | B | 812 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | 92 | 601 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | L | 203 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | A | 823 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | B | 802 | CLA | MG-NB | -5.30 | 1.95 | 2.05 |
| 21 | 72 | 602 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | B2 | 834 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | K | 203 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | 5 | 602 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | 52 | 602 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | 3 | 613 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | 32 | 613 | CLA | MG-NB | -5.29 | 1.95 | 2.05 |
| 21 | 92 | 611 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | 52 | 621 | CLA | C1D-ND | 5.28 | 1.44 | 1.37 |
| 21 | 8 | 603 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | A2 | 807 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | B2 | 837 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | 12 | 603 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | A2 | 823 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | Z | 609 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | 6 | 602 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | 12 | 609 | CLA | MG-NB | -5.28 | 1.95 | 2.05 |
| 21 | A | 836 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | 1 | 609 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | 42 | 612 | CLA | C1D-ND | 5.27 | 1.44 | 1.37 |
| 21 | 6 | 617 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | 12 | 608 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | A2 | 840 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | Z | 608 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | 6 | 611 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | A2 | 826 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | B2 | 831 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | 62 | 602 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | A | 826 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | Z2 | 609 | CLA | MG-NB | -5.27 | 1.95 | 2.05 |
| 21 | 3 | 615 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | 1 | 604 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | J2 | 101 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | Z | 612 | CLA | C1D-ND | 5.26 | 1.44 | 1.37 |
| 21 | Z2 | 612 | CLA | C1D-ND | 5.26 | 1.44 | 1.37 |
| 21 | 72 | 608 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | L2 | 203 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | A2 | 815 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | 7 | 614 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | 82 | 610 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | 62 | 617 | CLA | MG-NB | -5.26 | 1.95 | 2.05 |
| 21 | 12 | 604 | CLA | MG-NB | -5.25 | 1.95 | 2.05 |
| 21 | A | 840 | CLA | MG-NB | -5.25 | 1.95 | 2.05 |
| 21 | B | 831 | CLA | MG-NB | -5.25 | 1.95 | 2.05 |
| 21 | 72 | 614 | CLA | MG-NB | -5.25 | 1.95 | 2.05 |
| 21 | A | 822 | CLA | MG-NB | -5.25 | 1.95 | 2.05 |
| 21 | 52 | 603 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | 1 | 603 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | B2 | 810 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | A2 | 822 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | K | 206 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | 32 | 615 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | 12 | 611 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | B2 | 806 | CLA | MG-NB | -5.24 | 1.95 | 2.05 |
| 21 | 5 | 603 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 8 | 610 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | Z | 616 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | G2 | 204 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 6 | 614 | CLA | C1D-ND | 5.23 | 1.44 | 1.37 |
| 21 | 62 | 614 | CLA | C1D-ND | 5.23 | 1.44 | 1.37 |
| 21 | 82 | 608 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 1 | 608 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | K2 | 203 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 72 | 603 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 92 | 613 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 52 | 610 | CLA | MG-NB | -5.23 | 1.95 | 2.05 |
| 21 | 7 | 603 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |
| 21 | 4 | 603 | CLA | C1D-ND | 5.22 | 1.44 | 1.37 |
| 21 | 5 | 610 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |
| 21 | B | 811 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |
| 21 | 62 | 611 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 604 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |
| 21 | 52 | 604 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |
| 21 | 7 | 608 | CLA | MG-NB | -5.22 | 1.95 | 2.05 |
| 21 | L2 | 204 | CLA | C1D-ND | 5.22 | 1.44 | 1.37 |
| 21 | A | 808 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | A | 843 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | 3 | 604 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | 32 | 604 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | A | 821 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | B2 | 804 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | A2 | 843 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | 9 | 609 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | Z | 603 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | B | 806 | CLA | MG-NB | -5.21 | 1.95 | 2.05 |
| 21 | 42 | 610 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | B | 817 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | 6 | 612 | CLA | C1D-ND | 5.20 | 1.44 | 1.37 |
| 21 | 62 | 612 | CLA | C1D-ND | 5.20 | 1.44 | 1.37 |
| 21 | A | 842 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | 8 | 608 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | 7 | 616 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | 8 | 611 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | 82 | 611 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | K2 | 206 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | 9 | 613 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | A | 815 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 21 | G | 204 | CLA | MG-NB | -5.20 | 1.95 | 2.05 |
| 20 | A | 801 | CL0 | C3A-C2A | -5.19 | 1.50 | 1.54 |
| 21 | 32 | 614 | CLA | MG-NB | -5.19 | 1.95 | 2.05 |
| 21 | G | 203 | CLA | MG-NB | -5.19 | 1.95 | 2.05 |
| 21 | 8 | 613 | CLA | MG-NB | -5.19 | 1.95 | 2.05 |
| 21 | 62 | 610 | CLA | MG-NB | -5.19 | 1.95 | 2.05 |
| 21 | 1 | 611 | CLA | MG-NB | -5.19 | 1.95 | 2.05 |
| 21 | 3 | 611 | CLA | MG-NB | -5.19 | 1.95 | 2.05 |
| 21 | 5 | 612 | CLA | C1D-ND | 5.18 | 1.44 | 1.37 |
| 21 | 82 | 613 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | 7 | 613 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | Z2 | 616 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | 62 | 603 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | B2 | 835 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | 3 | 614 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | B | 810 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 42 | 611 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | B2 | 823 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | K | 204 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | 42 | 613 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | 42 | 603 | CLA | C1D-ND | 5.18 | 1.44 | 1.37 |
| 21 | B | 804 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | A2 | 821 | CLA | MG-NB | -5.18 | 1.95 | 2.05 |
| 21 | A2 | 824 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | A2 | 842 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | B2 | 811 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | 92 | 609 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | A | 824 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | F | 304 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 21 | F2 | 304 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 21 | L2 | 204 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | 1 | 614 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | B | 823 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | Z | 610 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | 72 | 613 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | 6 | 610 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | K2 | 204 | CLA | MG-NB | -5.17 | 1.95 | 2.05 |
| 21 | 82 | 612 | CLA | C1D-ND | 5.17 | 1.44 | 1.37 |
| 21 | 4 | 610 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | B2 | 817 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | 3 | 617 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | Z | 603 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 21 | A | 845 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | G2 | 203 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | 72 | 616 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | B | 824 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 21 | 5 | 601 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 21 | 52 | 601 | CLA | C1D-ND | 5.16 | 1.44 | 1.37 |
| 21 | K | 201 | CLA | MG-NB | -5.16 | 1.95 | 2.05 |
| 21 | 12 | 614 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 20 | A2 | 801 | CL0 | C3A-C2A | -5.15 | 1.50 | 1.54 |
| 21 | Z2 | 604 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 21 | Z2 | 610 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 21 | B | 840 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 21 | L | 204 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 21 | A2 | 845 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 21 | 3 | 607 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 21 | 32 | 607 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 614 | CLA | C1D-ND | 5.15 | 1.44 | 1.37 |
| 21 | 72 | 611 | CLA | MG-NB | -5.15 | 1.95 | 2.05 |
| 21 | B | 825 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | Z2 | 603 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | A2 | 808 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | F2 | 301 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 1 | 613 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 4 | 611 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 8 | 614 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | A | 813 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 7 | 611 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 8 | 604 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | B | 835 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 4 | 613 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | K2 | 201 | CLA | MG-NB | -5.14 | 1.95 | 2.05 |
| 21 | 32 | 617 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 6 | 603 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 12 | 613 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | A | 835 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | A2 | 835 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 9 | 610 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 82 | 614 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 52 | 612 | CLA | C1D-ND | 5.13 | 1.44 | 1.37 |
| 21 | 4 | 614 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | Z | 604 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 92 | 610 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 6 | 604 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | A2 | 804 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | B2 | 825 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | K2 | 206 | CLA | C1D-ND | 5.13 | 1.44 | 1.37 |
| 21 | 82 | 608 | CLA | C1D-ND | 5.13 | 1.44 | 1.37 |
| 21 | L | 204 | CLA | MG-NB | -5.13 | 1.95 | 2.05 |
| 21 | 8 | 612 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 21 | 5 | 616 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 21 | 52 | 616 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 21 | 5 | 611 | CLA | MG-NB | -5.12 | 1.95 | 2.05 |
| 21 | B2 | 824 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 21 | 4 | 604 | CLA | MG-NB | -5.12 | 1.95 | 2.05 |
| 21 | 42 | 604 | CLA | MG-NB | -5.12 | 1.95 | 2.05 |
| 21 | B | 827 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 21 | 72 | 620 | CLA | C1D-ND | 5.12 | 1.44 | 1.37 |
| 21 | 42 | 614 | CLA | MG-NB | -5.12 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 92 | 603 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 21 | A | 802 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | A | 830 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | B2 | 827 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 21 | B | 826 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | B2 | 826 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | 82 | 604 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | 52 | 611 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | A2 | 812 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | 7 | 620 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | 92 | 601 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 21 | A | 806 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | K2 | 203 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 21 | Z2 | 603 | CLA | C1D-ND | 5.11 | 1.44 | 1.37 |
| 21 | F | 301 | CLA | MG-NB | -5.11 | 1.95 | 2.05 |
| 21 | A2 | 830 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | 6 | 613 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | 72 | 604 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | B | 813 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | A2 | 841 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | B2 | 813 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | 52 | 614 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | A | 826 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | G2 | 204 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | 72 | 620 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | 12 | 612 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | 32 | 611 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | A2 | 817 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | 6 | 604 | CLA | C1D-ND | 5.10 | 1.44 | 1.37 |
| 21 | A | 804 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | B | 815 | CLA | MG-NB | -5.10 | 1.95 | 2.05 |
| 21 | 1 | 612 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 21 | 6 | 611 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 21 | 52 | 603 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 21 | B2 | 833 | CLA | MG-NB | -5.09 | 1.95 | 2.05 |
| 21 | 8 | 608 | CLA | C1D-ND | 5.09 | 1.44 | 1.37 |
| 21 | 5 | 616 | CLA | MG-NB | -5.09 | 1.95 | 2.05 |
| 21 | A2 | 813 | CLA | MG-NB | -5.09 | 1.95 | 2.05 |
| 21 | B2 | 815 | CLA | MG-NB | -5.09 | 1.95 | 2.05 |
| 21 | B2 | 840 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | J | 101 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | Z | 611 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 614 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | A2 | 828 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | 52 | 614 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | Z | 616 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | Z2 | 616 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | A2 | 839 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | 62 | 613 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | A2 | 806 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | 9 | 603 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | Z2 | 611 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | 62 | 604 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | K | 203 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | 3 | 615 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | 7 | 614 | CLA | C1D-ND | 5.08 | 1.44 | 1.37 |
| 21 | 62 | 609 | CLA | MG-NB | -5.08 | 1.95 | 2.05 |
| 21 | 5 | 603 | CLA | C1D-ND | 5.07 | 1.44 | 1.37 |
| 21 | A2 | 802 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | 52 | 621 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | A | 828 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | 4 | 616 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | A | 820 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | A | 812 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | A2 | 827 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | 5 | 613 | CLA | MG-NB | -5.07 | 1.95 | 2.05 |
| 21 | B | 839 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 21 | J2 | 101 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 21 | 52 | 613 | CLA | MG-NB | -5.06 | 1.95 | 2.05 |
| 21 | 9 | 601 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 21 | 62 | 611 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 21 | 4 | 616 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 21 | 42 | 616 | CLA | C1D-ND | 5.06 | 1.44 | 1.37 |
| 21 | B | 833 | CLA | MG-NB | -5.06 | 1.95 | 2.05 |
| 21 | 6 | 609 | CLA | MG-NB | -5.06 | 1.95 | 2.05 |
| 21 | A | 839 | CLA | MG-NB | -5.06 | 1.95 | 2.05 |
| 21 | B | 816 | CLA | MG-NB | -5.06 | 1.95 | 2.05 |
| 21 | A | 841 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |
| 21 | 42 | 616 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |
| 21 | A2 | 820 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |
| 21 | 82 | 603 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 21 | 92 | 614 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 21 | B2 | 816 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |
| 21 | 5 | 621 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 7 | 620 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 21 | B2 | 839 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |
| 21 | Z | 614 | CLA | MG-NB | -5.05 | 1.95 | 2.05 |
| 21 | 82 | 614 | CLA | C1D-ND | 5.05 | 1.44 | 1.37 |
| 21 | B | 814 | CLA | MG-NB | -5.04 | 1.95 | 2.05 |
| 21 | 52 | 616 | CLA | MG-NB | -5.04 | 1.95 | 2.05 |
| 21 | 7 | 604 | CLA | MG-NB | -5.04 | 1.95 | 2.05 |
| 21 | A2 | 826 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | 42 | 614 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | A | 832 | CLA | MG-NB | -5.04 | 1.95 | 2.05 |
| 21 | A | 816 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | G | 204 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | B2 | 814 | CLA | MG-NB | -5.04 | 1.95 | 2.05 |
| 21 | 62 | 604 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | A2 | 816 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | Z2 | 614 | CLA | C1D-ND | 5.04 | 1.44 | 1.37 |
| 21 | 6 | 603 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 21 | 9 | 614 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 21 | A2 | 832 | CLA | MG-NB | -5.03 | 1.95 | 2.05 |
| 21 | A | 827 | CLA | MG-NB | -5.03 | 1.95 | 2.05 |
| 21 | 12 | 608 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 21 | 32 | 615 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 21 | 6 | 622 | CLA | C1D-ND | 5.03 | 1.44 | 1.37 |
| 21 | A2 | 814 | CLA | MG-NB | -5.02 | 1.95 | 2.05 |
| 21 | A | 811 | CLA | MG-NB | -5.02 | 1.95 | 2.05 |
| 21 | A2 | 845 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | 8 | 616 | CLA | MG-NB | -5.02 | 1.95 | 2.05 |
| 21 | K2 | 201 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | A | 817 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | B2 | 839 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | 3 | 612 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | F2 | 303 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | K | 206 | CLA | C1D-ND | 5.02 | 1.44 | 1.37 |
| 21 | A2 | 818 | CLA | MG-NB | -5.01 | 1.95 | 2.05 |
| 21 | Z2 | 613 | CLA | MG-NB | -5.01 | 1.95 | 2.05 |
| 21 | 3 | 604 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 21 | 6 | 602 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 21 | A | 838 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 21 | A2 | 838 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 21 | 3 | 614 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 21 | A2 | 835 | CLA | C1D-ND | 5.01 | 1.44 | 1.37 |
| 21 | 9 | 604 | CLA | MG-NB | -5.00 | 1.95 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 1 | 614 | CLA | C1D-ND | 5.00 | 1.44 | 1.37 |
| 21 | A | 818 | CLA | MG-NB | -5.00 | 1.95 | 2.05 |
| 21 | A | 814 | CLA | MG-NB | -5.00 | 1.95 | 2.05 |
| 21 | 7 | 612 | CLA | C1D-ND | 5.00 | 1.44 | 1.37 |
| 21 | 92 | 612 | CLA | C1D-ND | 5.00 | 1.44 | 1.37 |
| 21 | 72 | 612 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 82 | 616 | CLA | MG-NB | -4.99 | 1.95 | 2.05 |
| 21 | 32 | 604 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | Z | 609 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | B | 835 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 5 | 611 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 62 | 602 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 62 | 603 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 4 | 610 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 4 | 614 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | 42 | 610 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | B | 828 | CLA | MG-NB | -4.99 | 1.95 | 2.05 |
| 21 | A2 | 811 | CLA | MG-NB | -4.99 | 1.95 | 2.05 |
| 21 | Z2 | 609 | CLA | C1D-ND | 4.99 | 1.44 | 1.37 |
| 21 | B2 | 822 | CLA | MG-NB | -4.98 | 1.95 | 2.05 |
| 21 | 62 | 622 | CLA | C1D-ND | 4.98 | 1.44 | 1.37 |
| 21 | Z | 614 | CLA | C1D-ND | 4.98 | 1.44 | 1.37 |
| 21 | 72 | 614 | CLA | C1D-ND | 4.98 | 1.44 | 1.37 |
| 21 | 6 | 613 | CLA | MG-NB | -4.98 | 1.95 | 2.05 |
| 21 | 62 | 613 | CLA | MG-NB | -4.98 | 1.95 | 2.05 |
| 21 | Z2 | 604 | CLA | C1D-ND | 4.98 | 1.44 | 1.37 |
| 21 | Z | 613 | CLA | MG-NB | -4.98 | 1.95 | 2.05 |
| 21 | 5 | 613 | CLA | C1D-ND | 4.98 | 1.44 | 1.37 |
| 21 | B | 839 | CLA | MG-NB | -4.98 | 1.95 | 2.05 |
| 21 | B | 822 | CLA | MG-NB | -4.98 | 1.95 | 2.05 |
| 21 | Z2 | 614 | CLA | MG-NB | -4.97 | 1.95 | 2.05 |
| 21 | 4 | 604 | CLA | C1D-ND | 4.97 | 1.44 | 1.37 |
| 21 | 62 | 614 | CLA | MG-NB | -4.97 | 1.95 | 2.05 |
| 21 | 32 | 614 | CLA | C1D-ND | 4.97 | 1.44 | 1.37 |
| 21 | 3 | 606 | CLA | C1D-ND | 4.97 | 1.44 | 1.37 |
| 21 | 52 | 602 | CLA | C1D-ND | 4.97 | 1.44 | 1.37 |
| 21 | F | 303 | CLA | C1D-ND | 4.97 | 1.44 | 1.37 |
| 21 | 6 | 614 | CLA | MG-NB | -4.97 | 1.95 | 2.05 |
| 21 | 42 | 604 | CLA | C1D-ND | 4.97 | 1.44 | 1.37 |
| 21 | F | 303 | CLA | MG-NB | -4.96 | 1.95 | 2.05 |
| 21 | 5 | 617 | CLA | MG-NB | -4.96 | 1.96 | 2.05 |
| 21 | 52 | 617 | CLA | MG-NB | -4.96 | 1.96 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 92 | 604 | CLA | MG-NB | -4.96 | 1.96 | 2.05 |
| 21 | B2 | 807 | CLA | C1D-ND | 4.96 | 1.44 | 1.37 |
| 21 | 32 | 612 | CLA | C1D-ND | 4.96 | 1.44 | 1.37 |
| 21 | B | 814 | CLA | C1D-ND | 4.96 | 1.44 | 1.37 |
| 21 | B | 830 | CLA | MG-NB | -4.96 | 1.96 | 2.05 |
| 21 | B2 | 830 | CLA | MG-NB | -4.96 | 1.96 | 2.05 |
| 21 | 6 | 617 | CLA | C1D-ND | 4.96 | 1.44 | 1.37 |
| 21 | 12 | 614 | CLA | C1D-ND | 4.96 | 1.44 | 1.37 |
| 21 | A | 815 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | K | 201 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | A2 | 815 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | A2 | 809 | CLA | MG-NB | -4.95 | 1.96 | 2.05 |
| 21 | Z | 611 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | A | 840 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | B | 810 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | B2 | 832 | CLA | MG-NB | -4.95 | 1.96 | 2.05 |
| 21 | A | 819 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | 8 | 603 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | F | 304 | CLA | MG-NB | -4.95 | 1.96 | 2.05 |
| 21 | A | 845 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | 4 | 611 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | 42 | 611 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | B2 | 805 | CLA | MG-NB | -4.95 | 1.96 | 2.05 |
| 21 | B2 | 828 | CLA | MG-NB | -4.95 | 1.96 | 2.05 |
| 21 | 8 | 614 | CLA | C1D-ND | 4.95 | 1.44 | 1.37 |
| 21 | F2 | 303 | CLA | MG-NB | -4.94 | 1.96 | 2.05 |
| 21 | 5 | 609 | CLA | MG-NB | -4.94 | 1.96 | 2.05 |
| 21 | 52 | 609 | CLA | MG-NB | -4.94 | 1.96 | 2.05 |
| 21 | 9 | 612 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | B | 804 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | B | 808 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | 52 | 611 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | B2 | 835 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | 3 | 611 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | A | 834 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | A2 | 834 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | 1 | 612 | CLA | MG-NB | -4.94 | 1.96 | 2.05 |
| 21 | K | 204 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | Z | 602 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | Z2 | 602 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | 1 | 608 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | 32 | 606 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B2 | 836 | CLA | MG-NB | -4.94 | 1.96 | 2.05 |
| 21 | 12 | 612 | CLA | MG-NB | -4.94 | 1.96 | 2.05 |
| 21 | A2 | 831 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | 52 | 617 | CLA | C1D-ND | 4.94 | 1.44 | 1.37 |
| 21 | A | 835 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | 62 | 610 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | A | 839 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | Z | 604 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | Z2 | 611 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | F2 | 304 | CLA | MG-NB | -4.93 | 1.96 | 2.05 |
| 21 | B | 811 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | 1 | 609 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | 12 | 609 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | B | 807 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | A2 | 839 | CLA | C1D-ND | 4.93 | 1.44 | 1.37 |
| 21 | B | 805 | CLA | MG-NB | -4.93 | 1.96 | 2.05 |
| 21 | B | 832 | CLA | MG-NB | -4.92 | 1.96 | 2.05 |
| 21 | 6 | 610 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | A2 | 832 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | A | 832 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | B2 | 814 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | A2 | 840 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | 52 | 613 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | B | 822 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | B2 | 822 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | A | 809 | CLA | MG-NB | -4.92 | 1.96 | 2.05 |
| 21 | 7 | 613 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | A | 828 | CLA | C1D-ND | 4.92 | 1.44 | 1.37 |
| 21 | B | 836 | CLA | MG-NB | -4.91 | 1.96 | 2.05 |
| 21 | 32 | 612 | CLA | MG-NB | -4.91 | 1.96 | 2.05 |
| 21 | 5 | 601 | CLA | MG-NB | -4.91 | 1.96 | 2.05 |
| 21 | 72 | 613 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | 5 | 604 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | 52 | 604 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | B2 | 836 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | 52 | 609 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | 82 | 602 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | A | 831 | CLA | C1D-ND | 4.91 | 1.44 | 1.37 |
| 21 | 8 | 611 | CLA | C1D-ND | 4.90 | 1.44 | 1.37 |
| 21 | A2 | 816 | CLA | MG-NB | -4.90 | 1.96 | 2.05 |
| 21 | 7 | 603 | CLA | C1D-ND | 4.90 | 1.44 | 1.37 |
| 21 | A | 816 | CLA | MG-NB | -4.90 | 1.96 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 9 | 603 | CLA | MG-NB | -4.90 | 1.96 | 2.05 |
| 21 | A | 830 | CLA | C1D-ND | 4.90 | 1.44 | 1.37 |
| 21 | 92 | 603 | CLA | MG-NB | -4.90 | 1.96 | 2.05 |
| 21 | B2 | 808 | CLA | C1D-ND | 4.90 | 1.44 | 1.37 |
| 21 | A | 818 | CLA | C1D-ND | 4.90 | 1.44 | 1.37 |
| 21 | 4 | 613 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 5 | 602 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | B2 | 804 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 72 | 611 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 72 | 602 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 32 | 611 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 92 | 612 | CLA | MG-NB | -4.89 | 1.96 | 2.05 |
| 21 | B | 836 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | B | 812 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 1 | 603 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | B2 | 812 | CLA | C1D-ND | 4.89 | 1.44 | 1.37 |
| 21 | 8 | 616 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 21 | 82 | 616 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 21 | 92 | 609 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 21 | 9 | 612 | CLA | MG-NB | -4.88 | 1.96 | 2.05 |
| 21 | 8 | 613 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 21 | 3 | 612 | CLA | MG-NB | -4.88 | 1.96 | 2.05 |
| 21 | 82 | 613 | CLA | C1D-ND | 4.88 | 1.44 | 1.37 |
| 21 | 8 | 602 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | Z2 | 613 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | 72 | 604 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | B | 815 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | Z | 613 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | B2 | 815 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | 12 | 603 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | 7 | 604 | CLA | C1D-ND | 4.87 | 1.44 | 1.37 |
| 21 | 7 | 611 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | A2 | 819 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | B2 | 810 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | A2 | 828 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | 72 | 603 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | 42 | 613 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | 62 | 617 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | 9 | 604 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | A | 813 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | A2 | 813 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |
| 21 | B | 816 | CLA | C1D-ND | 4.86 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 617 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | A2 | 820 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | B | 809 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | A2 | 854 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | B | 820 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | B2 | 811 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | 82 | 611 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | 5 | 612 | CLA | MG-NB | -4.85 | 1.96 | 2.05 |
| 21 | 52 | 612 | CLA | MG-NB | -4.85 | 1.96 | 2.05 |
| 21 | B2 | 820 | CLA | C1D-ND | 4.85 | 1.44 | 1.37 |
| 21 | 6 | 612 | CLA | MG-NB | -4.84 | 1.96 | 2.05 |
| 21 | 62 | 612 | CLA | MG-NB | -4.84 | 1.96 | 2.05 |
| 21 | 1 | 613 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 21 | 12 | 613 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 21 | K2 | 204 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 21 | 52 | 601 | CLA | MG-NB | -4.84 | 1.96 | 2.05 |
| 21 | 72 | 608 | CLA | C1D-ND | 4.84 | 1.44 | 1.37 |
| 21 | 3 | 613 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | 82 | 609 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | A2 | 830 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | 32 | 613 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | A2 | 814 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | A | 827 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | 7 | 602 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | B2 | 809 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | B | 808 | CLA | MG-NB | -4.83 | 1.96 | 2.05 |
| 21 | B2 | 808 | CLA | MG-NB | -4.83 | 1.96 | 2.05 |
| 21 | 52 | 610 | CLA | C1D-ND | 4.83 | 1.44 | 1.37 |
| 21 | B | 837 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 21 | A | 814 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 21 | G2 | 203 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 21 | A | 854 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 21 | 9 | 609 | CLA | C1D-ND | 4.82 | 1.44 | 1.37 |
| 21 | A2 | 838 | CLA | MG-NB | -4.82 | 1.96 | 2.05 |
| 21 | A | 838 | CLA | MG-NB | -4.81 | 1.96 | 2.05 |
| 21 | B | 813 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | B2 | 813 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | 1 | 604 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | 3 | 607 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | 12 | 604 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | B2 | 841 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | A | 831 | CLA | MG-NB | -4.81 | 1.96 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 609 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | B2 | 816 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | 92 | 604 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | G | 203 | CLA | C1D-ND | 4.81 | 1.44 | 1.37 |
| 21 | 32 | 617 | CLA | C1D-ND | 4.80 | 1.44 | 1.37 |
| 21 | 4 | 603 | CLA | MG-NB | -4.80 | 1.96 | 2.05 |
| 21 | 3 | 602 | CLA | C1D-ND | 4.80 | 1.44 | 1.37 |
| 21 | 72 | 612 | CLA | MG-NB | -4.80 | 1.96 | 2.05 |
| 21 | 8 | 609 | CLA | C1D-ND | 4.80 | 1.44 | 1.37 |
| 21 | 1 | 611 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | 72 | 616 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | B | 828 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | A | 822 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | A2 | 822 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | A2 | 831 | CLA | MG-NB | -4.79 | 1.96 | 2.05 |
| 21 | 42 | 609 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | 32 | 607 | CLA | C1D-ND | 4.79 | 1.44 | 1.37 |
| 21 | 7 | 612 | CLA | MG-NB | -4.78 | 1.96 | 2.05 |
| 21 | A2 | 821 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | 3 | 617 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | 62 | 609 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | 5 | 610 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | A | 808 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | 4 | 602 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | 42 | 602 | CLA | C1D-ND | 4.78 | 1.44 | 1.37 |
| 21 | B | 841 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 21 | A | 829 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 21 | B2 | 806 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 21 | 12 | 611 | CLA | C1D-ND | 4.77 | 1.44 | 1.37 |
| 21 | 42 | 612 | CLA | MG-NB | -4.77 | 1.96 | 2.05 |
| 21 | 7 | 608 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | 42 | 603 | CLA | MG-NB | -4.76 | 1.96 | 2.05 |
| 21 | 4 | 609 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | A2 | 829 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | 92 | 602 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | 7 | 609 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | B2 | 837 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | Z2 | 608 | CLA | C1D-ND | 4.76 | 1.44 | 1.37 |
| 21 | 82 | 612 | CLA | MG-NB | -4.75 | 1.96 | 2.05 |
| 21 | 7 | 616 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |
| 21 | Z | 608 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |
| 21 | 6 | 609 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | Z2 | 610 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |
| 21 | B2 | 802 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |
| 21 | A | 820 | CLA | C1D-ND | 4.75 | 1.44 | 1.37 |
| 21 | 4 | 612 | CLA | MG-NB | -4.75 | 1.96 | 2.05 |
| 21 | A2 | 827 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 21 | L2 | 203 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 21 | A2 | 841 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 21 | 9 | 610 | CLA | C1D-ND | 4.74 | 1.44 | 1.37 |
| 30 | 5 | 607 | CHL | C3A-C2A | -4.74 | 1.50 | 1.54 |
| 30 | 52 | 607 | CHL | C3A-C2A | -4.74 | 1.50 | 1.54 |
| 21 | B2 | 828 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | A2 | 808 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | B | 826 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | A2 | 836 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | A | 841 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | L | 203 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | A2 | 818 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | 8 | 604 | CLA | C1D-ND | 4.73 | 1.44 | 1.37 |
| 21 | A | 811 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 21 | A | 807 | CLA | C1D-ND | 4.72 | 1.44 | 1.37 |
| 21 | A2 | 811 | CLA | C1D-ND | 4.71 | 1.44 | 1.37 |
| 21 | B2 | 805 | CLA | C1D-ND | 4.71 | 1.44 | 1.37 |
| 21 | A | 821 | CLA | C1D-ND | 4.71 | 1.44 | 1.37 |
| 21 | B2 | 826 | CLA | C1D-ND | 4.71 | 1.44 | 1.37 |
| 21 | 82 | 604 | CLA | C1D-ND | 4.71 | 1.44 | 1.37 |
| 21 | A | 804 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | A | 824 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | 32 | 602 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | B2 | 834 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | 8 | 612 | CLA | MG-NB | -4.70 | 1.96 | 2.05 |
| 21 | 92 | 610 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | 32 | 603 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | A | 805 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | A2 | 824 | CLA | C1D-ND | 4.70 | 1.44 | 1.37 |
| 21 | B | 806 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 21 | A | 833 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 21 | 9 | 613 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 21 | 92 | 613 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 21 | 72 | 609 | CLA | C1D-ND | 4.69 | 1.44 | 1.37 |
| 21 | 3 | 610 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 21 | B2 | 817 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 21 | 32 | 610 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 833 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 21 | 9 | 602 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 21 | A | 836 | CLA | C1D-ND | 4.68 | 1.44 | 1.37 |
| 21 | A2 | 807 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 21 | A | 843 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 21 | A2 | 843 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 21 | A | 810 | CLA | MG-ND | -4.67 | 1.96 | 2.05 |
| 21 | 3 | 609 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 21 | B2 | 819 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 21 | 32 | 609 | CLA | C1D-ND | 4.67 | 1.44 | 1.37 |
| 21 | A2 | 804 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 21 | B2 | 832 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 21 | A2 | 837 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 21 | B | 802 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 21 | B | 838 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 21 | B2 | 838 | CLA | C1D-ND | 4.66 | 1.44 | 1.37 |
| 30 | 62 | 601 | CHL | C3A-C2A | -4.66 | 1.50 | 1.54 |
| 21 | A2 | 803 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 21 | F2 | 301 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 21 | B | 819 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 21 | B | 831 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 21 | B | 834 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 21 | 9 | 611 | CLA | C1D-ND | 4.65 | 1.44 | 1.37 |
| 21 | A2 | 810 | CLA | MG-ND | -4.65 | 1.96 | 2.05 |
| 21 | A | 837 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 21 | 8 | 610 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 21 | A | 825 | CLA | C1D-ND | 4.64 | 1.44 | 1.37 |
| 20 | A2 | 801 | CL0 | MG-ND | -4.63 | 1.96 | 2.05 |
| 21 | B | 840 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 21 | B2 | 840 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 21 | Z | 610 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 21 | A | 809 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 21 | A2 | 809 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 21 | B | 818 | CLA | C1D-ND | 4.63 | 1.43 | 1.37 |
| 21 | A2 | 805 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 20 | A | 801 | CL0 | MG-ND | -4.62 | 1.96 | 2.05 |
| 21 | 12 | 602 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 21 | 82 | 610 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 21 | A2 | 825 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 21 | B2 | 818 | CLA | C1D-ND | 4.62 | 1.43 | 1.37 |
| 21 | Z | 612 | CLA | MG-NB | -4.62 | 1.96 | 2.05 |
| 21 | A2 | 837 | CLA | MG-ND | -4.61 | 1.96 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 803 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 21 | B | 817 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 21 | B2 | 821 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 21 | 3 | 603 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 21 | A2 | 823 | CLA | C1D-ND | 4.61 | 1.43 | 1.37 |
| 21 | 1 | 616 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 21 | A2 | 806 | CLA | C1D-ND | 4.60 | 1.43 | 1.37 |
| 21 | 92 | 611 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 21 | B2 | 831 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 21 | A2 | 854 | CLA | MG-ND | -4.59 | 1.96 | 2.05 |
| 21 | A | 810 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 21 | A | 823 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 21 | A2 | 842 | CLA | C1D-ND | 4.59 | 1.43 | 1.37 |
| 21 | Z2 | 612 | CLA | MG-NB | -4.58 | 1.96 | 2.05 |
| 30 | 52 | 607 | CHL | CHB-C4A | -4.58 | 1.33 | 1.38 |
| 21 | 12 | 610 | CLA | C1D-ND | 4.58 | 1.43 | 1.37 |
| 21 | 1 | 602 | CLA | C1D-ND | 4.58 | 1.43 | 1.37 |
| 30 | 72 | 601 | CHL | CHB-C4A | -4.58 | 1.33 | 1.38 |
| 21 | B | 805 | CLA | C1D-ND | 4.57 | 1.43 | 1.37 |
| 21 | A2 | 810 | CLA | C1D-ND | 4.57 | 1.43 | 1.37 |
| 30 | 32 | 608 | CHL | C3A-C2A | -4.57 | 1.50 | 1.54 |
| 21 | F | 301 | CLA | C1D-ND | 4.57 | 1.43 | 1.37 |
| 21 | 1 | 610 | CLA | C1D-ND | 4.56 | 1.43 | 1.37 |
| 21 | 12 | 616 | CLA | C1D-ND | 4.56 | 1.43 | 1.37 |
| 21 | B | 832 | CLA | C1D-ND | 4.56 | 1.43 | 1.37 |
| 21 | B2 | 803 | CLA | C1D-ND | 4.56 | 1.43 | 1.37 |
| 21 | A | 812 | CLA | C1D-ND | 4.56 | 1.43 | 1.37 |
| 21 | A2 | 812 | CLA | C1D-ND | 4.56 | 1.43 | 1.37 |
| 21 | B2 | 830 | CLA | C1D-ND | 4.55 | 1.43 | 1.37 |
| 30 | 6 | 601 | CHL | C3A-C2A | -4.55 | 1.50 | 1.54 |
| 21 | A | 837 | CLA | MG-ND | -4.55 | 1.96 | 2.05 |
| 21 | B | 838 | CLA | MG-ND | -4.55 | 1.96 | 2.05 |
| 30 | 3 | 608 | CHL | C3A-C2A | -4.55 | 1.50 | 1.54 |
| 21 | B | 821 | CLA | MG-ND | -4.55 | 1.96 | 2.05 |
| 21 | B2 | 821 | CLA | MG-ND | -4.55 | 1.96 | 2.05 |
| 21 | A | 854 | CLA | MG-ND | -4.55 | 1.96 | 2.05 |
| 21 | A | 806 | CLA | C1D-ND | 4.54 | 1.43 | 1.37 |
| 21 | A | 829 | CLA | MG-ND | -4.53 | 1.96 | 2.05 |
| 21 | 7 | 610 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 21 | 72 | 610 | CLA | C1D-ND | 4.53 | 1.43 | 1.37 |
| 21 | K | 201 | CLA | MG-ND | -4.53 | 1.96 | 2.05 |
| 21 | B2 | 838 | CLA | MG-ND | -4.53 | 1.96 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 7 | 601 | CHL | CHB-C4A | -4.53 | 1.33 | 1.38 |
| 21 | B | 803 | CLA | MG-ND | -4.52 | 1.96 | 2.05 |
| 30 | 6 | 607 | CHL | CHB-C4A | -4.52 | 1.33 | 1.38 |
| 21 | B | 803 | CLA | C1D-ND | 4.52 | 1.43 | 1.37 |
| 30 | 1 | 607 | CHL | CHB-C4A | -4.51 | 1.33 | 1.38 |
| 21 | B2 | 803 | CLA | MG-ND | -4.51 | 1.96 | 2.05 |
| 30 | 62 | 607 | CHL | CHB-C4A | -4.51 | 1.33 | 1.38 |
| 21 | B | 821 | CLA | C1D-ND | 4.51 | 1.43 | 1.37 |
| 30 | 5 | 607 | CHL | CHB-C4A | -4.50 | 1.33 | 1.38 |
| 30 | 12 | 607 | CHL | CHB-C4A | -4.50 | 1.33 | 1.38 |
| 30 | 8 | 606 | CHL | CHB-C4A | -4.49 | 1.33 | 1.38 |
| 21 | 1 | 616 | CLA | MG-ND | -4.49 | 1.96 | 2.05 |
| 21 | A2 | 823 | CLA | MG-ND | -4.48 | 1.96 | 2.05 |
| 21 | 72 | 610 | CLA | MG-ND | -4.48 | 1.96 | 2.05 |
| 21 | A | 842 | CLA | C1D-ND | 4.48 | 1.43 | 1.37 |
| 21 | A | 803 | CLA | MG-ND | -4.48 | 1.96 | 2.05 |
| 21 | A2 | 803 | CLA | MG-ND | -4.48 | 1.96 | 2.05 |
| 21 | K2 | 201 | CLA | MG-ND | -4.48 | 1.96 | 2.05 |
| 21 | 72 | 609 | CLA | MG-ND | -4.48 | 1.96 | 2.05 |
| 21 | A2 | 829 | CLA | MG-ND | -4.47 | 1.96 | 2.05 |
| 21 | B | 830 | CLA | C1D-ND | 4.47 | 1.43 | 1.37 |
| 21 | B | 806 | CLA | MG-ND | -4.47 | 1.96 | 2.05 |
| 30 | 12 | 606 | CHL | CHB-C4A | -4.47 | 1.33 | 1.38 |
| 21 | 7 | 610 | CLA | MG-ND | -4.46 | 1.96 | 2.05 |
| 21 | A | 823 | CLA | MG-ND | -4.46 | 1.97 | 2.05 |
| 30 | 42 | 606 | CHL | CHB-C4A | -4.46 | 1.33 | 1.38 |
| 30 | 62 | 608 | CHL | CHB-C4A | -4.45 | 1.33 | 1.38 |
| 30 | 5 | 608 | CHL | CHB-C4A | -4.45 | 1.33 | 1.38 |
| 30 | 52 | 608 | CHL | CHB-C4A | -4.45 | 1.33 | 1.38 |
| 30 | 1 | 606 | CHL | CHB-C4A | -4.44 | 1.33 | 1.38 |
| 21 | B2 | 806 | CLA | MG-ND | -4.44 | 1.97 | 2.05 |
| 30 | 62 | 616 | CHL | CHB-C4A | -4.43 | 1.33 | 1.38 |
| 21 | A | 819 | CLA | MG-ND | -4.43 | 1.97 | 2.05 |
| 30 | 12 | 606 | CHL | C3A-C2A | -4.42 | 1.50 | 1.54 |
| 21 | A | 825 | CLA | MG-ND | -4.42 | 1.97 | 2.05 |
| 21 | A2 | 833 | CLA | MG-ND | -4.42 | 1.97 | 2.05 |
| 30 | 42 | 608 | CHL | C3A-C2A | -4.42 | 1.50 | 1.54 |
| 21 | 32 | 617 | CLA | MG-ND | -4.41 | 1.97 | 2.05 |
| 21 | A | 833 | CLA | MG-ND | -4.41 | 1.97 | 2.05 |
| 21 | B | 829 | CLA | MG-ND | -4.41 | 1.97 | 2.05 |
| 21 | A2 | 802 | CLA | MG-ND | -4.41 | 1.97 | 2.05 |
| 21 | 7 | 609 | CLA | MG-ND | -4.41 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 32 | 603 | CLA | MG-ND | -4.41 | 1.97 | 2.05 |
| 30 | 8 | 607 | CHL | CHB-C4A | -4.41 | 1.33 | 1.38 |
| 21 | 92 | 602 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 21 | A | 817 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 21 | B2 | 820 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 21 | B2 | 825 | CLA | C1D-ND | 4.40 | 1.43 | 1.37 |
| 21 | A2 | 825 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 30 | 4 | 606 | CHL | CHB-C4A | -4.40 | 1.33 | 1.38 |
| 21 | 3 | 603 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 21 | 12 | 616 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 21 | 9 | 602 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 21 | 5 | 621 | CLA | MG-ND | -4.40 | 1.97 | 2.05 |
| 30 | 6 | 616 | CHL | CHB-C4A | -4.39 | 1.33 | 1.38 |
| 21 | 52 | 621 | CLA | MG-ND | -4.39 | 1.97 | 2.05 |
| 30 | 6 | 608 | CHL | CHB-C4A | -4.39 | 1.33 | 1.38 |
| 21 | A | 802 | CLA | MG-ND | -4.39 | 1.97 | 2.05 |
| 30 | 82 | 606 | CHL | CHB-C4A | -4.39 | 1.33 | 1.38 |
| 21 | B | 839 | CLA | MG-ND | -4.38 | 1.97 | 2.05 |
| 21 | A2 | 817 | CLA | MG-ND | -4.38 | 1.97 | 2.05 |
| 21 | A2 | 819 | CLA | MG-ND | -4.38 | 1.97 | 2.05 |
| 21 | 3 | 617 | CLA | MG-ND | -4.37 | 1.97 | 2.05 |
| 21 | B2 | 839 | CLA | MG-ND | -4.37 | 1.97 | 2.05 |
| 21 | B | 820 | CLA | MG-ND | -4.37 | 1.97 | 2.05 |
| 30 | 4 | 608 | CHL | C3A-C2A | -4.37 | 1.50 | 1.54 |
| 21 | B2 | 817 | CLA | MG-ND | -4.37 | 1.97 | 2.05 |
| 21 | 72 | 608 | CLA | MG-ND | -4.37 | 1.97 | 2.05 |
| 21 | B2 | 823 | CLA | C1D-ND | 4.36 | 1.43 | 1.37 |
| 21 | 7 | 608 | CLA | MG-ND | -4.36 | 1.97 | 2.05 |
| 21 | B | 825 | CLA | C1D-ND | 4.35 | 1.43 | 1.37 |
| 21 | B2 | 829 | CLA | MG-ND | -4.35 | 1.97 | 2.05 |
| 21 | Z | 608 | CLA | MG-ND | -4.35 | 1.97 | 2.05 |
| 30 | 6 | 606 | CHL | CHB-C4A | -4.35 | 1.33 | 1.38 |
| 30 | 62 | 606 | CHL | CHB-C4A | -4.35 | 1.33 | 1.38 |
| 21 | 4 | 609 | CLA | MG-ND | -4.34 | 1.97 | 2.05 |
| 21 | 82 | 602 | CLA | MG-ND | -4.34 | 1.97 | 2.05 |
| 21 | B | 829 | CLA | C1D-ND | 4.34 | 1.43 | 1.37 |
| 21 | B | 818 | CLA | MG-ND | -4.34 | 1.97 | 2.05 |
| 21 | Z2 | 609 | CLA | MG-ND | -4.34 | 1.97 | 2.05 |
| 30 | 72 | 606 | CHL | CHB-C4A | -4.34 | 1.33 | 1.38 |
| 21 | A2 | 808 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |
| 21 | A2 | 828 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |
| 21 | 82 | 610 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 82 | 607 | CHL | CHB-C4A | -4.33 | 1.33 | 1.38 |
| 21 | 32 | 611 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |
| 21 | A2 | 843 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |
| 21 | A | 802 | CLA | C1D-ND | 4.33 | 1.43 | 1.37 |
| 30 | Z2 | 607 | CHL | CHB-C4A | -4.33 | 1.33 | 1.38 |
| 30 | 92 | 606 | CHL | CHB-C4A | -4.33 | 1.33 | 1.38 |
| 21 | Z2 | 608 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |
| 21 | A | 828 | CLA | MG-ND | -4.33 | 1.97 | 2.05 |
| 21 | 8 | 602 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 21 | A | 843 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 21 | B2 | 819 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 21 | B | 833 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 21 | B2 | 833 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 21 | 1 | 602 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 21 | 12 | 602 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 21 | B | 823 | CLA | C1D-ND | 4.32 | 1.43 | 1.37 |
| 21 | B | 819 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 21 | A2 | 813 | CLA | MG-ND | -4.32 | 1.97 | 2.05 |
| 30 | 7 | 601 | CHL | C3A-C2A | -4.31 | 1.51 | 1.54 |
| 21 | A | 836 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 21 | B2 | 818 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 30 | Z | 607 | CHL | CHB-C4A | -4.31 | 1.33 | 1.38 |
| 21 | A2 | 836 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 21 | B2 | 829 | CLA | C1D-ND | 4.31 | 1.43 | 1.37 |
| 21 | 72 | 613 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 21 | 1 | 608 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 21 | 1 | 611 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 21 | 42 | 609 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 30 | 7 | 606 | CHL | CHB-C4A | -4.31 | 1.33 | 1.38 |
| 21 | B2 | 823 | CLA | MG-ND | -4.31 | 1.97 | 2.05 |
| 21 | A | 808 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | B2 | 809 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 30 | 9 | 606 | CHL | CHB-C4A | -4.30 | 1.33 | 1.38 |
| 21 | 3 | 611 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | B2 | 812 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 30 | 42 | 607 | CHL | CHB-C4A | -4.30 | 1.33 | 1.38 |
| 21 | A | 813 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | 3 | 609 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | 32 | 609 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 30 | 5 | 608 | CHL | C3A-C2A | -4.30 | 1.51 | 1.54 |
| 30 | 52 | 608 | CHL | C3A-C2A | -4.30 | 1.51 | 1.54 |
| 30 | 62 | 618 | CHL | CHB-C4A | -4.30 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | G2 | 203 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | 82 | 604 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | 12 | 611 | CLA | MG-ND | -4.30 | 1.97 | 2.05 |
| 21 | 7 | 613 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | 32 | 607 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | A2 | 802 | CLA | C1D-ND | 4.29 | 1.43 | 1.37 |
| 21 | B | 823 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | 32 | 610 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | A | 815 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | Z | 609 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | 4 | 602 | CLA | MG-ND | -4.29 | 1.97 | 2.05 |
| 21 | B | 807 | CLA | MG-ND | -4.28 | 1.97 | 2.05 |
| 21 | 12 | 608 | CLA | MG-ND | -4.28 | 1.97 | 2.05 |
| 21 | B | 812 | CLA | MG-ND | -4.28 | 1.97 | 2.05 |
| 30 | 72 | 607 | CHL | CHB-C4A | -4.28 | 1.33 | 1.38 |
| 21 | B | 817 | CLA | MG-ND | -4.28 | 1.97 | 2.05 |
| 21 | 52 | 602 | CLA | MG-ND | -4.28 | 1.97 | 2.05 |
| 21 | G | 203 | CLA | MG-ND | -4.28 | 1.97 | 2.05 |
| 21 | K2 | 203 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | B2 | 826 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | A | 807 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | A2 | 807 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | 8 | 610 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | 42 | 602 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | B | 813 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 21 | 3 | 607 | CLA | MG-ND | -4.27 | 1.97 | 2.05 |
| 30 | 1 | 606 | CHL | C3A-C2A | -4.26 | 1.51 | 1.54 |
| 21 | B2 | 813 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 30 | 6 | 616 | CHL | C3A-C2A | -4.26 | 1.51 | 1.54 |
| 21 | A | 814 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | B | 809 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | 32 | 613 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | 92 | 611 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | A | 824 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | A2 | 815 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | 5 | 602 | CLA | MG-ND | -4.26 | 1.97 | 2.05 |
| 21 | 8 | 604 | CLA | MG-ND | -4.25 | 1.97 | 2.05 |
| 21 | L2 | 203 | CLA | MG-ND | -4.25 | 1.97 | 2.05 |
| 21 | 9 | 613 | CLA | MG-ND | -4.25 | 1.97 | 2.05 |
| 21 | A2 | 821 | CLA | MG-ND | -4.25 | 1.97 | 2.05 |
| 21 | 3 | 613 | CLA | MG-ND | -4.25 | 1.97 | 2.05 |
| 21 | A2 | 814 | CLA | MG-ND | -4.25 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 610 | CLA | MG-ND | -4.24 | 1.97 | 2.05 |
| 21 | 4 | 613 | CLA | MG-ND | -4.24 | 1.97 | 2.05 |
| 30 | 72 | 601 | CHL | C3A-C2A | -4.24 | 1.51 | 1.54 |
| 21 | 92 | 601 | CLA | MG-ND | -4.24 | 1.97 | 2.05 |
| 21 | A | 826 | CLA | MG-ND | -4.24 | 1.97 | 2.05 |
| 21 | 8 | 603 | CLA | MG-ND | -4.24 | 1.97 | 2.05 |
| 21 | 82 | 603 | CLA | MG-ND | -4.24 | 1.97 | 2.05 |
| 30 | 6 | 608 | CHL | C3A-C2A | -4.24 | 1.51 | 1.54 |
| 30 | 62 | 608 | CHL | C3A-C2A | -4.24 | 1.51 | 1.54 |
| 21 | 1 | 610 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | B | 826 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | A2 | 826 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | 72 | 604 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | 92 | 613 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | 32 | 606 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | 6 | 617 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | Z2 | 602 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | 62 | 617 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 30 | 82 | 606 | CHL | C3A-C2A | -4.23 | 1.51 | 1.54 |
| 21 | 9 | 610 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 21 | A | 821 | CLA | MG-ND | -4.23 | 1.97 | 2.05 |
| 30 | 4 | 607 | CHL | CHB-C4A | -4.22 | 1.33 | 1.38 |
| 21 | 9 | 601 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 3 | 615 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | B2 | 807 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 32 | 615 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | J2 | 101 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 3 | 606 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | B2 | 837 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | B | 835 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | K | 203 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 5 | 604 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 9 | 611 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 52 | 604 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | B | 833 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | B | 837 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | A2 | 839 | CLA | MG-ND | -4.22 | 1.97 | 2.05 |
| 21 | 32 | 602 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | A | 805 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 1 | 603 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | Z | 603 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 5 | 611 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 5 | 607 | CHL | C1A-CHA | -4.21 | 1.35 | 1.40 |
| 21 | 72 | 602 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 3 | 602 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 12 | 604 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 1 | 614 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | A2 | 824 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | B | 815 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 30 | 42 | 608 | CHL | CHB-C4A | -4.21 | 1.33 | 1.38 |
| 21 | 12 | 614 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | L | 203 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 1 | 609 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | 82 | 608 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 21 | B | 834 | CLA | MG-ND | -4.21 | 1.97 | 2.05 |
| 30 | 8 | 606 | CHL | C3A-C2A | -4.20 | 1.51 | 1.54 |
| 21 | A | 839 | CLA | MG-ND | -4.20 | 1.97 | 2.05 |
| 21 | 8 | 611 | CLA | MG-ND | -4.20 | 1.97 | 2.05 |
| 21 | 82 | 611 | CLA | MG-ND | -4.20 | 1.97 | 2.05 |
| 21 | B2 | 811 | CLA | MG-ND | -4.20 | 1.97 | 2.05 |
| 21 | A2 | 834 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | B2 | 833 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | B | 841 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 72 | 614 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | A2 | 822 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 8 | 608 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | B2 | 834 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 52 | 611 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | A | 834 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 6 | 622 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 82 | 609 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 42 | 616 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | A | 831 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 52 | 601 | CLA | MG-ND | -4.19 | 1.97 | 2.05 |
| 21 | 42 | 613 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 62 | 613 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 92 | 610 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 9 | 604 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 30 | 62 | 616 | CHL | C3A-C2A | -4.18 | 1.51 | 1.54 |
| 30 | 7 | 607 | CHL | CHB-C4A | -4.18 | 1.33 | 1.38 |
| 30 | 6 | 618 | CHL | CHB-C4A | -4.18 | 1.33 | 1.38 |
| 21 | B | 811 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 3 | 612 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | A2 | 805 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | Z2 | 603 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | Z | 602 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 7 | 604 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 92 | 609 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 30 | 62 | 601 | CHL | CHB-C4A | -4.18 | 1.33 | 1.38 |
| 21 | K | 204 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 7 | 611 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | B2 | 830 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 32 | 604 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | 12 | 610 | CLA | MG-ND | -4.18 | 1.97 | 2.05 |
| 21 | B2 | 815 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | B | 825 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 4 | 616 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 6 | 613 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | Z2 | 616 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 92 | 604 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 7 | 614 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 7 | 612 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 72 | 616 | CLA | MG-ND | -4.17 | 1.97 | 2.05 |
| 21 | 9 | 609 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | B2 | 841 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 32 | 612 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 12 | 603 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | B2 | 825 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | A | 822 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | F | 303 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 92 | 612 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | F2 | 301 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 12 | 609 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | F2 | 303 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 30 | 5 | 606 | CHL | CHB-C4A | -4.16 | 1.33 | 1.38 |
| 30 | 52 | 606 | CHL | CHB-C4A | -4.16 | 1.33 | 1.38 |
| 21 | F | 301 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | J | 101 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | A2 | 831 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 42 | 603 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | Z | 610 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 4 | 603 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | Z2 | 610 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 92 | 614 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 72 | 611 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 42 | 604 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B2 | 835 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 9 | 612 | CLA | MG-ND | -4.16 | 1.97 | 2.05 |
| 21 | 3 | 614 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 1 | 604 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 7 | 602 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 8 | 609 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 4 | 614 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 42 | 614 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | K2 | 206 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 9 | 614 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | A | 804 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | B | 810 | CLA | MG-ND | -4.15 | 1.97 | 2.05 |
| 21 | 6 | 610 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 32 | 614 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 3 | 604 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | B2 | 804 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 30 | 52 | 607 | CHL | C1A-CHA | -4.14 | 1.35 | 1.40 |
| 21 | 6 | 604 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 4 | 611 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 8 | 614 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 82 | 614 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 62 | 622 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 5 | 614 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 4 | 604 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | A2 | 845 | CLA | MG-ND | -4.14 | 1.97 | 2.05 |
| 21 | 12 | 612 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | Z | 604 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | Z | 613 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | A2 | 809 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | A | 841 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | 42 | 611 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | 62 | 611 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 30 | 4 | 607 | CHL | C1A-CHA | -4.13 | 1.35 | 1.40 |
| 30 | 42 | 607 | CHL | C1A-CHA | -4.13 | 1.35 | 1.40 |
| 21 | B | 804 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 30 | 4 | 608 | CHL | CHB-C4A | -4.13 | 1.33 | 1.38 |
| 21 | 6 | 603 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | Z2 | 614 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | Z2 | 613 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | 62 | 610 | CLA | MG-ND | -4.13 | 1.97 | 2.05 |
| 21 | 7 | 616 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | A | 832 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 611 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | B2 | 824 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | 1 | 612 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | 6 | 609 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | A | 818 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | Z | 616 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | 72 | 612 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 30 | 12 | 601 | CHL | CHB-C4A | -4.12 | 1.33 | 1.38 |
| 21 | Z2 | 604 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | 62 | 604 | CLA | MG-ND | -4.12 | 1.97 | 2.05 |
| 21 | 5 | 601 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | K2 | 204 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | B | 830 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 30 | 6 | 601 | CHL | CHB-C4A | -4.11 | 1.33 | 1.38 |
| 21 | B | 831 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | 52 | 614 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | 62 | 609 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | A2 | 835 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | A | 811 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | A2 | 804 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | B2 | 828 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | 4 | 612 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | 12 | 613 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 30 | 3 | 608 | CHL | CHB-C4A | -4.11 | 1.33 | 1.38 |
| 21 | 1 | 613 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | A2 | 841 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 21 | 52 | 610 | CLA | MG-ND | -4.11 | 1.97 | 2.05 |
| 30 | 1 | 607 | CHL | C3A-C2A | -4.11 | 1.51 | 1.54 |
| 21 | A | 845 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | B2 | 822 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | 72 | 620 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | A2 | 840 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | B | 822 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | K | 206 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | 8 | 613 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | 82 | 613 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | A2 | 832 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | A | 809 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | Z | 614 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | B2 | 810 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | A2 | 811 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | 52 | 616 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 824 | CLA | MG-ND | -4.10 | 1.97 | 2.05 |
| 21 | 5 | 610 | CLA | MG-ND | -4.09 | 1.97 | 2.05 |
| 21 | 7 | 620 | CLA | MG-ND | -4.09 | 1.97 | 2.05 |
| 21 | 7 | 603 | CLA | MG-ND | -4.09 | 1.97 | 2.05 |
| 21 | 62 | 603 | CLA | MG-ND | -4.09 | 1.97 | 2.05 |
| 21 | 52 | 612 | CLA | MG-ND | -4.09 | 1.97 | 2.05 |
| 21 | B2 | 832 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | B | 816 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | Z | 611 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | A | 835 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | B2 | 816 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 30 | 72 | 607 | CHL | C3A-C2A | -4.08 | 1.51 | 1.54 |
| 21 | A2 | 818 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | G | 204 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 30 | 32 | 608 | CHL | CHB-C4A | -4.08 | 1.33 | 1.38 |
| 21 | A | 827 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | Z2 | 611 | CLA | MG-ND | -4.08 | 1.97 | 2.05 |
| 21 | 4 | 610 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | 6 | 602 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | A2 | 827 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | 62 | 602 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | A2 | 816 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | A | 816 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 30 | 7 | 607 | CHL | C3A-C2A | -4.07 | 1.51 | 1.54 |
| 21 | A | 840 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 30 | 8 | 606 | CHL | C1A-CHA | -4.07 | 1.35 | 1.40 |
| 21 | 52 | 609 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | 82 | 616 | CLA | MG-ND | -4.07 | 1.97 | 2.05 |
| 21 | B | 827 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | B2 | 827 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | B | 832 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | B | 802 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | B2 | 836 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | B2 | 805 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | A | 838 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 30 | Z | 606 | CHL | C1A-CHA | -4.06 | 1.35 | 1.40 |
| 30 | Z2 | 606 | CHL | C1A-CHA | -4.06 | 1.35 | 1.40 |
| 21 | B | 828 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | 52 | 617 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 21 | 92 | 603 | CLA | MG-ND | -4.06 | 1.97 | 2.05 |
| 30 | 62 | 616 | CHL | C1A-CHA | -4.06 | 1.35 | 1.40 |
| 30 | 72 | 601 | CHL | C1A-CHA | -4.05 | 1.35 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 609 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | A | 830 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | B2 | 802 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | A | 820 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | B | 836 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | G2 | 204 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 5 | 612 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 5 | 616 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | A2 | 820 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 5 | 613 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 52 | 613 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 42 | 612 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 42 | 610 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 21 | 6 | 612 | CLA | MG-ND | -4.05 | 1.97 | 2.05 |
| 30 | 5 | 618 | CHL | CHB-C4A | -4.04 | 1.33 | 1.38 |
| 21 | 72 | 603 | CLA | MG-ND | -4.04 | 1.97 | 2.05 |
| 30 | 4 | 608 | CHL | C1A-CHA | -4.04 | 1.35 | 1.40 |
| 21 | F | 304 | CLA | MG-ND | -4.04 | 1.97 | 2.05 |
| 21 | 8 | 616 | CLA | MG-ND | -4.04 | 1.97 | 2.05 |
| 21 | F2 | 304 | CLA | MG-ND | -4.04 | 1.97 | 2.05 |
| 30 | 42 | 618 | CHL | C1A-CHA | -4.04 | 1.35 | 1.40 |
| 30 | 9 | 606 | CHL | C1A-CHA | -4.04 | 1.35 | 1.40 |
| 30 | 1 | 601 | CHL | CHB-C4A | -4.04 | 1.33 | 1.38 |
| 30 | 9 | 606 | CHL | C2A-C3A | -4.04 | 1.51 | 1.54 |
| 21 | 9 | 603 | CLA | MG-ND | -4.03 | 1.97 | 2.05 |
| 21 | A2 | 830 | CLA | MG-ND | -4.03 | 1.97 | 2.05 |
| 21 | B2 | 831 | CLA | MG-ND | -4.03 | 1.97 | 2.05 |
| 30 | 7 | 606 | CHL | C1A-CHA | -4.03 | 1.35 | 1.40 |
| 30 | 4 | 607 | CHL | C3A-C2A | -4.03 | 1.51 | 1.54 |
| 30 | 92 | 606 | CHL | C2A-C3A | -4.03 | 1.51 | 1.54 |
| 30 | 4 | 618 | CHL | CHB-C4A | -4.03 | 1.33 | 1.38 |
| 21 | B2 | 840 | CLA | MG-ND | -4.03 | 1.97 | 2.05 |
| 30 | 62 | 608 | CHL | C1A-CHA | -4.03 | 1.35 | 1.40 |
| 21 | 5 | 617 | CLA | MG-ND | -4.03 | 1.97 | 2.05 |
| 30 | 52 | 608 | CHL | C1A-CHA | -4.02 | 1.35 | 1.40 |
| 30 | 6 | 607 | CHL | C1A-CHA | -4.02 | 1.35 | 1.40 |
| 30 | 62 | 607 | CHL | C1A-CHA | -4.02 | 1.35 | 1.40 |
| 21 | L | 204 | CLA | MG-ND | -4.02 | 1.97 | 2.05 |
| 30 | Z2 | 607 | CHL | C1A-CHA | -4.02 | 1.35 | 1.40 |
| 30 | 92 | 607 | CHL | C1A-CHA | -4.01 | 1.35 | 1.40 |
| 21 | B | 805 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 30 | 42 | 607 | CHL | C3A-C2A | -4.01 | 1.51 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 842 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 21 | A | 812 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 21 | B | 840 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 21 | A2 | 812 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 21 | A | 842 | CLA | MG-ND | -4.01 | 1.97 | 2.05 |
| 30 | 12 | 601 | CHL | C1A-CHA | -4.01 | 1.35 | 1.40 |
| 30 | 82 | 606 | CHL | C1A-CHA | -4.00 | 1.35 | 1.40 |
| 30 | 1 | 607 | CHL | C1A-CHA | -4.00 | 1.35 | 1.40 |
| 30 | 12 | 607 | CHL | C1A-CHA | -4.00 | 1.35 | 1.40 |
| 21 | A2 | 806 | CLA | MG-ND | -4.00 | 1.97 | 2.05 |
| 30 | 4 | 618 | CHL | C1A-CHA | -4.00 | 1.35 | 1.40 |
| 21 | A2 | 838 | CLA | MG-ND | -3.99 | 1.97 | 2.05 |
| 21 | B | 808 | CLA | MG-ND | -3.99 | 1.97 | 2.05 |
| 21 | B2 | 814 | CLA | MG-ND | -3.99 | 1.97 | 2.05 |
| 21 | 62 | 612 | CLA | MG-ND | -3.99 | 1.97 | 2.05 |
| 30 | 52 | 618 | CHL | CHB-C4A | -3.99 | 1.33 | 1.38 |
| 30 | 6 | 607 | CHL | C3A-C2A | -3.99 | 1.51 | 1.54 |
| 30 | 12 | 607 | CHL | C3A-C2A | -3.99 | 1.51 | 1.54 |
| 30 | 72 | 606 | CHL | C1A-CHA | -3.99 | 1.35 | 1.40 |
| 30 | 42 | 608 | CHL | C1A-CHA | -3.98 | 1.35 | 1.40 |
| 21 | B | 814 | CLA | MG-ND | -3.98 | 1.97 | 2.05 |
| 21 | B2 | 808 | CLA | MG-ND | -3.98 | 1.97 | 2.05 |
| 30 | 62 | 607 | CHL | C3A-C2A | -3.98 | 1.51 | 1.54 |
| 30 | Z2 | 606 | CHL | CHB-C4A | -3.98 | 1.33 | 1.38 |
| 30 | 52 | 618 | CHL | C1A-CHA | -3.98 | 1.35 | 1.40 |
| 30 | 42 | 618 | CHL | CHB-C4A | -3.97 | 1.33 | 1.38 |
| 30 | 4 | 606 | CHL | C1A-CHA | -3.97 | 1.35 | 1.40 |
| 30 | 6 | 616 | CHL | C1A-CHA | -3.97 | 1.35 | 1.40 |
| 30 | 42 | 606 | CHL | C1A-CHA | -3.97 | 1.35 | 1.40 |
| 21 | L2 | 204 | CLA | MG-ND | -3.97 | 1.97 | 2.05 |
| 30 | 6 | 608 | CHL | C1A-CHA | -3.97 | 1.35 | 1.40 |
| 30 | 72 | 606 | CHL | C3A-C2A | -3.97 | 1.51 | 1.54 |
| 30 | 32 | 608 | CHL | C1A-CHA | -3.97 | 1.35 | 1.40 |
| 30 | Z | 607 | CHL | C1A-CHA | -3.96 | 1.35 | 1.40 |
| 30 | 42 | 601 | CHL | C1A-CHA | -3.95 | 1.35 | 1.40 |
| 30 | 92 | 606 | CHL | C1A-CHA | -3.95 | 1.35 | 1.40 |
| 21 | A | 806 | CLA | MG-ND | -3.95 | 1.98 | 2.05 |
| 30 | 6 | 618 | CHL | C1A-CHA | -3.94 | 1.35 | 1.40 |
| 30 | 62 | 618 | CHL | C1A-CHA | -3.94 | 1.35 | 1.40 |
| 21 | 6 | 614 | CLA | MG-ND | -3.94 | 1.98 | 2.05 |
| 21 | 62 | 614 | CLA | MG-ND | -3.94 | 1.98 | 2.05 |
| 30 | 72 | 607 | CHL | C1A-CHA | -3.93 | 1.35 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 5 | 608 | CHL | C1A-CHA | -3.93 | 1.35 | 1.40 |
| 21 | Z2 | 612 | CLA | MG-ND | -3.93 | 1.98 | 2.05 |
| 21 | 5 | 603 | CLA | MG-ND | -3.93 | 1.98 | 2.05 |
| 21 | 52 | 603 | CLA | MG-ND | -3.93 | 1.98 | 2.05 |
| 30 | 62 | 606 | CHL | C1A-CHA | -3.92 | 1.35 | 1.40 |
| 30 | 8 | 601 | CHL | C1A-CHA | -3.92 | 1.35 | 1.40 |
| 30 | 1 | 601 | CHL | C1A-CHA | -3.92 | 1.35 | 1.40 |
| 30 | 5 | 606 | CHL | C3A-C2A | -3.92 | 1.51 | 1.54 |
| 30 | 52 | 606 | CHL | C3A-C2A | -3.92 | 1.51 | 1.54 |
| 30 | 1 | 606 | CHL | C1A-CHA | -3.91 | 1.35 | 1.40 |
| 30 | 5 | 606 | CHL | C1A-CHA | -3.91 | 1.35 | 1.40 |
| 30 | 12 | 606 | CHL | C1A-CHA | -3.91 | 1.35 | 1.40 |
| 30 | 3 | 608 | CHL | C1A-CHA | -3.91 | 1.35 | 1.40 |
| 30 | 5 | 618 | CHL | C1A-CHA | -3.91 | 1.35 | 1.40 |
| 21 | 8 | 612 | CLA | MG-ND | -3.91 | 1.98 | 2.05 |
| 30 | 7 | 601 | CHL | C1A-CHA | -3.91 | 1.35 | 1.40 |
| 21 | 82 | 612 | CLA | MG-ND | -3.91 | 1.98 | 2.05 |
| 30 | 42 | 606 | CHL | C3A-C2A | -3.90 | 1.51 | 1.54 |
| 30 | Z | 601 | CHL | C1A-CHA | -3.90 | 1.35 | 1.40 |
| 30 | 6 | 606 | CHL | C1A-CHA | -3.90 | 1.35 | 1.40 |
| 30 | 8 | 601 | CHL | CHB-C4A | -3.89 | 1.33 | 1.38 |
| 30 | 62 | 601 | CHL | C1A-CHA | -3.89 | 1.35 | 1.40 |
| 30 | 62 | 606 | CHL | C3A-C2A | -3.88 | 1.51 | 1.54 |
| 30 | 7 | 607 | CHL | C1A-CHA | -3.88 | 1.35 | 1.40 |
| 30 | 4 | 601 | CHL | C1A-CHA | -3.88 | 1.35 | 1.40 |
| 30 | 6 | 606 | CHL | C3A-C2A | -3.88 | 1.51 | 1.54 |
| 30 | 82 | 601 | CHL | CHB-C4A | -3.88 | 1.34 | 1.38 |
| 30 | Z | 606 | CHL | CHB-C4A | -3.88 | 1.34 | 1.38 |
| 30 | 82 | 601 | CHL | C1A-CHA | -3.87 | 1.35 | 1.40 |
| 30 | 52 | 606 | CHL | C1A-CHA | -3.87 | 1.35 | 1.40 |
| 30 | 6 | 601 | CHL | C1A-CHA | -3.86 | 1.35 | 1.40 |
| 21 | Z | 612 | CLA | MG-ND | -3.86 | 1.98 | 2.05 |
| 30 | Z2 | 607 | CHL | C3A-C2A | -3.86 | 1.51 | 1.54 |
| 30 | Z2 | 601 | CHL | C1A-CHA | -3.85 | 1.35 | 1.40 |
| 20 | A | 801 | CL0 | C1A-CHA | -3.85 | 1.35 | 1.40 |
| 20 | A2 | 801 | CL0 | C1A-CHA | -3.85 | 1.35 | 1.40 |
| 30 | Z | 607 | CHL | C3A-C2A | -3.84 | 1.51 | 1.54 |
| 30 | 4 | 601 | CHL | C3A-C2A | -3.84 | 1.51 | 1.54 |
| 30 | 92 | 607 | CHL | CHB-C4A | -3.84 | 1.34 | 1.38 |
| 30 | 9 | 607 | CHL | C1A-CHA | -3.84 | 1.35 | 1.40 |
| 30 | 6 | 616 | CHL | C3B-C4B | 3.83 | 1.45 | 1.41 |
| 30 | 7 | 606 | CHL | C3A-C2A | -3.83 | 1.51 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 42 | 601 | CHL | C3A-C2A | -3.81 | 1.51 | 1.54 |
| 30 | Z2 | 601 | CHL | CHB-C4A | -3.81 | 1.34 | 1.38 |
| 30 | 6 | 618 | CHL | C3A-C2A | -3.80 | 1.51 | 1.54 |
| 30 | 62 | 618 | CHL | C3A-C2A | -3.77 | 1.51 | 1.54 |
| 30 | 8 | 607 | CHL | C1A-CHA | -3.76 | 1.35 | 1.40 |
| 30 | 62 | 616 | CHL | C3B-C4B | 3.73 | 1.45 | 1.41 |
| 30 | 4 | 601 | CHL | CHB-C4A | -3.73 | 1.34 | 1.38 |
| 30 | Z | 601 | CHL | CHB-C4A | -3.73 | 1.34 | 1.38 |
| 30 | 12 | 606 | CHL | C3B-C4B | 3.71 | 1.45 | 1.41 |
| 30 | 4 | 606 | CHL | C3A-C2A | -3.71 | 1.51 | 1.54 |
| 30 | 82 | 607 | CHL | C1A-CHA | -3.70 | 1.35 | 1.40 |
| 30 | 62 | 608 | CHL | C3B-C4B | 3.69 | 1.45 | 1.41 |
| 30 | 42 | 601 | CHL | CHB-C4A | -3.69 | 1.34 | 1.38 |
| 30 | 1 | 606 | CHL | C3B-C4B | 3.68 | 1.45 | 1.41 |
| 30 | 62 | 601 | CHL | C3B-C4B | 3.68 | 1.45 | 1.41 |
| 30 | 5 | 607 | CHL | C3B-C4B | 3.68 | 1.45 | 1.41 |
| 30 | 4 | 606 | CHL | C3B-C4B | 3.67 | 1.45 | 1.41 |
| 30 | 6 | 607 | CHL | C3B-C4B | 3.67 | 1.45 | 1.41 |
| 30 | 42 | 606 | CHL | C3B-C4B | 3.67 | 1.45 | 1.41 |
| 30 | 72 | 606 | CHL | C3B-C4B | 3.66 | 1.45 | 1.41 |
| 30 | 5 | 618 | CHL | C3B-C4B | 3.66 | 1.44 | 1.41 |
| 30 | 52 | 607 | CHL | C3B-C4B | 3.64 | 1.44 | 1.41 |
| 30 | 5 | 608 | CHL | C3B-C4B | 3.64 | 1.44 | 1.41 |
| 30 | 52 | 608 | CHL | C3B-C4B | 3.64 | 1.44 | 1.41 |
| 30 | 4 | 601 | CHL | C3B-C4B | 3.64 | 1.44 | 1.41 |
| 30 | 42 | 601 | CHL | C3B-C4B | 3.64 | 1.44 | 1.41 |
| 30 | 6 | 601 | CHL | C3B-C4B | 3.62 | 1.44 | 1.41 |
| 30 | 62 | 607 | CHL | C3B-C4B | 3.62 | 1.44 | 1.41 |
| 30 | 62 | 618 | CHL | C3B-C4B | 3.60 | 1.44 | 1.41 |
| 30 | 4 | 618 | CHL | C3B-C4B | 3.59 | 1.44 | 1.41 |
| 30 | 7 | 606 | CHL | C3B-C4B | 3.58 | 1.44 | 1.41 |
| 30 | 52 | 618 | CHL | C3B-C4B | 3.57 | 1.44 | 1.41 |
| 30 | 4 | 608 | CHL | C3B-C4B | 3.57 | 1.44 | 1.41 |
| 30 | 42 | 618 | CHL | C3B-C4B | 3.56 | 1.44 | 1.41 |
| 30 | 6 | 608 | CHL | C3B-C4B | 3.56 | 1.44 | 1.41 |
| 30 | 5 | 618 | CHL | C3A-C2A | -3.55 | 1.51 | 1.54 |
| 30 | 6 | 606 | CHL | C3B-C4B | 3.55 | 1.44 | 1.41 |
| 30 | 62 | 606 | CHL | C3B-C4B | 3.55 | 1.44 | 1.41 |
| 30 | Z | 606 | CHL | C3B-C4B | 3.54 | 1.44 | 1.41 |
| 30 | 6 | 618 | CHL | C3B-C4B | 3.53 | 1.44 | 1.41 |
| 30 | 3 | 608 | CHL | C3B-C4B | 3.52 | 1.44 | 1.41 |
| 30 | 32 | 608 | CHL | C3B-C4B | 3.52 | 1.44 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 52 | 618 | CHL | C3A-C2A | -3.51 | 1.51 | 1.54 |
| 30 | 8 | 606 | CHL | C3B-C4B | 3.50 | 1.44 | 1.41 |
| 30 | 82 | 606 | CHL | C3B-C4B | 3.50 | 1.44 | 1.41 |
| 30 | Z2 | 607 | CHL | C3B-C4B | 3.49 | 1.44 | 1.41 |
| 30 | 92 | 606 | CHL | C3B-C4B | 3.49 | 1.44 | 1.41 |
| 30 | 42 | 608 | CHL | C3B-C4B | 3.48 | 1.44 | 1.41 |
| 30 | 52 | 606 | CHL | C3B-C4B | 3.47 | 1.44 | 1.41 |
| 30 | 5 | 606 | CHL | C3B-C4B | 3.46 | 1.44 | 1.41 |
| 30 | 4 | 607 | CHL | C3B-C4B | 3.45 | 1.44 | 1.41 |
| 30 | 72 | 607 | CHL | C3B-C4B | 3.44 | 1.44 | 1.41 |
| 30 | 1 | 607 | CHL | C3B-C4B | 3.42 | 1.44 | 1.41 |
| 30 | Z2 | 606 | CHL | C3B-C4B | 3.42 | 1.44 | 1.41 |
| 30 | 7 | 607 | CHL | C3B-C4B | 3.42 | 1.44 | 1.41 |
| 30 | Z | 601 | CHL | C3B-C4B | 3.41 | 1.44 | 1.41 |
| 30 | Z2 | 601 | CHL | C3B-C4B | 3.41 | 1.44 | 1.41 |
| 30 | Z | 607 | CHL | C3B-C4B | 3.41 | 1.44 | 1.41 |
| 30 | 42 | 607 | CHL | C3B-C4B | 3.41 | 1.44 | 1.41 |
| 30 | 4 | 618 | CHL | C3A-C2A | -3.41 | 1.51 | 1.54 |
| 30 | 42 | 618 | CHL | C3A-C2A | -3.41 | 1.51 | 1.54 |
| 30 | 92 | 607 | CHL | C3A-C2A | -3.38 | 1.51 | 1.54 |
| 30 | 12 | 607 | CHL | C3B-C4B | 3.38 | 1.44 | 1.41 |
| 30 | 82 | 607 | CHL | C3B-C4B | 3.38 | 1.44 | 1.41 |
| 30 | 72 | 601 | CHL | C3B-C4B | 3.37 | 1.44 | 1.41 |
| 30 | 9 | 606 | CHL | C3B-C4B | 3.36 | 1.44 | 1.41 |
| 30 | Z | 601 | CHL | C3A-C2A | -3.36 | 1.51 | 1.54 |
| 30 | Z2 | 601 | CHL | C3A-C2A | -3.36 | 1.51 | 1.54 |
| 30 | 9 | 607 | CHL | CHB-C4A | -3.34 | 1.34 | 1.38 |
| 30 | 1 | 601 | CHL | C3B-C4B | 3.33 | 1.44 | 1.41 |
| 30 | 12 | 601 | CHL | C3B-C4B | 3.33 | 1.44 | 1.41 |
| 30 | 7 | 601 | CHL | C3B-C4B | 3.33 | 1.44 | 1.41 |
| 30 | 92 | 607 | CHL | C3B-C4B | 3.32 | 1.44 | 1.41 |
| 30 | 82 | 601 | CHL | C3B-C4B | 3.32 | 1.44 | 1.41 |
| 30 | 8 | 601 | CHL | C3B-C4B | 3.32 | 1.44 | 1.41 |
| 30 | 1 | 601 | CHL | C3A-C2A | -3.31 | 1.51 | 1.54 |
| 30 | 8 | 607 | CHL | C3B-C4B | 3.31 | 1.44 | 1.41 |
| 30 | 12 | 601 | CHL | C3A-C2A | -3.27 | 1.51 | 1.54 |
| 30 | 7 | 607 | CHL | C3B-C2B | -3.20 | 1.36 | 1.40 |
| 32 | 5 | 625 | NEX | C1-C6 | -3.20 | 1.49 | 1.54 |
| 30 | 9 | 607 | CHL | C3A-C2A | -3.20 | 1.52 | 1.54 |
| 30 | 1 | 601 | CHL | C3B-C2B | -3.20 | 1.36 | 1.40 |
| 30 | 9 | 607 | CHL | C3B-C4B | 3.19 | 1.44 | 1.41 |
| 30 | 82 | 607 | CHL | C3B-C2B | -3.19 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 8 | 607 | CHL | C3B-C2B | -3.17 | 1.36 | 1.40 |
| 30 | 12 | 601 | CHL | C3B-C2B | -3.16 | 1.36 | 1.40 |
| 30 | 72 | 607 | CHL | C3B-C2B | -3.12 | 1.36 | 1.40 |
| 30 | 32 | 608 | CHL | C3B-C2B | -3.12 | 1.36 | 1.40 |
| 30 | 3 | 608 | CHL | C3B-C2B | -3.11 | 1.36 | 1.40 |
| 30 | 1 | 607 | CHL | C3B-C2B | -3.11 | 1.36 | 1.40 |
| 30 | 52 | 606 | CHL | C3B-C2B | -3.11 | 1.36 | 1.40 |
| 30 | Z2 | 607 | CHL | C3B-C2B | -3.10 | 1.36 | 1.40 |
| 30 | 92 | 606 | CHL | C3B-C2B | -3.10 | 1.36 | 1.40 |
| 30 | 5 | 607 | CHL | C3B-C2B | -3.09 | 1.36 | 1.40 |
| 30 | 1 | 606 | CHL | C3B-C2B | -3.08 | 1.36 | 1.40 |
| 30 | 12 | 607 | CHL | C3B-C2B | -3.07 | 1.36 | 1.40 |
| 30 | 42 | 607 | CHL | C3B-C2B | -3.07 | 1.36 | 1.40 |
| 30 | Z | 607 | CHL | C3B-C2B | -3.07 | 1.36 | 1.40 |
| 30 | 62 | 606 | CHL | C3B-C2B | -3.06 | 1.36 | 1.40 |
| 30 | Z | 606 | CHL | C3B-C2B | -3.06 | 1.36 | 1.40 |
| 30 | 9 | 606 | CHL | C3B-C2B | -3.05 | 1.36 | 1.40 |
| 30 | 12 | 606 | CHL | C3B-C2B | -3.04 | 1.36 | 1.40 |
| 30 | 52 | 607 | CHL | C3B-C2B | -3.03 | 1.36 | 1.40 |
| 30 | 4 | 607 | CHL | C3B-C2B | -3.03 | 1.36 | 1.40 |
| 30 | 5 | 606 | CHL | C3B-C2B | -3.03 | 1.36 | 1.40 |
| 30 | 52 | 608 | CHL | C3B-C2B | -3.03 | 1.36 | 1.40 |
| 30 | 6 | 606 | CHL | C3B-C2B | -3.02 | 1.36 | 1.40 |
| 30 | 5 | 608 | CHL | C3B-C2B | -3.01 | 1.36 | 1.40 |
| 30 | Z2 | 606 | CHL | C3B-C2B | -3.01 | 1.36 | 1.40 |
| 30 | Z | 606 | CHL | C3A-C2A | -3.01 | 1.52 | 1.54 |
| 30 | Z2 | 606 | CHL | C3A-C2A | -3.01 | 1.52 | 1.54 |
| 30 | 6 | 616 | CHL | C3B-C2B | -3.01 | 1.36 | 1.40 |
| 30 | 52 | 618 | CHL | C3B-C2B | -2.99 | 1.36 | 1.40 |
| 30 | 6 | 607 | CHL | C3B-C2B | -2.99 | 1.36 | 1.40 |
| 30 | 62 | 607 | CHL | C3B-C2B | -2.99 | 1.36 | 1.40 |
| 30 | 5 | 618 | CHL | C3B-C2B | -2.98 | 1.36 | 1.40 |
| 30 | 4 | 608 | CHL | C3B-C2B | -2.98 | 1.36 | 1.40 |
| 30 | 7 | 606 | CHL | C3B-C2B | -2.97 | 1.36 | 1.40 |
| 30 | 72 | 606 | CHL | C3B-C2B | -2.97 | 1.36 | 1.40 |
| 30 | 62 | 616 | CHL | C3B-C2B | -2.97 | 1.36 | 1.40 |
| 30 | 42 | 618 | CHL | C3B-C2B | -2.97 | 1.36 | 1.40 |
| 30 | 8 | 601 | CHL | C3A-C2A | -2.97 | 1.52 | 1.54 |
| 30 | 6 | 608 | CHL | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 30 | 62 | 608 | CHL | C3B-C2B | -2.96 | 1.36 | 1.40 |
| 30 | 82 | 607 | CHL | C3A-C2A | -2.96 | 1.52 | 1.54 |
| 30 | 42 | 608 | CHL | C3B-C2B | -2.95 | 1.36 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 4 | 618 | CHL | C3B-C2B | -2.94 | 1.36 | 1.40 |
| 30 | 8 | 607 | CHL | C3A-C2A | -2.94 | 1.52 | 1.54 |
| 30 | 7 | 601 | CHL | C3B-C2B | -2.94 | 1.36 | 1.40 |
| 30 | 62 | 618 | CHL | C3B-C2B | -2.94 | 1.36 | 1.40 |
| 30 | 42 | 606 | CHL | C3B-C2B | -2.94 | 1.36 | 1.40 |
| 30 | 4 | 606 | CHL | C3B-C2B | -2.94 | 1.36 | 1.40 |
| 30 | 82 | 601 | CHL | C3A-C2A | -2.94 | 1.52 | 1.54 |
| 30 | 8 | 601 | CHL | C3B-C2B | -2.93 | 1.36 | 1.40 |
| 30 | 82 | 601 | CHL | C3B-C2B | -2.93 | 1.36 | 1.40 |
| 30 | Z | 601 | CHL | C3B-C2B | -2.93 | 1.36 | 1.40 |
| 30 | Z2 | 601 | CHL | C3B-C2B | -2.93 | 1.36 | 1.40 |
| 30 | 4 | 601 | CHL | C3B-C2B | -2.92 | 1.36 | 1.40 |
| 30 | 42 | 601 | CHL | C3B-C2B | -2.92 | 1.36 | 1.40 |
| 30 | 6 | 618 | CHL | C3B-C2B | -2.92 | 1.36 | 1.40 |
| 30 | 72 | 601 | CHL | C3B-C2B | -2.91 | 1.36 | 1.40 |
| 30 | 92 | 607 | CHL | C3B-C2B | -2.91 | 1.36 | 1.40 |
| 30 | 8 | 606 | CHL | C3B-C2B | -2.91 | 1.36 | 1.40 |
| 30 | 82 | 606 | CHL | C3B-C2B | -2.91 | 1.36 | 1.40 |
| 30 | 6 | 601 | CHL | C3B-C2B | -2.85 | 1.36 | 1.40 |
| 30 | 62 | 601 | CHL | C3B-C2B | -2.85 | 1.36 | 1.40 |
| 30 | 9 | 607 | CHL | C3B-C2B | -2.71 | 1.36 | 1.40 |
| 32 | 52 | 625 | NEX | C1-C6 | -2.71 | 1.50 | 1.54 |
| 30 | 1 | 607 | CHL | CHC-C4B | -2.63 | 1.35 | 1.39 |
| 30 | 12 | 607 | CHL | CHC-C4B | -2.63 | 1.35 | 1.39 |
| 30 | Z | 601 | CHL | CHC-C4B | -2.60 | 1.35 | 1.39 |
| 30 | 12 | 601 | CHL | CHC-C4B | -2.57 | 1.35 | 1.39 |
| 30 | 82 | 607 | CHL | CHC-C4B | -2.56 | 1.35 | 1.39 |
| 21 | A2 | 829 | CLA | C1D-C2D | -2.56 | 1.40 | 1.45 |
| 21 | A | 829 | CLA | C1D-C2D | -2.56 | 1.40 | 1.45 |
| 30 | 1 | 601 | CHL | CHC-C4B | -2.56 | 1.35 | 1.39 |
| 21 | B | 806 | CLA | C1D-C2D | -2.55 | 1.40 | 1.45 |
| 21 | A | 802 | CLA | C1D-C2D | -2.55 | 1.40 | 1.45 |
| 30 | 8 | 607 | CHL | CHC-C4B | -2.55 | 1.35 | 1.39 |
| 30 | Z2 | 601 | CHL | CHC-C4B | -2.55 | 1.35 | 1.39 |
| 20 | A2 | 801 | CL0 | CHB-C4A | -2.55 | 1.35 | 1.38 |
| 21 | B2 | 802 | CLA | C1D-C2D | -2.54 | 1.40 | 1.45 |
| 21 | B2 | 806 | CLA | C1D-C2D | -2.53 | 1.40 | 1.45 |
| 21 | B | 802 | CLA | C1D-C2D | -2.53 | 1.40 | 1.45 |
| 21 | A2 | 802 | CLA | C1D-C2D | -2.52 | 1.40 | 1.45 |
| 21 | A | 828 | CLA | C1D-C2D | -2.51 | 1.40 | 1.45 |
| 21 | K2 | 201 | CLA | C1D-C2D | -2.51 | 1.40 | 1.45 |
| 30 | 8 | 607 | CHL | CHB-C1B | -2.50 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 82 | 607 | CHL | CHB-C1B | -2.50 | 1.35 | 1.39 |
| 21 | A2 | 828 | CLA | C1D-C2D | -2.50 | 1.40 | 1.45 |
| 21 | A | 819 | CLA | C1D-C2D | -2.50 | 1.40 | 1.45 |
| 20 | A | 801 | CL0 | CHB-C4A | -2.50 | 1.35 | 1.38 |
| 21 | B2 | 803 | CLA | C1D-C2D | -2.50 | 1.40 | 1.45 |
| 30 | 3 | 608 | CHL | CHC-C4B | -2.50 | 1.35 | 1.39 |
| 21 | B | 803 | CLA | C1D-C2D | -2.50 | 1.40 | 1.45 |
| 21 | A2 | 854 | CLA | C1D-C2D | -2.49 | 1.40 | 1.45 |
| 21 | K | 201 | CLA | C1D-C2D | -2.49 | 1.40 | 1.45 |
| 21 | A2 | 810 | CLA | C1D-C2D | -2.49 | 1.40 | 1.45 |
| 21 | 7 | 612 | CLA | C1D-C2D | -2.49 | 1.40 | 1.45 |
| 30 | 5 | 606 | CHL | CHC-C4B | -2.49 | 1.35 | 1.39 |
| 30 | 72 | 606 | CHL | CHC-C4B | -2.49 | 1.35 | 1.39 |
| 30 | Z | 607 | CHL | CHC-C4B | -2.49 | 1.35 | 1.39 |
| 21 | A | 807 | CLA | C1D-C2D | -2.49 | 1.40 | 1.45 |
| 21 | A2 | 842 | CLA | C1D-C2D | -2.48 | 1.40 | 1.45 |
| 30 | 8 | 601 | CHL | CHC-C4B | -2.48 | 1.35 | 1.39 |
| 30 | 8 | 606 | CHL | CHC-C4B | -2.48 | 1.35 | 1.39 |
| 30 | 82 | 601 | CHL | CHC-C4B | -2.48 | 1.35 | 1.39 |
| 21 | B | 838 | CLA | C1D-C2D | -2.48 | 1.40 | 1.45 |
| 21 | 32 | 603 | CLA | C1D-C2D | -2.48 | 1.40 | 1.45 |
| 30 | 7 | 607 | CHL | CHC-C4B | -2.48 | 1.35 | 1.39 |
| 30 | 72 | 607 | CHL | CHC-C4B | -2.48 | 1.35 | 1.39 |
| 21 | A | 854 | CLA | C1D-C2D | -2.47 | 1.40 | 1.45 |
| 21 | A2 | 826 | CLA | C1D-C2D | -2.47 | 1.40 | 1.45 |
| 21 | F | 301 | CLA | C1D-C2D | -2.47 | 1.40 | 1.45 |
| 21 | F2 | 301 | CLA | C1D-C2D | -2.47 | 1.40 | 1.45 |
| 30 | 52 | 606 | CHL | CHC-C4B | -2.47 | 1.35 | 1.39 |
| 21 | A2 | 807 | CLA | C1D-C2D | -2.47 | 1.40 | 1.45 |
| 30 | 5 | 608 | CHL | CHC-C4B | -2.47 | 1.35 | 1.39 |
| 21 | A | 826 | CLA | C1D-C2D | -2.47 | 1.40 | 1.45 |
| 21 | 5 | 621 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 30 | 7 | 606 | CHL | CHC-C4B | -2.46 | 1.35 | 1.39 |
| 21 | 8 | 610 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 21 | B2 | 824 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 30 | 9 | 606 | CHL | CHC-C4B | -2.46 | 1.35 | 1.39 |
| 30 | Z2 | 607 | CHL | CHC-C4B | -2.46 | 1.35 | 1.39 |
| 21 | A | 814 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 21 | 3 | 603 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 21 | A2 | 814 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 21 | B | 824 | CLA | C1D-C2D | -2.46 | 1.40 | 1.45 |
| 30 | 42 | 606 | CHL | CHC-C4B | -2.45 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 809 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 30 | 4 | 606 | CHL | CHC-C4B | -2.45 | 1.35 | 1.39 |
| 21 | 8 | 608 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 21 | B2 | 838 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 21 | A2 | 838 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 21 | 72 | 612 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 21 | A | 813 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 21 | A | 810 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 21 | A | 830 | CLA | C1D-C2D | -2.45 | 1.40 | 1.45 |
| 30 | 92 | 606 | CHL | CHC-C4B | -2.44 | 1.35 | 1.39 |
| 21 | A | 821 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 21 | B2 | 825 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 21 | A2 | 808 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 21 | A | 808 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 21 | B2 | 809 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 30 | 32 | 608 | CHL | CHC-C4B | -2.44 | 1.35 | 1.39 |
| 21 | A | 842 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 21 | A2 | 805 | CLA | C1D-C2D | -2.44 | 1.40 | 1.45 |
| 21 | A | 812 | CLA | C1D-C2D | -2.43 | 1.40 | 1.45 |
| 21 | A2 | 819 | CLA | C1D-C2D | -2.43 | 1.40 | 1.45 |
| 30 | 5 | 618 | CHL | CHC-C4B | -2.43 | 1.35 | 1.39 |
| 21 | A | 805 | CLA | C1D-C2D | -2.43 | 1.40 | 1.45 |
| 30 | 42 | 607 | CHL | CHC-C4B | -2.43 | 1.35 | 1.39 |
| 30 | 1 | 606 | CHL | CHC-C4B | -2.43 | 1.35 | 1.39 |
| 21 | B | 825 | CLA | C1D-C2D | -2.43 | 1.40 | 1.45 |
| 30 | 82 | 606 | CHL | CHC-C4B | -2.43 | 1.35 | 1.39 |
| 21 | A | 818 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | B | 835 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | 52 | 621 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 30 | 52 | 608 | CHL | CHC-C4B | -2.42 | 1.35 | 1.39 |
| 21 | A | 843 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | A2 | 845 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | B | 813 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | B | 829 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | B2 | 829 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | 82 | 608 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | B2 | 820 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | 1 | 612 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | A2 | 818 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 30 | Z | 606 | CHL | CHC-C4B | -2.42 | 1.35 | 1.39 |
| 21 | A2 | 830 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | A2 | 815 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 1 | 606 | CHL | CHB-C1B | -2.42 | 1.35 | 1.39 |
| 21 | A | 845 | CLA | C1D-C2D | -2.42 | 1.40 | 1.45 |
| 21 | B2 | 827 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | A | 815 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | B | 808 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | A | 827 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | B2 | 808 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | 9 | 602 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | 82 | 612 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 30 | 4 | 608 | CHL | CHC-C4B | -2.41 | 1.35 | 1.39 |
| 21 | B | 827 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 30 | 62 | 608 | CHL | CHC-C4B | -2.41 | 1.35 | 1.39 |
| 21 | B2 | 813 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | A2 | 813 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | A2 | 821 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 30 | 4 | 607 | CHL | CHC-C4B | -2.41 | 1.35 | 1.39 |
| 21 | B | 816 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | A | 834 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | B | 805 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | 7 | 608 | CLA | C1D-C2D | -2.41 | 1.40 | 1.45 |
| 21 | 8 | 602 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | A2 | 806 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | 32 | 615 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | K2 | 203 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | Z2 | 609 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | K | 203 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | A2 | 834 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | J | 101 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | J2 | 101 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 30 | 72 | 601 | CHL | CHC-C4B | -2.40 | 1.35 | 1.39 |
| 21 | 1 | 616 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | 12 | 616 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 30 | 6 | 607 | CHL | CHB-C1B | -2.40 | 1.35 | 1.39 |
| 30 | 62 | 607 | CHL | CHB-C1B | -2.40 | 1.35 | 1.39 |
| 21 | B | 840 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | F | 303 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | F2 | 303 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | A | 804 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | 5 | 602 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | 3 | 615 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | A2 | 839 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |
| 21 | 12 | 612 | CLA | C1D-C2D | -2.40 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 819 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | 8 | 612 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 30 | 42 | 606 | CHL | CHB-C1B | -2.39 | 1.35 | 1.39 |
| 21 | B2 | 837 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | B2 | 834 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 30 | 4 | 606 | CHL | CHB-C1B | -2.39 | 1.35 | 1.39 |
| 21 | A | 833 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | A | 822 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | 3 | 606 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | 12 | 614 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | 52 | 602 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 30 | Z2 | 606 | CHL | CHC-C4B | -2.39 | 1.35 | 1.39 |
| 21 | 1 | 611 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | 42 | 603 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 30 | 6 | 606 | CHL | CHC-C4B | -2.39 | 1.35 | 1.39 |
| 30 | 62 | 606 | CHL | CHC-C4B | -2.39 | 1.35 | 1.39 |
| 21 | A | 820 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | A2 | 843 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | 92 | 603 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | B | 832 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | G | 203 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 30 | 5 | 607 | CHL | CHC-C4B | -2.39 | 1.35 | 1.39 |
| 21 | A2 | 817 | CLA | C1D-C2D | -2.39 | 1.40 | 1.45 |
| 21 | A | 838 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | B | 841 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | A2 | 812 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | B2 | 835 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | 12 | 611 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | A | 817 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | A2 | 827 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | 3 | 613 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 30 | 52 | 618 | CHL | CHC-C4B | -2.38 | 1.35 | 1.39 |
| 21 | A | 841 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | 42 | 609 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | 72 | 613 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 30 | 62 | 601 | CHL | CHC-C4B | -2.38 | 1.35 | 1.39 |
| 21 | A2 | 809 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 21 | A | 840 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 30 | 62 | 618 | CHL | CHB-C1B | -2.38 | 1.35 | 1.39 |
| 21 | Z | 612 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 30 | 52 | 607 | CHL | CHC-C4B | -2.38 | 1.35 | 1.39 |
| 21 | A | 806 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 820 | CLA | C1D-C2D | -2.38 | 1.40 | 1.45 |
| 30 | 7 | 606 | CHL | CHB-C1B | -2.38 | 1.35 | 1.39 |
| 21 | B | 818 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 7 | 614 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | Z | 609 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 4 | 602 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B2 | 818 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 30 | 7 | 601 | CHL | CHB-C1B | -2.37 | 1.35 | 1.39 |
| 30 | 62 | 618 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |
| 21 | B2 | 816 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 82 | 610 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 30 | 9 | 607 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |
| 30 | 72 | 606 | CHL | CHB-C1B | -2.37 | 1.35 | 1.39 |
| 21 | A2 | 841 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B | 836 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 72 | 609 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 3 | 617 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B2 | 819 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 32 | 612 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 1 | 609 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 1 | 613 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 6 | 622 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | A2 | 837 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 12 | 609 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 12 | 613 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 62 | 622 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B2 | 805 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | A | 832 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | A2 | 820 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | A2 | 831 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 92 | 602 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 30 | 4 | 618 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |
| 21 | B | 811 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B | 821 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | Z | 603 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B2 | 811 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B2 | 821 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | Z2 | 603 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 52 | 617 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 7 | 602 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | B2 | 828 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 30 | 6 | 607 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 6 | 608 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |
| 21 | A | 831 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 7 | 620 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 21 | 72 | 620 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 30 | 42 | 601 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |
| 21 | B2 | 815 | CLA | C1D-C2D | -2.37 | 1.40 | 1.45 |
| 30 | 6 | 616 | CHL | CHC-C4B | -2.37 | 1.35 | 1.39 |
| 21 | 82 | 609 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B2 | 831 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B2 | 832 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 32 | 604 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 82 | 602 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 82 | 613 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B | 828 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B | 837 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 7 | 611 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 72 | 611 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 30 | 72 | 601 | CHL | CHB-C1B | -2.36 | 1.35 | 1.39 |
| 21 | 1 | 603 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 8 | 603 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 82 | 603 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | F | 304 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | F2 | 304 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 52 | 616 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 3 | 610 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 30 | 42 | 618 | CHL | CHC-C4B | -2.36 | 1.35 | 1.39 |
| 21 | A2 | 822 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B2 | 833 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 7 | 616 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 4 | 603 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 6 | 603 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | A | 825 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B | 804 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | A2 | 803 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | A2 | 823 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | A2 | 840 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | A2 | 825 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | A2 | 804 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | G2 | 203 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 5 | 614 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | B2 | 830 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 52 | 614 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 52 | 613 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 7 | 613 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 5 | 601 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | K | 204 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 32 | 606 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 72 | 608 | CLA | C1D-C2D | -2.36 | 1.40 | 1.45 |
| 21 | 9 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | A2 | 836 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 92 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 5 | 617 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 52 | 610 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 4 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 42 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | A | 811 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 30 | 42 | 608 | CHL | CHC-C4B | -2.35 | 1.35 | 1.39 |
| 21 | 42 | 602 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 30 | 12 | 606 | CHL | CHC-C4B | -2.35 | 1.35 | 1.39 |
| 21 | B | 815 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 8 | 614 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 82 | 614 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 52 | 601 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 32 | 613 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 30 | 1 | 601 | CHL | CHB-C1B | -2.35 | 1.35 | 1.39 |
| 30 | 7 | 607 | CHL | CHB-C1B | -2.35 | 1.35 | 1.39 |
| 21 | 3 | 609 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 8 | 609 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | B | 826 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 32 | 602 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 7 | 604 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 3 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 72 | 602 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 3 | 604 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | Z2 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | A | 839 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | B | 839 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 1 | 614 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 6 | 609 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 62 | 612 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 30 | 7 | 601 | CHL | CHC-C4B | -2.35 | 1.35 | 1.39 |
| 21 | B | 834 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 1 | 602 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | A2 | 832 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 12 | 602 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 30 | 6 | 618 | CHL | CHB-C1B | -2.35 | 1.35 | 1.39 |
| 21 | B2 | 836 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | B2 | 841 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 7 | 609 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | K2 | 206 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 21 | 62 | 609 | CLA | C1D-C2D | -2.35 | 1.40 | 1.45 |
| 30 | 6 | 618 | CHL | CHC-C4B | -2.34 | 1.35 | 1.39 |
| 21 | 9 | 603 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 52 | 612 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | B2 | 812 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 6 | 602 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | B2 | 840 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | B | 831 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | B2 | 817 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | A | 836 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 3 | 614 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 30 | Z2 | 607 | CHL | CHB-C1B | -2.34 | 1.35 | 1.39 |
| 21 | 8 | 604 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 5 | 610 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 62 | 603 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 8 | 613 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 12 | 610 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | Z2 | 616 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | 5 | 613 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | A | 824 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | Z | 616 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | B2 | 804 | CLA | C1D-C2D | -2.34 | 1.40 | 1.45 |
| 21 | K | 206 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B2 | 807 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B2 | 814 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 30 | 4 | 601 | CHL | CHC-C4B | -2.33 | 1.35 | 1.39 |
| 21 | B | 812 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B | 817 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | A2 | 833 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 6 | 612 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 32 | 610 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 92 | 609 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | A2 | 824 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 30 | 6 | 601 | CHL | CHC-C4B | -2.33 | 1.35 | 1.39 |
| 21 | 7 | 610 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 5 | 611 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 72 | 610 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 52 | 611 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 30 | 12 | 606 | CHL | CHB-C1B | -2.33 | 1.35 | 1.39 |
| 30 | 52 | 606 | CHL | CHB-C1B | -2.33 | 1.35 | 1.39 |
| 21 | 4 | 613 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | A | 809 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B | 823 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 32 | 617 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 30 | 5 | 608 | CHL | CHB-C1B | -2.33 | 1.35 | 1.39 |
| 30 | 52 | 608 | CHL | CHB-C1B | -2.33 | 1.35 | 1.39 |
| 21 | 9 | 611 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | A | 837 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 12 | 608 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 42 | 616 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 72 | 604 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B | 833 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 5 | 609 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 6 | 604 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B2 | 826 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 52 | 609 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 62 | 604 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | A | 803 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 3 | 602 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | B2 | 823 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 32 | 609 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 92 | 613 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 5 | 616 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | Z2 | 608 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 1 | 610 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 5 | 604 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 72 | 614 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | Z2 | 614 | CLA | C1D-C2D | -2.33 | 1.40 | 1.45 |
| 21 | 5 | 612 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | G | 204 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | 6 | 611 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 30 | 6 | 606 | CHL | CHB-C1B | -2.32 | 1.35 | 1.39 |
| 21 | Z | 602 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | 12 | 603 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | 72 | 616 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | L2 | 203 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 30 | 62 | 616 | CHL | CHC-C4B | -2.32 | 1.35 | 1.39 |
| 21 | 92 | 604 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 6 | 616 | CHL | CHB-C1B | -2.32 | 1.35 | 1.39 |
| 30 | 62 | 616 | CHL | CHB-C1B | -2.32 | 1.35 | 1.39 |
| 21 | A2 | 816 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | 4 | 616 | CLA | C1D-C2D | -2.32 | 1.40 | 1.45 |
| 21 | A | 823 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 30 | 6 | 608 | CHL | CHB-C1B | -2.31 | 1.35 | 1.39 |
| 21 | Z | 613 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | 6 | 613 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | 9 | 613 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | B | 807 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 30 | 5 | 618 | CHL | CHB-C1B | -2.31 | 1.35 | 1.39 |
| 21 | A | 816 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | B2 | 822 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | 62 | 614 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 30 | 42 | 618 | CHL | CHB-C1B | -2.31 | 1.35 | 1.39 |
| 21 | A | 835 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | 4 | 614 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 21 | 42 | 614 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 30 | 9 | 606 | CHL | CHB-C1B | -2.31 | 1.35 | 1.39 |
| 21 | 42 | 613 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 30 | 72 | 607 | CHL | CHB-C1B | -2.31 | 1.35 | 1.39 |
| 21 | B2 | 810 | CLA | C1D-C2D | -2.31 | 1.40 | 1.45 |
| 30 | 62 | 607 | CHL | CHC-C4B | -2.31 | 1.35 | 1.39 |
| 21 | G2 | 204 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | K2 | 204 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 7 | 603 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 30 | 62 | 606 | CHL | CHB-C1B | -2.30 | 1.35 | 1.39 |
| 21 | B | 830 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 3 | 611 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | A2 | 811 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 62 | 610 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | Z | 611 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | L | 203 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 62 | 602 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 42 | 610 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 42 | 604 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 52 | 604 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 6 | 617 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 62 | 617 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 30 | 5 | 606 | CHL | CHB-C1B | -2.30 | 1.35 | 1.39 |
| 30 | 12 | 607 | CHL | CHB-C1B | -2.30 | 1.35 | 1.39 |
| 21 | B2 | 839 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 822 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 8 | 611 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 21 | 82 | 611 | CLA | C1D-C2D | -2.30 | 1.40 | 1.45 |
| 30 | 1 | 607 | CHL | CHB-C1B | -2.30 | 1.35 | 1.39 |
| 30 | 52 | 618 | CHL | CHB-C1B | -2.30 | 1.35 | 1.39 |
| 21 | 4 | 611 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | 42 | 611 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 30 | 12 | 601 | CHL | CHB-C1B | -2.29 | 1.35 | 1.39 |
| 21 | 1 | 608 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | 9 | 604 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | 9 | 609 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 30 | 92 | 607 | CHL | CHC-C4B | -2.29 | 1.35 | 1.39 |
| 21 | B | 810 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 30 | 8 | 606 | CHL | CHB-C1B | -2.29 | 1.35 | 1.39 |
| 30 | 82 | 606 | CHL | CHB-C1B | -2.29 | 1.35 | 1.39 |
| 21 | 92 | 614 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | Z | 610 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | Z2 | 610 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | Z2 | 613 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | 92 | 610 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | 92 | 601 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | A2 | 835 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | Z2 | 602 | CLA | C1D-C2D | -2.29 | 1.40 | 1.45 |
| 21 | 32 | 614 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 5 | 603 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 52 | 603 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 4 | 604 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 6 | 610 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 8 | 616 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 82 | 616 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 30 | 8 | 601 | CHL | CHB-C1B | -2.28 | 1.35 | 1.39 |
| 30 | 82 | 601 | CHL | CHB-C1B | -2.28 | 1.35 | 1.39 |
| 21 | 62 | 611 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 1 | 604 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | Z | 608 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 72 | 603 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | Z2 | 611 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 4 | 610 | CLA | C1D-C2D | -2.28 | 1.40 | 1.45 |
| 21 | 32 | 607 | CLA | C1D-C2D | -2.27 | 1.40 | 1.45 |
| 21 | 4 | 609 | CLA | C1D-C2D | -2.27 | 1.40 | 1.45 |
| 30 | Z | 607 | CHL | CHB-C1B | -2.27 | 1.36 | 1.39 |
| 21 | 82 | 604 | CLA | C1D-C2D | -2.27 | 1.40 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 30 | 62 | 608 | CHL | CHB-C1B | -2.27 | 1.36 | 1.39 |
| 21 | 32 | 611 | CLA | C1D-C2D | -2.27 | 1.40 | 1.45 |
| 30 | 4 | 607 | CHL | CHB-C1B | -2.27 | 1.36 | 1.39 |
| 21 | Z | 614 | CLA | C1D-C2D | -2.27 | 1.40 | 1.45 |
| 21 | 9 | 614 | CLA | C1D-C2D | -2.27 | 1.40 | 1.45 |
| 30 | 4 | 608 | CHL | CHB-C1B | -2.26 | 1.36 | 1.39 |
| 30 | 42 | 608 | CHL | CHB-C1B | -2.26 | 1.36 | 1.39 |
| 21 | 3 | 607 | CLA | C1D-C2D | -2.26 | 1.40 | 1.45 |
| 21 | 6 | 614 | CLA | C1D-C2D | -2.26 | 1.40 | 1.45 |
| 30 | 3 | 608 | CHL | CHB-C1B | -2.26 | 1.36 | 1.39 |
| 21 | 9 | 601 | CLA | C1D-C2D | -2.26 | 1.40 | 1.45 |
| 30 | 92 | 606 | CHL | CHB-C1B | -2.26 | 1.36 | 1.39 |
| 21 | B | 814 | CLA | C1D-C2D | -2.26 | 1.40 | 1.45 |
| 21 | 92 | 611 | CLA | C1D-C2D | -2.26 | 1.40 | 1.45 |
| 30 | Z2 | 606 | CHL | CHB-C1B | -2.26 | 1.36 | 1.39 |
| 21 | 62 | 613 | CLA | C1D-C2D | -2.26 | 1.40 | 1.45 |
| 30 | 52 | 607 | CHL | CHB-C1B | -2.25 | 1.36 | 1.39 |
| 21 | Z | 604 | CLA | C1D-C2D | -2.25 | 1.40 | 1.45 |
| 21 | Z2 | 604 | CLA | C1D-C2D | -2.25 | 1.40 | 1.45 |
| 30 | Z | 601 | CHL | CHB-C1B | -2.25 | 1.36 | 1.39 |
| 30 | 5 | 607 | CHL | CHB-C1B | -2.25 | 1.36 | 1.39 |
| 21 | 9 | 610 | CLA | C1D-C2D | -2.25 | 1.40 | 1.45 |
| 21 | L | 204 | CLA | C1D-C2D | -2.24 | 1.40 | 1.45 |
| 21 | L2 | 204 | CLA | C1D-C2D | -2.24 | 1.40 | 1.45 |
| 30 | 62 | 601 | CHL | CHB-C1B | -2.24 | 1.36 | 1.39 |
| 30 | Z | 606 | CHL | CHB-C1B | -2.24 | 1.36 | 1.39 |
| 21 | 12 | 604 | CLA | C1D-C2D | -2.23 | 1.40 | 1.45 |
| 30 | 4 | 618 | CHL | CHB-C1B | -2.23 | 1.36 | 1.39 |
| 30 | 42 | 607 | CHL | CHB-C1B | -2.23 | 1.36 | 1.39 |
| 30 | 32 | 608 | CHL | CHB-C1B | -2.22 | 1.36 | 1.39 |
| 30 | 6 | 601 | CHL | CHB-C1B | -2.22 | 1.36 | 1.39 |
| 30 | 42 | 601 | CHL | CHB-C1B | -2.21 | 1.36 | 1.39 |
| 30 | 92 | 607 | CHL | CHB-C1B | -2.19 | 1.36 | 1.39 |
| 30 | Z2 | 601 | CHL | CHB-C1B | -2.16 | 1.36 | 1.39 |
| 30 | 4 | 601 | CHL | CHB-C1B | -2.15 | 1.36 | 1.39 |
| 21 | B2 | 840 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 21 | B | 840 | CLA | C3D-C4D | -2.11 | 1.39 | 1.44 |
| 21 | A | 806 | CLA | C3D-C4D | -2.09 | 1.39 | 1.44 |
| 21 | A2 | 806 | CLA | C3D-C4D | -2.09 | 1.39 | 1.44 |
| 21 | A2 | 827 | CLA | C3D-C4D | -2.09 | 1.39 | 1.44 |
| 21 | A | 833 | CLA | C3D-C4D | -2.09 | 1.39 | 1.44 |
| 21 | B2 | 830 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | 92 | 610 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 21 | B2 | 829 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 21 | 9 | 610 | CLA | C3D-C4D | -2.08 | 1.39 | 1.44 |
| 21 | A | 809 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | B2 | 825 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | B2 | 831 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | A2 | 842 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 20 | A | 801 | CL0 | CHD-C4C | -2.07 | 1.35 | 1.39 |
| 21 | A | 842 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | B | 833 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | 12 | 602 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | A | 803 | CLA | C3D-C4D | -2.07 | 1.39 | 1.44 |
| 21 | 1 | 602 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A | 802 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A | 805 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A | 822 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A2 | 822 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A | 827 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | B | 837 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | B | 823 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A | 843 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | B2 | 833 | CLA | C3D-C4D | -2.06 | 1.39 | 1.44 |
| 21 | A | 834 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | B | 825 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | B2 | 823 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | B | 830 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A2 | 803 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | 12 | 610 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A | 808 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A | 812 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A | 841 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A2 | 841 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | B | 829 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | B | 831 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 20 | A2 | 801 | CL0 | CHD-C4C | -2.05 | 1.35 | 1.39 |
| 21 | B2 | 818 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A2 | 809 | CLA | C3D-C4D | -2.05 | 1.39 | 1.44 |
| 21 | A2 | 839 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | B2 | 837 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | 32 | 610 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 30 | 9 | 607 | CHL | CHB-C1B | -2.04 | 1.36 | 1.39 |
| 21 | 4 | 603 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | B | 821 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | 9 | 604 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | B2 | 821 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | 82 | 602 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | 92 | 604 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | A | 825 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | A2 | 833 | CLA | C3D-C4D | -2.04 | 1.39 | 1.44 |
| 21 | A | 839 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 805 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | B2 | 832 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | B | 812 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | B2 | 812 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | B2 | 819 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A | 820 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 802 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 843 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 812 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 820 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | B | 832 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | 82 | 603 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A | 836 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A | 807 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 807 | CLA | C3D-C4D | -2.03 | 1.39 | 1.44 |
| 21 | A2 | 824 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 1 | 613 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A2 | 831 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 12 | 613 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 9 | 603 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 9 | 602 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A2 | 823 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A | 837 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A2 | 836 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A | 811 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | B | 805 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A2 | 811 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A | 832 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | B | 811 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 3 | 602 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 8 | 602 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 82 | 604 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | A | 804 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |
| 21 | 42 | 603 | CLA | C3D-C4D | -2.02 | 1.39 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | A | 854 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | 7 | 616 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | B2 | 817 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A2 | 804 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A2 | 821 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A2 | 834 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | B | 819 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | K | 204 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | Z | 603 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | B2 | 802 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | Z2 | 603 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A | 813 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | B | 808 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A2 | 813 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A | 823 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | B2 | 806 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | Z | 613 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | 8 | 616 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | B2 | 835 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | 82 | 616 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | 1 | 608 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A | 821 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | A | 829 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | L | 203 | CLA | C3D-C4D | -2.01 | 1.39 | 1.44 |
| 21 | 92 | 609 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 72 | 603 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | B | 834 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | B | 802 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 7 | 603 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 3 | 610 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 1 | 610 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | A | 831 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 8 | 611 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | B2 | 805 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | B2 | 808 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 72 | 602 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | B | 813 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | A2 | 832 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | L2 | 203 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | B | 806 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |
| 21 | 92 | 603 | CLA | C3D-C4D | -2.00 | 1.39 | 1.44 |

All (1399) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | A2 | 801 | CL0 | C1B-CHB-C4A | 10.02 | 127.77 | 121.32 |
| 20 | A | 801 | CL0 | C1B-CHB-C4A | 10.01 | 127.76 | 121.32 |
| 30 | 8 | 601 | CHL | C1B-CHB-C4A | 4.95 | 124.51 | 121.32 |
| 30 | 82 | 601 | CHL | C1B-CHB-C4A | 4.92 | 124.49 | 121.32 |
| 30 | 82 | 607 | CHL | C1B-CHB-C4A | 4.79 | 124.41 | 121.32 |
| 30 | 42 | 601 | CHL | C1B-CHB-C4A | 4.76 | 124.39 | 121.32 |
| 30 | 8 | 607 | CHL | C1B-CHB-C4A | 4.74 | 124.37 | 121.32 |
| 30 | 32 | 608 | CHL | C1B-CHB-C4A | 4.73 | 124.37 | 121.32 |
| 30 | 3 | 608 | CHL | C1B-CHB-C4A | 4.71 | 124.36 | 121.32 |
| 30 | 4 | 601 | CHL | C1B-CHB-C4A | 4.70 | 124.35 | 121.32 |
| 30 | 8 | 606 | CHL | C1B-CHB-C4A | 4.63 | 124.30 | 121.32 |
| 30 | 82 | 606 | CHL | C1B-CHB-C4A | 4.59 | 124.28 | 121.32 |
| 30 | 7 | 606 | CHL | C1B-CHB-C4A | 4.58 | 124.27 | 121.32 |
| 30 | Z | 601 | CHL | C1B-CHB-C4A | 4.56 | 124.25 | 121.32 |
| 21 | 92 | 610 | CLA | C1D-ND-C4D | -4.55 | 103.12 | 106.31 |
| 30 | Z2 | 606 | CHL | C1B-CHB-C4A | 4.53 | 124.24 | 121.32 |
| 30 | 52 | 606 | CHL | C1B-CHB-C4A | 4.53 | 124.23 | 121.32 |
| 21 | 9 | 610 | CLA | C1D-ND-C4D | -4.53 | 103.14 | 106.31 |
| 30 | 5 | 606 | CHL | C1B-CHB-C4A | 4.52 | 124.23 | 121.32 |
| 30 | 72 | 607 | CHL | C1B-CHB-C4A | 4.51 | 124.22 | 121.32 |
| 30 | Z | 606 | CHL | C1B-CHB-C4A | 4.50 | 124.22 | 121.32 |
| 30 | Z2 | 601 | CHL | C1B-CHB-C4A | 4.49 | 124.21 | 121.32 |
| 30 | 72 | 606 | CHL | C1B-CHB-C4A | 4.44 | 124.18 | 121.32 |
| 21 | Z | 613 | CLA | C1D-ND-C4D | -4.43 | 103.20 | 106.31 |
| 30 | 7 | 607 | CHL | C1B-CHB-C4A | 4.41 | 124.16 | 121.32 |
| 21 | 9 | 604 | CLA | C1D-ND-C4D | -4.41 | 103.22 | 106.31 |
| 21 | 92 | 604 | CLA | C1D-ND-C4D | -4.38 | 103.24 | 106.31 |
| 30 | 4 | 606 | CHL | C1B-CHB-C4A | 4.38 | 124.14 | 121.32 |
| 21 | 5 | 603 | CLA | C1D-ND-C4D | -4.36 | 103.25 | 106.31 |
| 21 | 8 | 616 | CLA | C1D-ND-C4D | -4.36 | 103.25 | 106.31 |
| 21 | 82 | 616 | CLA | C1D-ND-C4D | -4.36 | 103.25 | 106.31 |
| 21 | B2 | 814 | CLA | C1D-ND-C4D | -4.36 | 103.26 | 106.31 |
| 21 | Z2 | 613 | CLA | C1D-ND-C4D | -4.35 | 103.26 | 106.31 |
| 21 | K | 204 | CLA | C1D-ND-C4D | -4.35 | 103.26 | 106.31 |
| 21 | 92 | 603 | CLA | C1D-ND-C4D | -4.35 | 103.26 | 106.31 |
| 21 | 1 | 613 | CLA | C1D-ND-C4D | -4.35 | 103.26 | 106.31 |
| 21 | 12 | 613 | CLA | C1D-ND-C4D | -4.35 | 103.26 | 106.31 |
| 21 | 5 | 609 | CLA | C1D-ND-C4D | -4.34 | 103.27 | 106.31 |
| 21 | A | 816 | CLA | C1D-ND-C4D | -4.34 | 103.27 | 106.31 |
| 21 | 6 | 614 | CLA | C1D-ND-C4D | -4.34 | 103.27 | 106.31 |
| 21 | 52 | 609 | CLA | C1D-ND-C4D | -4.34 | 103.27 | 106.31 |
| 21 | 62 | 614 | CLA | C1D-ND-C4D | -4.34 | 103.27 | 106.31 |
| 21 | 42 | 604 | CLA | C1D-ND-C4D | -4.34 | 103.27 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 52 | 603 | CLA | C1D-ND-C4D | -4.33 | 103.27 | 106.31 |
| 30 | 42 | 606 | CHL | C1B-CHB-C4A | 4.33 | 124.11 | 121.32 |
| 21 | B | 840 | CLA | C1D-ND-C4D | -4.32 | 103.28 | 106.31 |
| 21 | B | 808 | CLA | C1D-ND-C4D | -4.32 | 103.28 | 106.31 |
| 21 | 5 | 617 | CLA | C1D-ND-C4D | -4.32 | 103.28 | 106.31 |
| 21 | 52 | 617 | CLA | C1D-ND-C4D | -4.32 | 103.28 | 106.31 |
| 30 | 12 | 606 | CHL | C1B-CHB-C4A | 4.32 | 124.10 | 121.32 |
| 30 | 62 | 618 | CHL | C1B-CHB-C4A | 4.31 | 124.10 | 121.32 |
| 21 | 8 | 611 | CLA | C1D-ND-C4D | -4.31 | 103.29 | 106.31 |
| 21 | 5 | 614 | CLA | C1D-ND-C4D | -4.31 | 103.29 | 106.31 |
| 21 | Z | 611 | CLA | C1D-ND-C4D | -4.31 | 103.29 | 106.31 |
| 21 | B2 | 840 | CLA | C1D-ND-C4D | -4.30 | 103.29 | 106.31 |
| 21 | Z2 | 611 | CLA | C1D-ND-C4D | -4.30 | 103.29 | 106.31 |
| 21 | 5 | 613 | CLA | C1D-ND-C4D | -4.30 | 103.30 | 106.31 |
| 21 | 92 | 609 | CLA | C1D-ND-C4D | -4.30 | 103.30 | 106.31 |
| 30 | 1 | 606 | CHL | C1B-CHB-C4A | 4.30 | 124.09 | 121.32 |
| 21 | B | 814 | CLA | C1D-ND-C4D | -4.29 | 103.30 | 106.31 |
| 21 | 9 | 603 | CLA | C1D-ND-C4D | -4.29 | 103.30 | 106.31 |
| 21 | Z | 614 | CLA | C1D-ND-C4D | -4.29 | 103.30 | 106.31 |
| 21 | 3 | 614 | CLA | C1D-ND-C4D | -4.29 | 103.30 | 106.31 |
| 21 | 82 | 611 | CLA | C1D-ND-C4D | -4.29 | 103.30 | 106.31 |
| 21 | F | 303 | CLA | C1D-ND-C4D | -4.29 | 103.31 | 106.31 |
| 21 | A | 809 | CLA | C1D-ND-C4D | -4.28 | 103.31 | 106.31 |
| 21 | B | 822 | CLA | C1D-ND-C4D | -4.28 | 103.31 | 106.31 |
| 21 | 32 | 607 | CLA | C1D-ND-C4D | -4.28 | 103.31 | 106.31 |
| 21 | 4 | 616 | CLA | C1D-ND-C4D | -4.28 | 103.31 | 106.31 |
| 21 | 6 | 609 | CLA | C1D-ND-C4D | -4.28 | 103.31 | 106.31 |
| 21 | 52 | 613 | CLA | C1D-ND-C4D | -4.28 | 103.31 | 106.31 |
| 21 | A2 | 816 | CLA | C1D-ND-C4D | -4.27 | 103.31 | 106.31 |
| 21 | 82 | 613 | CLA | C1D-ND-C4D | -4.27 | 103.31 | 106.31 |
| 21 | B2 | 822 | CLA | C1D-ND-C4D | -4.27 | 103.31 | 106.31 |
| 21 | 4 | 604 | CLA | C1D-ND-C4D | -4.27 | 103.31 | 106.31 |
| 21 | A2 | 806 | CLA | C1D-ND-C4D | -4.27 | 103.32 | 106.31 |
| 21 | 52 | 614 | CLA | C1D-ND-C4D | -4.27 | 103.32 | 106.31 |
| 30 | 6 | 618 | CHL | C1B-CHB-C4A | 4.27 | 124.07 | 121.32 |
| 21 | 7 | 603 | CLA | C1D-ND-C4D | -4.27 | 103.32 | 106.31 |
| 21 | 62 | 609 | CLA | C1D-ND-C4D | -4.27 | 103.32 | 106.31 |
| 21 | 62 | 612 | CLA | C1D-ND-C4D | -4.26 | 103.32 | 106.31 |
| 21 | B2 | 808 | CLA | C1D-ND-C4D | -4.26 | 103.32 | 106.31 |
| 21 | L | 204 | CLA | C1D-ND-C4D | -4.26 | 103.32 | 106.31 |
| 21 | A | 820 | CLA | C1D-ND-C4D | -4.26 | 103.32 | 106.31 |
| 21 | K2 | 204 | CLA | C1D-ND-C4D | -4.26 | 103.33 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 602 | CLA | C1D-ND-C4D | -4.25 | 103.33 | 106.31 |
| 21 | Z2 | 614 | CLA | C1D-ND-C4D | -4.25 | 103.33 | 106.31 |
| 21 | 4 | 612 | CLA | C1D-ND-C4D | -4.25 | 103.33 | 106.31 |
| 21 | A2 | 809 | CLA | C1D-ND-C4D | -4.24 | 103.33 | 106.31 |
| 30 | 5 | 608 | CHL | C1B-CHB-C4A | 4.24 | 124.05 | 121.32 |
| 30 | 52 | 608 | CHL | C1B-CHB-C4A | 4.24 | 124.05 | 121.32 |
| 21 | 6 | 613 | CLA | C1D-ND-C4D | -4.24 | 103.33 | 106.31 |
| 21 | 5 | 611 | CLA | C1D-ND-C4D | -4.24 | 103.34 | 106.31 |
| 21 | A2 | 839 | CLA | C1D-ND-C4D | -4.24 | 103.34 | 106.31 |
| 21 | L2 | 204 | CLA | C1D-ND-C4D | -4.24 | 103.34 | 106.31 |
| 21 | 72 | 614 | CLA | C1D-ND-C4D | -4.24 | 103.34 | 106.31 |
| 30 | 5 | 618 | CHL | C1B-CHB-C4A | 4.24 | 124.05 | 121.32 |
| 21 | 4 | 611 | CLA | C1D-ND-C4D | -4.24 | 103.34 | 106.31 |
| 21 | 42 | 611 | CLA | C1D-ND-C4D | -4.24 | 103.34 | 106.31 |
| 21 | 32 | 614 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | 42 | 616 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | 32 | 610 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | F | 304 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | Z | 612 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | 6 | 617 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | 72 | 604 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | Z2 | 612 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | B | 836 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | 6 | 610 | CLA | C1D-ND-C4D | -4.23 | 103.34 | 106.31 |
| 21 | 3 | 612 | CLA | C1D-ND-C4D | -4.23 | 103.35 | 106.31 |
| 21 | 9 | 614 | CLA | C1D-ND-C4D | -4.23 | 103.35 | 106.31 |
| 21 | 72 | 603 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 21 | 9 | 609 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 21 | A2 | 822 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 21 | F2 | 303 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 21 | B | 816 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 30 | 9 | 606 | CHL | C1B-CHB-C4A | 4.22 | 124.04 | 121.32 |
| 21 | 3 | 604 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 21 | A2 | 820 | CLA | C1D-ND-C4D | -4.22 | 103.35 | 106.31 |
| 21 | 62 | 610 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | 1 | 602 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | 32 | 602 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | A | 804 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | 52 | 611 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | 3 | 607 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | 7 | 614 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | A | 822 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 612 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 30 | 62 | 606 | CHL | C1B-CHB-C4A | 4.21 | 124.03 | 121.32 |
| 21 | A | 818 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 21 | 3 | 602 | CLA | C1D-ND-C4D | -4.21 | 103.36 | 106.31 |
| 30 | 52 | 618 | CHL | C1B-CHB-C4A | 4.21 | 124.03 | 121.32 |
| 21 | F2 | 304 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | Z2 | 604 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | 1 | 616 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | 62 | 602 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | A | 835 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | 62 | 617 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | B | 810 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | 62 | 613 | CLA | C1D-ND-C4D | -4.20 | 103.36 | 106.31 |
| 21 | A2 | 831 | CLA | C1D-ND-C4D | -4.20 | 103.37 | 106.31 |
| 21 | 62 | 611 | CLA | C1D-ND-C4D | -4.20 | 103.37 | 106.31 |
| 21 | 8 | 613 | CLA | C1D-ND-C4D | -4.20 | 103.37 | 106.31 |
| 21 | 32 | 612 | CLA | C1D-ND-C4D | -4.20 | 103.37 | 106.31 |
| 21 | B | 807 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 1 | 614 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 92 | 614 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 72 | 616 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | A | 834 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 8 | 612 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 4 | 614 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 52 | 616 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 12 | 614 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | 72 | 602 | CLA | C1D-ND-C4D | -4.19 | 103.37 | 106.31 |
| 21 | Z | 604 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 42 | 603 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 1 | 610 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | B2 | 810 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 30 | 4 | 618 | CHL | C1B-CHB-C4A | 4.18 | 124.01 | 121.32 |
| 21 | A | 831 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 1 | 609 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 82 | 603 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 5 | 612 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | B2 | 816 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | K2 | 206 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 30 | 6 | 606 | CHL | C1B-CHB-C4A | 4.18 | 124.01 | 121.32 |
| 21 | B | 813 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 9 | 601 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 3 | 610 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 12 | 601 | CHL | C1B-CHB-C4A | 4.18 | 124.01 | 121.32 |
| 21 | B | 831 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | B | 833 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | 6 | 604 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 21 | B2 | 836 | CLA | C1D-ND-C4D | -4.18 | 103.38 | 106.31 |
| 30 | 42 | 618 | CHL | C1B-CHB-C4A | 4.18 | 124.01 | 121.32 |
| 21 | 32 | 604 | CLA | C1D-ND-C4D | -4.17 | 103.38 | 106.31 |
| 21 | A | 832 | CLA | C1D-ND-C4D | -4.17 | 103.38 | 106.31 |
| 21 | B2 | 834 | CLA | C1D-ND-C4D | -4.17 | 103.38 | 106.31 |
| 21 | A | 830 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | B | 834 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | 6 | 611 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | B2 | 833 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | 42 | 612 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | B | 839 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | Z | 610 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | B2 | 831 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | A2 | 841 | CLA | C1D-ND-C4D | -4.17 | 103.39 | 106.31 |
| 21 | A | 811 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | A2 | 834 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | A | 806 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | A | 841 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | 3 | 611 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | 4 | 603 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | 92 | 601 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 30 | 1 | 601 | CHL | C1B-CHB-C4A | 4.16 | 124.00 | 121.32 |
| 21 | G2 | 204 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | 12 | 609 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | 7 | 612 | CLA | C1D-ND-C4D | -4.16 | 103.39 | 106.31 |
| 21 | A2 | 832 | CLA | C1D-ND-C4D | -4.16 | 103.40 | 106.31 |
| 21 | A | 813 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | A | 838 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | A2 | 813 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | 12 | 610 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | A2 | 804 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | B2 | 835 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | Z2 | 616 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | 32 | 611 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | 5 | 616 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | A2 | 830 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | 12 | 604 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | A | 823 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 827 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 30 | 92 | 606 | CHL | C1B-CHB-C4A | 4.15 | 123.99 | 121.32 |
| 21 | 12 | 602 | CLA | C1D-ND-C4D | -4.15 | 103.40 | 106.31 |
| 21 | B | 811 | CLA | C1D-ND-C4D | -4.14 | 103.40 | 106.31 |
| 21 | A | 839 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | B | 835 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | A2 | 818 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | 7 | 616 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | 82 | 608 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | 1 | 611 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | B | 837 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | 7 | 604 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | Z | 616 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | A2 | 824 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | A2 | 835 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | B2 | 830 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | 4 | 602 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | B2 | 805 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | 12 | 612 | CLA | C1D-ND-C4D | -4.14 | 103.41 | 106.31 |
| 21 | A | 827 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | B | 828 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | A2 | 842 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | 72 | 611 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | 1 | 612 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | B2 | 813 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | 72 | 613 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | 72 | 620 | CLA | C1D-ND-C4D | -4.13 | 103.41 | 106.31 |
| 21 | Z | 602 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | Z | 608 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | B2 | 827 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | 5 | 610 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | 82 | 612 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | 52 | 612 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | B2 | 837 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | 52 | 604 | CLA | C1D-ND-C4D | -4.13 | 103.42 | 106.31 |
| 21 | A | 812 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | Z2 | 610 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 62 | 603 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 12 | 611 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 82 | 614 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | Z2 | 602 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | A | 808 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 812 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | B2 | 812 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 9 | 613 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 92 | 602 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 4 | 610 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | A2 | 823 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | 42 | 610 | CLA | C1D-ND-C4D | -4.12 | 103.42 | 106.31 |
| 21 | G | 204 | CLA | C1D-ND-C4D | -4.11 | 103.42 | 106.31 |
| 21 | 3 | 606 | CLA | C1D-ND-C4D | -4.11 | 103.42 | 106.31 |
| 21 | B2 | 828 | CLA | C1D-ND-C4D | -4.11 | 103.42 | 106.31 |
| 21 | 12 | 608 | CLA | C1D-ND-C4D | -4.11 | 103.42 | 106.31 |
| 30 | 62 | 616 | CHL | C1B-CHB-C4A | 4.11 | 123.97 | 121.32 |
| 21 | B | 805 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | B2 | 807 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | 8 | 603 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | Z2 | 603 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | 42 | 614 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | 7 | 608 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | 7 | 611 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | 7 | 602 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | 7 | 620 | CLA | C1D-ND-C4D | -4.11 | 103.43 | 106.31 |
| 21 | L2 | 203 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | 72 | 612 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | 92 | 613 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | 1 | 604 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | A | 843 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | B2 | 819 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | B2 | 839 | CLA | C1D-ND-C4D | -4.10 | 103.43 | 106.31 |
| 21 | 7 | 613 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | Z | 603 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | K2 | 203 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | A | 833 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | 8 | 614 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | 42 | 602 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | 92 | 612 | CLA | C1D-ND-C4D | -4.10 | 103.44 | 106.31 |
| 21 | 32 | 606 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | B2 | 818 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | A | 824 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | 9 | 602 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | A2 | 843 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | 62 | 604 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | 1 | 608 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 811 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | 52 | 601 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | B | 841 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | B2 | 832 | CLA | C1D-ND-C4D | -4.09 | 103.44 | 106.31 |
| 21 | 5 | 604 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | 52 | 610 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 30 | 6 | 616 | CHL | C1B-CHB-C4A | 4.08 | 123.95 | 121.32 |
| 21 | B2 | 811 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | Z2 | 608 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | B | 827 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | 9 | 612 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | A2 | 833 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | 12 | 616 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | B | 819 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | K | 203 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | A2 | 838 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | 52 | 602 | CLA | C1D-ND-C4D | -4.08 | 103.45 | 106.31 |
| 21 | B | 832 | CLA | C1D-ND-C4D | -4.07 | 103.45 | 106.31 |
| 21 | A2 | 821 | CLA | C1D-ND-C4D | -4.07 | 103.46 | 106.31 |
| 21 | 8 | 604 | CLA | C1D-ND-C4D | -4.07 | 103.46 | 106.31 |
| 21 | 6 | 603 | CLA | C1D-ND-C4D | -4.07 | 103.46 | 106.31 |
| 21 | 3 | 613 | CLA | C1D-ND-C4D | -4.07 | 103.46 | 106.31 |
| 21 | 8 | 609 | CLA | C1D-ND-C4D | -4.07 | 103.46 | 106.31 |
| 21 | A | 842 | CLA | C1D-ND-C4D | -4.06 | 103.46 | 106.31 |
| 21 | 82 | 604 | CLA | C1D-ND-C4D | -4.06 | 103.46 | 106.31 |
| 21 | 6 | 622 | CLA | C1D-ND-C4D | -4.06 | 103.46 | 106.31 |
| 21 | 32 | 613 | CLA | C1D-ND-C4D | -4.06 | 103.46 | 106.31 |
| 21 | B | 818 | CLA | C1D-ND-C4D | -4.06 | 103.47 | 106.31 |
| 21 | B | 804 | CLA | C1D-ND-C4D | -4.06 | 103.47 | 106.31 |
| 21 | A2 | 845 | CLA | C1D-ND-C4D | -4.06 | 103.47 | 106.31 |
| 21 | 9 | 611 | CLA | C1D-ND-C4D | -4.05 | 103.47 | 106.31 |
| 21 | 82 | 602 | CLA | C1D-ND-C4D | -4.05 | 103.47 | 106.31 |
| 21 | A | 814 | CLA | C1D-ND-C4D | -4.05 | 103.47 | 106.31 |
| 21 | K | 206 | CLA | C1D-ND-C4D | -4.05 | 103.47 | 106.31 |
| 21 | A2 | 812 | CLA | C1D-ND-C4D | -4.05 | 103.47 | 106.31 |
| 30 | 6 | 608 | CHL | C1B-CHB-C4A | 4.05 | 123.92 | 121.32 |
| 21 | B2 | 804 | CLA | C1D-ND-C4D | -4.04 | 103.47 | 106.31 |
| 21 | A | 821 | CLA | C1D-ND-C4D | -4.04 | 103.47 | 106.31 |
| 21 | A | 845 | CLA | C1D-ND-C4D | -4.04 | 103.47 | 106.31 |
| 21 | B2 | 823 | CLA | C1D-ND-C4D | -4.04 | 103.47 | 106.31 |
| 21 | B2 | 841 | CLA | C1D-ND-C4D | -4.04 | 103.48 | 106.31 |
| 21 | 5 | 602 | CLA | C1D-ND-C4D | -4.04 | 103.48 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 42 | 608 | CHL | C1B-CHB-C4A | 4.04 | 123.92 | 121.32 |
| 21 | 1 | 603 | CLA | C1D-ND-C4D | -4.04 | 103.48 | 106.31 |
| 21 | J2 | 101 | CLA | C1D-ND-C4D | -4.04 | 103.48 | 106.31 |
| 30 | 4 | 608 | CHL | C1B-CHB-C4A | 4.04 | 123.92 | 121.32 |
| 21 | 3 | 609 | CLA | C1D-ND-C4D | -4.03 | 103.48 | 106.31 |
| 21 | 5 | 601 | CLA | C1D-ND-C4D | -4.03 | 103.48 | 106.31 |
| 21 | L | 203 | CLA | C1D-ND-C4D | -4.03 | 103.48 | 106.31 |
| 21 | A2 | 840 | CLA | C1D-ND-C4D | -4.03 | 103.48 | 106.31 |
| 21 | B | 825 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | 32 | 609 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | B2 | 820 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | 92 | 611 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | 72 | 608 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | 4 | 613 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | A | 840 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | A2 | 808 | CLA | C1D-ND-C4D | -4.02 | 103.49 | 106.31 |
| 21 | 82 | 609 | CLA | C1D-ND-C4D | -4.01 | 103.50 | 106.31 |
| 21 | 8 | 602 | CLA | C1D-ND-C4D | -4.01 | 103.50 | 106.31 |
| 21 | 8 | 608 | CLA | C1D-ND-C4D | -4.01 | 103.50 | 106.31 |
| 21 | 12 | 603 | CLA | C1D-ND-C4D | -4.01 | 103.50 | 106.31 |
| 21 | 8 | 610 | CLA | C1D-ND-C4D | -4.01 | 103.50 | 106.31 |
| 21 | 72 | 609 | CLA | C1D-ND-C4D | -4.01 | 103.50 | 106.31 |
| 21 | B | 823 | CLA | C1D-ND-C4D | -4.00 | 103.50 | 106.31 |
| 21 | A2 | 814 | CLA | C1D-ND-C4D | -4.00 | 103.51 | 106.31 |
| 21 | 62 | 622 | CLA | C1D-ND-C4D | -3.99 | 103.51 | 106.31 |
| 30 | 62 | 608 | CHL | C1B-CHB-C4A | 3.99 | 123.89 | 121.32 |
| 21 | A | 817 | CLA | C1D-ND-C4D | -3.99 | 103.51 | 106.31 |
| 21 | B2 | 815 | CLA | C1D-ND-C4D | -3.99 | 103.51 | 106.31 |
| 21 | B | 829 | CLA | C1D-ND-C4D | -3.99 | 103.52 | 106.31 |
| 21 | A2 | 825 | CLA | C1D-ND-C4D | -3.99 | 103.52 | 106.31 |
| 21 | A | 836 | CLA | C1D-ND-C4D | -3.98 | 103.52 | 106.31 |
| 21 | 3 | 615 | CLA | C1D-ND-C4D | -3.98 | 103.52 | 106.31 |
| 30 | 7 | 601 | CHL | C1B-CHB-C4A | 3.98 | 123.89 | 121.32 |
| 21 | F | 301 | CLA | C1D-ND-C4D | -3.98 | 103.52 | 106.31 |
| 21 | B | 815 | CLA | C1D-ND-C4D | -3.98 | 103.52 | 106.31 |
| 21 | B2 | 825 | CLA | C1D-ND-C4D | -3.98 | 103.52 | 106.31 |
| 30 | Z2 | 607 | CHL | C1B-CHB-C4A | 3.98 | 123.88 | 121.32 |
| 21 | B2 | 821 | CLA | C1D-ND-C4D | -3.97 | 103.53 | 106.31 |
| 21 | A | 825 | CLA | C1D-ND-C4D | -3.97 | 103.53 | 106.31 |
| 21 | B | 820 | CLA | C1D-ND-C4D | -3.97 | 103.53 | 106.31 |
| 21 | J | 101 | CLA | C1D-ND-C4D | -3.96 | 103.53 | 106.31 |
| 30 | 62 | 607 | CHL | C1B-CHB-C4A | 3.96 | 123.87 | 121.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B | 830 | CLA | C1D-ND-C4D | -3.96 | 103.53 | 106.31 |
| 21 | A | 815 | CLA | C1D-ND-C4D | -3.96 | 103.53 | 106.31 |
| 21 | A2 | 836 | CLA | C1D-ND-C4D | -3.96 | 103.53 | 106.31 |
| 21 | B2 | 829 | CLA | C1D-ND-C4D | -3.95 | 103.54 | 106.31 |
| 21 | B | 826 | CLA | C1D-ND-C4D | -3.95 | 103.54 | 106.31 |
| 21 | B2 | 817 | CLA | C1D-ND-C4D | -3.95 | 103.54 | 106.31 |
| 21 | A | 803 | CLA | C1D-ND-C4D | -3.95 | 103.54 | 106.31 |
| 21 | A | 819 | CLA | C1D-ND-C4D | -3.95 | 103.54 | 106.31 |
| 21 | A | 828 | CLA | C1D-ND-C4D | -3.94 | 103.55 | 106.31 |
| 21 | A2 | 805 | CLA | C1D-ND-C4D | -3.94 | 103.55 | 106.31 |
| 21 | A2 | 815 | CLA | C1D-ND-C4D | -3.94 | 103.55 | 106.31 |
| 21 | F2 | 301 | CLA | C1D-ND-C4D | -3.94 | 103.55 | 106.31 |
| 21 | 42 | 609 | CLA | C1D-ND-C4D | -3.94 | 103.55 | 106.31 |
| 21 | 32 | 617 | CLA | C1D-ND-C4D | -3.93 | 103.55 | 106.31 |
| 21 | A | 805 | CLA | C1D-ND-C4D | -3.93 | 103.55 | 106.31 |
| 30 | Z | 607 | CHL | C1B-CHB-C4A | 3.93 | 123.85 | 121.32 |
| 21 | 82 | 610 | CLA | C1D-ND-C4D | -3.93 | 103.55 | 106.31 |
| 21 | 4 | 609 | CLA | C1D-ND-C4D | -3.92 | 103.56 | 106.31 |
| 21 | B | 821 | CLA | C1D-ND-C4D | -3.92 | 103.56 | 106.31 |
| 21 | B2 | 824 | CLA | C1D-ND-C4D | -3.91 | 103.57 | 106.31 |
| 21 | 7 | 609 | CLA | C1D-ND-C4D | -3.91 | 103.57 | 106.31 |
| 32 | 62 | 625 | NEX | C5-C6-C1 | 3.91 | 123.58 | 119.70 |
| 21 | 32 | 615 | CLA | C1D-ND-C4D | -3.91 | 103.57 | 106.31 |
| 21 | A2 | 817 | CLA | C1D-ND-C4D | -3.91 | 103.57 | 106.31 |
| 21 | B2 | 809 | CLA | C1D-ND-C4D | -3.91 | 103.57 | 106.31 |
| 21 | 42 | 613 | CLA | C1D-ND-C4D | -3.90 | 103.57 | 106.31 |
| 21 | B2 | 826 | CLA | C1D-ND-C4D | -3.90 | 103.58 | 106.31 |
| 21 | B | 809 | CLA | C1D-ND-C4D | -3.90 | 103.58 | 106.31 |
| 30 | 6 | 607 | CHL | C1B-CHB-C4A | 3.89 | 123.83 | 121.32 |
| 21 | B | 817 | CLA | C1D-ND-C4D | -3.89 | 103.58 | 106.31 |
| 21 | A2 | 803 | CLA | C1D-ND-C4D | -3.89 | 103.58 | 106.31 |
| 21 | B | 824 | CLA | C1D-ND-C4D | -3.89 | 103.58 | 106.31 |
| 21 | 3 | 617 | CLA | C1D-ND-C4D | -3.89 | 103.59 | 106.31 |
| 21 | Z2 | 609 | CLA | C1D-ND-C4D | -3.87 | 103.60 | 106.31 |
| 30 | 72 | 601 | CHL | C1B-CHB-C4A | 3.87 | 123.81 | 121.32 |
| 21 | A2 | 828 | CLA | C1D-ND-C4D | -3.87 | 103.60 | 106.31 |
| 21 | A2 | 819 | CLA | C1D-ND-C4D | -3.86 | 103.60 | 106.31 |
| 21 | G2 | 203 | CLA | C1D-ND-C4D | -3.85 | 103.61 | 106.31 |
| 21 | A2 | 837 | CLA | C1D-ND-C4D | -3.85 | 103.61 | 106.31 |
| 21 | G | 203 | CLA | C1D-ND-C4D | -3.84 | 103.62 | 106.31 |
| 21 | A2 | 807 | CLA | C1D-ND-C4D | -3.83 | 103.63 | 106.31 |
| 21 | A | 826 | CLA | C1D-ND-C4D | -3.82 | 103.63 | 106.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 826 | CLA | C1D-ND-C4D | -3.82 | 103.63 | 106.31 |
| 21 | A2 | 854 | CLA | C1D-ND-C4D | -3.82 | 103.63 | 106.31 |
| 21 | A | 807 | CLA | C1D-ND-C4D | -3.81 | 103.64 | 106.31 |
| 21 | 32 | 603 | CLA | C1D-ND-C4D | -3.80 | 103.65 | 106.31 |
| 21 | Z | 609 | CLA | C1D-ND-C4D | -3.79 | 103.65 | 106.31 |
| 21 | A | 854 | CLA | C1D-ND-C4D | -3.77 | 103.67 | 106.31 |
| 21 | B2 | 802 | CLA | C1D-ND-C4D | -3.76 | 103.67 | 106.31 |
| 32 | 6 | 625 | NEX | C5-C6-C1 | 3.76 | 123.43 | 119.70 |
| 21 | 3 | 603 | CLA | C1D-ND-C4D | -3.76 | 103.67 | 106.31 |
| 30 | 42 | 607 | CHL | C1B-CHB-C4A | 3.76 | 123.74 | 121.32 |
| 21 | A | 837 | CLA | C1D-ND-C4D | -3.75 | 103.68 | 106.31 |
| 21 | B | 838 | CLA | C1D-ND-C4D | -3.74 | 103.69 | 106.31 |
| 21 | A | 802 | CLA | C1D-ND-C4D | -3.74 | 103.69 | 106.31 |
| 21 | A2 | 829 | CLA | C1D-ND-C4D | -3.73 | 103.69 | 106.31 |
| 21 | B | 802 | CLA | C1D-ND-C4D | -3.73 | 103.69 | 106.31 |
| 21 | A2 | 802 | CLA | C1D-ND-C4D | -3.70 | 103.72 | 106.31 |
| 30 | 1 | 607 | CHL | C1B-CHB-C4A | 3.69 | 123.70 | 121.32 |
| 21 | K | 201 | CLA | C1D-ND-C4D | -3.69 | 103.72 | 106.31 |
| 21 | 72 | 610 | CLA | C1D-ND-C4D | -3.68 | 103.73 | 106.31 |
| 30 | 4 | 607 | CHL | C1B-CHB-C4A | 3.68 | 123.69 | 121.32 |
| 21 | A2 | 810 | CLA | C1D-ND-C4D | -3.67 | 103.73 | 106.31 |
| 21 | B2 | 806 | CLA | C1D-ND-C4D | -3.67 | 103.74 | 106.31 |
| 21 | B2 | 838 | CLA | C1D-ND-C4D | -3.67 | 103.74 | 106.31 |
| 21 | 5 | 621 | CLA | C1D-ND-C4D | -3.66 | 103.75 | 106.31 |
| 21 | B | 806 | CLA | C1D-ND-C4D | -3.64 | 103.76 | 106.31 |
| 21 | A | 829 | CLA | C1D-ND-C4D | -3.62 | 103.77 | 106.31 |
| 21 | A | 810 | CLA | C1D-ND-C4D | -3.62 | 103.77 | 106.31 |
| 21 | 7 | 610 | CLA | C1D-ND-C4D | -3.62 | 103.77 | 106.31 |
| 21 | 52 | 621 | CLA | C1D-ND-C4D | -3.60 | 103.78 | 106.31 |
| 30 | 12 | 607 | CHL | C1B-CHB-C4A | 3.60 | 123.64 | 121.32 |
| 21 | K2 | 201 | CLA | C1D-ND-C4D | -3.58 | 103.80 | 106.31 |
| 21 | B2 | 803 | CLA | C1D-ND-C4D | -3.41 | 103.92 | 106.31 |
| 30 | 62 | 601 | CHL | C1B-CHB-C4A | 3.39 | 123.50 | 121.32 |
| 21 | B | 803 | CLA | C1D-ND-C4D | -3.37 | 103.94 | 106.31 |
| 30 | 7 | 606 | CHL | CHA-C1A-C2A | -3.32 | 125.52 | 133.31 |
| 30 | 72 | 606 | CHL | CHA-C1A-C2A | -3.28 | 125.60 | 133.31 |
| 30 | 6 | 601 | CHL | C1B-CHB-C4A | 3.26 | 123.42 | 121.32 |
| 30 | Z | 606 | CHL | CHA-C1A-C2A | -3.25 | 125.67 | 133.31 |
| 30 | Z2 | 606 | CHL | CHA-C1A-C2A | -3.24 | 125.71 | 133.31 |
| 20 | A | 801 | CL0 | CHA-C1A-C2A | -3.19 | 125.82 | 133.31 |
| 20 | A2 | 801 | CL0 | CHA-C1A-C2A | -3.18 | 125.83 | 133.31 |
| 30 | 8 | 606 | CHL | CHA-C1A-C2A | -3.18 | 125.83 | 133.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | 52 | 625 | NEX | O24-C25-C24 | -3.18 | 110.51 | 113.49 |
| 30 | 5 | 608 | CHL | CHA-C1A-C2A | -3.18 | 125.84 | 133.31 |
| 30 | 82 | 606 | CHL | CHA-C1A-C2A | -3.18 | 125.85 | 133.31 |
| 30 | 52 | 608 | CHL | CHA-C1A-C2A | -3.16 | 125.88 | 133.31 |
| 30 | 4 | 601 | CHL | CHA-C1A-C2A | -3.15 | 125.92 | 133.31 |
| 30 | 32 | 608 | CHL | CHA-C1A-C2A | -3.14 | 125.92 | 133.31 |
| 30 | 3 | 608 | CHL | CHA-C1A-C2A | -3.14 | 125.92 | 133.31 |
| 30 | 42 | 601 | CHL | CHA-C1A-C2A | -3.14 | 125.93 | 133.31 |
| 30 | 4 | 606 | CHL | CHA-C1A-C2A | -3.14 | 125.93 | 133.31 |
| 30 | 6 | 607 | CHL | CHA-C1A-C2A | -3.14 | 125.94 | 133.31 |
| 30 | 12 | 601 | CHL | CHA-C1A-C2A | -3.14 | 125.94 | 133.31 |
| 30 | 42 | 606 | CHL | CHA-C1A-C2A | -3.13 | 125.95 | 133.31 |
| 30 | 7 | 601 | CHL | CHA-C1A-C2A | -3.13 | 125.95 | 133.31 |
| 30 | 7 | 607 | CHL | CHA-C1A-C2A | -3.13 | 125.95 | 133.31 |
| 30 | 92 | 607 | CHL | C1B-CHB-C4A | 3.13 | 123.34 | 121.32 |
| 32 | 5 | 625 | NEX | O24-C25-C24 | -3.13 | 110.56 | 113.49 |
| 30 | 72 | 601 | CHL | CHA-C1A-C2A | -3.13 | 125.97 | 133.31 |
| 30 | 62 | 607 | CHL | CHA-C1A-C2A | -3.12 | 125.97 | 133.31 |
| 30 | 1 | 601 | CHL | CHA-C1A-C2A | -3.12 | 125.98 | 133.31 |
| 30 | 62 | 618 | CHL | CHA-C1A-C2A | -3.12 | 125.98 | 133.31 |
| 30 | 6 | 618 | CHL | CHA-C1A-C2A | -3.12 | 125.99 | 133.31 |
| 30 | 72 | 607 | CHL | CHA-C1A-C2A | -3.12 | 125.99 | 133.31 |
| 30 | 6 | 608 | CHL | CHA-C1A-C2A | -3.11 | 126.00 | 133.31 |
| 30 | 4 | 608 | CHL | CHA-C1A-C2A | -3.10 | 126.03 | 133.31 |
| 30 | 42 | 608 | CHL | CHA-C1A-C2A | -3.09 | 126.05 | 133.31 |
| 30 | 62 | 608 | CHL | CHA-C1A-C2A | -3.08 | 126.07 | 133.31 |
| 30 | Z2 | 607 | CHL | CHA-C1A-C2A | -3.07 | 126.09 | 133.31 |
| 30 | Z | 607 | CHL | CHA-C1A-C2A | -3.06 | 126.12 | 133.31 |
| 30 | 62 | 606 | CHL | CHA-C1A-C2A | -3.06 | 126.13 | 133.31 |
| 30 | 52 | 607 | CHL | C1B-CHB-C4A | 3.05 | 123.29 | 121.32 |
| 30 | 1 | 606 | CHL | CHA-C1A-C2A | -3.05 | 126.14 | 133.31 |
| 30 | 12 | 606 | CHL | CHA-C1A-C2A | -3.05 | 126.14 | 133.31 |
| 30 | 6 | 606 | CHL | CHA-C1A-C2A | -3.05 | 126.15 | 133.31 |
| 30 | 5 | 606 | CHL | CHA-C1A-C2A | -3.03 | 126.19 | 133.31 |
| 30 | 62 | 616 | CHL | CHA-C1A-C2A | -3.03 | 126.20 | 133.31 |
| 30 | 6 | 616 | CHL | CHA-C1A-C2A | -3.02 | 126.22 | 133.31 |
| 30 | 9 | 607 | CHL | CHA-C1A-C2A | -3.02 | 126.23 | 133.31 |
| 30 | 52 | 606 | CHL | CHA-C1A-C2A | -2.99 | 126.29 | 133.31 |
| 30 | 5 | 607 | CHL | C1B-CHB-C4A | 2.98 | 123.24 | 121.32 |
| 30 | 5 | 618 | CHL | CHA-C1A-C2A | -2.98 | 126.31 | 133.31 |
| 30 | 52 | 618 | CHL | CHA-C1A-C2A | -2.98 | 126.31 | 133.31 |
| 30 | 4 | 607 | CHL | CHA-C1A-C2A | -2.96 | 126.35 | 133.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 42 | 607 | CHL | CHA-C1A-C2A | -2.96 | 126.35 | 133.31 |
| 30 | 92 | 607 | CHL | CHA-C1A-C2A | -2.96 | 126.35 | 133.31 |
| 30 | 42 | 618 | CHL | CHA-C1A-C2A | -2.95 | 126.39 | 133.31 |
| 30 | 4 | 618 | CHL | CHA-C1A-C2A | -2.93 | 126.42 | 133.31 |
| 30 | Z2 | 601 | CHL | CHA-C1A-C2A | -2.93 | 126.43 | 133.31 |
| 30 | Z | 601 | CHL | CHA-C1A-C2A | -2.93 | 126.43 | 133.31 |
| 30 | 82 | 601 | CHL | CHA-C1A-C2A | -2.89 | 126.53 | 133.31 |
| 32 | 62 | 625 | NEX | O24-C25-C24 | -2.88 | 110.79 | 113.49 |
| 30 | 8 | 601 | CHL | CHA-C1A-C2A | -2.88 | 126.54 | 133.31 |
| 32 | 6 | 625 | NEX | O24-C25-C24 | -2.86 | 110.81 | 113.49 |
| 30 | 8 | 607 | CHL | C3D-C4D-CHA | 2.80 | 112.79 | 108.54 |
| 30 | 82 | 607 | CHL | C3D-C4D-CHA | 2.78 | 112.76 | 108.54 |
| 30 | Z | 601 | CHL | C3D-C4D-CHA | 2.75 | 112.72 | 108.54 |
| 30 | 6 | 601 | CHL | C3D-C4D-CHA | 2.75 | 112.71 | 108.54 |
| 30 | 62 | 601 | CHL | C3D-C4D-CHA | 2.74 | 112.70 | 108.54 |
| 30 | 62 | 606 | CHL | C3D-C4D-CHA | 2.73 | 112.69 | 108.54 |
| 30 | Z2 | 601 | CHL | C3D-C4D-CHA | 2.73 | 112.69 | 108.54 |
| 30 | 12 | 607 | CHL | C3D-C4D-CHA | 2.73 | 112.69 | 108.54 |
| 21 | 72 | 610 | CLA | CHD-C1D-ND | -2.73 | 120.97 | 124.80 |
| 21 | 7 | 610 | CLA | CHD-C1D-ND | -2.72 | 120.97 | 124.80 |
| 30 | 6 | 606 | CHL | C3D-C4D-CHA | 2.72 | 112.67 | 108.54 |
| 30 | 1 | 607 | CHL | C3D-C4D-CHA | 2.71 | 112.66 | 108.54 |
| 30 | 72 | 601 | CHL | C3D-C4D-CHA | 2.71 | 112.66 | 108.54 |
| 30 | 7 | 601 | CHL | C3D-C4D-CHA | 2.71 | 112.65 | 108.54 |
| 30 | 82 | 607 | CHL | CHA-C1A-C2A | -2.70 | 126.98 | 133.31 |
| 30 | 42 | 618 | CHL | C3D-C4D-CHA | 2.69 | 112.63 | 108.54 |
| 30 | 4 | 618 | CHL | C3D-C4D-CHA | 2.69 | 112.63 | 108.54 |
| 30 | 6 | 607 | CHL | C3D-C4D-CHA | 2.67 | 112.61 | 108.54 |
| 30 | 62 | 607 | CHL | C3D-C4D-CHA | 2.67 | 112.61 | 108.54 |
| 30 | 6 | 618 | CHL | C3D-C4D-CHA | 2.67 | 112.60 | 108.54 |
| 30 | 1 | 606 | CHL | C3D-C4D-CHA | 2.67 | 112.60 | 108.54 |
| 21 | B | 833 | CLA | CHD-C1D-ND | -2.67 | 121.05 | 124.80 |
| 21 | B2 | 833 | CLA | CHD-C1D-ND | -2.67 | 121.05 | 124.80 |
| 30 | 8 | 607 | CHL | CHA-C1A-C2A | -2.67 | 127.04 | 133.31 |
| 30 | 7 | 607 | CHL | C3D-C4D-CHA | 2.67 | 112.59 | 108.54 |
| 30 | Z2 | 606 | CHL | C3D-C4D-CHA | 2.66 | 112.59 | 108.54 |
| 30 | 92 | 606 | CHL | C3D-C4D-CHA | 2.66 | 112.59 | 108.54 |
| 30 | 52 | 606 | CHL | C3D-C4D-CHA | 2.66 | 112.59 | 108.54 |
| 30 | 8 | 601 | CHL | C3D-C4D-CHA | 2.66 | 112.58 | 108.54 |
| 30 | 62 | 618 | CHL | C3D-C4D-CHA | 2.66 | 112.58 | 108.54 |
| 30 | Z | 607 | CHL | C3D-C4D-CHA | 2.65 | 112.57 | 108.54 |
| 30 | 5 | 606 | CHL | C3D-C4D-CHA | 2.65 | 112.57 | 108.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 9 | 606 | CHL | C3D-C4D-CHA | 2.65 | 112.56 | 108.54 |
| 30 | 5 | 618 | CHL | C3D-C4D-CHA | 2.65 | 112.56 | 108.54 |
| 30 | Z2 | 607 | CHL | C3D-C4D-CHA | 2.65 | 112.56 | 108.54 |
| 30 | 72 | 607 | CHL | C3D-C4D-CHA | 2.65 | 112.56 | 108.54 |
| 30 | 82 | 601 | CHL | C3D-C4D-CHA | 2.64 | 112.56 | 108.54 |
| 30 | 4 | 606 | CHL | C3D-C4D-CHA | 2.64 | 112.55 | 108.54 |
| 30 | Z | 606 | CHL | C3D-C4D-CHA | 2.64 | 112.55 | 108.54 |
| 30 | 9 | 607 | CHL | C3D-C4D-CHA | 2.64 | 112.55 | 108.54 |
| 30 | 52 | 618 | CHL | C3D-C4D-CHA | 2.63 | 112.54 | 108.54 |
| 30 | 12 | 606 | CHL | C3D-C4D-CHA | 2.63 | 112.54 | 108.54 |
| 30 | 42 | 606 | CHL | C3D-C4D-CHA | 2.63 | 112.53 | 108.54 |
| 30 | 4 | 608 | CHL | C3D-C4D-CHA | 2.63 | 112.53 | 108.54 |
| 30 | 52 | 608 | CHL | C3D-C4D-CHA | 2.62 | 112.52 | 108.54 |
| 21 | A2 | 823 | CLA | CHD-C1D-ND | -2.61 | 121.12 | 124.80 |
| 30 | 42 | 608 | CHL | C3D-C4D-CHA | 2.61 | 112.50 | 108.54 |
| 30 | 8 | 606 | CHL | C3D-C4D-CHA | 2.60 | 112.50 | 108.54 |
| 30 | 1 | 601 | CHL | C3D-C4D-CHA | 2.60 | 112.50 | 108.54 |
| 30 | 12 | 601 | CHL | C3D-C4D-CHA | 2.60 | 112.50 | 108.54 |
| 21 | A2 | 806 | CLA | CHD-C1D-ND | -2.60 | 121.14 | 124.80 |
| 30 | 42 | 601 | CHL | C3D-C4D-CHA | 2.60 | 112.49 | 108.54 |
| 30 | 4 | 607 | CHL | C3D-C4D-CHA | 2.60 | 112.49 | 108.54 |
| 30 | 5 | 607 | CHL | C3D-C4D-CHA | 2.60 | 112.49 | 108.54 |
| 21 | A | 823 | CLA | CHD-C1D-ND | -2.60 | 121.15 | 124.80 |
| 30 | 42 | 607 | CHL | C3D-C4D-CHA | 2.60 | 112.49 | 108.54 |
| 21 | 1 | 604 | CLA | CHD-C1D-ND | -2.60 | 121.15 | 124.80 |
| 21 | 92 | 610 | CLA | CHD-C1D-ND | -2.59 | 121.16 | 124.80 |
| 30 | 4 | 601 | CHL | C3D-C4D-CHA | 2.59 | 112.47 | 108.54 |
| 30 | 5 | 608 | CHL | C3D-C4D-CHA | 2.58 | 112.47 | 108.54 |
| 21 | 12 | 604 | CLA | CHD-C1D-ND | -2.58 | 121.17 | 124.80 |
| 21 | A2 | 809 | CLA | CHD-C1D-ND | -2.58 | 121.17 | 124.80 |
| 30 | 62 | 616 | CHL | C3D-C4D-CHA | 2.58 | 112.46 | 108.54 |
| 21 | A | 809 | CLA | CHD-C1D-ND | -2.58 | 121.18 | 124.80 |
| 30 | 52 | 607 | CHL | C3D-C4D-CHA | 2.57 | 112.45 | 108.54 |
| 21 | 5 | 616 | CLA | CHD-C1D-ND | -2.57 | 121.19 | 124.80 |
| 30 | 72 | 606 | CHL | C3D-C4D-CHA | 2.57 | 112.44 | 108.54 |
| 21 | B2 | 834 | CLA | CHD-C1D-ND | -2.56 | 121.19 | 124.80 |
| 30 | 82 | 606 | CHL | C3D-C4D-CHA | 2.56 | 112.43 | 108.54 |
| 21 | A | 806 | CLA | CHD-C1D-ND | -2.56 | 121.20 | 124.80 |
| 30 | 92 | 607 | CHL | C3D-C4D-CHA | 2.56 | 112.42 | 108.54 |
| 21 | B2 | 830 | CLA | CHD-C1D-ND | -2.56 | 121.20 | 124.80 |
| 21 | 52 | 616 | CLA | CHD-C1D-ND | -2.56 | 121.21 | 124.80 |
| 21 | B | 803 | CLA | CHD-C1D-ND | -2.55 | 121.21 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 9 | 610 | CLA | CHD-C1D-ND | -2.55 | 121.21 | 124.80 |
| 30 | 62 | 608 | CHL | C3D-C4D-CHA | 2.55 | 112.42 | 108.54 |
| 30 | 6 | 616 | CHL | C3D-C4D-CHA | 2.55 | 112.42 | 108.54 |
| 21 | 62 | 614 | CLA | CHD-C1D-ND | -2.55 | 121.22 | 124.80 |
| 21 | B2 | 803 | CLA | CHD-C1D-ND | -2.55 | 121.22 | 124.80 |
| 21 | 12 | 608 | CLA | CHD-C1D-ND | -2.54 | 121.22 | 124.80 |
| 21 | 82 | 616 | CLA | CHD-C1D-ND | -2.54 | 121.22 | 124.80 |
| 21 | 42 | 610 | CLA | CHD-C1D-ND | -2.54 | 121.23 | 124.80 |
| 30 | 52 | 607 | CHL | CHA-C1A-C2A | -2.54 | 127.35 | 133.31 |
| 21 | 6 | 614 | CLA | CHD-C1D-ND | -2.54 | 121.23 | 124.80 |
| 30 | 6 | 608 | CHL | C3D-C4D-CHA | 2.54 | 112.39 | 108.54 |
| 21 | 1 | 610 | CLA | CHD-C1D-ND | -2.53 | 121.23 | 124.80 |
| 30 | 5 | 607 | CHL | CHA-C1A-C2A | -2.53 | 127.36 | 133.31 |
| 30 | 7 | 606 | CHL | C3D-C4D-CHA | 2.53 | 112.39 | 108.54 |
| 21 | 5 | 610 | CLA | CHD-C1D-ND | -2.53 | 121.24 | 124.80 |
| 21 | 6 | 610 | CLA | CHD-C1D-ND | -2.53 | 121.24 | 124.80 |
| 21 | B | 829 | CLA | CHD-C1D-ND | -2.53 | 121.25 | 124.80 |
| 21 | B2 | 829 | CLA | CHD-C1D-ND | -2.52 | 121.25 | 124.80 |
| 21 | 8 | 616 | CLA | CHD-C1D-ND | -2.52 | 121.25 | 124.80 |
| 21 | 4 | 610 | CLA | CHD-C1D-ND | -2.52 | 121.26 | 124.80 |
| 21 | B | 841 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 30 | 3 | 608 | CHL | C3D-C4D-CHA | 2.51 | 112.36 | 108.54 |
| 21 | 9 | 604 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | A | 812 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | A2 | 812 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | B | 834 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | L2 | 203 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | 12 | 610 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | 62 | 610 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | 5 | 613 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | A2 | 841 | CLA | CHD-C1D-ND | -2.51 | 121.27 | 124.80 |
| 21 | A | 827 | CLA | CHD-C1D-ND | -2.51 | 121.28 | 124.80 |
| 21 | B | 830 | CLA | CHD-C1D-ND | -2.50 | 121.28 | 124.80 |
| 21 | A | 836 | CLA | CHD-C1D-ND | -2.50 | 121.28 | 124.80 |
| 21 | 42 | 604 | CLA | CHD-C1D-ND | -2.50 | 121.28 | 124.80 |
| 30 | 32 | 608 | CHL | C3D-C4D-CHA | 2.50 | 112.34 | 108.54 |
| 21 | 52 | 610 | CLA | CHD-C1D-ND | -2.50 | 121.28 | 124.80 |
| 21 | A | 841 | CLA | CHD-C1D-ND | -2.50 | 121.29 | 124.80 |
| 21 | 92 | 609 | CLA | CHD-C1D-ND | -2.50 | 121.29 | 124.80 |
| 21 | 9 | 611 | CLA | CHD-C1D-ND | -2.50 | 121.29 | 124.80 |
| 21 | A | 811 | CLA | CHD-C1D-ND | -2.49 | 121.29 | 124.80 |
| 21 | Z | 604 | CLA | CHD-C1D-ND | -2.49 | 121.29 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 62 | 609 | CLA | CHD-C1D-ND | -2.49 | 121.29 | 124.80 |
| 21 | 92 | 604 | CLA | CHD-C1D-ND | -2.49 | 121.29 | 124.80 |
| 21 | Z | 613 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B2 | 805 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | A | 804 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B2 | 841 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B | 805 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | 5 | 603 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | Z2 | 614 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B | 822 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | A2 | 836 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B2 | 822 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | 3 | 614 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | Z2 | 604 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | L | 203 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B2 | 823 | CLA | CHD-C1D-ND | -2.49 | 121.30 | 124.80 |
| 21 | B2 | 840 | CLA | CHD-C1D-ND | -2.49 | 121.31 | 124.80 |
| 21 | 7 | 603 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | 52 | 613 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | B | 840 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | A2 | 827 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | 6 | 617 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | Z | 610 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | A2 | 820 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | 1 | 608 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | A2 | 837 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | B2 | 814 | CLA | CHD-C1D-ND | -2.48 | 121.31 | 124.80 |
| 21 | 6 | 609 | CLA | CHD-C1D-ND | -2.48 | 121.32 | 124.80 |
| 21 | A | 809 | CLA | C1-C2-C3 | -2.48 | 122.14 | 126.20 |
| 21 | B2 | 828 | CLA | CHD-C1D-ND | -2.48 | 121.32 | 124.80 |
| 21 | 72 | 616 | CLA | CHD-C1D-ND | -2.48 | 121.32 | 124.80 |
| 21 | 92 | 611 | CLA | CHD-C1D-ND | -2.47 | 121.32 | 124.80 |
| 21 | B2 | 837 | CLA | CHD-C1D-ND | -2.47 | 121.32 | 124.80 |
| 21 | B | 839 | CLA | CHD-C1D-ND | -2.47 | 121.32 | 124.80 |
| 21 | B | 828 | CLA | CHD-C1D-ND | -2.47 | 121.32 | 124.80 |
| 21 | 52 | 621 | CLA | C2A-C1A-CHA | 2.47 | 128.16 | 123.87 |
| 21 | A2 | 831 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | 72 | 603 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 26 | B2 | 853 | LMU | C1B-O5B-C5B | 2.47 | 118.54 | 113.72 |
| 21 | A2 | 809 | CLA | C1-C2-C3 | -2.47 | 122.15 | 126.20 |
| 21 | 9 | 613 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | 62 | 617 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | Z | 614 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | B2 | 819 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | B | 831 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | 32 | 602 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | 8 | 604 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | 9 | 609 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | Z2 | 610 | CLA | CHD-C1D-ND | -2.47 | 121.33 | 124.80 |
| 21 | A | 802 | CLA | CHD-C1D-ND | -2.46 | 121.33 | 124.80 |
| 21 | 9 | 614 | CLA | CHD-C1D-ND | -2.46 | 121.33 | 124.80 |
| 21 | 32 | 614 | CLA | CHD-C1D-ND | -2.46 | 121.33 | 124.80 |
| 21 | A | 831 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | A2 | 811 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | 6 | 602 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | 52 | 603 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | L | 204 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | 4 | 604 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | Z2 | 608 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | A | 830 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | B | 807 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | Z | 608 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | 5 | 617 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | 5 | 621 | CLA | C2A-C1A-CHA | 2.46 | 128.13 | 123.87 |
| 21 | A | 803 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | 7 | 616 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | B | 812 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | B | 819 | CLA | CHD-C1D-ND | -2.46 | 121.34 | 124.80 |
| 21 | Z | 602 | CLA | CHD-C1D-ND | -2.46 | 121.35 | 124.80 |
| 21 | 4 | 616 | CLA | CHD-C1D-ND | -2.46 | 121.35 | 124.80 |
| 21 | A2 | 832 | CLA | CHD-C1D-ND | -2.46 | 121.35 | 124.80 |
| 21 | 82 | 602 | CLA | CHD-C1D-ND | -2.46 | 121.35 | 124.80 |
| 21 | 52 | 617 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | A | 820 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | 4 | 613 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | B2 | 807 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | 1 | 603 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | 8 | 602 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | 72 | 611 | CLA | CHD-C1D-ND | -2.45 | 121.35 | 124.80 |
| 21 | B2 | 821 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | L2 | 204 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | Z2 | 613 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | 42 | 616 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | A | 837 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | B2 | 831 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | 92 | 613 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | A2 | 803 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 21 | A | 833 | CLA | CHD-C1D-ND | -2.45 | 121.36 | 124.80 |
| 26 | B | 853 | LMU | C1B-O5B-C5B | 2.44 | 118.49 | 113.72 |
| 21 | 7 | 608 | CLA | CHD-C1D-ND | -2.44 | 121.36 | 124.80 |
| 21 | 92 | 614 | CLA | CHD-C1D-ND | -2.44 | 121.36 | 124.80 |
| 21 | B | 823 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | A2 | 816 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | B2 | 832 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | A2 | 830 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 3 | 610 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 1 | 609 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | A2 | 833 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 82 | 604 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | A2 | 804 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 12 | 609 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 82 | 614 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 6 | 613 | CLA | CHD-C1D-ND | -2.44 | 121.37 | 124.80 |
| 21 | 42 | 614 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | 7 | 611 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | 4 | 614 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | 6 | 622 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | B | 814 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | B | 837 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | 32 | 604 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | B2 | 839 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | A2 | 802 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | 8 | 614 | CLA | CHD-C1D-ND | -2.43 | 121.38 | 124.80 |
| 21 | 82 | 613 | CLA | CHD-C1D-ND | -2.43 | 121.39 | 124.80 |
| 21 | 5 | 609 | CLA | CHD-C1D-ND | -2.43 | 121.39 | 124.80 |
| 21 | 3 | 604 | CLA | CHD-C1D-ND | -2.43 | 121.39 | 124.80 |
| 21 | A2 | 835 | CLA | CHD-C1D-ND | -2.43 | 121.39 | 124.80 |
| 21 | A | 816 | CLA | CHD-C1D-ND | -2.43 | 121.39 | 124.80 |
| 21 | 62 | 622 | CLA | CHD-C1D-ND | -2.43 | 121.39 | 124.80 |
| 21 | 3 | 602 | CLA | CHD-C1D-ND | -2.42 | 121.39 | 124.80 |
| 21 | Z2 | 602 | CLA | CHD-C1D-ND | -2.42 | 121.39 | 124.80 |
| 21 | B | 821 | CLA | CHD-C1D-ND | -2.42 | 121.39 | 124.80 |
| 21 | 52 | 614 | CLA | CHD-C1D-ND | -2.42 | 121.39 | 124.80 |
| 21 | Z | 603 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | B | 835 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 52 | 604 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 835 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 20 | A2 | 801 | CL0 | C3D-C4D-CHA | 2.42 | 112.22 | 108.54 |
| 21 | A | 821 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | B | 810 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 8 | 613 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 5 | 614 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 42 | 611 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 52 | 609 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 5 | 604 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | Z2 | 603 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 1 | 613 | CLA | CHD-C1D-ND | -2.42 | 121.40 | 124.80 |
| 21 | 72 | 608 | CLA | CHD-C1D-ND | -2.41 | 121.40 | 124.80 |
| 21 | 42 | 609 | CLA | CHD-C1D-ND | -2.41 | 121.41 | 124.80 |
| 21 | A | 832 | CLA | CHD-C1D-ND | -2.41 | 121.41 | 124.80 |
| 21 | 32 | 610 | CLA | CHD-C1D-ND | -2.41 | 121.41 | 124.80 |
| 30 | 9 | 607 | CHL | C1B-CHB-C4A | 2.41 | 122.87 | 121.32 |
| 21 | A | 840 | CLA | CHD-C1D-ND | -2.41 | 121.41 | 124.80 |
| 21 | 12 | 613 | CLA | CHD-C1D-ND | -2.41 | 121.41 | 124.80 |
| 21 | B2 | 812 | CLA | CHD-C1D-ND | -2.41 | 121.41 | 124.80 |
| 21 | K | 204 | CLA | CHD-C1D-ND | -2.41 | 121.42 | 124.80 |
| 21 | A2 | 821 | CLA | CHD-C1D-ND | -2.41 | 121.42 | 124.80 |
| 21 | A2 | 840 | CLA | CHD-C1D-ND | -2.41 | 121.42 | 124.80 |
| 21 | B | 804 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 21 | 72 | 609 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 20 | A | 801 | CL0 | C3D-C4D-CHA | 2.40 | 112.19 | 108.54 |
| 21 | 42 | 613 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 21 | 62 | 602 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 21 | 8 | 610 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 21 | 32 | 611 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 21 | B | 832 | CLA | CHD-C1D-ND | -2.40 | 121.42 | 124.80 |
| 30 | 6 | 616 | CHL | C1-C2-C3 | -2.40 | 122.27 | 126.20 |
| 21 | B | 838 | CLA | CHD-C1D-ND | -2.40 | 121.43 | 124.80 |
| 21 | B2 | 838 | CLA | CHD-C1D-ND | -2.40 | 121.43 | 124.80 |
| 21 | 82 | 603 | CLA | CHD-C1D-ND | -2.40 | 121.43 | 124.80 |
| 21 | 3 | 611 | CLA | CHD-C1D-ND | -2.40 | 121.43 | 124.80 |
| 21 | 82 | 609 | CLA | CHD-C1D-ND | -2.40 | 121.43 | 124.80 |
| 21 | 4 | 611 | CLA | CHD-C1D-ND | -2.40 | 121.43 | 124.80 |
| 21 | 12 | 603 | CLA | CHD-C1D-ND | -2.39 | 121.43 | 124.80 |
| 32 | 5 | 625 | NEX | C2-C1-C6 | -2.39 | 106.89 | 109.21 |
| 21 | A | 843 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | B | 818 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 30 | 12 | 607 | CHL | CHA-C1A-C2A | -2.39 | 127.69 | 133.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A2 | 824 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | 8 | 611 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 30 | 1 | 607 | CHL | CHA-C1A-C2A | -2.39 | 127.70 | 133.31 |
| 21 | A | 822 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | A | 824 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | 3 | 609 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | B2 | 810 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | 8 | 603 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | 62 | 613 | CLA | CHD-C1D-ND | -2.39 | 121.44 | 124.80 |
| 21 | 6 | 611 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | B2 | 835 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | B | 825 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | 12 | 614 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | 8 | 609 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | B | 816 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | 82 | 611 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 31 | 12 | 618 | XAT | C7-C8-C9 | 2.38 | 129.22 | 125.53 |
| 21 | K2 | 204 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | A2 | 825 | CLA | CHD-C1D-ND | -2.38 | 121.45 | 124.80 |
| 21 | A2 | 842 | CLA | CHD-C1D-ND | -2.38 | 121.46 | 124.80 |
| 21 | 3 | 612 | CLA | CHD-C1D-ND | -2.38 | 121.46 | 124.80 |
| 21 | B2 | 818 | CLA | CHD-C1D-ND | -2.38 | 121.46 | 124.80 |
| 21 | 4 | 609 | CLA | CHD-C1D-ND | -2.37 | 121.46 | 124.80 |
| 21 | 5 | 621 | CLA | CAA-C2A-C1A | 2.37 | 119.75 | 111.97 |
| 21 | F | 303 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | A2 | 839 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 92 | 603 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 4 | 602 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 32 | 607 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 28 | F | 305 | LUT | C8-C7-C6 | 2.37 | 133.32 | 127.00 |
| 21 | K | 203 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 7 | 609 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 32 | 609 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | B | 811 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 3 | 607 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 52 | 621 | CLA | CAA-C2A-C1A | 2.37 | 119.73 | 111.97 |
| 21 | B | 836 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 30 | 62 | 616 | CHL | C1-C2-C3 | -2.37 | 122.32 | 126.20 |
| 21 | B2 | 811 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | Z2 | 616 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | 1 | 602 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |
| 21 | F2 | 303 | CLA | CHD-C1D-ND | -2.37 | 121.47 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 615 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | A2 | 843 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | B2 | 804 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 1 | 614 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 92 | 601 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 42 | 602 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | A | 818 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 3 | 606 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | K2 | 206 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | B2 | 816 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | B2 | 825 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | B | 815 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | B2 | 815 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 72 | 602 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | A2 | 807 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | A2 | 822 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 82 | 610 | CLA | CHD-C1D-ND | -2.36 | 121.48 | 124.80 |
| 21 | 6 | 604 | CLA | CHD-C1D-ND | -2.36 | 121.49 | 124.80 |
| 21 | 32 | 612 | CLA | CHD-C1D-ND | -2.36 | 121.49 | 124.80 |
| 21 | B | 826 | CLA | CHD-C1D-ND | -2.35 | 121.49 | 124.80 |
| 21 | A | 808 | CLA | CHD-C1D-ND | -2.35 | 121.49 | 124.80 |
| 21 | 12 | 602 | CLA | CHD-C1D-ND | -2.35 | 121.49 | 124.80 |
| 21 | Z | 609 | CLA | CHD-C1D-ND | -2.35 | 121.49 | 124.80 |
| 21 | 92 | 602 | CLA | CHD-C1D-ND | -2.35 | 121.49 | 124.80 |
| 21 | A | 815 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | 7 | 614 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | Z2 | 611 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | K2 | 203 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | 52 | 611 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | 62 | 603 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | 72 | 614 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | B2 | 826 | CLA | CHD-C1D-ND | -2.35 | 121.50 | 124.80 |
| 21 | A | 825 | CLA | CHD-C1D-ND | -2.34 | 121.50 | 124.80 |
| 21 | 9 | 601 | CLA | CHD-C1D-ND | -2.34 | 121.50 | 124.80 |
| 21 | 8 | 612 | CLA | CHD-C1D-ND | -2.34 | 121.50 | 124.80 |
| 21 | G2 | 203 | CLA | CHD-C1D-ND | -2.34 | 121.50 | 124.80 |
| 21 | 7 | 602 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 21 | B2 | 827 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 21 | Z | 616 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 21 | A | 834 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 21 | B | 827 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 21 | A2 | 834 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 5 | 611 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 21 | 62 | 611 | CLA | CHD-C1D-ND | -2.34 | 121.51 | 124.80 |
| 28 | F2 | 305 | LUT | C8-C7-C6 | 2.34 | 133.25 | 127.00 |
| 21 | A2 | 838 | CLA | CHD-C1D-ND | -2.34 | 121.52 | 124.80 |
| 21 | A2 | 815 | CLA | CHD-C1D-ND | -2.34 | 121.52 | 124.80 |
| 21 | 6 | 603 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | 9 | 602 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | Z | 612 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | B2 | 836 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | 32 | 606 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | A | 839 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | G | 203 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | Z | 611 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | A2 | 808 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | B2 | 802 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | Z2 | 609 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | A2 | 818 | CLA | CHD-C1D-ND | -2.33 | 121.52 | 124.80 |
| 21 | 92 | 612 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | A | 845 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | 32 | 615 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | 7 | 620 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | 82 | 612 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 30 | 4 | 606 | CHL | C1-C2-C3 | -2.33 | 122.39 | 126.20 |
| 21 | A | 807 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | 7 | 604 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | 82 | 608 | CLA | CHD-C1D-ND | -2.33 | 121.53 | 124.80 |
| 21 | A | 805 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 21 | A | 817 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 21 | 1 | 611 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 21 | 92 | 610 | CLA | C3D-C4D-ND | 2.32 | 113.77 | 109.99 |
| 21 | 12 | 611 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 21 | A2 | 805 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 21 | 1 | 612 | CLA | CHD-C1D-ND | -2.32 | 121.53 | 124.80 |
| 21 | F | 301 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 21 | B | 809 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 30 | 42 | 606 | CHL | C1-C2-C3 | -2.32 | 122.40 | 126.20 |
| 21 | 4 | 612 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 21 | 5 | 612 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 21 | 72 | 604 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 21 | 62 | 604 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 21 | 9 | 603 | CLA | CHD-C1D-ND | -2.32 | 121.54 | 124.80 |
| 21 | B | 802 | CLA | CHD-C1D-ND | -2.31 | 121.55 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 3 | 613 | CLA | CHD-C1D-ND | -2.31 | 121.55 | 124.80 |
| 21 | B | 808 | CLA | CHD-C1D-ND | -2.31 | 121.55 | 124.80 |
| 21 | A | 842 | CLA | CHD-C1D-ND | -2.31 | 121.55 | 124.80 |
| 21 | 9 | 610 | CLA | C3D-C4D-ND | 2.31 | 113.74 | 109.99 |
| 21 | B | 817 | CLA | CHD-C1D-ND | -2.31 | 121.56 | 124.80 |
| 21 | B2 | 809 | CLA | CHD-C1D-ND | -2.31 | 121.56 | 124.80 |
| 21 | 1 | 616 | CLA | CHD-C1D-ND | -2.31 | 121.56 | 124.80 |
| 21 | 72 | 620 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 21 | Z2 | 612 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 31 | 1 | 618 | XAT | C7-C8-C9 | 2.30 | 129.10 | 125.53 |
| 21 | 8 | 608 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 21 | 42 | 603 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 21 | A | 838 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 21 | 7 | 613 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 21 | 52 | 602 | CLA | CHD-C1D-ND | -2.30 | 121.56 | 124.80 |
| 21 | K | 206 | CLA | CHD-C1D-ND | -2.30 | 121.57 | 124.80 |
| 21 | 72 | 613 | CLA | CHD-C1D-ND | -2.30 | 121.57 | 124.80 |
| 21 | B2 | 817 | CLA | CHD-C1D-ND | -2.30 | 121.57 | 124.80 |
| 30 | 6 | 607 | CHL | C1-C2-C3 | -2.30 | 122.44 | 126.20 |
| 21 | 42 | 612 | CLA | CHD-C1D-ND | -2.29 | 121.57 | 124.80 |
| 21 | 9 | 612 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | A2 | 845 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | 32 | 613 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | A2 | 854 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 30 | 42 | 601 | CHL | C1A-CHA-C4D | 2.29 | 122.80 | 118.98 |
| 21 | A2 | 826 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | A | 828 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | B2 | 820 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | F2 | 301 | CLA | CHD-C1D-ND | -2.29 | 121.58 | 124.80 |
| 21 | A | 813 | CLA | CHD-C1D-ND | -2.28 | 121.59 | 124.80 |
| 21 | A2 | 813 | CLA | CHD-C1D-ND | -2.28 | 121.59 | 124.80 |
| 21 | 52 | 612 | CLA | CHD-C1D-ND | -2.28 | 121.59 | 124.80 |
| 21 | G2 | 204 | CLA | CHD-C1D-ND | -2.28 | 121.59 | 124.80 |
| 32 | 52 | 625 | NEX | C2-C1-C6 | -2.28 | 106.99 | 109.21 |
| 21 | 5 | 602 | CLA | CHD-C1D-ND | -2.28 | 121.59 | 124.80 |
| 21 | A2 | 828 | CLA | CHD-C1D-ND | -2.28 | 121.59 | 124.80 |
| 21 | 12 | 612 | CLA | CHD-C1D-ND | -2.28 | 121.60 | 124.80 |
| 32 | 52 | 625 | NEX | O24-C26-C27 | -2.28 | 110.35 | 116.88 |
| 21 | G | 204 | CLA | CHD-C1D-ND | -2.28 | 121.60 | 124.80 |
| 32 | 5 | 625 | NEX | O24-C26-C27 | -2.28 | 110.36 | 116.88 |
| 21 | A2 | 817 | CLA | CHD-C1D-ND | -2.28 | 121.60 | 124.80 |
| 21 | 7 | 612 | CLA | CHD-C1D-ND | -2.27 | 121.60 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 4 | 601 | CHL | C1A-CHA-C4D | 2.27 | 122.78 | 118.98 |
| 21 | J2 | 101 | CLA | CHD-C1D-ND | -2.27 | 121.60 | 124.80 |
| 21 | 32 | 617 | CLA | CHD-C1D-ND | -2.27 | 121.60 | 124.80 |
| 21 | A | 826 | CLA | CHD-C1D-ND | -2.27 | 121.61 | 124.80 |
| 21 | 5 | 601 | CLA | CHD-C1D-ND | -2.27 | 121.61 | 124.80 |
| 21 | 52 | 601 | CLA | CHD-C1D-ND | -2.27 | 121.61 | 124.80 |
| 21 | B2 | 808 | CLA | CHD-C1D-ND | -2.27 | 121.61 | 124.80 |
| 30 | 52 | 608 | CHL | C1A-CHA-C4D | 2.27 | 122.76 | 118.98 |
| 21 | 4 | 603 | CLA | CHD-C1D-ND | -2.27 | 121.61 | 124.80 |
| 30 | 62 | 608 | CHL | C1A-CHA-C4D | 2.26 | 122.76 | 118.98 |
| 21 | 3 | 617 | CLA | CHD-C1D-ND | -2.26 | 121.62 | 124.80 |
| 30 | 62 | 607 | CHL | C1-C2-C3 | -2.26 | 122.49 | 126.20 |
| 21 | J | 101 | CLA | CHD-C1D-ND | -2.26 | 121.62 | 124.80 |
| 30 | 1 | 606 | CHL | C1A-CHA-C4D | 2.26 | 122.75 | 118.98 |
| 21 | B | 820 | CLA | CHD-C1D-ND | -2.26 | 121.62 | 124.80 |
| 21 | A | 814 | CLA | CHD-C1D-ND | -2.26 | 121.63 | 124.80 |
| 21 | A2 | 814 | CLA | CHD-C1D-ND | -2.25 | 121.63 | 124.80 |
| 30 | 6 | 618 | CHL | C1A-CHA-C4D | 2.25 | 122.74 | 118.98 |
| 30 | 5 | 608 | CHL | C1A-CHA-C4D | 2.25 | 122.74 | 118.98 |
| 21 | A2 | 810 | CLA | CHD-C1D-ND | -2.25 | 121.64 | 124.80 |
| 30 | 4 | 607 | CHL | C4C-CHD-C1D | 2.25 | 124.11 | 116.07 |
| 28 | F2 | 305 | LUT | C27-C28-C29 | 2.25 | 131.16 | 126.32 |
| 21 | A | 854 | CLA | CHD-C1D-ND | -2.25 | 121.64 | 124.80 |
| 21 | B | 813 | CLA | CHD-C1D-ND | -2.25 | 121.64 | 124.80 |
| 21 | 12 | 616 | CLA | CHD-C1D-ND | -2.25 | 121.64 | 124.80 |
| 30 | 6 | 607 | CHL | C1A-CHA-C4D | 2.25 | 122.73 | 118.98 |
| 30 | 62 | 607 | CHL | C1A-CHA-C4D | 2.25 | 122.73 | 118.98 |
| 21 | A | 810 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |
| 21 | F | 304 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |
| 21 | B2 | 824 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |
| 21 | F2 | 304 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |
| 30 | Z2 | 606 | CHL | C1A-CHA-C4D | 2.24 | 122.72 | 118.98 |
| 30 | 12 | 606 | CHL | C1A-CHA-C4D | 2.24 | 122.72 | 118.98 |
| 30 | 6 | 601 | CHL | CHA-C1A-C2A | -2.24 | 128.05 | 133.31 |
| 21 | 62 | 612 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |
| 30 | 42 | 607 | CHL | C4C-CHD-C1D | 2.24 | 124.08 | 116.07 |
| 30 | Z2 | 607 | CHL | C4C-CHD-C1D | 2.24 | 124.08 | 116.07 |
| 30 | Z | 606 | CHL | C1A-CHA-C4D | 2.24 | 122.72 | 118.98 |
| 30 | 6 | 606 | CHL | C4C-CHD-C1D | 2.24 | 124.08 | 116.07 |
| 21 | A2 | 829 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |
| 30 | 7 | 601 | CHL | C4C-CHD-C1D | 2.24 | 124.08 | 116.07 |
| 21 | 6 | 612 | CLA | CHD-C1D-ND | -2.24 | 121.65 | 124.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 62 | 618 | CHL | C1A-CHA-C4D | 2.24 | 122.71 | 118.98 |
| 30 | Z | 607 | CHL | C4C-CHD-C1D | 2.24 | 124.07 | 116.07 |
| 30 | 72 | 601 | CHL | C4C-CHD-C1D | 2.23 | 124.06 | 116.07 |
| 30 | 72 | 607 | CHL | C1A-CHA-C4D | 2.23 | 122.71 | 118.98 |
| 21 | 72 | 612 | CLA | CHD-C1D-ND | -2.23 | 121.66 | 124.80 |
| 30 | 52 | 606 | CHL | C1A-CHA-C4D | 2.23 | 122.71 | 118.98 |
| 21 | B2 | 813 | CLA | CHD-C1D-ND | -2.23 | 121.67 | 124.80 |
| 30 | 62 | 616 | CHL | C4C-CHD-C1D | 2.23 | 124.04 | 116.07 |
| 30 | 42 | 606 | CHL | C1A-CHA-C4D | 2.23 | 122.70 | 118.98 |
| 21 | Z | 613 | CLA | C3D-C4D-ND | 2.23 | 113.60 | 109.99 |
| 30 | 62 | 606 | CHL | C4C-CHD-C1D | 2.23 | 124.03 | 116.07 |
| 30 | 6 | 616 | CHL | C4C-CHD-C1D | 2.22 | 124.01 | 116.07 |
| 30 | Z | 601 | CHL | C1A-CHA-C4D | 2.22 | 122.69 | 118.98 |
| 30 | 6 | 608 | CHL | C1A-CHA-C4D | 2.22 | 122.69 | 118.98 |
| 30 | 6 | 601 | CHL | C4C-CHD-C1D | 2.22 | 124.01 | 116.07 |
| 30 | Z2 | 601 | CHL | C1A-CHA-C4D | 2.22 | 122.69 | 118.98 |
| 21 | 32 | 607 | CLA | C3D-C4D-ND | 2.22 | 113.59 | 109.99 |
| 30 | 1 | 606 | CHL | C4C-CHD-C1D | 2.22 | 124.01 | 116.07 |
| 30 | 62 | 601 | CHL | C4C-CHD-C1D | 2.22 | 124.00 | 116.07 |
| 30 | 4 | 606 | CHL | C1A-CHA-C4D | 2.22 | 122.68 | 118.98 |
| 30 | 42 | 606 | CHL | C4C-CHD-C1D | 2.22 | 124.00 | 116.07 |
| 30 | 62 | 601 | CHL | CHA-C1A-C2A | -2.22 | 128.10 | 133.31 |
| 30 | 5 | 607 | CHL | C4C-CHD-C1D | 2.22 | 123.99 | 116.07 |
| 28 | F | 305 | LUT | C27-C28-C29 | 2.21 | 131.09 | 126.32 |
| 30 | 4 | 606 | CHL | C4C-CHD-C1D | 2.21 | 123.99 | 116.07 |
| 30 | 8 | 606 | CHL | C4C-CHD-C1D | 2.21 | 123.98 | 116.07 |
| 30 | 52 | 607 | CHL | C4C-CHD-C1D | 2.21 | 123.98 | 116.07 |
| 30 | 82 | 606 | CHL | C4C-CHD-C1D | 2.21 | 123.98 | 116.07 |
| 30 | 92 | 606 | CHL | C4C-CHD-C1D | 2.21 | 123.98 | 116.07 |
| 30 | 52 | 618 | CHL | C4C-CHD-C1D | 2.21 | 123.97 | 116.07 |
| 30 | 7 | 607 | CHL | C1A-CHA-C4D | 2.21 | 122.67 | 118.98 |
| 30 | 3 | 608 | CHL | C4C-CHD-C1D | 2.21 | 123.96 | 116.07 |
| 21 | Z2 | 613 | CLA | C3D-C4D-ND | 2.21 | 113.57 | 109.99 |
| 30 | 9 | 606 | CHL | C4C-CHD-C1D | 2.20 | 123.96 | 116.07 |
| 30 | 1 | 601 | CHL | C4C-CHD-C1D | 2.20 | 123.95 | 116.07 |
| 30 | 62 | 618 | CHL | C4C-CHD-C1D | 2.20 | 123.95 | 116.07 |
| 30 | 8 | 607 | CHL | C1A-CHA-C4D | 2.20 | 122.66 | 118.98 |
| 30 | 42 | 618 | CHL | C4C-CHD-C1D | 2.20 | 123.95 | 116.07 |
| 21 | A | 829 | CLA | CHD-C1D-ND | -2.20 | 121.70 | 124.80 |
| 21 | B | 824 | CLA | CHD-C1D-ND | -2.20 | 121.70 | 124.80 |
| 21 | A2 | 806 | CLA | C3D-C4D-ND | 2.20 | 113.56 | 109.99 |
| 30 | 12 | 606 | CHL | C4C-CHD-C1D | 2.20 | 123.94 | 116.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | 82 | 601 | CHL | C4C-CHD-C1D | 2.20 | 123.94 | 116.07 |
| 21 | 32 | 603 | CLA | CHD-C1D-ND | -2.20 | 121.71 | 124.80 |
| 30 | Z2 | 606 | CHL | C4C-CHD-C1D | 2.20 | 123.93 | 116.07 |
| 30 | 5 | 606 | CHL | C1A-CHA-C4D | 2.20 | 122.65 | 118.98 |
| 30 | 4 | 618 | CHL | C4C-CHD-C1D | 2.20 | 123.93 | 116.07 |
| 30 | 72 | 606 | CHL | C4C-CHD-C1D | 2.20 | 123.93 | 116.07 |
| 30 | 7 | 607 | CHL | C4C-CHD-C1D | 2.20 | 123.92 | 116.07 |
| 30 | 8 | 601 | CHL | C4C-CHD-C1D | 2.20 | 123.92 | 116.07 |
| 30 | Z | 606 | CHL | C4C-CHD-C1D | 2.19 | 123.92 | 116.07 |
| 30 | 5 | 618 | CHL | C4C-CHD-C1D | 2.19 | 123.92 | 116.07 |
| 21 | 3 | 603 | CLA | CHD-C1D-ND | -2.19 | 121.72 | 124.80 |
| 30 | 6 | 618 | CHL | C4C-CHD-C1D | 2.19 | 123.92 | 116.07 |
| 30 | 12 | 601 | CHL | C4C-CHD-C1D | 2.19 | 123.92 | 116.07 |
| 21 | 4 | 604 | CLA | C3D-C4D-ND | 2.19 | 113.55 | 109.99 |
| 30 | 5 | 608 | CHL | C4C-CHD-C1D | 2.19 | 123.91 | 116.07 |
| 30 | 42 | 608 | CHL | C4C-CHD-C1D | 2.19 | 123.91 | 116.07 |
| 21 | B | 826 | CLA | C3B-C4B-NB | -2.19 | 108.57 | 110.53 |
| 21 | B2 | 806 | CLA | CHD-C1D-ND | -2.19 | 121.72 | 124.80 |
| 30 | 32 | 608 | CHL | C4C-CHD-C1D | 2.19 | 123.91 | 116.07 |
| 30 | 7 | 606 | CHL | C4C-CHD-C1D | 2.19 | 123.90 | 116.07 |
| 30 | 8 | 606 | CHL | C1A-CHA-C4D | 2.19 | 122.63 | 118.98 |
| 21 | B | 814 | CLA | C3D-C4D-ND | 2.19 | 113.54 | 109.99 |
| 21 | 6 | 617 | CLA | C3D-C4D-ND | 2.18 | 113.54 | 109.99 |
| 21 | 82 | 611 | CLA | C3D-C4D-ND | 2.18 | 113.54 | 109.99 |
| 30 | 5 | 606 | CHL | C4C-CHD-C1D | 2.18 | 123.88 | 116.07 |
| 30 | 4 | 608 | CHL | C1A-CHA-C4D | 2.18 | 122.62 | 118.98 |
| 30 | 92 | 606 | CHL | C1A-CHA-C4D | 2.18 | 122.62 | 118.98 |
| 30 | 4 | 608 | CHL | C4C-CHD-C1D | 2.18 | 123.88 | 116.07 |
| 30 | 72 | 607 | CHL | C4C-CHD-C1D | 2.18 | 123.88 | 116.07 |
| 30 | 52 | 606 | CHL | C4C-CHD-C1D | 2.18 | 123.88 | 116.07 |
| 30 | 42 | 608 | CHL | C1A-CHA-C4D | 2.18 | 122.62 | 118.98 |
| 21 | 8 | 616 | CLA | C3D-C4D-ND | 2.18 | 113.53 | 109.99 |
| 21 | B2 | 814 | CLA | C3D-C4D-ND | 2.18 | 113.53 | 109.99 |
| 21 | B2 | 831 | CLA | C3D-C4D-ND | 2.18 | 113.53 | 109.99 |
| 21 | 82 | 616 | CLA | C3D-C4D-ND | 2.18 | 113.53 | 109.99 |
| 30 | 9 | 606 | CHL | C1A-CHA-C4D | 2.18 | 122.62 | 118.98 |
| 21 | 3 | 607 | CLA | C3D-C4D-ND | 2.18 | 113.53 | 109.99 |
| 21 | 8 | 611 | CLA | C3D-C4D-ND | 2.18 | 113.53 | 109.99 |
| 30 | 3 | 608 | CHL | C1A-CHA-C4D | 2.18 | 122.61 | 118.98 |
| 30 | 6 | 608 | CHL | C4C-CHD-C1D | 2.18 | 123.86 | 116.07 |
| 21 | Z | 614 | CLA | C3D-C4D-ND | 2.18 | 113.52 | 109.99 |
| 21 | 9 | 604 | CLA | C3D-C4D-ND | 2.18 | 113.52 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 30 | Z2 | 601 | CHL | C4C-CHD-C1D | 2.17 | 123.85 | 116.07 |
| 21 | 42 | 604 | CLA | C3D-C4D-ND | 2.17 | 113.52 | 109.99 |
| 21 | B2 | 826 | CLA | C3B-C4B-NB | -2.17 | 108.59 | 110.53 |
| 21 | A | 823 | CLA | C3D-C4D-ND | 2.17 | 113.52 | 109.99 |
| 21 | K | 204 | CLA | C3D-C4D-ND | 2.17 | 113.52 | 109.99 |
| 30 | 52 | 608 | CHL | C4C-CHD-C1D | 2.17 | 123.84 | 116.07 |
| 21 | A | 820 | CLA | C3D-C4D-ND | 2.17 | 113.52 | 109.99 |
| 21 | B | 831 | CLA | C3D-C4D-ND | 2.17 | 113.52 | 109.99 |
| 30 | Z | 601 | CHL | C4C-CHD-C1D | 2.17 | 123.83 | 116.07 |
| 30 | 4 | 601 | CHL | C4C-CHD-C1D | 2.17 | 123.83 | 116.07 |
| 21 | A | 806 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 30 | 6 | 606 | CHL | C1A-CHA-C4D | 2.17 | 122.60 | 118.98 |
| 30 | 6 | 607 | CHL | C4C-CHD-C1D | 2.17 | 123.83 | 116.07 |
| 21 | 5 | 609 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 21 | 4 | 611 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 21 | 42 | 611 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 30 | 32 | 608 | CHL | C1A-CHA-C4D | 2.17 | 122.60 | 118.98 |
| 30 | 82 | 607 | CHL | C1A-CHA-C4D | 2.17 | 122.60 | 118.98 |
| 30 | 62 | 608 | CHL | C4C-CHD-C1D | 2.17 | 123.82 | 116.07 |
| 21 | A | 809 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 21 | 52 | 609 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 21 | 92 | 604 | CLA | C3D-C4D-ND | 2.17 | 113.51 | 109.99 |
| 30 | 82 | 607 | CHL | C4C-CHD-C1D | 2.17 | 123.82 | 116.07 |
| 30 | 42 | 601 | CHL | C4C-CHD-C1D | 2.16 | 123.81 | 116.07 |
| 30 | 62 | 606 | CHL | C1A-CHA-C4D | 2.16 | 122.59 | 118.98 |
| 30 | 62 | 607 | CHL | C4C-CHD-C1D | 2.16 | 123.80 | 116.07 |
| 30 | 82 | 606 | CHL | C1A-CHA-C4D | 2.16 | 122.59 | 118.98 |
| 21 | 52 | 603 | CLA | C3D-C4D-ND | 2.16 | 113.50 | 109.99 |
| 21 | A | 819 | CLA | CHD-C1D-ND | -2.16 | 121.76 | 124.80 |
| 30 | 92 | 607 | CHL | C1-C2-C3 | -2.16 | 123.27 | 126.76 |
| 21 | A | 803 | CLA | C3B-C4B-NB | -2.16 | 108.60 | 110.53 |
| 30 | 8 | 607 | CHL | C4C-CHD-C1D | 2.16 | 123.79 | 116.07 |
| 21 | B2 | 833 | CLA | C3D-C4D-ND | 2.16 | 113.50 | 109.99 |
| 21 | B | 841 | CLA | C1-C2-C3 | -2.16 | 122.67 | 126.20 |
| 21 | B2 | 841 | CLA | C1-C2-C3 | -2.15 | 122.67 | 126.20 |
| 30 | 9 | 607 | CHL | C1-C2-C3 | -2.15 | 123.28 | 126.76 |
| 21 | Z2 | 614 | CLA | C3D-C4D-ND | 2.15 | 113.48 | 109.99 |
| 30 | Z | 607 | CHL | C1A-CHA-C4D | 2.15 | 122.57 | 118.98 |
| 21 | L | 204 | CLA | C3D-C4D-ND | 2.15 | 113.48 | 109.99 |
| 21 | L2 | 204 | CLA | C3D-C4D-ND | 2.15 | 113.48 | 109.99 |
| 21 | 92 | 609 | CLA | C3D-C4D-ND | 2.15 | 113.48 | 109.99 |
| 30 | 5 | 618 | CHL | C1A-CHA-C4D | 2.15 | 122.56 | 118.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 92 | 614 | CLA | C3D-C4D-ND | 2.15 | 113.47 | 109.99 |
| 30 | Z2 | 607 | CHL | C1A-CHA-C4D | 2.15 | 122.56 | 118.98 |
| 21 | A2 | 823 | CLA | C3D-C4D-ND | 2.14 | 113.47 | 109.99 |
| 30 | 12 | 607 | CHL | C4C-CHD-C1D | 2.14 | 123.74 | 116.07 |
| 30 | 62 | 616 | CHL | C1A-CHA-C4D | 2.14 | 122.56 | 118.98 |
| 21 | 52 | 621 | CLA | CHA-C1A-NA | -2.14 | 121.54 | 126.39 |
| 21 | B | 833 | CLA | C3D-C4D-ND | 2.14 | 113.47 | 109.99 |
| 21 | Z2 | 611 | CLA | C3D-C4D-ND | 2.14 | 113.47 | 109.99 |
| 21 | Z | 611 | CLA | C3D-C4D-ND | 2.14 | 113.47 | 109.99 |
| 30 | 4 | 618 | CHL | C1A-CHA-C4D | 2.14 | 122.55 | 118.98 |
| 21 | Z | 610 | CLA | C3D-C4D-ND | 2.14 | 113.47 | 109.99 |
| 21 | A | 829 | CLA | C3B-C4B-NB | -2.14 | 108.62 | 110.53 |
| 21 | B | 806 | CLA | CHD-C1D-ND | -2.14 | 121.79 | 124.80 |
| 21 | 32 | 614 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 9 | 603 | CLA | CHC-C4B-NB | 2.14 | 127.26 | 124.05 |
| 30 | Z2 | 607 | CHL | C1-C2-C3 | -2.14 | 122.69 | 126.20 |
| 21 | B | 823 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 1 | 613 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | A2 | 820 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 12 | 613 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | Z2 | 604 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 62 | 609 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 3 | 614 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 1 | 602 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 5 | 617 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 21 | 9 | 614 | CLA | C3D-C4D-ND | 2.14 | 113.46 | 109.99 |
| 30 | 1 | 607 | CHL | C4C-CHD-C1D | 2.14 | 123.71 | 116.07 |
| 21 | K2 | 204 | CLA | C3D-C4D-ND | 2.13 | 113.45 | 109.99 |
| 21 | A2 | 822 | CLA | C3D-C4D-ND | 2.13 | 113.45 | 109.99 |
| 21 | 5 | 603 | CLA | C3D-C4D-ND | 2.13 | 113.45 | 109.99 |
| 21 | A | 816 | CLA | C3D-C4D-ND | 2.13 | 113.45 | 109.99 |
| 21 | 6 | 609 | CLA | C3D-C4D-ND | 2.13 | 113.45 | 109.99 |
| 21 | A2 | 803 | CLA | C3B-C4B-NB | -2.13 | 108.63 | 110.53 |
| 21 | 52 | 617 | CLA | C3D-C4D-ND | 2.13 | 113.45 | 109.99 |
| 21 | A | 822 | CLA | C3D-C4D-ND | 2.13 | 113.44 | 109.99 |
| 21 | 82 | 613 | CLA | C3D-C4D-ND | 2.13 | 113.44 | 109.99 |
| 21 | B2 | 823 | CLA | C3D-C4D-ND | 2.13 | 113.44 | 109.99 |
| 21 | 72 | 614 | CLA | C3D-C4D-ND | 2.13 | 113.44 | 109.99 |
| 21 | A | 835 | CLA | C3D-C4D-ND | 2.13 | 113.44 | 109.99 |
| 21 | 62 | 617 | CLA | C3D-C4D-ND | 2.13 | 113.44 | 109.99 |
| 30 | 42 | 618 | CHL | C1A-CHA-C4D | 2.12 | 122.53 | 118.98 |
| 30 | 72 | 606 | CHL | C1A-CHA-C4D | 2.12 | 122.53 | 118.98 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 9 | 609 | CLA | C3D-C4D-ND | 2.12 | 113.44 | 109.99 |
| 21 | 5 | 621 | CLA | CHA-C1A-NA | -2.12 | 121.58 | 126.39 |
| 21 | B | 840 | CLA | C3D-C4D-ND | 2.12 | 113.44 | 109.99 |
| 21 | 3 | 602 | CLA | C3D-C4D-ND | 2.12 | 113.44 | 109.99 |
| 21 | 3 | 611 | CLA | C3D-C4D-ND | 2.12 | 113.44 | 109.99 |
| 21 | 8 | 613 | CLA | C3D-C4D-ND | 2.12 | 113.44 | 109.99 |
| 30 | 72 | 601 | CHL | C1A-CHA-C4D | 2.12 | 122.52 | 118.98 |
| 30 | 52 | 618 | CHL | C1A-CHA-C4D | 2.12 | 122.52 | 118.98 |
| 30 | 6 | 616 | CHL | C1A-CHA-C4D | 2.12 | 122.52 | 118.98 |
| 21 | A2 | 819 | CLA | CHD-C1D-ND | -2.12 | 121.82 | 124.80 |
| 26 | B2 | 853 | LMU | C1B-O1B-C4' | 2.12 | 123.00 | 117.98 |
| 21 | 7 | 614 | CLA | C3D-C4D-ND | 2.12 | 113.43 | 109.99 |
| 21 | 92 | 613 | CLA | C3D-C4D-ND | 2.12 | 113.43 | 109.99 |
| 26 | B | 853 | LMU | C1B-O1B-C4' | 2.12 | 122.99 | 117.98 |
| 21 | 5 | 613 | CLA | C3D-C4D-ND | 2.11 | 113.42 | 109.99 |
| 21 | 52 | 613 | CLA | C3D-C4D-ND | 2.11 | 113.42 | 109.99 |
| 21 | 5 | 614 | CLA | C3D-C4D-ND | 2.11 | 113.42 | 109.99 |
| 21 | Z2 | 610 | CLA | C3D-C4D-ND | 2.11 | 113.42 | 109.99 |
| 30 | Z | 607 | CHL | C1-C2-C3 | -2.11 | 122.73 | 126.20 |
| 21 | A2 | 804 | CLA | C3D-C4D-ND | 2.11 | 113.42 | 109.99 |
| 21 | 1 | 604 | CLA | C3D-C4D-ND | 2.11 | 113.41 | 109.99 |
| 21 | A2 | 809 | CLA | C3D-C4D-ND | 2.11 | 113.41 | 109.99 |
| 21 | 92 | 603 | CLA | CHC-C4B-NB | 2.11 | 127.21 | 124.05 |
| 21 | 12 | 604 | CLA | C3D-C4D-ND | 2.10 | 113.41 | 109.99 |
| 21 | Z | 604 | CLA | C3D-C4D-ND | 2.10 | 113.41 | 109.99 |
| 21 | 9 | 603 | CLA | C3D-C4D-ND | 2.10 | 113.41 | 109.99 |
| 21 | A2 | 816 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | A | 804 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | 1 | 610 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | 92 | 601 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | B | 807 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | B2 | 818 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | 12 | 602 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | 82 | 604 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | 72 | 604 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 21 | A | 837 | CLA | C3B-C4B-NB | -2.10 | 108.66 | 110.53 |
| 21 | 62 | 613 | CLA | C3D-C4D-ND | 2.10 | 113.40 | 109.99 |
| 30 | 7 | 601 | CHL | C1A-CHA-C4D | 2.10 | 122.48 | 118.98 |
| 21 | 7 | 616 | CLA | C3D-C4D-ND | 2.10 | 113.39 | 109.99 |
| 21 | 32 | 602 | CLA | C3D-C4D-ND | 2.10 | 113.39 | 109.99 |
| 21 | B2 | 810 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |
| 21 | 52 | 614 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 62 | 610 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |
| 32 | 6 | 625 | NEX | O24-C26-C27 | -2.09 | 110.88 | 116.88 |
| 21 | 9 | 613 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |
| 21 | B2 | 840 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |
| 21 | 32 | 611 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |
| 21 | 72 | 616 | CLA | C3D-C4D-ND | 2.09 | 113.39 | 109.99 |
| 21 | A2 | 835 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | B2 | 807 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | 32 | 610 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | B2 | 830 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | 7 | 604 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | 5 | 611 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | 92 | 603 | CLA | C3D-C4D-ND | 2.09 | 113.38 | 109.99 |
| 21 | L | 203 | CLA | C3D-C4D-ND | 2.08 | 113.38 | 109.99 |
| 21 | 1 | 614 | CLA | C3D-C4D-ND | 2.08 | 113.38 | 109.99 |
| 21 | A | 827 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | B | 841 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 32 | 62 | 625 | NEX | O24-C26-C27 | -2.08 | 110.91 | 116.88 |
| 21 | 1 | 616 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | A2 | 839 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 12 | 611 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | A2 | 837 | CLA | C3B-C4B-NB | -2.08 | 108.67 | 110.53 |
| 21 | B | 822 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | F | 303 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 9 | 601 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 92 | 611 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 5 | 621 | CLA | CHD-C1D-ND | -2.08 | 121.87 | 124.80 |
| 21 | B | 836 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | B2 | 819 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 30 | 9 | 607 | CHL | C4C-CHD-C1D | 2.08 | 123.51 | 116.07 |
| 21 | 7 | 603 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | Z | 608 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 6 | 613 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 12 | 610 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 6 | 614 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | A2 | 834 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 62 | 614 | CLA | C3D-C4D-ND | 2.08 | 113.37 | 109.99 |
| 21 | 4 | 616 | CLA | C3D-C4D-ND | 2.08 | 113.36 | 109.99 |
| 21 | A | 811 | CLA | C3D-C4D-ND | 2.08 | 113.36 | 109.99 |
| 30 | 7 | 606 | CHL | C1A-CHA-C4D | 2.08 | 122.45 | 118.98 |
| 21 | B | 834 | CLA | C3D-C4D-ND | 2.08 | 113.36 | 109.99 |
| 21 | A | 834 | CLA | C3D-C4D-ND | 2.07 | 113.36 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 843 | CLA | C3D-C4D-ND | 2.07 | 113.36 | 109.99 |
| 21 | 62 | 609 | CLA | CAA-C2A-C1A | -2.07 | 105.18 | 111.97 |
| 21 | 62 | 602 | CLA | C3D-C4D-ND | 2.07 | 113.36 | 109.99 |
| 21 | B | 810 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | A2 | 843 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | A2 | 824 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | 72 | 611 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | 1 | 611 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | 52 | 611 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | A | 824 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 21 | 6 | 610 | CLA | C3D-C4D-ND | 2.07 | 113.35 | 109.99 |
| 30 | 92 | 607 | CHL | C4C-CHD-C1D | 2.07 | 123.47 | 116.07 |
| 21 | 52 | 621 | CLA | CHD-C1D-ND | -2.07 | 121.89 | 124.80 |
| 21 | B | 819 | CLA | C3D-C4D-ND | 2.07 | 113.34 | 109.99 |
| 21 | B | 825 | CLA | C3D-C4D-ND | 2.07 | 113.34 | 109.99 |
| 21 | B2 | 834 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | L2 | 203 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | 72 | 603 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | 6 | 609 | CLA | CAA-C2A-C1A | -2.06 | 105.21 | 111.97 |
| 21 | 9 | 611 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | 6 | 602 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | B2 | 822 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | B | 808 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | 8 | 604 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | F2 | 303 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | B2 | 825 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | Z2 | 616 | CLA | C3D-C4D-ND | 2.06 | 113.34 | 109.99 |
| 21 | A | 812 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | B2 | 836 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | 42 | 602 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | 1 | 609 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | 42 | 616 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | Z2 | 608 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | 4 | 602 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | A2 | 827 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | 42 | 614 | CLA | C3D-C4D-ND | 2.06 | 113.33 | 109.99 |
| 21 | B2 | 805 | CLA | C3D-C4D-ND | 2.05 | 113.33 | 109.99 |
| 21 | Z | 616 | CLA | C3D-C4D-ND | 2.05 | 113.33 | 109.99 |
| 21 | B | 837 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | A2 | 811 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | 7 | 611 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | B | 818 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | A | 839 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | B2 | 841 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | 3 | 604 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | B | 805 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | B | 839 | CLA | C3D-C4D-ND | 2.05 | 113.32 | 109.99 |
| 21 | A | 803 | CLA | C3D-C4D-ND | 2.05 | 113.31 | 109.99 |
| 21 | 3 | 612 | CLA | C3D-C4D-ND | 2.05 | 113.31 | 109.99 |
| 21 | 12 | 616 | CLA | C3D-C4D-ND | 2.05 | 113.31 | 109.99 |
| 21 | 52 | 604 | CLA | C3D-C4D-ND | 2.05 | 113.31 | 109.99 |
| 21 | 62 | 612 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | 12 | 614 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | A | 818 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | B2 | 839 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | 72 | 602 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | B | 828 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | 72 | 614 | CLA | CHC-C4B-NB | 2.04 | 127.11 | 124.05 |
| 21 | 4 | 614 | CLA | C3D-C4D-ND | 2.04 | 113.31 | 109.99 |
| 21 | 72 | 610 | CLA | C3B-C4B-NB | -2.04 | 108.71 | 110.53 |
| 21 | F | 304 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | B | 811 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | 9 | 602 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | A2 | 839 | CLA | CHC-C4B-NB | 2.04 | 127.11 | 124.05 |
| 21 | Z | 602 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | F2 | 304 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | B | 813 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | B | 816 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | 3 | 610 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | Z2 | 602 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | 6 | 604 | CLA | C3D-C4D-ND | 2.04 | 113.30 | 109.99 |
| 21 | A2 | 803 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | A | 833 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | 7 | 602 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | A | 841 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | A2 | 812 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | B2 | 816 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | B2 | 817 | CLA | C3D-C4D-ND | 2.03 | 113.29 | 109.99 |
| 21 | 1 | 612 | CLA | CHC-C4B-NB | 2.03 | 127.09 | 124.05 |
| 21 | A | 813 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |
| 21 | A2 | 813 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |
| 21 | A2 | 833 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |
| 21 | 3 | 613 | CLA | CHC-C4B-NB | 2.03 | 127.09 | 124.05 |
| 21 | 62 | 611 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 7 | 610 | CLA | C3B-C4B-NB | -2.03 | 108.72 | 110.53 |
| 21 | B | 830 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |
| 21 | G2 | 204 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |
| 21 | B2 | 828 | CLA | C3D-C4D-ND | 2.03 | 113.28 | 109.99 |
| 21 | 3 | 615 | CLA | CHC-C4B-NB | 2.03 | 127.09 | 124.05 |
| 21 | K | 201 | CLA | CHD-C1D-ND | -2.03 | 121.95 | 124.80 |
| 21 | 7 | 609 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | 5 | 610 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | 52 | 610 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | 62 | 604 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | A2 | 829 | CLA | C3B-C4B-NB | -2.02 | 108.72 | 110.53 |
| 21 | A | 825 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | A2 | 841 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | 72 | 613 | CLA | C3D-C4D-ND | 2.02 | 113.28 | 109.99 |
| 21 | 8 | 612 | CLA | CHC-C4B-NB | 2.02 | 127.08 | 124.05 |
| 31 | 12 | 618 | XAT | O4-C5-C4 | -2.02 | 111.59 | 113.49 |
| 21 | 6 | 612 | CLA | C3D-C4D-ND | 2.02 | 113.27 | 109.99 |
| 30 | 92 | 607 | CHL | CMA-C3A-C4A | -2.02 | 110.25 | 114.61 |
| 21 | 32 | 613 | CLA | CHC-C4B-NB | 2.02 | 127.08 | 124.05 |
| 21 | A2 | 818 | CLA | C3D-C4D-ND | 2.02 | 113.27 | 109.99 |
| 21 | B2 | 821 | CLA | C3D-C4D-ND | 2.02 | 113.27 | 109.99 |
| 21 | K2 | 206 | CLA | C3D-C4D-ND | 2.02 | 113.27 | 109.99 |
| 21 | 7 | 608 | CLA | C3D-C4D-ND | 2.02 | 113.27 | 109.99 |
| 21 | A2 | 812 | CLA | CHC-C4B-NB | 2.02 | 127.08 | 124.05 |
| 21 | B | 817 | CLA | C3D-C4D-ND | 2.02 | 113.27 | 109.99 |
| 21 | A | 812 | CLA | CHC-C4B-NB | 2.02 | 127.07 | 124.05 |
| 21 | 4 | 612 | CLA | C3D-C4D-ND | 2.02 | 113.26 | 109.99 |
| 21 | 12 | 609 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | 72 | 609 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | B2 | 808 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | 5 | 604 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | 32 | 604 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | 82 | 603 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | 4 | 610 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | A | 839 | CLA | CHC-C4B-NB | 2.01 | 127.07 | 124.05 |
| 21 | B2 | 837 | CLA | C3D-C4D-ND | 2.01 | 113.26 | 109.99 |
| 21 | B | 832 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | 92 | 613 | CLA | CHC-C4B-NB | 2.01 | 127.06 | 124.05 |
| 21 | A2 | 830 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | A | 832 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | A2 | 825 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | 92 | 602 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | 6 | 611 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | A | 830 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | A2 | 831 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | B2 | 835 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | 12 | 608 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 21 | 32 | 612 | CLA | C3D-C4D-ND | 2.01 | 113.25 | 109.99 |
| 30 | 92 | 607 | CHL | C1A-CHA-C4D | 2.00 | 122.33 | 118.98 |
| 21 | 42 | 610 | CLA | C3D-C4D-ND | 2.00 | 113.25 | 109.99 |
| 21 | 72 | 608 | CLA | C3D-C4D-ND | 2.00 | 113.24 | 109.99 |
| 21 | 5 | 602 | CLA | CHC-C4B-NB | 2.00 | 127.05 | 124.05 |
| 21 | 8 | 609 | CLA | C3D-C4D-ND | 2.00 | 113.24 | 109.99 |
| 30 | 9 | 607 | CHL | CMA-C3A-C4A | -2.00 | 110.30 | 114.61 |

All (584) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 20 | A | 801 | CL0 | NC |
| 20 | A | 801 | CL0 | ND |
| 20 | A | 801 | CL0 | NA |
| 20 | A2 | 801 | CL0 | NC |
| 20 | A2 | 801 | CL0 | ND |
| 20 | A2 | 801 | CL0 | NA |
| 21 | A | 802 | CLA | ND |
| 21 | A | 803 | CLA | ND |
| 21 | A | 804 | CLA | ND |
| 21 | A | 805 | CLA | ND |
| 21 | A | 806 | CLA | ND |
| 21 | A | 807 | CLA | ND |
| 21 | A | 808 | CLA | ND |
| 21 | A | 809 | CLA | ND |
| 21 | A | 810 | CLA | ND |
| 21 | A | 811 | CLA | ND |
| 21 | A | 812 | CLA | ND |
| 21 | A | 813 | CLA | ND |
| 21 | A | 814 | CLA | ND |
| 21 | A | 815 | CLA | ND |
| 21 | A | 816 | CLA | ND |
| 21 | A | 817 | CLA | ND |
| 21 | A | 818 | CLA | ND |
| 21 | A | 819 | CLA | ND |
| 21 | A | 820 | CLA | ND |
| 21 | A | 821 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | A | 822 | CLA | ND |
| 21 | A | 823 | CLA | ND |
| 21 | A | 824 | CLA | ND |
| 21 | A | 825 | CLA | ND |
| 21 | A | 826 | CLA | ND |
| 21 | A | 827 | CLA | ND |
| 21 | A | 828 | CLA | ND |
| 21 | A | 829 | CLA | ND |
| 21 | A | 830 | CLA | ND |
| 21 | A | 831 | CLA | ND |
| 21 | A | 832 | CLA | ND |
| 21 | A | 833 | CLA | ND |
| 21 | A | 834 | CLA | ND |
| 21 | A | 835 | CLA | ND |
| 21 | A | 836 | CLA | ND |
| 21 | A | 837 | CLA | ND |
| 21 | A | 838 | CLA | ND |
| 21 | A | 839 | CLA | ND |
| 21 | A | 840 | CLA | ND |
| 21 | A | 841 | CLA | ND |
| 21 | A | 842 | CLA | ND |
| 21 | A | 843 | CLA | ND |
| 21 | A | 845 | CLA | ND |
| 21 | A | 854 | CLA | ND |
| 21 | B | 802 | CLA | ND |
| 21 | B | 803 | CLA | ND |
| 21 | B | 804 | CLA | ND |
| 21 | B | 805 | CLA | ND |
| 21 | B | 806 | CLA | ND |
| 21 | B | 807 | CLA | ND |
| 21 | B | 808 | CLA | ND |
| 21 | B | 809 | CLA | ND |
| 21 | B | 810 | CLA | ND |
| 21 | B | 811 | CLA | ND |
| 21 | B | 812 | CLA | ND |
| 21 | B | 813 | CLA | ND |
| 21 | B | 814 | CLA | ND |
| 21 | B | 815 | CLA | ND |
| 21 | B | 816 | CLA | ND |
| 21 | B | 817 | CLA | ND |
| 21 | B | 818 | CLA | ND |
| 21 | B | 819 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | B | 820 | CLA | ND |
| 21 | B | 821 | CLA | ND |
| 21 | B | 822 | CLA | ND |
| 21 | B | 823 | CLA | ND |
| 21 | B | 824 | CLA | ND |
| 21 | B | 825 | CLA | ND |
| 21 | B | 826 | CLA | ND |
| 21 | B | 827 | CLA | ND |
| 21 | B | 828 | CLA | ND |
| 21 | B | 829 | CLA | ND |
| 21 | B | 830 | CLA | ND |
| 21 | B | 831 | CLA | ND |
| 21 | B | 832 | CLA | ND |
| 21 | B | 833 | CLA | ND |
| 21 | B | 834 | CLA | ND |
| 21 | B | 835 | CLA | ND |
| 21 | B | 836 | CLA | ND |
| 21 | B | 837 | CLA | ND |
| 21 | B | 838 | CLA | ND |
| 21 | B | 839 | CLA | ND |
| 21 | B | 840 | CLA | ND |
| 21 | B | 841 | CLA | ND |
| 21 | F | 301 | CLA | ND |
| 21 | F | 303 | CLA | ND |
| 21 | F | 304 | CLA | ND |
| 21 | G | 203 | CLA | ND |
| 21 | G | 204 | CLA | ND |
| 21 | J | 101 | CLA | ND |
| 21 | L | 203 | CLA | ND |
| 21 | L | 204 | CLA | ND |
| 21 | K | 201 | CLA | ND |
| 21 | K | 203 | CLA | ND |
| 21 | K | 204 | CLA | ND |
| 21 | K | 206 | CLA | ND |
| 21 | 1 | 602 | CLA | ND |
| 21 | 1 | 603 | CLA | ND |
| 21 | 1 | 604 | CLA | ND |
| 21 | 1 | 608 | CLA | ND |
| 21 | 1 | 609 | CLA | ND |
| 21 | 1 | 610 | CLA | ND |
| 21 | 1 | 611 | CLA | ND |
| 21 | 1 | 612 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | 1 | 613 | CLA | ND |
| 21 | 1 | 614 | CLA | ND |
| 21 | 1 | 616 | CLA | ND |
| 21 | 3 | 602 | CLA | ND |
| 21 | 3 | 603 | CLA | ND |
| 21 | 3 | 604 | CLA | ND |
| 21 | 3 | 606 | CLA | ND |
| 21 | 3 | 607 | CLA | ND |
| 21 | 3 | 609 | CLA | ND |
| 21 | 3 | 610 | CLA | ND |
| 21 | 3 | 611 | CLA | ND |
| 21 | 3 | 612 | CLA | ND |
| 21 | 3 | 613 | CLA | ND |
| 21 | 3 | 614 | CLA | ND |
| 21 | 3 | 617 | CLA | ND |
| 21 | 3 | 615 | CLA | ND |
| 21 | 7 | 602 | CLA | ND |
| 21 | 7 | 603 | CLA | ND |
| 21 | 7 | 604 | CLA | ND |
| 21 | 7 | 608 | CLA | ND |
| 21 | 7 | 609 | CLA | ND |
| 21 | 7 | 610 | CLA | ND |
| 21 | 7 | 611 | CLA | ND |
| 21 | 7 | 612 | CLA | ND |
| 21 | 7 | 613 | CLA | ND |
| 21 | 7 | 614 | CLA | ND |
| 21 | 7 | 616 | CLA | ND |
| 21 | 7 | 620 | CLA | ND |
| 21 | 8 | 602 | CLA | ND |
| 21 | 8 | 603 | CLA | ND |
| 21 | 8 | 604 | CLA | ND |
| 21 | 8 | 608 | CLA | ND |
| 21 | 8 | 609 | CLA | ND |
| 21 | 8 | 610 | CLA | ND |
| 21 | 8 | 611 | CLA | ND |
| 21 | 8 | 612 | CLA | ND |
| 21 | 8 | 613 | CLA | ND |
| 21 | 8 | 614 | CLA | ND |
| 21 | 8 | 616 | CLA | ND |
| 21 | Z | 602 | CLA | ND |
| 21 | Z | 603 | CLA | ND |
| 21 | Z | 604 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | Z | 608 | CLA | ND |
| 21 | Z | 609 | CLA | ND |
| 21 | Z | 610 | CLA | ND |
| 21 | Z | 611 | CLA | ND |
| 21 | Z | 612 | CLA | ND |
| 21 | Z | 613 | CLA | ND |
| 21 | Z | 614 | CLA | ND |
| 21 | Z | 616 | CLA | ND |
| 21 | 4 | 602 | CLA | ND |
| 21 | 4 | 603 | CLA | ND |
| 21 | 4 | 604 | CLA | ND |
| 21 | 4 | 609 | CLA | ND |
| 21 | 4 | 610 | CLA | ND |
| 21 | 4 | 611 | CLA | ND |
| 21 | 4 | 612 | CLA | ND |
| 21 | 4 | 613 | CLA | ND |
| 21 | 4 | 614 | CLA | ND |
| 21 | 4 | 616 | CLA | ND |
| 21 | 5 | 601 | CLA | ND |
| 21 | 5 | 602 | CLA | ND |
| 21 | 5 | 603 | CLA | ND |
| 21 | 5 | 604 | CLA | ND |
| 21 | 5 | 609 | CLA | ND |
| 21 | 5 | 610 | CLA | ND |
| 21 | 5 | 611 | CLA | ND |
| 21 | 5 | 612 | CLA | ND |
| 21 | 5 | 613 | CLA | ND |
| 21 | 5 | 614 | CLA | ND |
| 21 | 5 | 616 | CLA | ND |
| 21 | 5 | 617 | CLA | ND |
| 21 | 5 | 621 | CLA | ND |
| 21 | 6 | 602 | CLA | ND |
| 21 | 6 | 603 | CLA | ND |
| 21 | 6 | 604 | CLA | ND |
| 21 | 6 | 609 | CLA | ND |
| 21 | 6 | 610 | CLA | ND |
| 21 | 6 | 611 | CLA | ND |
| 21 | 6 | 612 | CLA | ND |
| 21 | 6 | 613 | CLA | ND |
| 21 | 6 | 614 | CLA | ND |
| 21 | 6 | 617 | CLA | ND |
| 21 | 6 | 622 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | 9 | 601 | CLA | ND |
| 21 | 9 | 602 | CLA | ND |
| 21 | 9 | 603 | CLA | ND |
| 21 | 9 | 604 | CLA | ND |
| 21 | 9 | 609 | CLA | ND |
| 21 | 9 | 610 | CLA | ND |
| 21 | 9 | 611 | CLA | ND |
| 21 | 9 | 612 | CLA | ND |
| 21 | 9 | 613 | CLA | ND |
| 21 | 9 | 614 | CLA | ND |
| 21 | A2 | 802 | CLA | ND |
| 21 | A2 | 803 | CLA | ND |
| 21 | A2 | 804 | CLA | ND |
| 21 | A2 | 805 | CLA | ND |
| 21 | A2 | 806 | CLA | ND |
| 21 | A2 | 807 | CLA | ND |
| 21 | A2 | 808 | CLA | ND |
| 21 | A2 | 809 | CLA | ND |
| 21 | A2 | 810 | CLA | ND |
| 21 | A2 | 811 | CLA | ND |
| 21 | A2 | 812 | CLA | ND |
| 21 | A2 | 813 | CLA | ND |
| 21 | A2 | 814 | CLA | ND |
| 21 | A2 | 815 | CLA | ND |
| 21 | A2 | 816 | CLA | ND |
| 21 | A2 | 817 | CLA | ND |
| 21 | A2 | 818 | CLA | ND |
| 21 | A2 | 819 | CLA | ND |
| 21 | A2 | 820 | CLA | ND |
| 21 | A2 | 821 | CLA | ND |
| 21 | A2 | 822 | CLA | ND |
| 21 | A2 | 823 | CLA | ND |
| 21 | A2 | 824 | CLA | ND |
| 21 | A2 | 825 | CLA | ND |
| 21 | A2 | 826 | CLA | ND |
| 21 | A2 | 827 | CLA | ND |
| 21 | A2 | 828 | CLA | ND |
| 21 | A2 | 829 | CLA | ND |
| 21 | A2 | 830 | CLA | ND |
| 21 | A2 | 831 | CLA | ND |
| 21 | A2 | 832 | CLA | ND |
| 21 | A2 | 833 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | A2 | 834 | CLA | ND |
| 21 | A2 | 835 | CLA | ND |
| 21 | A2 | 836 | CLA | ND |
| 21 | A2 | 837 | CLA | ND |
| 21 | A2 | 838 | CLA | ND |
| 21 | A2 | 839 | CLA | ND |
| 21 | A2 | 840 | CLA | ND |
| 21 | A2 | 841 | CLA | ND |
| 21 | A2 | 842 | CLA | ND |
| 21 | A2 | 843 | CLA | ND |
| 21 | A2 | 845 | CLA | ND |
| 21 | A2 | 854 | CLA | ND |
| 21 | B2 | 802 | CLA | ND |
| 21 | B2 | 803 | CLA | ND |
| 21 | B2 | 804 | CLA | ND |
| 21 | B2 | 805 | CLA | ND |
| 21 | B2 | 806 | CLA | ND |
| 21 | B2 | 807 | CLA | ND |
| 21 | B2 | 808 | CLA | ND |
| 21 | B2 | 809 | CLA | ND |
| 21 | B2 | 810 | CLA | ND |
| 21 | B2 | 811 | CLA | ND |
| 21 | B2 | 812 | CLA | ND |
| 21 | B2 | 813 | CLA | ND |
| 21 | B2 | 814 | CLA | ND |
| 21 | B2 | 815 | CLA | ND |
| 21 | B2 | 816 | CLA | ND |
| 21 | B2 | 817 | CLA | ND |
| 21 | B2 | 818 | CLA | ND |
| 21 | B2 | 819 | CLA | ND |
| 21 | B2 | 820 | CLA | ND |
| 21 | B2 | 821 | CLA | ND |
| 21 | B2 | 822 | CLA | ND |
| 21 | B2 | 823 | CLA | ND |
| 21 | B2 | 824 | CLA | ND |
| 21 | B2 | 825 | CLA | ND |
| 21 | B2 | 826 | CLA | ND |
| 21 | B2 | 827 | CLA | ND |
| 21 | B2 | 828 | CLA | ND |
| 21 | B2 | 829 | CLA | ND |
| 21 | B2 | 830 | CLA | ND |
| 21 | B2 | 831 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | B2 | 832 | CLA | ND |
| 21 | B2 | 833 | CLA | ND |
| 21 | B2 | 834 | CLA | ND |
| 21 | B2 | 835 | CLA | ND |
| 21 | B2 | 836 | CLA | ND |
| 21 | B2 | 837 | CLA | ND |
| 21 | B2 | 838 | CLA | ND |
| 21 | B2 | 839 | CLA | ND |
| 21 | B2 | 840 | CLA | ND |
| 21 | B2 | 841 | CLA | ND |
| 21 | F2 | 301 | CLA | ND |
| 21 | F2 | 303 | CLA | ND |
| 21 | F2 | 304 | CLA | ND |
| 21 | G2 | 203 | CLA | ND |
| 21 | G2 | 204 | CLA | ND |
| 21 | J2 | 101 | CLA | ND |
| 21 | L2 | 203 | CLA | ND |
| 21 | L2 | 204 | CLA | ND |
| 21 | K2 | 201 | CLA | ND |
| 21 | K2 | 203 | CLA | ND |
| 21 | K2 | 204 | CLA | ND |
| 21 | K2 | 206 | CLA | ND |
| 21 | 12 | 602 | CLA | ND |
| 21 | 12 | 603 | CLA | ND |
| 21 | 12 | 604 | CLA | ND |
| 21 | 12 | 608 | CLA | ND |
| 21 | 12 | 609 | CLA | ND |
| 21 | 12 | 610 | CLA | ND |
| 21 | 12 | 611 | CLA | ND |
| 21 | 12 | 612 | CLA | ND |
| 21 | 12 | 613 | CLA | ND |
| 21 | 12 | 614 | CLA | ND |
| 21 | 12 | 616 | CLA | ND |
| 21 | 32 | 602 | CLA | ND |
| 21 | 32 | 603 | CLA | ND |
| 21 | 32 | 604 | CLA | ND |
| 21 | 32 | 606 | CLA | ND |
| 21 | 32 | 607 | CLA | ND |
| 21 | 32 | 609 | CLA | ND |
| 21 | 32 | 610 | CLA | ND |
| 21 | 32 | 611 | CLA | ND |
| 21 | 32 | 612 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | 32 | 613 | CLA | ND |
| 21 | 32 | 614 | CLA | ND |
| 21 | 32 | 617 | CLA | ND |
| 21 | 32 | 615 | CLA | ND |
| 21 | 72 | 602 | CLA | ND |
| 21 | 72 | 603 | CLA | ND |
| 21 | 72 | 604 | CLA | ND |
| 21 | 72 | 608 | CLA | ND |
| 21 | 72 | 609 | CLA | ND |
| 21 | 72 | 610 | CLA | ND |
| 21 | 72 | 611 | CLA | ND |
| 21 | 72 | 612 | CLA | ND |
| 21 | 72 | 613 | CLA | ND |
| 21 | 72 | 614 | CLA | ND |
| 21 | 72 | 616 | CLA | ND |
| 21 | 72 | 620 | CLA | ND |
| 21 | 82 | 602 | CLA | ND |
| 21 | 82 | 603 | CLA | ND |
| 21 | 82 | 604 | CLA | ND |
| 21 | 82 | 608 | CLA | ND |
| 21 | 82 | 609 | CLA | ND |
| 21 | 82 | 610 | CLA | ND |
| 21 | 82 | 611 | CLA | ND |
| 21 | 82 | 612 | CLA | ND |
| 21 | 82 | 613 | CLA | ND |
| 21 | 82 | 614 | CLA | ND |
| 21 | 82 | 616 | CLA | ND |
| 21 | Z2 | 602 | CLA | ND |
| 21 | Z2 | 603 | CLA | ND |
| 21 | Z2 | 604 | CLA | ND |
| 21 | Z2 | 608 | CLA | ND |
| 21 | Z2 | 609 | CLA | ND |
| 21 | Z2 | 610 | CLA | ND |
| 21 | Z2 | 611 | CLA | ND |
| 21 | Z2 | 612 | CLA | ND |
| 21 | Z2 | 613 | CLA | ND |
| 21 | Z2 | 614 | CLA | ND |
| 21 | Z2 | 616 | CLA | ND |
| 21 | 42 | 602 | CLA | ND |
| 21 | 42 | 603 | CLA | ND |
| 21 | 42 | 604 | CLA | ND |
| 21 | 42 | 609 | CLA | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | 42 | 610 | CLA | ND |
| 21 | 42 | 611 | CLA | ND |
| 21 | 42 | 612 | CLA | ND |
| 21 | 42 | 613 | CLA | ND |
| 21 | 42 | 614 | CLA | ND |
| 21 | 42 | 616 | CLA | ND |
| 21 | 52 | 601 | CLA | ND |
| 21 | 52 | 602 | CLA | ND |
| 21 | 52 | 603 | CLA | ND |
| 21 | 52 | 604 | CLA | ND |
| 21 | 52 | 609 | CLA | ND |
| 21 | 52 | 610 | CLA | ND |
| 21 | 52 | 611 | CLA | ND |
| 21 | 52 | 612 | CLA | ND |
| 21 | 52 | 613 | CLA | ND |
| 21 | 52 | 614 | CLA | ND |
| 21 | 52 | 616 | CLA | ND |
| 21 | 52 | 617 | CLA | ND |
| 21 | 52 | 621 | CLA | ND |
| 21 | 62 | 602 | CLA | ND |
| 21 | 62 | 603 | CLA | ND |
| 21 | 62 | 604 | CLA | ND |
| 21 | 62 | 609 | CLA | ND |
| 21 | 62 | 610 | CLA | ND |
| 21 | 62 | 611 | CLA | ND |
| 21 | 62 | 612 | CLA | ND |
| 21 | 62 | 613 | CLA | ND |
| 21 | 62 | 614 | CLA | ND |
| 21 | 62 | 617 | CLA | ND |
| 21 | 62 | 622 | CLA | ND |
| 21 | 92 | 601 | CLA | ND |
| 21 | 92 | 602 | CLA | ND |
| 21 | 92 | 603 | CLA | ND |
| 21 | 92 | 604 | CLA | ND |
| 21 | 92 | 609 | CLA | ND |
| 21 | 92 | 610 | CLA | ND |
| 21 | 92 | 611 | CLA | ND |
| 21 | 92 | 612 | CLA | ND |
| 21 | 92 | 613 | CLA | ND |
| 21 | 92 | 614 | CLA | ND |
| 30 | 1 | 601 | CHL | NC |
| 30 | 1 | 601 | CHL | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 30 | 1 | 601 | CHL | NA |
| 30 | 1 | 606 | CHL | NC |
| 30 | 1 | 606 | CHL | ND |
| 30 | 1 | 606 | CHL | NA |
| 30 | 1 | 607 | CHL | NC |
| 30 | 1 | 607 | CHL | ND |
| 30 | 1 | 607 | CHL | NA |
| 30 | 3 | 608 | CHL | NC |
| 30 | 3 | 608 | CHL | ND |
| 30 | 3 | 608 | CHL | NA |
| 30 | 7 | 601 | CHL | NC |
| 30 | 7 | 601 | CHL | ND |
| 30 | 7 | 601 | CHL | NA |
| 30 | 7 | 606 | CHL | NC |
| 30 | 7 | 606 | CHL | ND |
| 30 | 7 | 606 | CHL | NA |
| 30 | 7 | 607 | CHL | NC |
| 30 | 7 | 607 | CHL | ND |
| 30 | 7 | 607 | CHL | NA |
| 30 | 8 | 601 | CHL | NC |
| 30 | 8 | 601 | CHL | ND |
| 30 | 8 | 601 | CHL | NA |
| 30 | 8 | 606 | CHL | NC |
| 30 | 8 | 606 | CHL | ND |
| 30 | 8 | 606 | CHL | NA |
| 30 | 8 | 607 | CHL | NC |
| 30 | 8 | 607 | CHL | ND |
| 30 | 8 | 607 | CHL | NA |
| 30 | Z | 601 | CHL | NC |
| 30 | Z | 601 | CHL | ND |
| 30 | Z | 601 | CHL | NA |
| 30 | Z | 606 | CHL | NC |
| 30 | Z | 606 | CHL | ND |
| 30 | Z | 606 | CHL | NA |
| 30 | Z | 607 | CHL | NC |
| 30 | Z | 607 | CHL | ND |
| 30 | Z | 607 | CHL | NA |
| 30 | 4 | 601 | CHL | NC |
| 30 | 4 | 601 | CHL | ND |
| 30 | 4 | 601 | CHL | NA |
| 30 | 4 | 606 | CHL | NC |
| 30 | 4 | 606 | CHL | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 30 | 4 | 606 | CHL | NA |
| 30 | 4 | 607 | CHL | NC |
| 30 | 4 | 607 | CHL | ND |
| 30 | 4 | 607 | CHL | NA |
| 30 | 4 | 608 | CHL | NC |
| 30 | 4 | 608 | CHL | ND |
| 30 | 4 | 608 | CHL | NA |
| 30 | 4 | 618 | CHL | NC |
| 30 | 4 | 618 | CHL | ND |
| 30 | 4 | 618 | CHL | NA |
| 30 | 5 | 606 | CHL | NC |
| 30 | 5 | 606 | CHL | ND |
| 30 | 5 | 606 | CHL | NA |
| 30 | 5 | 607 | CHL | NC |
| 30 | 5 | 607 | CHL | ND |
| 30 | 5 | 607 | CHL | NA |
| 30 | 5 | 608 | CHL | NC |
| 30 | 5 | 608 | CHL | ND |
| 30 | 5 | 608 | CHL | NA |
| 30 | 5 | 618 | CHL | NC |
| 30 | 5 | 618 | CHL | ND |
| 30 | 5 | 618 | CHL | NA |
| 30 | 6 | 601 | CHL | NC |
| 30 | 6 | 601 | CHL | ND |
| 30 | 6 | 601 | CHL | NA |
| 30 | 6 | 606 | CHL | NC |
| 30 | 6 | 606 | CHL | ND |
| 30 | 6 | 606 | CHL | NA |
| 30 | 6 | 607 | CHL | NC |
| 30 | 6 | 607 | CHL | ND |
| 30 | 6 | 607 | CHL | NA |
| 30 | 6 | 608 | CHL | NC |
| 30 | 6 | 608 | CHL | ND |
| 30 | 6 | 608 | CHL | NA |
| 30 | 6 | 616 | CHL | NC |
| 30 | 6 | 616 | CHL | ND |
| 30 | 6 | 616 | CHL | NA |
| 30 | 6 | 618 | CHL | NC |
| 30 | 6 | 618 | CHL | ND |
| 30 | 6 | 618 | CHL | NA |
| 30 | 9 | 606 | CHL | NC |
| 30 | 9 | 606 | CHL | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 30 | 9 | 606 | CHL | NA |
| 30 | 9 | 607 | CHL | NC |
| 30 | 9 | 607 | CHL | ND |
| 30 | 9 | 607 | CHL | NA |
| 30 | 12 | 601 | CHL | NC |
| 30 | 12 | 601 | CHL | ND |
| 30 | 12 | 601 | CHL | NA |
| 30 | 12 | 606 | CHL | NC |
| 30 | 12 | 606 | CHL | ND |
| 30 | 12 | 606 | CHL | NA |
| 30 | 12 | 607 | CHL | NC |
| 30 | 12 | 607 | CHL | ND |
| 30 | 12 | 607 | CHL | NA |
| 30 | 32 | 608 | CHL | NC |
| 30 | 32 | 608 | CHL | ND |
| 30 | 32 | 608 | CHL | NA |
| 30 | 72 | 601 | CHL | NC |
| 30 | 72 | 601 | CHL | ND |
| 30 | 72 | 601 | CHL | NA |
| 30 | 72 | 606 | CHL | NC |
| 30 | 72 | 606 | CHL | ND |
| 30 | 72 | 606 | CHL | NA |
| 30 | 72 | 607 | CHL | NC |
| 30 | 72 | 607 | CHL | ND |
| 30 | 72 | 607 | CHL | NA |
| 30 | 82 | 601 | CHL | NC |
| 30 | 82 | 601 | CHL | ND |
| 30 | 82 | 601 | CHL | NA |
| 30 | 82 | 606 | CHL | NC |
| 30 | 82 | 606 | CHL | ND |
| 30 | 82 | 606 | CHL | NA |
| 30 | 82 | 607 | CHL | NC |
| 30 | 82 | 607 | CHL | ND |
| 30 | 82 | 607 | CHL | NA |
| 30 | Z2 | 601 | CHL | NC |
| 30 | Z2 | 601 | CHL | ND |
| 30 | Z2 | 601 | CHL | NA |
| 30 | Z2 | 606 | CHL | NC |
| 30 | Z2 | 606 | CHL | ND |
| 30 | Z2 | 606 | CHL | NA |
| 30 | Z2 | 607 | CHL | NC |
| 30 | Z2 | 607 | CHL | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 30 | Z2 | 607 | CHL | NA |
| 30 | 42 | 601 | CHL | NC |
| 30 | 42 | 601 | CHL | ND |
| 30 | 42 | 601 | CHL | NA |
| 30 | 42 | 606 | CHL | NC |
| 30 | 42 | 606 | CHL | ND |
| 30 | 42 | 606 | CHL | NA |
| 30 | 42 | 607 | CHL | NC |
| 30 | 42 | 607 | CHL | ND |
| 30 | 42 | 607 | CHL | NA |
| 30 | 42 | 608 | CHL | NC |
| 30 | 42 | 608 | CHL | ND |
| 30 | 42 | 608 | CHL | NA |
| 30 | 42 | 618 | CHL | NC |
| 30 | 42 | 618 | CHL | ND |
| 30 | 42 | 618 | CHL | NA |
| 30 | 52 | 606 | CHL | NC |
| 30 | 52 | 606 | CHL | ND |
| 30 | 52 | 606 | CHL | NA |
| 30 | 52 | 607 | CHL | NC |
| 30 | 52 | 607 | CHL | ND |
| 30 | 52 | 607 | CHL | NA |
| 30 | 52 | 608 | CHL | NC |
| 30 | 52 | 608 | CHL | ND |
| 30 | 52 | 608 | CHL | NA |
| 30 | 52 | 618 | CHL | NC |
| 30 | 52 | 618 | CHL | ND |
| 30 | 52 | 618 | CHL | NA |
| 30 | 62 | 601 | CHL | NC |
| 30 | 62 | 601 | CHL | ND |
| 30 | 62 | 601 | CHL | NA |
| 30 | 62 | 606 | CHL | NC |
| 30 | 62 | 606 | CHL | ND |
| 30 | 62 | 606 | CHL | NA |
| 30 | 62 | 607 | CHL | NC |
| 30 | 62 | 607 | CHL | ND |
| 30 | 62 | 607 | CHL | NA |
| 30 | 62 | 608 | CHL | NC |
| 30 | 62 | 608 | CHL | ND |
| 30 | 62 | 608 | CHL | NA |
| 30 | 62 | 616 | CHL | NC |
| 30 | 62 | 616 | CHL | ND |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 30 | 62 | 616 | CHL | NA |
| 30 | 62 | 618 | CHL | NC |
| 30 | 62 | 618 | CHL | ND |
| 30 | 62 | 618 | CHL | NA |
| 30 | 92 | 606 | CHL | NC |
| 30 | 92 | 606 | CHL | ND |
| 30 | 92 | 606 | CHL | NA |
| 30 | 92 | 607 | CHL | NC |
| 30 | 92 | 607 | CHL | ND |
| 30 | 92 | 607 | CHL | NA |
| 31 | 5 | 624 | XAT | C26 |
| 31 | 52 | 624 | XAT | C26 |

All (2606) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 806 | CLA | CAD-CBD-CGD-O1D |
| 21 | A | 806 | CLA | CAD-CBD-CGD-O2D |
| 21 | A | 806 | CLA | C4-C3-C5-C6 |
| 21 | A | 809 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 809 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 816 | CLA | O2A-C1-C2-C3 |
| 21 | A | 817 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 817 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 821 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 821 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 823 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 823 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 825 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 831 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 831 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 834 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 834 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 835 | CLA | CHA-CBD-CGD-O1D |
| 21 | A | 835 | CLA | CHA-CBD-CGD-O2D |
| 21 | A | 841 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 841 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 842 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 842 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 845 | CLA | CAD-CBD-CGD-O1D |
| 21 | A | 845 | CLA | CAD-CBD-CGD-O2D |
| 21 | B | 804 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 804 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 808 | CLA | CHA-CBD-CGD-O1D |
| 21 | B | 808 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 815 | CLA | CHA-CBD-CGD-O1D |
| 21 | B | 815 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 817 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 817 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 819 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 819 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 821 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 825 | CLA | CHA-CBD-CGD-O1D |
| 21 | B | 825 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 828 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 833 | CLA | CHA-CBD-CGD-O1D |
| 21 | B | 833 | CLA | CHA-CBD-CGD-O2D |
| 21 | F | 304 | CLA | C1A-C2A-CAA-CBA |
| 21 | F | 304 | CLA | C2-C1-O2A-CGA |
| 21 | G | 204 | CLA | CHA-CBD-CGD-O1D |
| 21 | G | 204 | CLA | CHA-CBD-CGD-O2D |
| 21 | K | 201 | CLA | C2B-C3B-CAB-CBB |
| 21 | K | 201 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 610 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 7 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 7 | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | 7 | 610 | CLA | C3A-C2A-CAA-CBA |
| 21 | 7 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 614 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 7 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 620 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 620 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 8 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 8 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 8 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 8 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | Z | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 4 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 4 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 610 | CLA | C4-C3-C5-C6 |
| 21 | 4 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 4 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 4 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 4 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 5 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 6 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 6 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 6 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 9 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 9 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 609 | CLA | C4-C3-C5-C6 |
| 21 | 9 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 9 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 9 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 806 | CLA | CAD-CBD-CGD-O1D |
| 21 | A2 | 806 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 806 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 809 | CLA | CHA-CBD-CGD-O1D |
| 21 | A2 | 809 | CLA | CHA-CBD-CGD-O2D |
| 21 | A2 | 816 | CLA | O2A-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A2 | 817 | CLA | CHA-CBD-CGD-O1D |
| 21 | A2 | 817 | CLA | CHA-CBD-CGD-O2D |
| 21 | A2 | 821 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 821 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 823 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 823 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 825 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 831 | CLA | CHA-CBD-CGD-O1D |
| 21 | A2 | 831 | CLA | CHA-CBD-CGD-O2D |
| 21 | A2 | 834 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 834 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 835 | CLA | CHA-CBD-CGD-O1D |
| 21 | A2 | 835 | CLA | CHA-CBD-CGD-O2D |
| 21 | A2 | 841 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 841 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 842 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 842 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 845 | CLA | CAD-CBD-CGD-O1D |
| 21 | A2 | 845 | CLA | CAD-CBD-CGD-O2D |
| 21 | B2 | 804 | CLA | CHA-CBD-CGD-O1D |
| 21 | B2 | 804 | CLA | CHA-CBD-CGD-O2D |
| 21 | B2 | 808 | CLA | CHA-CBD-CGD-O1D |
| 21 | B2 | 808 | CLA | CHA-CBD-CGD-O2D |
| 21 | B2 | 815 | CLA | CHA-CBD-CGD-O1D |
| 21 | B2 | 815 | CLA | CHA-CBD-CGD-O2D |
| 21 | B2 | 817 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 817 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 819 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 819 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 821 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 825 | CLA | CHA-CBD-CGD-O1D |
| 21 | B2 | 825 | CLA | CHA-CBD-CGD-O2D |
| 21 | B2 | 828 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 833 | CLA | CHA-CBD-CGD-O1D |
| 21 | B2 | 833 | CLA | CHA-CBD-CGD-O2D |
| 21 | F2 | 304 | CLA | C1A-C2A-CAA-CBA |
| 21 | F2 | 304 | CLA | C2-C1-O2A-CGA |
| 21 | G2 | 204 | CLA | CHA-CBD-CGD-O1D |
| 21 | G2 | 204 | CLA | CHA-CBD-CGD-O2D |
| 21 | K2 | 201 | CLA | C2B-C3B-CAB-CBB |
| 21 | K2 | 201 | CLA | C4B-C3B-CAB-CBB |
| 21 | 12 | 610 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 12 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 12 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 12 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 12 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 12 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 12 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 12 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 32 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 32 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 32 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 32 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 32 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 72 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 72 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 72 | 610 | CLA | C1A-C2A-CAA-CBA |
| 21 | 72 | 610 | CLA | C3A-C2A-CAA-CBA |
| 21 | 72 | 610 | CLA | C4B-C3B-CAB-CBB |
| 21 | 72 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 72 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 72 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 72 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 72 | 620 | CLA | C2B-C3B-CAB-CBB |
| 21 | 72 | 620 | CLA | C4B-C3B-CAB-CBB |
| 21 | 82 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 82 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 82 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 82 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 82 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z2 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | Z2 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 42 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 42 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 42 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 42 | 610 | CLA | C4-C3-C5-C6 |
| 21 | 42 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 42 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 42 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 42 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 42 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 52 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 62 | 602 | CLA | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 62 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 62 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | 62 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 92 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 92 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 92 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | 92 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 92 | 609 | CLA | C4-C3-C5-C6 |
| 21 | 92 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 92 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 92 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 92 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 92 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 92 | 614 | CLA | C4B-C3B-CAB-CBB |
| 23 | A | 846 | LHG | C3-O3-P-O5 |
| 23 | A | 846 | LHG | C4-O6-P-O3 |
| 23 | A | 846 | LHG | C4-O6-P-O5 |
| 23 | A | 847 | LHG | C4-O6-P-O3 |
| 23 | 1 | 620 | LHG | C3-O3-P-O6 |
| 23 | 3 | 721 | LHG | C2-C3-O3-P |
| 23 | 3 | 721 | LHG | C3-O3-P-O4 |
| 23 | 3 | 721 | LHG | C4-O6-P-O3 |
| 23 | 3 | 721 | LHG | C4-O6-P-O5 |
| 23 | 3 | 623 | LHG | O2-C2-C3-O3 |
| 23 | 3 | 623 | LHG | C3-O3-P-O5 |
| 23 | 3 | 623 | LHG | C3-O3-P-O6 |
| 23 | 3 | 623 | LHG | O6-C4-C5-O7 |
| 23 | 7 | 625 | LHG | C1-C2-C3-O3 |
| 23 | 7 | 625 | LHG | C3-O3-P-O4 |
| 23 | 7 | 625 | LHG | C3-O3-P-O5 |
| 23 | 7 | 625 | LHG | C3-O3-P-O6 |
| 23 | 8 | 620 | LHG | C3-O3-P-O5 |
| 23 | 8 | 620 | LHG | C3-O3-P-O6 |
| 23 | 8 | 620 | LHG | C4-O6-P-O3 |
| 23 | 8 | 620 | LHG | C4-O6-P-O4 |
| 23 | 4 | 622 | LHG | C2-C3-O3-P |
| 23 | 4 | 622 | LHG | C3-O3-P-O4 |
| 23 | 4 | 622 | LHG | C3-O3-P-O6 |
| 23 | 4 | 623 | LHG | C3-O3-P-O4 |
| 23 | 4 | 623 | LHG | C3-O3-P-O5 |
| 23 | 4 | 623 | LHG | C3-O3-P-O6 |
| 23 | 4 | 623 | LHG | C4-O6-P-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | 4 | 623 | LHG | C4-O6-P-O4 |
| 23 | 4 | 623 | LHG | C4-O6-P-O5 |
| 23 | 5 | 623 | LHG | C3-O3-P-O5 |
| 23 | 5 | 623 | LHG | C3-O3-P-O6 |
| 23 | 5 | 623 | LHG | C4-O6-P-O3 |
| 23 | 5 | 623 | LHG | C4-O6-P-O4 |
| 23 | 5 | 623 | LHG | C4-O6-P-O5 |
| 23 | 6 | 629 | LHG | C1-C2-C3-O3 |
| 23 | 6 | 629 | LHG | C4-O6-P-O3 |
| 23 | 6 | 629 | LHG | C4-O6-P-O4 |
| 23 | 6 | 629 | LHG | C4-O6-P-O5 |
| 23 | 9 | 622 | LHG | C1-C2-C3-O3 |
| 23 | 9 | 622 | LHG | C4-O6-P-O4 |
| 23 | A2 | 846 | LHG | C3-O3-P-O5 |
| 23 | A2 | 846 | LHG | C4-O6-P-O3 |
| 23 | A2 | 846 | LHG | C4-O6-P-O5 |
| 23 | A2 | 847 | LHG | C4-O6-P-O3 |
| 23 | 12 | 620 | LHG | C3-O3-P-O6 |
| 23 | 32 | 721 | LHG | C2-C3-O3-P |
| 23 | 32 | 721 | LHG | C3-O3-P-O4 |
| 23 | 32 | 721 | LHG | C4-O6-P-O3 |
| 23 | 32 | 721 | LHG | C4-O6-P-O5 |
| 23 | 32 | 623 | LHG | O2-C2-C3-O3 |
| 23 | 32 | 623 | LHG | C3-O3-P-O5 |
| 23 | 32 | 623 | LHG | C3-O3-P-O6 |
| 23 | 32 | 623 | LHG | O6-C4-C5-O7 |
| 23 | 72 | 625 | LHG | C1-C2-C3-O3 |
| 23 | 72 | 625 | LHG | C3-O3-P-O4 |
| 23 | 72 | 625 | LHG | C3-O3-P-O5 |
| 23 | 72 | 625 | LHG | C3-O3-P-O6 |
| 23 | 82 | 620 | LHG | C3-O3-P-O5 |
| 23 | 82 | 620 | LHG | C3-O3-P-O6 |
| 23 | 82 | 620 | LHG | C4-O6-P-O3 |
| 23 | 82 | 620 | LHG | C4-O6-P-O4 |
| 23 | 42 | 622 | LHG | C2-C3-O3-P |
| 23 | 42 | 622 | LHG | C3-O3-P-O4 |
| 23 | 42 | 622 | LHG | C3-O3-P-O6 |
| 23 | 42 | 623 | LHG | C3-O3-P-O4 |
| 23 | 42 | 623 | LHG | C3-O3-P-O5 |
| 23 | 42 | 623 | LHG | C3-O3-P-O6 |
| 23 | 42 | 623 | LHG | C4-O6-P-O3 |
| 23 | 42 | 623 | LHG | C4-O6-P-O4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | 42 | 623 | LHG | C4-O6-P-O5 |
| 23 | 52 | 623 | LHG | C3-O3-P-O5 |
| 23 | 52 | 623 | LHG | C3-O3-P-O6 |
| 23 | 52 | 623 | LHG | C4-O6-P-O3 |
| 23 | 52 | 623 | LHG | C4-O6-P-O4 |
| 23 | 52 | 623 | LHG | C4-O6-P-O5 |
| 23 | 62 | 629 | LHG | C1-C2-C3-O3 |
| 23 | 62 | 629 | LHG | C4-O6-P-O3 |
| 23 | 62 | 629 | LHG | C4-O6-P-O4 |
| 23 | 62 | 629 | LHG | C4-O6-P-O5 |
| 23 | 92 | 622 | LHG | C1-C2-C3-O3 |
| 23 | 92 | 622 | LHG | C3-O3-P-O5 |
| 23 | 92 | 622 | LHG | C4-O6-P-O4 |
| 24 | A | 851 | BCR | C23-C24-C25-C26 |
| 24 | A | 851 | BCR | C23-C24-C25-C30 |
| 24 | J | 102 | BCR | C23-C24-C25-C26 |
| 24 | 3 | 620 | BCR | C1-C6-C7-C8 |
| 24 | 3 | 620 | BCR | C5-C6-C7-C8 |
| 24 | 8 | 619 | BCR | C1-C6-C7-C8 |
| 24 | 8 | 619 | BCR | C5-C6-C7-C8 |
| 24 | 9 | 623 | BCR | C23-C24-C25-C26 |
| 24 | A2 | 851 | BCR | C23-C24-C25-C26 |
| 24 | A2 | 851 | BCR | C23-C24-C25-C30 |
| 24 | J2 | 102 | BCR | C23-C24-C25-C26 |
| 24 | 32 | 620 | BCR | C1-C6-C7-C8 |
| 24 | 32 | 620 | BCR | C5-C6-C7-C8 |
| 24 | 82 | 619 | BCR | C1-C6-C7-C8 |
| 24 | 82 | 619 | BCR | C5-C6-C7-C8 |
| 24 | 92 | 623 | BCR | C23-C24-C25-C26 |
| 26 | A | 858 | LMU | O5'-C1'-O1'-C1 |
| 26 | A | 865 | LMU | C2'-C1'-O1'-C1 |
| 26 | A | 865 | LMU | O5'-C1'-O1'-C1 |
| 26 | A | 864 | LMU | O5'-C1'-O1'-C1 |
| 26 | B | 853 | LMU | O5'-C1'-O1'-C1 |
| 26 | 1 | 627 | LMU | C2'-C1'-O1'-C1 |
| 26 | 1 | 627 | LMU | O5'-C1'-O1'-C1 |
| 26 | 7 | 628 | LMU | C2'-C1'-O1'-C1 |
| 26 | 7 | 628 | LMU | O5'-C1'-O1'-C1 |
| 26 | 7 | 628 | LMU | C2-C1-O1'-C1' |
| 26 | 7 | 629 | LMU | C2'-C1'-O1'-C1 |
| 26 | 7 | 629 | LMU | O5'-C1'-O1'-C1 |
| 26 | 5 | 627 | LMU | C2-C1-O1'-C1' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | 6 | 632 | LMU | C2'-C1'-O1'-C1 |
| 26 | 6 | 632 | LMU | O5'-C1'-O1'-C1 |
| 26 | 6 | 632 | LMU | C2-C1-O1'-C1' |
| 26 | 6 | 628 | LMU | O5'-C1'-O1'-C1 |
| 26 | A2 | 858 | LMU | O5'-C1'-O1'-C1 |
| 26 | A2 | 865 | LMU | C2'-C1'-O1'-C1 |
| 26 | A2 | 865 | LMU | O5'-C1'-O1'-C1 |
| 26 | A2 | 864 | LMU | O5'-C1'-O1'-C1 |
| 26 | B2 | 853 | LMU | O5'-C1'-O1'-C1 |
| 26 | 12 | 627 | LMU | C2'-C1'-O1'-C1 |
| 26 | 12 | 627 | LMU | O5'-C1'-O1'-C1 |
| 26 | 72 | 628 | LMU | C2'-C1'-O1'-C1 |
| 26 | 72 | 628 | LMU | O5'-C1'-O1'-C1 |
| 26 | 72 | 628 | LMU | C2-C1-O1'-C1' |
| 26 | 72 | 629 | LMU | C2'-C1'-O1'-C1 |
| 26 | 72 | 629 | LMU | O5'-C1'-O1'-C1 |
| 26 | 52 | 627 | LMU | C2-C1-O1'-C1' |
| 26 | 62 | 632 | LMU | C2'-C1'-O1'-C1 |
| 26 | 62 | 632 | LMU | O5'-C1'-O1'-C1 |
| 26 | 62 | 632 | LMU | C2-C1-O1'-C1' |
| 26 | 62 | 628 | LMU | O5'-C1'-O1'-C1 |
| 27 | A | 859 | LMG | O6-C1-O1-C7 |
| 27 | B | 854 | LMG | C2-C1-O1-C7 |
| 27 | B | 854 | LMG | O6-C1-O1-C7 |
| 27 | 7 | 626 | LMG | O6-C1-O1-C7 |
| 27 | 8 | 626 | LMG | C2-C1-O1-C7 |
| 27 | 8 | 626 | LMG | O6-C1-O1-C7 |
| 27 | 8 | 629 | LMG | C2-C1-O1-C7 |
| 27 | 8 | 629 | LMG | O6-C1-O1-C7 |
| 27 | 4 | 624 | LMG | O6-C1-O1-C7 |
| 27 | A2 | 859 | LMG | O6-C1-O1-C7 |
| 27 | B2 | 854 | LMG | C2-C1-O1-C7 |
| 27 | B2 | 854 | LMG | O6-C1-O1-C7 |
| 27 | 72 | 626 | LMG | O6-C1-O1-C7 |
| 27 | 82 | 626 | LMG | C2-C1-O1-C7 |
| 27 | 82 | 626 | LMG | O6-C1-O1-C7 |
| 27 | 82 | 629 | LMG | C2-C1-O1-C7 |
| 27 | 82 | 629 | LMG | O6-C1-O1-C7 |
| 27 | 42 | 624 | LMG | O6-C1-O1-C7 |
| 28 | A | 856 | LUT | C5-C6-C7-C8 |
| 28 | A | 856 | LUT | C21-C26-C27-C28 |
| 28 | A | 856 | LUT | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | F | 305 | LUT | C1-C6-C7-C8 |
| 28 | F | 305 | LUT | C5-C6-C7-C8 |
| 28 | F | 305 | LUT | C25-C26-C27-C28 |
| 28 | 7 | 624 | LUT | C21-C26-C27-C28 |
| 28 | 7 | 624 | LUT | C25-C26-C27-C28 |
| 28 | 7 | 624 | LUT | C27-C28-C29-C30 |
| 28 | 5 | 626 | LUT | C25-C26-C27-C28 |
| 28 | A2 | 856 | LUT | C1-C6-C7-C8 |
| 28 | A2 | 856 | LUT | C5-C6-C7-C8 |
| 28 | A2 | 856 | LUT | C21-C26-C27-C28 |
| 28 | A2 | 856 | LUT | C25-C26-C27-C28 |
| 28 | F2 | 305 | LUT | C1-C6-C7-C8 |
| 28 | F2 | 305 | LUT | C5-C6-C7-C8 |
| 28 | F2 | 305 | LUT | C25-C26-C27-C28 |
| 28 | 72 | 624 | LUT | C21-C26-C27-C28 |
| 28 | 72 | 624 | LUT | C25-C26-C27-C28 |
| 28 | 72 | 624 | LUT | C27-C28-C29-C30 |
| 28 | 52 | 626 | LUT | C25-C26-C27-C28 |
| 29 | B | 850 | DGD | O6D-C1D-O3G-C3G |
| 29 | B2 | 850 | DGD | O6D-C1D-O3G-C3G |
| 30 | 8 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 8 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 5 | 607 | CHL | CHA-CBD-CGD-O1D |
| 30 | 5 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 9 | 607 | CHL | C1A-C2A-CAA-CBA |
| 30 | 82 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 82 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 52 | 607 | CHL | CHA-CBD-CGD-O1D |
| 30 | 52 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 92 | 607 | CHL | C1A-C2A-CAA-CBA |
| 26 | A | 858 | LMU | O5B-C1B-O1B-C4' |
| 26 | A2 | 858 | LMU | O5B-C1B-O1B-C4' |
| 26 | A | 858 | LMU | C2B-C1B-O1B-C4' |
| 26 | A2 | 858 | LMU | C2B-C1B-O1B-C4' |
| 26 | 8 | 627 | LMU | O5B-C1B-O1B-C4' |
| 26 | 82 | 627 | LMU | O5B-C1B-O1B-C4' |
| 21 | B | 806 | CLA | C3-C5-C6-C7 |
| 21 | B2 | 806 | CLA | C3-C5-C6-C7 |
| 30 | 9 | 607 | CHL | CBD-CGD-O2D-CED |
| 26 | A | 863 | LMU | O5B-C1B-O1B-C4' |
| 26 | A2 | 863 | LMU | O5B-C1B-O1B-C4' |
| 21 | B | 822 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 840 | CLA | C4-C3-C5-C6 |
| 21 | J | 101 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 611 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 617 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 822 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 840 | CLA | C4-C3-C5-C6 |
| 21 | J2 | 101 | CLA | C4-C3-C5-C6 |
| 21 | 12 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 611 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 617 | CLA | C4-C3-C5-C6 |
| 30 | 1 | 601 | CHL | C4-C3-C5-C6 |
| 30 | 8 | 607 | CHL | C4-C3-C5-C6 |
| 30 | 12 | 601 | CHL | C4-C3-C5-C6 |
| 30 | 82 | 607 | CHL | C4-C3-C5-C6 |
| 21 | A | 806 | CLA | C2-C3-C5-C6 |
| 21 | B | 822 | CLA | C2-C3-C5-C6 |
| 21 | J | 101 | CLA | C2-C3-C5-C6 |
| 21 | 1 | 603 | CLA | C2-C3-C5-C6 |
| 21 | 4 | 610 | CLA | C2-C3-C5-C6 |
| 21 | 4 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 611 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 617 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 806 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 822 | CLA | C2-C3-C5-C6 |
| 21 | J2 | 101 | CLA | C2-C3-C5-C6 |
| 21 | 12 | 603 | CLA | C2-C3-C5-C6 |
| 21 | 42 | 610 | CLA | C2-C3-C5-C6 |
| 21 | 42 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 52 | 611 | CLA | C2-C3-C5-C6 |
| 21 | 52 | 617 | CLA | C2-C3-C5-C6 |
| 30 | 1 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 8 | 607 | CHL | C2-C3-C5-C6 |
| 30 | 12 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 82 | 607 | CHL | C2-C3-C5-C6 |
| 21 | 5 | 603 | CLA | C2A-CAA-CBA-CGA |
| 21 | 52 | 603 | CLA | C2A-CAA-CBA-CGA |
| 26 | A | 863 | LMU | C2B-C1B-O1B-C4' |
| 26 | A2 | 863 | LMU | C2B-C1B-O1B-C4' |
| 26 | 8 | 627 | LMU | C2B-C1B-O1B-C4' |
| 26 | 82 | 627 | LMU | C2B-C1B-O1B-C4' |
| 21 | B | 808 | CLA | C3-C5-C6-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B2 | 808 | CLA | C3-C5-C6-C7 |
| 21 | 5 | 621 | CLA | C2C-C3C-CAC-CBC |
| 21 | 52 | 621 | CLA | C2C-C3C-CAC-CBC |
| 26 | B | 853 | LMU | C2B-C1B-O1B-C4' |
| 26 | B2 | 853 | LMU | C2B-C1B-O1B-C4' |
| 23 | 3 | 721 | LHG | O2-C2-C3-O3 |
| 23 | 7 | 625 | LHG | O2-C2-C3-O3 |
| 23 | 4 | 623 | LHG | O2-C2-C3-O3 |
| 23 | 6 | 629 | LHG | O2-C2-C3-O3 |
| 23 | 9 | 622 | LHG | O2-C2-C3-O3 |
| 23 | 32 | 721 | LHG | O2-C2-C3-O3 |
| 23 | 72 | 625 | LHG | O2-C2-C3-O3 |
| 23 | 42 | 623 | LHG | O2-C2-C3-O3 |
| 23 | 62 | 629 | LHG | O2-C2-C3-O3 |
| 23 | 92 | 622 | LHG | O2-C2-C3-O3 |
| 26 | 8 | 627 | LMU | C5'-C4'-O1B-C1B |
| 26 | 82 | 627 | LMU | C5'-C4'-O1B-C1B |
| 21 | A | 825 | CLA | C3-C5-C6-C7 |
| 21 | A2 | 825 | CLA | C3-C5-C6-C7 |
| 21 | A | 829 | CLA | C4-C3-C5-C6 |
| 21 | B | 833 | CLA | C4-C3-C5-C6 |
| 21 | L | 203 | CLA | C4-C3-C5-C6 |
| 21 | 8 | 612 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 829 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 833 | CLA | C4-C3-C5-C6 |
| 21 | L2 | 203 | CLA | C4-C3-C5-C6 |
| 21 | 82 | 612 | CLA | C4-C3-C5-C6 |
| 21 | A | 829 | CLA | C2-C3-C5-C6 |
| 21 | B | 833 | CLA | C2-C3-C5-C6 |
| 21 | B | 840 | CLA | C2-C3-C5-C6 |
| 21 | 7 | 612 | CLA | C2-C3-C5-C6 |
| 21 | 8 | 612 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 829 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 833 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 840 | CLA | C2-C3-C5-C6 |
| 21 | 72 | 612 | CLA | C2-C3-C5-C6 |
| 21 | 82 | 612 | CLA | C2-C3-C5-C6 |
| 23 | 6 | 629 | LHG | C2-C3-O3-P |
| 23 | 62 | 629 | LHG | C2-C3-O3-P |
| 26 | G | 206 | LMU | O5'-C1'-O1'-C1 |
| 26 | 1 | 622 | LMU | O5'-C1'-O1'-C1 |
| 26 | 7 | 627 | LMU | O5'-C1'-O1'-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | 8 | 628 | LMU | O5'-C1'-O1'-C1 |
| 26 | Z | 621 | LMU | O5'-C1'-O1'-C1 |
| 26 | 4 | 625 | LMU | O5'-C1'-O1'-C1 |
| 26 | 6 | 631 | LMU | O5'-C1'-O1'-C1 |
| 26 | G2 | 206 | LMU | O5'-C1'-O1'-C1 |
| 26 | 12 | 622 | LMU | O5'-C1'-O1'-C1 |
| 26 | 72 | 627 | LMU | O5'-C1'-O1'-C1 |
| 26 | 82 | 628 | LMU | O5'-C1'-O1'-C1 |
| 26 | Z2 | 621 | LMU | O5'-C1'-O1'-C1 |
| 26 | 42 | 625 | LMU | O5'-C1'-O1'-C1 |
| 26 | 62 | 631 | LMU | O5'-C1'-O1'-C1 |
| 27 | A | 860 | LMG | O6-C1-O1-C7 |
| 27 | 9 | 620 | LMG | O6-C1-O1-C7 |
| 27 | A2 | 860 | LMG | O6-C1-O1-C7 |
| 27 | 92 | 620 | LMG | O6-C1-O1-C7 |
| 23 | 1 | 620 | LHG | C1-C2-C3-O3 |
| 23 | 3 | 623 | LHG | C1-C2-C3-O3 |
| 23 | 12 | 620 | LHG | C1-C2-C3-O3 |
| 23 | 32 | 623 | LHG | C1-C2-C3-O3 |
| 21 | 7 | 612 | CLA | C4-C3-C5-C6 |
| 21 | Z | 603 | CLA | C4-C3-C5-C6 |
| 21 | 72 | 612 | CLA | C4-C3-C5-C6 |
| 21 | Z2 | 603 | CLA | C4-C3-C5-C6 |
| 21 | L | 203 | CLA | C2-C3-C5-C6 |
| 21 | Z | 603 | CLA | C2-C3-C5-C6 |
| 21 | L2 | 203 | CLA | C2-C3-C5-C6 |
| 21 | Z2 | 603 | CLA | C2-C3-C5-C6 |
| 21 | A | 806 | CLA | C11-C10-C8-C9 |
| 21 | B | 808 | CLA | C14-C13-C15-C16 |
| 21 | B | 809 | CLA | C6-C7-C8-C9 |
| 21 | G | 203 | CLA | C6-C7-C8-C9 |
| 21 | 1 | 609 | CLA | C11-C10-C8-C9 |
| 21 | 4 | 609 | CLA | C11-C10-C8-C9 |
| 21 | 5 | 603 | CLA | C11-C10-C8-C9 |
| 21 | 5 | 603 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 806 | CLA | C11-C10-C8-C9 |
| 21 | B2 | 808 | CLA | C14-C13-C15-C16 |
| 21 | B2 | 809 | CLA | C6-C7-C8-C9 |
| 21 | G2 | 203 | CLA | C6-C7-C8-C9 |
| 21 | 12 | 609 | CLA | C11-C10-C8-C9 |
| 21 | 42 | 609 | CLA | C11-C10-C8-C9 |
| 21 | 52 | 603 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 52 | 603 | CLA | C14-C13-C15-C16 |
| 30 | 1 | 601 | CHL | C6-C7-C8-C9 |
| 30 | 12 | 601 | CHL | C6-C7-C8-C9 |
| 26 | A | 858 | LMU | C2'-C1'-O1'-C1 |
| 26 | G | 206 | LMU | C2'-C1'-O1'-C1 |
| 26 | 1 | 622 | LMU | C2'-C1'-O1'-C1 |
| 26 | 7 | 627 | LMU | C2'-C1'-O1'-C1 |
| 26 | 8 | 628 | LMU | C2'-C1'-O1'-C1 |
| 26 | Z | 621 | LMU | C2'-C1'-O1'-C1 |
| 26 | 4 | 625 | LMU | C2'-C1'-O1'-C1 |
| 26 | 6 | 628 | LMU | C2'-C1'-O1'-C1 |
| 26 | 6 | 631 | LMU | C2'-C1'-O1'-C1 |
| 26 | A2 | 858 | LMU | C2'-C1'-O1'-C1 |
| 26 | G2 | 206 | LMU | C2'-C1'-O1'-C1 |
| 26 | 12 | 622 | LMU | C2'-C1'-O1'-C1 |
| 26 | 72 | 627 | LMU | C2'-C1'-O1'-C1 |
| 26 | 82 | 628 | LMU | C2'-C1'-O1'-C1 |
| 26 | Z2 | 621 | LMU | C2'-C1'-O1'-C1 |
| 26 | 42 | 625 | LMU | C2'-C1'-O1'-C1 |
| 26 | 62 | 628 | LMU | C2'-C1'-O1'-C1 |
| 26 | 62 | 631 | LMU | C2'-C1'-O1'-C1 |
| 27 | A | 859 | LMG | C2-C1-O1-C7 |
| 27 | A | 860 | LMG | C2-C1-O1-C7 |
| 27 | 7 | 626 | LMG | C2-C1-O1-C7 |
| 27 | 9 | 620 | LMG | C2-C1-O1-C7 |
| 27 | A2 | 859 | LMG | C2-C1-O1-C7 |
| 27 | A2 | 860 | LMG | C2-C1-O1-C7 |
| 27 | 72 | 626 | LMG | C2-C1-O1-C7 |
| 27 | 92 | 620 | LMG | C2-C1-O1-C7 |
| 29 | B | 850 | DGD | C2D-C1D-O3G-C3G |
| 29 | B2 | 850 | DGD | C2D-C1D-O3G-C3G |
| 23 | 1 | 620 | LHG | O2-C2-C3-O3 |
| 23 | 12 | 620 | LHG | O2-C2-C3-O3 |
| 28 | 7 | 624 | LUT | C27-C28-C29-C39 |
| 28 | 72 | 624 | LUT | C27-C28-C29-C39 |
| 21 | A | 830 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 830 | CLA | C2A-CAA-CBA-CGA |
| 30 | 6 | 616 | CHL | C8-C10-C11-C12 |
| 26 | B | 853 | LMU | O5B-C1B-O1B-C4' |
| 26 | B2 | 853 | LMU | O5B-C1B-O1B-C4' |
| 30 | 62 | 616 | CHL | C8-C10-C11-C12 |
| 21 | B | 839 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B2 | 839 | CLA | C2A-CAA-CBA-CGA |
| 21 | 12 | 611 | CLA | C5-C6-C7-C8 |
| 26 | A | 862 | LMU | O5'-C1'-O1'-C1 |
| 26 | A | 861 | LMU | O5'-C1'-O1'-C1 |
| 26 | A2 | 862 | LMU | O5'-C1'-O1'-C1 |
| 26 | A2 | 861 | LMU | O5'-C1'-O1'-C1 |
| 21 | B | 803 | CLA | C10-C11-C12-C13 |
| 21 | B | 818 | CLA | C13-C15-C16-C17 |
| 21 | 1 | 611 | CLA | C5-C6-C7-C8 |
| 21 | 5 | 617 | CLA | C8-C10-C11-C12 |
| 21 | B2 | 803 | CLA | C10-C11-C12-C13 |
| 21 | B2 | 818 | CLA | C13-C15-C16-C17 |
| 21 | 52 | 617 | CLA | C8-C10-C11-C12 |
| 23 | 8 | 620 | LHG | O2-C2-C3-O3 |
| 23 | 82 | 620 | LHG | O2-C2-C3-O3 |
| 27 | 4 | 624 | LMG | C10-C11-C12-C13 |
| 27 | 42 | 624 | LMG | C10-C11-C12-C13 |
| 21 | 5 | 609 | CLA | C10-C11-C12-C13 |
| 21 | 52 | 609 | CLA | C10-C11-C12-C13 |
| 26 | 8 | 627 | LMU | C3'-C4'-O1B-C1B |
| 21 | Z | 604 | CLA | C3-C5-C6-C7 |
| 21 | Z2 | 604 | CLA | C3-C5-C6-C7 |
| 30 | 9 | 607 | CHL | O1D-CGD-O2D-CED |
| 26 | 82 | 627 | LMU | C3'-C4'-O1B-C1B |
| 21 | 5 | 621 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 818 | CLA | C3-C5-C6-C7 |
| 21 | 4 | 603 | CLA | C3-C5-C6-C7 |
| 21 | A2 | 818 | CLA | C3-C5-C6-C7 |
| 21 | 42 | 603 | CLA | C3-C5-C6-C7 |
| 23 | 8 | 620 | LHG | C1-C2-C3-O3 |
| 23 | 4 | 623 | LHG | C1-C2-C3-O3 |
| 23 | 82 | 620 | LHG | C1-C2-C3-O3 |
| 23 | 42 | 623 | LHG | C1-C2-C3-O3 |
| 21 | 7 | 616 | CLA | C2A-CAA-CBA-CGA |
| 21 | 72 | 616 | CLA | C2A-CAA-CBA-CGA |
| 21 | 52 | 621 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 840 | CLA | C15-C16-C17-C18 |
| 21 | A2 | 840 | CLA | C15-C16-C17-C18 |
| 21 | A | 813 | CLA | C15-C16-C17-C18 |
| 21 | A2 | 813 | CLA | C15-C16-C17-C18 |
| 26 | A | 862 | LMU | C2'-C1'-O1'-C1 |
| 26 | A | 863 | LMU | C2'-C1'-O1'-C1 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | B | 853 | LMU | C2'-C1'-O1'-C1 |
| 26 | K | 208 | LMU | C2'-C1'-O1'-C1 |
| 26 | A2 | 862 | LMU | C2'-C1'-O1'-C1 |
| 26 | A2 | 863 | LMU | C2'-C1'-O1'-C1 |
| 26 | B2 | 853 | LMU | C2'-C1'-O1'-C1 |
| 26 | K2 | 208 | LMU | C2'-C1'-O1'-C1 |
| 23 | B | 851 | LHG | O2-C2-C3-O3 |
| 23 | B2 | 851 | LHG | O2-C2-C3-O3 |
| 21 | B | 823 | CLA | C2A-CAA-CBA-CGA |
| 21 | 1 | 614 | CLA | C2A-CAA-CBA-CGA |
| 21 | B2 | 823 | CLA | C2A-CAA-CBA-CGA |
| 21 | 12 | 614 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 843 | CLA | O2A-C1-C2-C3 |
| 21 | A2 | 843 | CLA | O2A-C1-C2-C3 |
| 29 | B | 850 | DGD | O6E-C5E-C6E-O5E |
| 30 | 9 | 607 | CHL | CBA-CGA-O2A-C1 |
| 21 | 3 | 603 | CLA | C8-C10-C11-C12 |
| 21 | 32 | 603 | CLA | C8-C10-C11-C12 |
| 30 | 92 | 607 | CHL | CBD-CGD-O2D-CED |
| 27 | 6 | 633 | LMG | C17-C18-C19-C20 |
| 27 | 62 | 633 | LMG | C17-C18-C19-C20 |
| 21 | B | 820 | CLA | C5-C6-C7-C8 |
| 30 | Z | 607 | CHL | C10-C11-C12-C13 |
| 30 | Z2 | 607 | CHL | C10-C11-C12-C13 |
| 23 | 42 | 622 | LHG | C9-C10-C11-C12 |
| 23 | 4 | 622 | LHG | C9-C10-C11-C12 |
| 29 | B | 850 | DGD | C3A-C4A-C5A-C6A |
| 26 | 7 | 629 | LMU | O5'-C5'-C6'-O6' |
| 26 | 1 | 627 | LMU | C2-C1-O1'-C1' |
| 26 | Z | 622 | LMU | C2-C1-O1'-C1' |
| 26 | G2 | 206 | LMU | C2-C1-O1'-C1' |
| 26 | 12 | 627 | LMU | C2-C1-O1'-C1' |
| 26 | Z2 | 622 | LMU | C2-C1-O1'-C1' |
| 21 | B2 | 820 | CLA | C5-C6-C7-C8 |
| 21 | A | 836 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 808 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 839 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 841 | CLA | C4B-C3B-CAB-CBB |
| 21 | F | 304 | CLA | C4B-C3B-CAB-CBB |
| 21 | K | 204 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z | 608 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 617 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 9 | 601 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 836 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 808 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 839 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 841 | CLA | C4B-C3B-CAB-CBB |
| 21 | F2 | 304 | CLA | C4B-C3B-CAB-CBB |
| 21 | K2 | 204 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z2 | 608 | CLA | C4B-C3B-CAB-CBB |
| 21 | 62 | 617 | CLA | C4B-C3B-CAB-CBB |
| 21 | 92 | 601 | CLA | C4B-C3B-CAB-CBB |
| 21 | 92 | 613 | CLA | C4B-C3B-CAB-CBB |
| 26 | 72 | 629 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 834 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 823 | CLA | C3A-C2A-CAA-CBA |
| 21 | 3 | 611 | CLA | C3A-C2A-CAA-CBA |
| 21 | 7 | 616 | CLA | C3A-C2A-CAA-CBA |
| 21 | 9 | 603 | CLA | C3A-C2A-CAA-CBA |
| 21 | A2 | 834 | CLA | C3A-C2A-CAA-CBA |
| 21 | B2 | 823 | CLA | C3A-C2A-CAA-CBA |
| 21 | 32 | 611 | CLA | C3A-C2A-CAA-CBA |
| 21 | 72 | 616 | CLA | C3A-C2A-CAA-CBA |
| 21 | 92 | 603 | CLA | C3A-C2A-CAA-CBA |
| 30 | Z | 606 | CHL | C3A-C2A-CAA-CBA |
| 30 | 9 | 607 | CHL | C3A-C2A-CAA-CBA |
| 30 | Z2 | 606 | CHL | C3A-C2A-CAA-CBA |
| 30 | 92 | 607 | CHL | C3A-C2A-CAA-CBA |
| 23 | B | 851 | LHG | C1-C2-C3-O3 |
| 23 | 4 | 622 | LHG | C1-C2-C3-O3 |
| 23 | B2 | 851 | LHG | C1-C2-C3-O3 |
| 23 | 42 | 622 | LHG | C1-C2-C3-O3 |
| 23 | 6 | 619 | LHG | C26-C27-C28-C29 |
| 23 | 62 | 619 | LHG | C26-C27-C28-C29 |
| 29 | B | 850 | DGD | CBB-CCB-CDB-CEB |
| 21 | A | 825 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 808 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 821 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 828 | CLA | C2B-C3B-CAB-CBB |
| 21 | F | 304 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 7 | 610 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z | 613 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 4 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 617 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 601 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 825 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 808 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 821 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 828 | CLA | C2B-C3B-CAB-CBB |
| 21 | F2 | 304 | CLA | C2B-C3B-CAB-CBB |
| 21 | 32 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 72 | 610 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z2 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 42 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | 62 | 617 | CLA | C2B-C3B-CAB-CBB |
| 21 | 92 | 601 | CLA | C2B-C3B-CAB-CBB |
| 24 | B | 846 | BCR | C23-C24-C25-C30 |
| 24 | B | 847 | BCR | C23-C24-C25-C30 |
| 24 | J | 102 | BCR | C23-C24-C25-C30 |
| 24 | K | 202 | BCR | C23-C24-C25-C26 |
| 24 | K | 202 | BCR | C23-C24-C25-C30 |
| 24 | K | 207 | BCR | C23-C24-C25-C26 |
| 24 | K | 207 | BCR | C23-C24-C25-C30 |
| 24 | 3 | 620 | BCR | C23-C24-C25-C26 |
| 24 | 3 | 620 | BCR | C23-C24-C25-C30 |
| 24 | 3 | 719 | BCR | C23-C24-C25-C26 |
| 24 | 3 | 719 | BCR | C23-C24-C25-C30 |
| 24 | 7 | 623 | BCR | C23-C24-C25-C30 |
| 24 | 8 | 619 | BCR | C23-C24-C25-C26 |
| 24 | 8 | 619 | BCR | C23-C24-C25-C30 |
| 24 | 4 | 621 | BCR | C23-C24-C25-C26 |
| 24 | 4 | 621 | BCR | C23-C24-C25-C30 |
| 24 | 5 | 622 | BCR | C23-C24-C25-C26 |
| 24 | 5 | 622 | BCR | C23-C24-C25-C30 |
| 24 | 6 | 623 | BCR | C23-C24-C25-C30 |
| 24 | 9 | 623 | BCR | C23-C24-C25-C30 |
| 24 | B2 | 846 | BCR | C23-C24-C25-C30 |
| 24 | B2 | 847 | BCR | C23-C24-C25-C30 |
| 24 | J2 | 102 | BCR | C23-C24-C25-C30 |
| 24 | K2 | 202 | BCR | C23-C24-C25-C26 |
| 24 | K2 | 202 | BCR | C23-C24-C25-C30 |
| 24 | K2 | 207 | BCR | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | K2 | 207 | BCR | C23-C24-C25-C30 |
| 24 | 32 | 620 | BCR | C23-C24-C25-C26 |
| 24 | 32 | 620 | BCR | C23-C24-C25-C30 |
| 24 | 32 | 719 | BCR | C23-C24-C25-C26 |
| 24 | 32 | 719 | BCR | C23-C24-C25-C30 |
| 24 | 72 | 623 | BCR | C23-C24-C25-C30 |
| 24 | 82 | 619 | BCR | C23-C24-C25-C26 |
| 24 | 82 | 619 | BCR | C23-C24-C25-C30 |
| 24 | 42 | 621 | BCR | C23-C24-C25-C26 |
| 24 | 42 | 621 | BCR | C23-C24-C25-C30 |
| 24 | 52 | 622 | BCR | C23-C24-C25-C26 |
| 24 | 52 | 622 | BCR | C23-C24-C25-C30 |
| 24 | 62 | 623 | BCR | C23-C24-C25-C30 |
| 24 | 92 | 623 | BCR | C23-C24-C25-C30 |
| 28 | A | 856 | LUT | C1-C6-C7-C8 |
| 28 | 1 | 619 | LUT | C1-C6-C7-C8 |
| 28 | Z | 619 | LUT | C1-C6-C7-C8 |
| 28 | Z | 619 | LUT | C5-C6-C7-C8 |
| 28 | 5 | 620 | LUT | C1-C6-C7-C8 |
| 28 | 5 | 626 | LUT | C1-C6-C7-C8 |
| 28 | 5 | 626 | LUT | C5-C6-C7-C8 |
| 28 | 9 | 616 | LUT | C1-C6-C7-C8 |
| 28 | 12 | 619 | LUT | C1-C6-C7-C8 |
| 28 | Z2 | 619 | LUT | C1-C6-C7-C8 |
| 28 | Z2 | 619 | LUT | C5-C6-C7-C8 |
| 28 | 52 | 620 | LUT | C1-C6-C7-C8 |
| 28 | 52 | 626 | LUT | C1-C6-C7-C8 |
| 28 | 52 | 626 | LUT | C5-C6-C7-C8 |
| 28 | 92 | 616 | LUT | C1-C6-C7-C8 |
| 21 | A | 806 | CLA | C5-C6-C7-C8 |
| 21 | 9 | 612 | CLA | C13-C15-C16-C17 |
| 21 | A2 | 806 | CLA | C5-C6-C7-C8 |
| 21 | 92 | 612 | CLA | C13-C15-C16-C17 |
| 23 | 8 | 620 | LHG | C23-C24-C25-C26 |
| 23 | 82 | 620 | LHG | C23-C24-C25-C26 |
| 21 | B | 829 | CLA | C5-C6-C7-C8 |
| 30 | 9 | 607 | CHL | O1A-CGA-O2A-C1 |
| 30 | 7 | 601 | CHL | C4-C3-C5-C6 |
| 30 | 72 | 601 | CHL | C4-C3-C5-C6 |
| 21 | 9 | 611 | CLA | C10-C11-C12-C13 |
| 21 | B2 | 829 | CLA | C5-C6-C7-C8 |
| 21 | 92 | 611 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 7 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 72 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 92 | 607 | CHL | CBA-CGA-O2A-C1 |
| 21 | 6 | 613 | CLA | C11-C10-C8-C9 |
| 21 | 62 | 613 | CLA | C11-C10-C8-C9 |
| 26 | A | 863 | LMU | O5'-C1'-O1'-C1 |
| 26 | K | 208 | LMU | O5'-C1'-O1'-C1 |
| 26 | A2 | 863 | LMU | O5'-C1'-O1'-C1 |
| 26 | K2 | 208 | LMU | O5'-C1'-O1'-C1 |
| 21 | 4 | 609 | CLA | C5-C6-C7-C8 |
| 21 | 3 | 607 | CLA | C2C-C3C-CAC-CBC |
| 21 | 42 | 609 | CLA | C5-C6-C7-C8 |
| 21 | 32 | 607 | CLA | C2C-C3C-CAC-CBC |
| 23 | A | 846 | LHG | C23-C24-C25-C26 |
| 23 | A2 | 846 | LHG | C23-C24-C25-C26 |
| 27 | A | 860 | LMG | C8-C7-O1-C1 |
| 27 | A2 | 860 | LMG | C8-C7-O1-C1 |
| 21 | B | 817 | CLA | C2C-C3C-CAC-CBC |
| 21 | B2 | 817 | CLA | C2C-C3C-CAC-CBC |
| 23 | 8 | 620 | LHG | C17-C18-C19-C20 |
| 23 | 82 | 620 | LHG | C17-C18-C19-C20 |
| 27 | B2 | 852 | LMG | C11-C12-C13-C14 |
| 21 | Z2 | 609 | CLA | C13-C15-C16-C17 |
| 27 | B | 852 | LMG | C11-C12-C13-C14 |
| 26 | A | 864 | LMU | O5'-C5'-C6'-O6' |
| 26 | B | 853 | LMU | O5'-C5'-C6'-O6' |
| 26 | 6 | 630 | LMU | O5'-C5'-C6'-O6' |
| 26 | A2 | 864 | LMU | O5'-C5'-C6'-O6' |
| 26 | B2 | 853 | LMU | O5'-C5'-C6'-O6' |
| 26 | 62 | 630 | LMU | O5'-C5'-C6'-O6' |
| 27 | 1 | 628 | LMG | O6-C5-C6-O5 |
| 27 | 7 | 626 | LMG | O6-C5-C6-O5 |
| 27 | 12 | 628 | LMG | O6-C5-C6-O5 |
| 27 | 72 | 626 | LMG | O6-C5-C6-O5 |
| 29 | B | 850 | DGD | C8B-C9B-CAB-CBB |
| 21 | Z | 609 | CLA | C13-C15-C16-C17 |
| 30 | 62 | 607 | CHL | C15-C16-C17-C18 |
| 30 | 92 | 607 | CHL | O1A-CGA-O2A-C1 |
| 26 | 12 | 621 | LMU | O5B-C1B-O1B-C4' |
| 30 | 6 | 607 | CHL | C15-C16-C17-C18 |
| 26 | 1 | 622 | LMU | O5'-C5'-C6'-O6' |
| 26 | 12 | 622 | LMU | O5'-C5'-C6'-O6' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | A | 860 | LMG | O6-C5-C6-O5 |
| 27 | 8 | 626 | LMG | O6-C5-C6-O5 |
| 27 | A2 | 860 | LMG | O6-C5-C6-O5 |
| 27 | 82 | 626 | LMG | O6-C5-C6-O5 |
| 21 | 5 | 603 | CLA | C3-C5-C6-C7 |
| 21 | 52 | 603 | CLA | C3-C5-C6-C7 |
| 23 | 5 | 623 | LHG | O7-C5-C6-O8 |
| 23 | 52 | 623 | LHG | O7-C5-C6-O8 |
| 26 | 1 | 621 | LMU | O5B-C1B-O1B-C4' |
| 27 | J | 104 | LMG | O6-C5-C6-O5 |
| 27 | 8 | 629 | LMG | O6-C5-C6-O5 |
| 27 | J2 | 104 | LMG | O6-C5-C6-O5 |
| 27 | 82 | 629 | LMG | O6-C5-C6-O5 |
| 21 | A | 806 | CLA | C2-C1-O2A-CGA |
| 21 | A2 | 806 | CLA | C2-C1-O2A-CGA |
| 26 | 1 | 625 | LMU | O5'-C5'-C6'-O6' |
| 26 | 12 | 625 | LMU | O5'-C5'-C6'-O6' |
| 27 | 9 | 620 | LMG | O6-C5-C6-O5 |
| 21 | B | 836 | CLA | C10-C11-C12-C13 |
| 26 | A | 861 | LMU | O5'-C5'-C6'-O6' |
| 26 | A2 | 861 | LMU | O5'-C5'-C6'-O6' |
| 27 | 92 | 620 | LMG | O6-C5-C6-O5 |
| 21 | B | 820 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 820 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 836 | CLA | C10-C11-C12-C13 |
| 23 | B | 851 | LHG | C17-C18-C19-C20 |
| 21 | A | 854 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 854 | CLA | C2A-CAA-CBA-CGA |
| 23 | B2 | 851 | LHG | C17-C18-C19-C20 |
| 21 | B | 824 | CLA | C8-C10-C11-C12 |
| 21 | B | 840 | CLA | C15-C16-C17-C18 |
| 21 | K | 203 | CLA | C5-C6-C7-C8 |
| 21 | B2 | 824 | CLA | C8-C10-C11-C12 |
| 21 | B2 | 840 | CLA | C15-C16-C17-C18 |
| 21 | K2 | 203 | CLA | C5-C6-C7-C8 |
| 21 | A2 | 836 | CLA | C8-C10-C11-C12 |
| 26 | 8 | 627 | LMU | O5B-C5B-C6B-O6B |
| 26 | 82 | 627 | LMU | O5B-C5B-C6B-O6B |
| 29 | B | 850 | DGD | C5A-C6A-C7A-C8A |
| 21 | A | 812 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 834 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 823 | CLA | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 838 | CLA | C1A-C2A-CAA-CBA |
| 21 | J | 101 | CLA | C1A-C2A-CAA-CBA |
| 21 | 1 | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | 3 | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | Z | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 9 | 603 | CLA | C1A-C2A-CAA-CBA |
| 21 | A2 | 812 | CLA | C1A-C2A-CAA-CBA |
| 21 | A2 | 834 | CLA | C1A-C2A-CAA-CBA |
| 21 | B2 | 823 | CLA | C1A-C2A-CAA-CBA |
| 21 | B2 | 838 | CLA | C1A-C2A-CAA-CBA |
| 21 | J2 | 101 | CLA | C1A-C2A-CAA-CBA |
| 21 | 12 | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | 32 | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | Z2 | 609 | CLA | C1A-C2A-CAA-CBA |
| 21 | 92 | 603 | CLA | C1A-C2A-CAA-CBA |
| 21 | A | 826 | CLA | C10-C11-C12-C13 |
| 21 | A | 836 | CLA | C8-C10-C11-C12 |
| 21 | 1 | 608 | CLA | C10-C11-C12-C13 |
| 21 | A2 | 826 | CLA | C10-C11-C12-C13 |
| 21 | 12 | 608 | CLA | C10-C11-C12-C13 |
| 30 | 4 | 608 | CHL | C15-C16-C17-C18 |
| 30 | 42 | 608 | CHL | C15-C16-C17-C18 |
| 23 | A | 847 | LHG | O6-C4-C5-C6 |
| 23 | 3 | 721 | LHG | O6-C4-C5-C6 |
| 23 | 5 | 623 | LHG | O6-C4-C5-C6 |
| 23 | A2 | 847 | LHG | O6-C4-C5-C6 |
| 23 | 32 | 721 | LHG | O6-C4-C5-C6 |
| 23 | 52 | 623 | LHG | O6-C4-C5-C6 |
| 26 | A | 857 | LMU | O5B-C5B-C6B-O6B |
| 26 | 8 | 625 | LMU | O5'-C5'-C6'-O6' |
| 26 | A2 | 857 | LMU | O5B-C5B-C6B-O6B |
| 26 | 82 | 625 | LMU | O5'-C5'-C6'-O6' |
| 21 | A | 833 | CLA | C3-C5-C6-C7 |
| 21 | B | 827 | CLA | C3-C5-C6-C7 |
| 21 | B2 | 827 | CLA | C3-C5-C6-C7 |
| 21 | A | 834 | CLA | C11-C10-C8-C7 |
| 21 | 1 | 614 | CLA | C6-C7-C8-C10 |
| 21 | 5 | 603 | CLA | C11-C10-C8-C7 |
| 21 | A2 | 834 | CLA | C11-C10-C8-C7 |
| 21 | 12 | 614 | CLA | C6-C7-C8-C10 |
| 21 | 52 | 603 | CLA | C11-C10-C8-C7 |
| 22 | A | 844 | PQN | C17-C18-C20-C21 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | A2 | 844 | PQN | C17-C18-C20-C21 |
| 21 | A | 826 | CLA | C4-C3-C5-C6 |
| 21 | A | 835 | CLA | C4-C3-C5-C6 |
| 21 | B | 820 | CLA | C4-C3-C5-C6 |
| 21 | B | 828 | CLA | C4-C3-C5-C6 |
| 21 | 9 | 611 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 826 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 835 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 820 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 828 | CLA | C4-C3-C5-C6 |
| 21 | 92 | 611 | CLA | C4-C3-C5-C6 |
| 21 | B | 828 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 835 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 828 | CLA | C2-C3-C5-C6 |
| 21 | 92 | 611 | CLA | C2-C3-C5-C6 |
| 26 | A2 | 858 | LMU | O5B-C5B-C6B-O6B |
| 26 | 9 | 624 | LMU | C4-C5-C6-C7 |
| 21 | A2 | 833 | CLA | C3-C5-C6-C7 |
| 21 | B | 805 | CLA | C14-C13-C15-C16 |
| 21 | B | 827 | CLA | C11-C10-C8-C9 |
| 21 | B | 834 | CLA | C11-C10-C8-C9 |
| 21 | Z | 609 | CLA | C11-C12-C13-C14 |
| 21 | B2 | 805 | CLA | C14-C13-C15-C16 |
| 21 | B2 | 827 | CLA | C11-C10-C8-C9 |
| 21 | B2 | 834 | CLA | C11-C10-C8-C9 |
| 21 | Z2 | 609 | CLA | C11-C12-C13-C14 |
| 30 | Z | 601 | CHL | C6-C7-C8-C9 |
| 30 | 5 | 607 | CHL | C6-C7-C8-C9 |
| 30 | Z2 | 601 | CHL | C6-C7-C8-C9 |
| 30 | 52 | 607 | CHL | C6-C7-C8-C9 |
| 26 | 92 | 624 | LMU | C4-C5-C6-C7 |
| 26 | A | 858 | LMU | O5B-C5B-C6B-O6B |
| 30 | 82 | 607 | CHL | C15-C16-C17-C18 |
| 21 | A | 834 | CLA | C13-C15-C16-C17 |
| 30 | 8 | 607 | CHL | C15-C16-C17-C18 |
| 23 | 7 | 625 | LHG | C4-C5-C6-O8 |
| 23 | 72 | 625 | LHG | C4-C5-C6-O8 |
| 27 | J | 104 | LMG | O1-C7-C8-C9 |
| 27 | J2 | 104 | LMG | O1-C7-C8-C9 |
| 26 | 8 | 628 | LMU | O5'-C5'-C6'-O6' |
| 26 | 82 | 628 | LMU | O5'-C5'-C6'-O6' |
| 27 | J2 | 103 | LMG | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A2 | 834 | CLA | C13-C15-C16-C17 |
| 27 | J | 103 | LMG | C16-C17-C18-C19 |
| 26 | G | 206 | LMU | O5'-C5'-C6'-O6' |
| 26 | G2 | 206 | LMU | O5'-C5'-C6'-O6' |
| 27 | 4 | 624 | LMG | O6-C5-C6-O5 |
| 27 | 42 | 624 | LMG | O6-C5-C6-O5 |
| 27 | 3 | 722 | LMG | C33-C34-C35-C36 |
| 27 | 32 | 722 | LMG | C33-C34-C35-C36 |
| 26 | 9 | 624 | LMU | O5'-C5'-C6'-O6' |
| 30 | 5 | 618 | CHL | CHA-CBD-CGD-O1D |
| 30 | 5 | 618 | CHL | CHA-CBD-CGD-O2D |
| 30 | 9 | 607 | CHL | CHA-CBD-CGD-O1D |
| 30 | 9 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 52 | 618 | CHL | CHA-CBD-CGD-O2D |
| 26 | 92 | 624 | LMU | O5'-C5'-C6'-O6' |
| 21 | 62 | 613 | CLA | C4-C3-C5-C6 |
| 30 | 6 | 607 | CHL | C4-C3-C5-C6 |
| 30 | 62 | 607 | CHL | C4-C3-C5-C6 |
| 21 | A | 826 | CLA | C2-C3-C5-C6 |
| 21 | A | 835 | CLA | C2-C3-C5-C6 |
| 21 | 6 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 9 | 611 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 826 | CLA | C2-C3-C5-C6 |
| 21 | 62 | 613 | CLA | C2-C3-C5-C6 |
| 21 | Z | 611 | CLA | C10-C11-C12-C13 |
| 21 | 5 | 601 | CLA | C10-C11-C12-C13 |
| 21 | Z2 | 611 | CLA | C10-C11-C12-C13 |
| 26 | 6 | 631 | LMU | O5'-C5'-C6'-O6' |
| 26 | 62 | 631 | LMU | O5'-C5'-C6'-O6' |
| 21 | 6 | 603 | CLA | C5-C6-C7-C8 |
| 21 | 52 | 601 | CLA | C10-C11-C12-C13 |
| 21 | 62 | 603 | CLA | C5-C6-C7-C8 |
| 21 | A | 810 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 810 | CLA | C2A-CAA-CBA-CGA |
| 21 | A | 826 | CLA | O2A-C1-C2-C3 |
| 21 | 9 | 609 | CLA | O2A-C1-C2-C3 |
| 21 | A2 | 826 | CLA | O2A-C1-C2-C3 |
| 21 | 92 | 609 | CLA | O2A-C1-C2-C3 |
| 30 | 4 | 606 | CHL | O2A-C1-C2-C3 |
| 30 | 42 | 606 | CHL | O2A-C1-C2-C3 |
| 21 | 8 | 603 | CLA | C15-C16-C17-C18 |
| 21 | 82 | 603 | CLA | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 6 | 613 | CLA | C4-C3-C5-C6 |
| 21 | B | 839 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 839 | CLA | C2-C3-C5-C6 |
| 30 | 6 | 607 | CHL | C2-C3-C5-C6 |
| 30 | 62 | 607 | CHL | C2-C3-C5-C6 |
| 26 | 12 | 623 | LMU | C11-C10-C9-C8 |
| 26 | 1 | 623 | LMU | C11-C10-C9-C8 |
| 27 | 1 | 628 | LMG | C12-C13-C14-C15 |
| 27 | 12 | 628 | LMG | C12-C13-C14-C15 |
| 23 | B | 851 | LHG | O7-C5-C6-O8 |
| 23 | B2 | 851 | LHG | O7-C5-C6-O8 |
| 23 | 5 | 623 | LHG | O2-C2-C3-O3 |
| 23 | 52 | 623 | LHG | O2-C2-C3-O3 |
| 29 | B | 850 | DGD | O2G-C1B-C2B-C3B |
| 30 | 5 | 607 | CHL | CAA-CBA-CGA-O2A |
| 30 | 52 | 607 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 806 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 806 | CLA | C2A-CAA-CBA-CGA |
| 21 | B | 811 | CLA | C15-C16-C17-C18 |
| 21 | 5 | 603 | CLA | C5-C6-C7-C8 |
| 21 | B2 | 811 | CLA | C15-C16-C17-C18 |
| 21 | 52 | 603 | CLA | C5-C6-C7-C8 |
| 21 | B | 817 | CLA | C13-C15-C16-C17 |
| 21 | B | 821 | CLA | C10-C11-C12-C13 |
| 21 | B2 | 817 | CLA | C13-C15-C16-C17 |
| 21 | B2 | 821 | CLA | C10-C11-C12-C13 |
| 21 | A | 820 | CLA | C4-C3-C5-C6 |
| 21 | A | 830 | CLA | C4-C3-C5-C6 |
| 21 | A | 840 | CLA | C4-C3-C5-C6 |
| 21 | B | 812 | CLA | C4-C3-C5-C6 |
| 21 | B | 829 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 614 | CLA | C4-C3-C5-C6 |
| 21 | 3 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 9 | 612 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 820 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 830 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 840 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 812 | CLA | C4-C3-C5-C6 |
| 21 | 12 | 614 | CLA | C4-C3-C5-C6 |
| 21 | 32 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 92 | 612 | CLA | C4-C3-C5-C6 |
| 30 | 6 | 601 | CHL | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 62 | 601 | CHL | C4-C3-C5-C6 |
| 29 | B2 | 850 | DGD | C2A-C3A-C4A-C5A |
| 26 | B | 853 | LMU | C2-C1-O1'-C1' |
| 26 | G | 206 | LMU | C2-C1-O1'-C1' |
| 26 | 1 | 621 | LMU | C2-C1-O1'-C1' |
| 26 | 1 | 622 | LMU | C2-C1-O1'-C1' |
| 26 | 8 | 625 | LMU | C2-C1-O1'-C1' |
| 26 | B2 | 853 | LMU | C2-C1-O1'-C1' |
| 26 | 12 | 621 | LMU | C2-C1-O1'-C1' |
| 26 | 12 | 622 | LMU | C2-C1-O1'-C1' |
| 26 | 82 | 625 | LMU | C2-C1-O1'-C1' |
| 22 | A | 844 | PQN | C19-C18-C20-C21 |
| 22 | A2 | 844 | PQN | C19-C18-C20-C21 |
| 21 | B | 826 | CLA | C8-C10-C11-C12 |
| 21 | 82 | 602 | CLA | C8-C10-C11-C12 |
| 21 | A | 835 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 818 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 832 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 834 | CLA | C4B-C3B-CAB-CBB |
| 21 | K | 206 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 4 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 835 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 818 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 832 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 834 | CLA | C4B-C3B-CAB-CBB |
| 21 | K2 | 206 | CLA | C4B-C3B-CAB-CBB |
| 21 | 32 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z2 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 42 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | 62 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 602 | CLA | C8-C10-C11-C12 |
| 21 | B2 | 826 | CLA | C8-C10-C11-C12 |
| 21 | A2 | 828 | CLA | C8-C10-C11-C12 |
| 23 | B | 851 | LHG | O6-C4-C5-C6 |
| 23 | Z | 620 | LHG | O6-C4-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | B2 | 851 | LHG | O6-C4-C5-C6 |
| 23 | Z2 | 620 | LHG | O6-C4-C5-C6 |
| 23 | B | 851 | LHG | O7-C7-C8-C9 |
| 23 | B2 | 851 | LHG | O7-C7-C8-C9 |
| 21 | A | 804 | CLA | C11-C12-C13-C15 |
| 21 | A | 811 | CLA | C6-C7-C8-C10 |
| 21 | A | 829 | CLA | C6-C7-C8-C10 |
| 21 | B | 827 | CLA | C11-C10-C8-C7 |
| 21 | B | 834 | CLA | C11-C10-C8-C7 |
| 21 | F | 301 | CLA | C11-C10-C8-C7 |
| 21 | Z | 609 | CLA | C11-C12-C13-C15 |
| 21 | A2 | 804 | CLA | C11-C12-C13-C15 |
| 21 | A2 | 811 | CLA | C6-C7-C8-C10 |
| 21 | A2 | 829 | CLA | C6-C7-C8-C10 |
| 21 | B2 | 827 | CLA | C11-C10-C8-C7 |
| 21 | B2 | 834 | CLA | C11-C10-C8-C7 |
| 21 | F2 | 301 | CLA | C11-C10-C8-C7 |
| 21 | Z2 | 609 | CLA | C11-C12-C13-C15 |
| 30 | 1 | 601 | CHL | C11-C12-C13-C15 |
| 30 | Z | 601 | CHL | C6-C7-C8-C10 |
| 30 | 12 | 601 | CHL | C11-C12-C13-C15 |
| 30 | Z2 | 601 | CHL | C6-C7-C8-C10 |
| 21 | A | 816 | CLA | C13-C15-C16-C17 |
| 21 | A | 828 | CLA | C8-C10-C11-C12 |
| 21 | 7 | 611 | CLA | C8-C10-C11-C12 |
| 21 | A2 | 816 | CLA | C13-C15-C16-C17 |
| 21 | 72 | 611 | CLA | C8-C10-C11-C12 |
| 23 | 4 | 622 | LHG | O2-C2-C3-O3 |
| 23 | 9 | 622 | LHG | C25-C26-C27-C28 |
| 23 | 92 | 622 | LHG | C25-C26-C27-C28 |
| 21 | A | 810 | CLA | C4-C3-C5-C6 |
| 21 | A | 817 | CLA | C4-C3-C5-C6 |
| 21 | A | 828 | CLA | C4-C3-C5-C6 |
| 21 | A | 841 | CLA | C4-C3-C5-C6 |
| 21 | B | 805 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 807 | CLA | C4-C3-C5-C6 |
| 21 | B | 808 | CLA | C4-C3-C5-C6 |
| 21 | B | 839 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 609 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 810 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 817 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 828 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A2 | 841 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 805 | CLA | C3A-C2A-CAA-CBA |
| 21 | B2 | 807 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 808 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 829 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 839 | CLA | C4-C3-C5-C6 |
| 21 | 12 | 609 | CLA | C4-C3-C5-C6 |
| 21 | A | 830 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 830 | CLA | C2-C3-C5-C6 |
| 27 | A | 859 | LMG | C40-C41-C42-C43 |
| 27 | A2 | 859 | LMG | C40-C41-C42-C43 |
| 27 | 4 | 624 | LMG | O1-C7-C8-C9 |
| 27 | 42 | 624 | LMG | O1-C7-C8-C9 |
| 30 | Z | 606 | CHL | C1A-C2A-CAA-CBA |
| 30 | Z2 | 606 | CHL | C1A-C2A-CAA-CBA |
| 23 | 4 | 623 | LHG | C13-C14-C15-C16 |
| 21 | A | 815 | CLA | C4-C3-C5-C6 |
| 21 | Z | 609 | CLA | C4-C3-C5-C6 |
| 23 | 42 | 623 | LHG | C13-C14-C15-C16 |
| 21 | A | 817 | CLA | C2-C3-C5-C6 |
| 21 | A | 840 | CLA | C2-C3-C5-C6 |
| 21 | A | 841 | CLA | C2-C3-C5-C6 |
| 21 | B | 808 | CLA | C2-C3-C5-C6 |
| 21 | B | 812 | CLA | C2-C3-C5-C6 |
| 21 | 9 | 612 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 817 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 840 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 808 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 829 | CLA | C2-C3-C5-C6 |
| 21 | 92 | 612 | CLA | C2-C3-C5-C6 |
| 21 | 32 | 603 | CLA | C2C-C3C-CAC-CBC |
| 21 | 3 | 603 | CLA | C2C-C3C-CAC-CBC |
| 27 | 1 | 628 | LMG | C14-C15-C16-C17 |
| 27 | 12 | 628 | LMG | C14-C15-C16-C17 |
| 23 | A | 847 | LHG | O6-C4-C5-O7 |
| 23 | B | 851 | LHG | O6-C4-C5-O7 |
| 23 | A2 | 847 | LHG | O6-C4-C5-O7 |
| 23 | B2 | 851 | LHG | O6-C4-C5-O7 |
| 21 | B | 832 | CLA | C2B-C3B-CAB-CBB |
| 21 | 3 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 4 | 611 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 6 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 832 | CLA | C2B-C3B-CAB-CBB |
| 21 | 32 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z2 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 42 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 62 | 611 | CLA | C2B-C3B-CAB-CBB |
| 24 | A | 848 | BCR | C1-C6-C7-C8 |
| 24 | B | 846 | BCR | C23-C24-C25-C26 |
| 24 | B | 848 | BCR | C1-C6-C7-C8 |
| 24 | L | 201 | BCR | C1-C6-C7-C8 |
| 24 | 3 | 718 | BCR | C23-C24-C25-C30 |
| 24 | A2 | 848 | BCR | C1-C6-C7-C8 |
| 24 | B2 | 848 | BCR | C1-C6-C7-C8 |
| 24 | L2 | 201 | BCR | C1-C6-C7-C8 |
| 24 | 32 | 718 | BCR | C23-C24-C25-C30 |
| 28 | 1 | 617 | LUT | C1-C6-C7-C8 |
| 28 | 3 | 621 | LUT | C1-C6-C7-C8 |
| 28 | 3 | 622 | LUT | C1-C6-C7-C8 |
| 28 | 8 | 617 | LUT | C1-C6-C7-C8 |
| 28 | Z | 617 | LUT | C1-C6-C7-C8 |
| 28 | 6 | 621 | LUT | C1-C6-C7-C8 |
| 28 | 12 | 617 | LUT | C1-C6-C7-C8 |
| 28 | 32 | 621 | LUT | C1-C6-C7-C8 |
| 28 | 32 | 622 | LUT | C1-C6-C7-C8 |
| 28 | 82 | 617 | LUT | C1-C6-C7-C8 |
| 28 | Z2 | 617 | LUT | C1-C6-C7-C8 |
| 28 | 62 | 621 | LUT | C1-C6-C7-C8 |
| 23 | 8 | 620 | LHG | C26-C27-C28-C29 |
| 23 | 42 | 622 | LHG | O2-C2-C3-O3 |
| 23 | 82 | 620 | LHG | C26-C27-C28-C29 |
| 21 | A | 809 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 809 | CLA | C2A-CAA-CBA-CGA |
| 21 | 12 | 609 | CLA | C15-C16-C17-C18 |
| 27 | 8 | 626 | LMG | O7-C8-C9-O8 |
| 27 | 82 | 626 | LMG | O7-C8-C9-O8 |
| 23 | A | 846 | LHG | C27-C28-C29-C30 |
| 21 | A2 | 815 | CLA | C4-C3-C5-C6 |
| 21 | Z2 | 609 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 609 | CLA | C15-C16-C17-C18 |
| 21 | A | 828 | CLA | C2-C3-C5-C6 |
| 21 | B | 807 | CLA | C2-C3-C5-C6 |
| 21 | B | 829 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 1 | 609 | CLA | C2-C3-C5-C6 |
| 21 | 1 | 614 | CLA | C2-C3-C5-C6 |
| 21 | 3 | 603 | CLA | C2-C3-C5-C6 |
| 21 | Z | 609 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 828 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 841 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 807 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 812 | CLA | C2-C3-C5-C6 |
| 21 | 12 | 609 | CLA | C2-C3-C5-C6 |
| 21 | 12 | 614 | CLA | C2-C3-C5-C6 |
| 21 | 32 | 603 | CLA | C2-C3-C5-C6 |
| 21 | Z2 | 609 | CLA | C2-C3-C5-C6 |
| 23 | A2 | 846 | LHG | C27-C28-C29-C30 |
| 30 | 92 | 607 | CHL | O1D-CGD-O2D-CED |
| 21 | A | 811 | CLA | C6-C7-C8-C9 |
| 21 | A | 828 | CLA | C14-C13-C15-C16 |
| 21 | A | 829 | CLA | C6-C7-C8-C9 |
| 21 | B | 802 | CLA | C11-C10-C8-C9 |
| 21 | A2 | 811 | CLA | C6-C7-C8-C9 |
| 21 | A2 | 828 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 829 | CLA | C6-C7-C8-C9 |
| 21 | B2 | 802 | CLA | C11-C10-C8-C9 |
| 27 | 3 | 722 | LMG | C8-C7-O1-C1 |
| 27 | 32 | 722 | LMG | C8-C7-O1-C1 |
| 21 | A | 812 | CLA | C15-C16-C17-C18 |
| 23 | 8 | 620 | LHG | C15-C16-C17-C18 |
| 23 | 82 | 620 | LHG | C15-C16-C17-C18 |
| 21 | A2 | 812 | CLA | C15-C16-C17-C18 |
| 30 | 6 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 62 | 601 | CHL | C2-C3-C5-C6 |
| 29 | B2 | 850 | DGD | C3A-C4A-C5A-C6A |
| 29 | B | 850 | DGD | C2A-C3A-C4A-C5A |
| 23 | 3 | 623 | LHG | O6-C4-C5-C6 |
| 23 | 32 | 623 | LHG | O6-C4-C5-C6 |
| 21 | A | 828 | CLA | C12-C13-C15-C16 |
| 21 | B | 819 | CLA | C11-C10-C8-C7 |
| 21 | B2 | 819 | CLA | C11-C10-C8-C7 |
| 30 | 8 | 607 | CHL | C6-C7-C8-C10 |
| 30 | 6 | 616 | CHL | C12-C13-C15-C16 |
| 30 | 82 | 607 | CHL | C6-C7-C8-C10 |
| 30 | 62 | 616 | CHL | C12-C13-C15-C16 |
| 27 | 7 | 626 | LMG | O8-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | 72 | 626 | LMG | O8-C28-C29-C30 |
| 27 | J | 104 | LMG | C8-C7-O1-C1 |
| 27 | J2 | 104 | LMG | C8-C7-O1-C1 |
| 21 | A | 803 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 803 | CLA | C2A-CAA-CBA-CGA |
| 21 | B2 | 815 | CLA | C4-C3-C5-C6 |
| 21 | A | 815 | CLA | C2-C3-C5-C6 |
| 21 | A | 820 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 815 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 820 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 617 | CLA | C10-C11-C12-C13 |
| 21 | 52 | 617 | CLA | C10-C11-C12-C13 |
| 23 | 62 | 619 | LHG | C9-C10-C11-C12 |
| 21 | 7 | 610 | CLA | CBA-CGA-O2A-C1 |
| 21 | 72 | 610 | CLA | CBA-CGA-O2A-C1 |
| 21 | A | 823 | CLA | O2A-C1-C2-C3 |
| 21 | A | 827 | CLA | O2A-C1-C2-C3 |
| 21 | 9 | 613 | CLA | O2A-C1-C2-C3 |
| 21 | A2 | 823 | CLA | O2A-C1-C2-C3 |
| 21 | A2 | 827 | CLA | O2A-C1-C2-C3 |
| 21 | 92 | 613 | CLA | O2A-C1-C2-C3 |
| 30 | 8 | 607 | CHL | O2A-C1-C2-C3 |
| 30 | Z | 601 | CHL | O2A-C1-C2-C3 |
| 30 | 82 | 607 | CHL | O2A-C1-C2-C3 |
| 30 | Z2 | 601 | CHL | O2A-C1-C2-C3 |
| 23 | 6 | 619 | LHG | C9-C10-C11-C12 |
| 26 | B | 853 | LMU | C2-C3-C4-C5 |
| 26 | B2 | 853 | LMU | C2-C3-C4-C5 |
| 30 | 32 | 608 | CHL | C15-C16-C17-C18 |
| 23 | Z | 620 | LHG | O6-C4-C5-O7 |
| 23 | 4 | 623 | LHG | O6-C4-C5-O7 |
| 23 | 6 | 629 | LHG | O6-C4-C5-O7 |
| 23 | Z2 | 620 | LHG | O6-C4-C5-O7 |
| 23 | 42 | 623 | LHG | O6-C4-C5-O7 |
| 23 | 62 | 629 | LHG | O6-C4-C5-O7 |
| 30 | 3 | 608 | CHL | C15-C16-C17-C18 |
| 21 | A | 811 | CLA | C4-C3-C5-C6 |
| 21 | B | 813 | CLA | C4-C3-C5-C6 |
| 21 | B | 815 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 811 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 813 | CLA | C4-C3-C5-C6 |
| 21 | B | 831 | CLA | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 9 | 613 | CLA | C2A-CAA-CBA-CGA |
| 21 | B2 | 831 | CLA | C2A-CAA-CBA-CGA |
| 21 | 92 | 613 | CLA | C2A-CAA-CBA-CGA |
| 27 | 3 | 722 | LMG | O8-C28-C29-C30 |
| 21 | A | 810 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 810 | CLA | C2-C3-C5-C6 |
| 26 | 4 | 625 | LMU | C3-C4-C5-C6 |
| 23 | 72 | 625 | LHG | C34-C35-C36-C37 |
| 21 | A | 812 | CLA | C13-C15-C16-C17 |
| 21 | Z | 611 | CLA | C5-C6-C7-C8 |
| 21 | Z2 | 611 | CLA | C5-C6-C7-C8 |
| 26 | 42 | 625 | LMU | C3-C4-C5-C6 |
| 23 | 7 | 625 | LHG | O7-C5-C6-O8 |
| 23 | 72 | 625 | LHG | O7-C5-C6-O8 |
| 27 | 4 | 624 | LMG | O1-C7-C8-O7 |
| 27 | 42 | 624 | LMG | O1-C7-C8-O7 |
| 30 | 8 | 607 | CHL | C6-C7-C8-C9 |
| 30 | 82 | 607 | CHL | C6-C7-C8-C9 |
| 23 | 7 | 625 | LHG | C34-C35-C36-C37 |
| 27 | 32 | 722 | LMG | O8-C28-C29-C30 |
| 23 | 42 | 622 | LHG | C19-C20-C21-C22 |
| 23 | 4 | 622 | LHG | C19-C20-C21-C22 |
| 21 | A | 829 | CLA | C8-C10-C11-C12 |
| 21 | A | 829 | CLA | C10-C11-C12-C13 |
| 21 | A2 | 812 | CLA | C13-C15-C16-C17 |
| 21 | A2 | 829 | CLA | C8-C10-C11-C12 |
| 21 | A2 | 829 | CLA | C10-C11-C12-C13 |
| 21 | 5 | 603 | CLA | C2-C1-O2A-CGA |
| 21 | 52 | 603 | CLA | C2-C1-O2A-CGA |
| 27 | A | 859 | LMG | C32-C33-C34-C35 |
| 27 | A2 | 859 | LMG | C32-C33-C34-C35 |
| 21 | A | 821 | CLA | C4-C3-C5-C6 |
| 21 | 1 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 610 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 821 | CLA | C4-C3-C5-C6 |
| 21 | 12 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 610 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 836 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 813 | CLA | C2-C3-C5-C6 |
| 21 | B | 815 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 813 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 815 | CLA | C2-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 3 | 607 | CLA | C4C-C3C-CAC-CBC |
| 30 | Z | 607 | CHL | C4C-C3C-CAC-CBC |
| 30 | 5 | 607 | CHL | C4C-C3C-CAC-CBC |
| 30 | Z2 | 607 | CHL | C4C-C3C-CAC-CBC |
| 30 | 52 | 607 | CHL | C4C-C3C-CAC-CBC |
| 23 | 4 | 623 | LHG | C9-C10-C11-C12 |
| 26 | 8 | 627 | LMU | C7-C8-C9-C10 |
| 21 | 32 | 607 | CLA | C4C-C3C-CAC-CBC |
| 23 | 42 | 623 | LHG | C9-C10-C11-C12 |
| 26 | A | 863 | LMU | C2-C1-O1'-C1' |
| 26 | 1 | 625 | LMU | C2-C1-O1'-C1' |
| 26 | 8 | 624 | LMU | C2-C1-O1'-C1' |
| 26 | A2 | 863 | LMU | C2-C1-O1'-C1' |
| 26 | 12 | 625 | LMU | C2-C1-O1'-C1' |
| 26 | 82 | 624 | LMU | C2-C1-O1'-C1' |
| 21 | 3 | 611 | CLA | C3-C5-C6-C7 |
| 21 | 32 | 611 | CLA | C3-C5-C6-C7 |
| 26 | 82 | 627 | LMU | C7-C8-C9-C10 |
| 21 | A | 819 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 805 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 826 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 827 | CLA | C1A-C2A-CAA-CBA |
| 21 | B | 840 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 616 | CLA | C1A-C2A-CAA-CBA |
| 21 | 4 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 616 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 617 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 621 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 819 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 805 | CLA | C1A-C2A-CAA-CBA |
| 21 | B2 | 826 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 827 | CLA | C1A-C2A-CAA-CBA |
| 21 | B2 | 840 | CLA | C4B-C3B-CAB-CBB |
| 21 | 72 | 616 | CLA | C1A-C2A-CAA-CBA |
| 21 | 42 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 616 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 617 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 621 | CLA | C4B-C3B-CAB-CBB |
| 21 | 3 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 7 | 620 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B2 | 805 | CLA | C4-C3-C5-C6 |
| 21 | 32 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 72 | 620 | CLA | C4-C3-C5-C6 |
| 21 | A | 836 | CLA | CAA-CBA-CGA-O2A |
| 23 | 1 | 620 | LHG | O6-C4-C5-C6 |
| 23 | 4 | 623 | LHG | O6-C4-C5-C6 |
| 23 | 6 | 629 | LHG | O6-C4-C5-C6 |
| 23 | 9 | 622 | LHG | O6-C4-C5-C6 |
| 23 | 12 | 620 | LHG | O6-C4-C5-C6 |
| 23 | 42 | 623 | LHG | O6-C4-C5-C6 |
| 23 | 62 | 629 | LHG | O6-C4-C5-C6 |
| 26 | A2 | 863 | LMU | C5'-C4'-O1B-C1B |
| 26 | A | 863 | LMU | C5'-C4'-O1B-C1B |
| 21 | A | 809 | CLA | C12-C13-C15-C16 |
| 21 | A | 816 | CLA | C12-C13-C15-C16 |
| 21 | A | 820 | CLA | C6-C7-C8-C10 |
| 21 | B | 802 | CLA | C11-C10-C8-C7 |
| 21 | 8 | 613 | CLA | C12-C13-C15-C16 |
| 21 | 4 | 609 | CLA | C11-C10-C8-C7 |
| 21 | A2 | 809 | CLA | C12-C13-C15-C16 |
| 21 | A2 | 816 | CLA | C12-C13-C15-C16 |
| 21 | A2 | 820 | CLA | C6-C7-C8-C10 |
| 21 | A2 | 828 | CLA | C12-C13-C15-C16 |
| 21 | B2 | 802 | CLA | C11-C10-C8-C7 |
| 21 | 82 | 613 | CLA | C12-C13-C15-C16 |
| 21 | 42 | 609 | CLA | C11-C10-C8-C7 |
| 30 | 4 | 601 | CHL | C11-C10-C8-C7 |
| 30 | 6 | 607 | CHL | C12-C13-C15-C16 |
| 30 | 42 | 601 | CHL | C11-C10-C8-C7 |
| 30 | 62 | 607 | CHL | C12-C13-C15-C16 |
| 23 | 7 | 625 | LHG | C31-C32-C33-C34 |
| 23 | 72 | 625 | LHG | C31-C32-C33-C34 |
| 21 | Z2 | 616 | CLA | C5-C6-C7-C8 |
| 21 | B | 805 | CLA | C4-C3-C5-C6 |
| 23 | 1 | 620 | LHG | O6-C4-C5-O7 |
| 23 | 5 | 623 | LHG | O6-C4-C5-O7 |
| 23 | 12 | 620 | LHG | O6-C4-C5-O7 |
| 23 | 52 | 623 | LHG | O6-C4-C5-O7 |
| 29 | B | 850 | DGD | C4E-C5E-C6E-O5E |
| 21 | A | 806 | CLA | C3-C5-C6-C7 |
| 21 | A2 | 806 | CLA | C3-C5-C6-C7 |
| 21 | B | 817 | CLA | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A | 804 | CLA | C11-C12-C13-C14 |
| 21 | B | 819 | CLA | C11-C10-C8-C9 |
| 21 | A2 | 804 | CLA | C11-C12-C13-C14 |
| 21 | B2 | 819 | CLA | C11-C10-C8-C9 |
| 21 | Z | 616 | CLA | C5-C6-C7-C8 |
| 21 | A | 830 | CLA | C13-C15-C16-C17 |
| 21 | A2 | 830 | CLA | C13-C15-C16-C17 |
| 21 | B2 | 817 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 812 | CLA | C3-C5-C6-C7 |
| 21 | A2 | 812 | CLA | C3-C5-C6-C7 |
| 27 | 8 | 626 | LMG | C7-C8-C9-O8 |
| 27 | 82 | 626 | LMG | C7-C8-C9-O8 |
| 21 | 6 | 604 | CLA | C4-C3-C5-C6 |
| 21 | 62 | 604 | CLA | C4-C3-C5-C6 |
| 21 | B | 826 | CLA | C13-C15-C16-C17 |
| 21 | A | 811 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 811 | CLA | C2-C3-C5-C6 |
| 21 | A | 804 | CLA | CAD-CBD-CGD-O2D |
| 21 | B | 805 | CLA | CAD-CBD-CGD-O2D |
| 21 | B | 841 | CLA | CAD-CBD-CGD-O2D |
| 21 | 7 | 614 | CLA | CAD-CBD-CGD-O2D |
| 21 | 7 | 620 | CLA | CAD-CBD-CGD-O2D |
| 21 | 6 | 622 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 804 | CLA | CAD-CBD-CGD-O2D |
| 21 | B2 | 805 | CLA | CAD-CBD-CGD-O2D |
| 21 | B2 | 841 | CLA | CAD-CBD-CGD-O2D |
| 21 | 72 | 614 | CLA | CAD-CBD-CGD-O2D |
| 21 | 72 | 620 | CLA | CAD-CBD-CGD-O2D |
| 21 | 62 | 622 | CLA | CAD-CBD-CGD-O2D |
| 30 | 1 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 1 | 607 | CHL | CAD-CBD-CGD-O2D |
| 30 | 7 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | Z | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 4 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 6 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 12 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 12 | 607 | CHL | CAD-CBD-CGD-O2D |
| 30 | 72 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | Z2 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 42 | 601 | CHL | CAD-CBD-CGD-O2D |
| 30 | 62 | 601 | CHL | CAD-CBD-CGD-O2D |
| 21 | B2 | 826 | CLA | C13-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | A2 | 859 | LMG | C12-C13-C14-C15 |
| 27 | A | 859 | LMG | C12-C13-C14-C15 |
| 21 | A | 841 | CLA | C16-C17-C18-C20 |
| 21 | A2 | 841 | CLA | C16-C17-C18-C20 |
| 21 | 6 | 609 | CLA | C2A-CAA-CBA-CGA |
| 21 | 62 | 609 | CLA | C2A-CAA-CBA-CGA |
| 30 | 4 | 608 | CHL | C2A-CAA-CBA-CGA |
| 30 | 42 | 608 | CHL | C2A-CAA-CBA-CGA |
| 23 | 32 | 623 | LHG | C32-C33-C34-C35 |
| 26 | A2 | 863 | LMU | C3'-C4'-O1B-C1B |
| 23 | 3 | 623 | LHG | C32-C33-C34-C35 |
| 26 | A | 863 | LMU | C3'-C4'-O1B-C1B |
| 20 | A | 801 | CL0 | CHA-CBD-CGD-O1D |
| 20 | A | 801 | CL0 | CHA-CBD-CGD-O2D |
| 20 | A2 | 801 | CL0 | CHA-CBD-CGD-O1D |
| 20 | A2 | 801 | CL0 | CHA-CBD-CGD-O2D |
| 21 | A | 804 | CLA | CAD-CBD-CGD-O1D |
| 21 | A | 814 | CLA | CAD-CBD-CGD-O1D |
| 21 | B | 805 | CLA | CAD-CBD-CGD-O1D |
| 21 | B | 821 | CLA | CHA-CBD-CGD-O1D |
| 21 | B | 821 | CLA | CHA-CBD-CGD-O2D |
| 21 | B | 841 | CLA | CAD-CBD-CGD-O1D |
| 21 | K | 204 | CLA | CHA-CBD-CGD-O1D |
| 21 | K | 204 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 1 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 1 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 1 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 1 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 3 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 3 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 7 | 614 | CLA | CAD-CBD-CGD-O1D |
| 21 | 7 | 620 | CLA | CAD-CBD-CGD-O1D |
| 21 | 8 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 8 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 8 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | Z | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | Z | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | Z | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | Z | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | Z | 612 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 5 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 5 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 5 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 5 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 6 | 603 | CLA | CAD-CBD-CGD-O1D |
| 21 | 6 | 622 | CLA | CAD-CBD-CGD-O1D |
| 21 | 9 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 9 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | A2 | 804 | CLA | CAD-CBD-CGD-O1D |
| 21 | A2 | 814 | CLA | CAD-CBD-CGD-O1D |
| 21 | B2 | 805 | CLA | CAD-CBD-CGD-O1D |
| 21 | B2 | 821 | CLA | CHA-CBD-CGD-O1D |
| 21 | B2 | 821 | CLA | CHA-CBD-CGD-O2D |
| 21 | B2 | 841 | CLA | CAD-CBD-CGD-O1D |
| 21 | K2 | 204 | CLA | CHA-CBD-CGD-O1D |
| 21 | K2 | 204 | CLA | CHA-CBD-CGD-O2D |
| 21 | 12 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 12 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 12 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 12 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | 12 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 12 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 32 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 32 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 72 | 614 | CLA | CAD-CBD-CGD-O1D |
| 21 | 72 | 620 | CLA | CAD-CBD-CGD-O1D |
| 21 | 82 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 82 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 82 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | Z2 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | Z2 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | Z2 | 603 | CLA | CHA-CBD-CGD-O2D |
| 21 | Z2 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | Z2 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 52 | 602 | CLA | CHA-CBD-CGD-O1D |
| 21 | 52 | 602 | CLA | CHA-CBD-CGD-O2D |
| 21 | 52 | 612 | CLA | CHA-CBD-CGD-O1D |
| 21 | 52 | 612 | CLA | CHA-CBD-CGD-O2D |
| 21 | 62 | 603 | CLA | CAD-CBD-CGD-O1D |
| 21 | 62 | 622 | CLA | CAD-CBD-CGD-O1D |
| 21 | 92 | 603 | CLA | CHA-CBD-CGD-O1D |
| 21 | 92 | 603 | CLA | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | A | 846 | LHG | C4-O6-P-O4 |
| 23 | A | 847 | LHG | C3-O3-P-O5 |
| 23 | 3 | 721 | LHG | C3-O3-P-O5 |
| 23 | 3 | 721 | LHG | C4-O6-P-O4 |
| 23 | 3 | 623 | LHG | C3-O3-P-O4 |
| 23 | 3 | 623 | LHG | C4-O6-P-O3 |
| 23 | 3 | 623 | LHG | C4-O6-P-O4 |
| 23 | 3 | 623 | LHG | C4-O6-P-O5 |
| 23 | 7 | 625 | LHG | C4-O6-P-O5 |
| 23 | 8 | 620 | LHG | C3-O3-P-O4 |
| 23 | 8 | 620 | LHG | C4-O6-P-O5 |
| 23 | Z | 620 | LHG | C4-O6-P-O3 |
| 23 | Z | 620 | LHG | C4-O6-P-O4 |
| 23 | Z | 620 | LHG | C4-O6-P-O5 |
| 23 | 9 | 622 | LHG | C3-O3-P-O5 |
| 23 | 9 | 622 | LHG | C4-O6-P-O5 |
| 23 | A2 | 846 | LHG | C4-O6-P-O4 |
| 23 | A2 | 847 | LHG | C3-O3-P-O5 |
| 23 | 32 | 721 | LHG | C3-O3-P-O5 |
| 23 | 32 | 721 | LHG | C4-O6-P-O4 |
| 23 | 32 | 623 | LHG | C3-O3-P-O4 |
| 23 | 32 | 623 | LHG | C4-O6-P-O3 |
| 23 | 32 | 623 | LHG | C4-O6-P-O4 |
| 23 | 32 | 623 | LHG | C4-O6-P-O5 |
| 23 | 72 | 625 | LHG | C4-O6-P-O5 |
| 23 | 82 | 620 | LHG | C3-O3-P-O4 |
| 23 | 82 | 620 | LHG | C4-O6-P-O5 |
| 23 | Z2 | 620 | LHG | C4-O6-P-O3 |
| 23 | Z2 | 620 | LHG | C4-O6-P-O4 |
| 23 | Z2 | 620 | LHG | C4-O6-P-O5 |
| 23 | 92 | 622 | LHG | C4-O6-P-O5 |
| 30 | 1 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 1 | 607 | CHL | CAD-CBD-CGD-O1D |
| 30 | 7 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 8 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | Z | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 4 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 4 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 4 | 608 | CHL | CHA-CBD-CGD-O2D |
| 30 | 6 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 12 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 12 | 607 | CHL | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 72 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 82 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | Z2 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 42 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 42 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 42 | 608 | CHL | CHA-CBD-CGD-O2D |
| 30 | 52 | 618 | CHL | CHA-CBD-CGD-O1D |
| 30 | 62 | 601 | CHL | CAD-CBD-CGD-O1D |
| 30 | 92 | 607 | CHL | CHA-CBD-CGD-O2D |
| 21 | B | 819 | CLA | C3-C5-C6-C7 |
| 21 | B2 | 819 | CLA | C3-C5-C6-C7 |
| 21 | B | 834 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 613 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 834 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 613 | CLA | C4-C3-C5-C6 |
| 21 | A | 819 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 836 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 834 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 839 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 840 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 841 | CLA | C2B-C3B-CAB-CBB |
| 21 | K | 204 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z | 608 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 819 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 836 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 834 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 839 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 841 | CLA | C2B-C3B-CAB-CBB |
| 21 | K2 | 204 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z2 | 608 | CLA | C2B-C3B-CAB-CBB |
| 21 | 92 | 613 | CLA | C2B-C3B-CAB-CBB |
| 24 | 7 | 623 | BCR | C23-C24-C25-C26 |
| 24 | B2 | 846 | BCR | C23-C24-C25-C26 |
| 24 | 72 | 623 | BCR | C23-C24-C25-C26 |
| 28 | 1 | 619 | LUT | C5-C6-C7-C8 |
| 28 | 12 | 619 | LUT | C5-C6-C7-C8 |
| 23 | 4 | 623 | LHG | C6-C5-O7-C7 |
| 23 | 42 | 623 | LHG | C6-C5-O7-C7 |
| 29 | B | 850 | DGD | C3G-C2G-O2G-C1B |
| 30 | 4 | 601 | CHL | C4-C3-C5-C6 |
| 30 | 42 | 601 | CHL | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | Z | 607 | CHL | CAA-CBA-CGA-O2A |
| 30 | Z2 | 607 | CHL | CAA-CBA-CGA-O2A |
| 21 | A | 829 | CLA | C5-C6-C7-C8 |
| 21 | A2 | 829 | CLA | C5-C6-C7-C8 |
| 23 | 92 | 622 | LHG | O6-C4-C5-C6 |
| 21 | A | 823 | CLA | C11-C12-C13-C14 |
| 21 | B | 841 | CLA | C14-C13-C15-C16 |
| 21 | 8 | 613 | CLA | C11-C12-C13-C14 |
| 21 | A2 | 823 | CLA | C11-C12-C13-C14 |
| 21 | B2 | 841 | CLA | C14-C13-C15-C16 |
| 21 | 82 | 613 | CLA | C11-C12-C13-C14 |
| 21 | 82 | 613 | CLA | C14-C13-C15-C16 |
| 30 | 1 | 601 | CHL | C11-C12-C13-C14 |
| 30 | 8 | 601 | CHL | C14-C13-C15-C16 |
| 30 | 6 | 607 | CHL | C6-C7-C8-C9 |
| 30 | 6 | 616 | CHL | C14-C13-C15-C16 |
| 30 | 12 | 601 | CHL | C11-C12-C13-C14 |
| 30 | 82 | 601 | CHL | C14-C13-C15-C16 |
| 30 | 62 | 607 | CHL | C6-C7-C8-C9 |
| 30 | 62 | 616 | CHL | C14-C13-C15-C16 |
| 29 | B | 850 | DGD | C7B-C8B-C9B-CAB |
| 23 | 3 | 721 | LHG | C1-C2-C3-O3 |
| 23 | 32 | 721 | LHG | C1-C2-C3-O3 |
| 23 | 3 | 721 | LHG | O6-C4-C5-O7 |
| 23 | 9 | 622 | LHG | O6-C4-C5-O7 |
| 23 | 32 | 721 | LHG | O6-C4-C5-O7 |
| 23 | 92 | 622 | LHG | O6-C4-C5-O7 |
| 23 | 6 | 629 | LHG | C13-C14-C15-C16 |
| 26 | 1 | 621 | LMU | O5'-C1'-O1'-C1 |
| 26 | 12 | 621 | LMU | O5'-C1'-O1'-C1 |
| 27 | B | 852 | LMG | O6-C1-O1-C7 |
| 27 | B2 | 852 | LMG | O6-C1-O1-C7 |
| 21 | 3 | 615 | CLA | CAA-CBA-CGA-O2A |
| 29 | B2 | 850 | DGD | O2G-C1B-C2B-C3B |
| 26 | 9 | 624 | LMU | C2'-C1'-O1'-C1 |
| 26 | 92 | 624 | LMU | C2'-C1'-O1'-C1 |
| 21 | 32 | 615 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 805 | CLA | C2-C3-C5-C6 |
| 21 | 72 | 620 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 601 | CLA | C16-C17-C18-C19 |
| 21 | 52 | 601 | CLA | C16-C17-C18-C19 |
| 23 | 62 | 629 | LHG | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | J | 104 | LMG | O1-C7-C8-O7 |
| 27 | J2 | 104 | LMG | O1-C7-C8-O7 |
| 21 | 32 | 607 | CLA | C4-C3-C5-C6 |
| 30 | 8 | 601 | CHL | C4-C3-C5-C6 |
| 30 | 82 | 601 | CHL | C4-C3-C5-C6 |
| 21 | 1 | 609 | CLA | CAA-CBA-CGA-O2A |
| 21 | 12 | 609 | CLA | CAA-CBA-CGA-O2A |
| 30 | 8 | 601 | CHL | CAA-CBA-CGA-O2A |
| 30 | 82 | 601 | CHL | CAA-CBA-CGA-O2A |
| 21 | B | 805 | CLA | C2-C3-C5-C6 |
| 21 | 7 | 620 | CLA | C2-C3-C5-C6 |
| 23 | 5 | 623 | LHG | C4-C5-C6-O8 |
| 23 | 52 | 623 | LHG | C4-C5-C6-O8 |
| 27 | 8 | 629 | LMG | C14-C15-C16-C17 |
| 27 | 82 | 629 | LMG | C14-C15-C16-C17 |
| 21 | B | 805 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 805 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 818 | CLA | C10-C11-C12-C13 |
| 21 | A | 823 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 823 | CLA | C2A-CAA-CBA-CGA |
| 21 | 3 | 607 | CLA | C4-C3-C5-C6 |
| 21 | 6 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 62 | 603 | CLA | C4-C3-C5-C6 |
| 21 | B | 818 | CLA | C10-C11-C12-C13 |
| 21 | 1 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 7 | 603 | CLA | C2-C3-C5-C6 |
| 21 | 12 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 72 | 603 | CLA | C2-C3-C5-C6 |
| 26 | A2 | 857 | LMU | O1'-C1-C2-C3 |
| 26 | A | 857 | LMU | C2-C1-O1'-C1' |
| 26 | A | 858 | LMU | C2-C1-O1'-C1' |
| 26 | 7 | 629 | LMU | C2-C1-O1'-C1' |
| 26 | 8 | 628 | LMU | C2-C1-O1'-C1' |
| 26 | 8 | 627 | LMU | C2-C1-O1'-C1' |
| 26 | A2 | 857 | LMU | C2-C1-O1'-C1' |
| 26 | A2 | 858 | LMU | C2-C1-O1'-C1' |
| 26 | 72 | 629 | LMU | C2-C1-O1'-C1' |
| 26 | 82 | 628 | LMU | C2-C1-O1'-C1' |
| 26 | 82 | 627 | LMU | C2-C1-O1'-C1' |
| 21 | A | 809 | CLA | C14-C13-C15-C16 |
| 21 | A | 840 | CLA | C14-C13-C15-C16 |
| 21 | F | 301 | CLA | C11-C10-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 7 | 611 | CLA | C6-C7-C8-C9 |
| 21 | 8 | 613 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 809 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 840 | CLA | C14-C13-C15-C16 |
| 21 | F2 | 301 | CLA | C11-C10-C8-C9 |
| 21 | 72 | 611 | CLA | C6-C7-C8-C9 |
| 21 | B | 802 | CLA | C4B-C3B-CAB-CBB |
| 21 | L | 203 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 802 | CLA | C4B-C3B-CAB-CBB |
| 21 | L2 | 203 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 832 | CLA | C15-C16-C17-C18 |
| 23 | B2 | 851 | LHG | C23-C24-C25-C26 |
| 26 | A | 857 | LMU | O1'-C1-C2-C3 |
| 26 | Z2 | 622 | LMU | C5'-C4'-O1B-C1B |
| 21 | 5 | 601 | CLA | C16-C17-C18-C20 |
| 21 | 52 | 601 | CLA | C16-C17-C18-C20 |
| 21 | B2 | 832 | CLA | C15-C16-C17-C18 |
| 21 | B | 810 | CLA | C4-C3-C5-C6 |
| 21 | 4 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 4 | 611 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 603 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 810 | CLA | C4-C3-C5-C6 |
| 21 | 42 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 42 | 611 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 603 | CLA | C4-C3-C5-C6 |
| 21 | B | 810 | CLA | C2-C3-C5-C6 |
| 21 | B | 834 | CLA | C2-C3-C5-C6 |
| 21 | 3 | 607 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 6 | 603 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 834 | CLA | C2-C3-C5-C6 |
| 21 | 32 | 607 | CLA | C2-C3-C5-C6 |
| 21 | 52 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 62 | 603 | CLA | C2-C3-C5-C6 |
| 26 | Z | 622 | LMU | C5'-C4'-O1B-C1B |
| 32 | 62 | 625 | NEX | C33-C34-C35-C15 |
| 21 | A | 840 | CLA | C12-C13-C15-C16 |
| 21 | 7 | 611 | CLA | C6-C7-C8-C10 |
| 21 | A2 | 840 | CLA | C12-C13-C15-C16 |
| 21 | 72 | 611 | CLA | C6-C7-C8-C10 |
| 30 | 8 | 601 | CHL | C11-C12-C13-C15 |
| 30 | 82 | 601 | CHL | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | A | 860 | LMG | O1-C7-C8-O7 |
| 27 | A2 | 860 | LMG | O1-C7-C8-O7 |
| 26 | 82 | 627 | LMU | C2-C3-C4-C5 |
| 21 | 4 | 609 | CLA | C3A-C2A-CAA-CBA |
| 21 | 5 | 621 | CLA | C3A-C2A-CAA-CBA |
| 21 | 42 | 609 | CLA | C3A-C2A-CAA-CBA |
| 21 | 52 | 621 | CLA | C3A-C2A-CAA-CBA |
| 30 | 5 | 607 | CHL | C4-C3-C5-C6 |
| 30 | 52 | 607 | CHL | C4-C3-C5-C6 |
| 26 | 8 | 627 | LMU | C2-C3-C4-C5 |
| 29 | B | 850 | DGD | CDB-CEB-CFB-CGB |
| 21 | A | 821 | CLA | C2-C3-C5-C6 |
| 21 | 6 | 604 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 810 | CLA | C2-C3-C5-C6 |
| 23 | B | 851 | LHG | C23-C24-C25-C26 |
| 21 | 6 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | 62 | 612 | CLA | CAA-CBA-CGA-O1A |
| 24 | A | 852 | BCR | C11-C10-C9-C34 |
| 24 | A | 852 | BCR | C16-C17-C18-C36 |
| 24 | B | 845 | BCR | C11-C10-C9-C34 |
| 24 | B | 845 | BCR | C20-C21-C22-C37 |
| 24 | L | 201 | BCR | C11-C10-C9-C34 |
| 24 | A2 | 852 | BCR | C11-C10-C9-C34 |
| 24 | A2 | 852 | BCR | C16-C17-C18-C36 |
| 24 | B2 | 845 | BCR | C11-C10-C9-C34 |
| 24 | B2 | 845 | BCR | C20-C21-C22-C37 |
| 24 | L2 | 201 | BCR | C11-C10-C9-C34 |
| 28 | F | 305 | LUT | C20-C13-C14-C15 |
| 28 | F2 | 305 | LUT | C20-C13-C14-C15 |
| 32 | 5 | 625 | NEX | C39-C29-C30-C31 |
| 32 | 6 | 625 | NEX | C39-C29-C30-C31 |
| 32 | 52 | 625 | NEX | C39-C29-C30-C31 |
| 32 | 62 | 625 | NEX | C39-C29-C30-C31 |
| 23 | B | 851 | LHG | O9-C7-C8-C9 |
| 23 | B2 | 851 | LHG | O9-C7-C8-C9 |
| 30 | 3 | 608 | CHL | C13-C15-C16-C17 |
| 30 | 32 | 608 | CHL | C13-C15-C16-C17 |
| 32 | 6 | 625 | NEX | C33-C34-C35-C15 |
| 21 | B | 840 | CLA | C10-C11-C12-C13 |
| 21 | 4 | 603 | CLA | C10-C11-C12-C13 |
| 21 | B2 | 840 | CLA | C10-C11-C12-C13 |
| 21 | 42 | 603 | CLA | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | 4 | 622 | LHG | C5-C4-O6-P |
| 23 | 42 | 622 | LHG | C5-C4-O6-P |
| 21 | 4 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | 42 | 612 | CLA | CAA-CBA-CGA-O1A |
| 27 | 8 | 629 | LMG | C13-C14-C15-C16 |
| 26 | Z2 | 622 | LMU | C3'-C4'-O1B-C1B |
| 21 | 7 | 604 | CLA | C4-C3-C5-C6 |
| 21 | 72 | 604 | CLA | C4-C3-C5-C6 |
| 21 | 82 | 611 | CLA | CAA-CBA-CGA-O1A |
| 21 | 7 | 603 | CLA | C4-C3-C5-C6 |
| 21 | 8 | 613 | CLA | C4-C3-C5-C6 |
| 21 | 72 | 603 | CLA | C4-C3-C5-C6 |
| 26 | Z | 622 | LMU | C3'-C4'-O1B-C1B |
| 21 | 3 | 613 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 821 | CLA | C2-C3-C5-C6 |
| 21 | 32 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 62 | 604 | CLA | C2-C3-C5-C6 |
| 30 | 42 | 601 | CHL | C2-C3-C5-C6 |
| 23 | 5 | 623 | LHG | C1-C2-C3-O3 |
| 23 | 52 | 623 | LHG | C1-C2-C3-O3 |
| 21 | B2 | 803 | CLA | C8-C10-C11-C12 |
| 21 | 8 | 611 | CLA | CAA-CBA-CGA-O1A |
| 23 | 42 | 622 | LHG | C27-C28-C29-C30 |
| 27 | 82 | 629 | LMG | C13-C14-C15-C16 |
| 21 | B | 803 | CLA | C8-C10-C11-C12 |
| 23 | B | 851 | LHG | C4-C5-C6-O8 |
| 23 | B2 | 851 | LHG | C4-C5-C6-O8 |
| 21 | A2 | 841 | CLA | C10-C11-C12-C13 |
| 23 | 4 | 622 | LHG | C27-C28-C29-C30 |
| 21 | A | 810 | CLA | C11-C10-C8-C9 |
| 21 | A | 812 | CLA | C14-C13-C15-C16 |
| 21 | A | 820 | CLA | C6-C7-C8-C9 |
| 21 | A | 820 | CLA | C11-C12-C13-C14 |
| 21 | B | 811 | CLA | C11-C10-C8-C9 |
| 21 | B | 817 | CLA | C11-C10-C8-C9 |
| 21 | B | 840 | CLA | C11-C12-C13-C14 |
| 21 | 7 | 611 | CLA | C11-C12-C13-C14 |
| 21 | 5 | 601 | CLA | C6-C7-C8-C9 |
| 21 | A2 | 810 | CLA | C11-C10-C8-C9 |
| 21 | A2 | 812 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 820 | CLA | C6-C7-C8-C9 |
| 21 | A2 | 820 | CLA | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B2 | 811 | CLA | C11-C10-C8-C9 |
| 21 | B2 | 817 | CLA | C11-C10-C8-C9 |
| 21 | B2 | 840 | CLA | C11-C12-C13-C14 |
| 21 | 72 | 611 | CLA | C11-C12-C13-C14 |
| 21 | 52 | 601 | CLA | C6-C7-C8-C9 |
| 30 | 4 | 601 | CHL | C11-C10-C8-C9 |
| 30 | 5 | 607 | CHL | C11-C10-C8-C9 |
| 30 | 42 | 601 | CHL | C11-C10-C8-C9 |
| 30 | 52 | 607 | CHL | C11-C10-C8-C9 |
| 21 | 3 | 603 | CLA | C4C-C3C-CAC-CBC |
| 21 | 32 | 603 | CLA | C4C-C3C-CAC-CBC |
| 21 | A2 | 810 | CLA | C5-C6-C7-C8 |
| 27 | 12 | 628 | LMG | C11-C12-C13-C14 |
| 23 | 4 | 623 | LHG | C4-C5-O7-C7 |
| 23 | 6 | 629 | LHG | C4-C5-O7-C7 |
| 23 | 42 | 623 | LHG | C4-C5-O7-C7 |
| 23 | 62 | 629 | LHG | C4-C5-O7-C7 |
| 29 | B2 | 850 | DGD | C1G-C2G-O2G-C1B |
| 21 | A | 810 | CLA | C5-C6-C7-C8 |
| 30 | 6 | 607 | CHL | C1A-C2A-CAA-CBA |
| 30 | 62 | 607 | CHL | C1A-C2A-CAA-CBA |
| 21 | A | 841 | CLA | C10-C11-C12-C13 |
| 21 | 1 | 612 | CLA | CAA-CBA-CGA-O2A |
| 27 | 1 | 628 | LMG | C11-C12-C13-C14 |
| 21 | B2 | 836 | CLA | C4-C3-C5-C6 |
| 21 | 82 | 613 | CLA | C4-C3-C5-C6 |
| 30 | 8 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 4 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 5 | 607 | CHL | C2-C3-C5-C6 |
| 30 | 82 | 601 | CHL | C2-C3-C5-C6 |
| 30 | 52 | 607 | CHL | C2-C3-C5-C6 |
| 21 | 7 | 610 | CLA | O1A-CGA-O2A-C1 |
| 21 | 72 | 610 | CLA | O1A-CGA-O2A-C1 |
| 21 | 12 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 819 | CLA | C1A-C2A-CAA-CBA |
| 21 | 7 | 614 | CLA | C1A-C2A-CAA-CBA |
| 21 | 5 | 621 | CLA | C1A-C2A-CAA-CBA |
| 21 | A2 | 819 | CLA | C1A-C2A-CAA-CBA |
| 21 | 72 | 614 | CLA | C1A-C2A-CAA-CBA |
| 21 | 52 | 621 | CLA | C1A-C2A-CAA-CBA |
| 24 | A | 852 | BCR | C11-C10-C9-C8 |
| 24 | A | 852 | BCR | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 24 | B | 845 | BCR | C11-C10-C9-C8 |
| 24 | B | 845 | BCR | C20-C21-C22-C23 |
| 24 | L | 201 | BCR | C11-C10-C9-C8 |
| 24 | A2 | 852 | BCR | C11-C10-C9-C8 |
| 24 | A2 | 852 | BCR | C16-C17-C18-C19 |
| 24 | B2 | 845 | BCR | C11-C10-C9-C8 |
| 24 | B2 | 845 | BCR | C20-C21-C22-C23 |
| 24 | L2 | 201 | BCR | C11-C10-C9-C8 |
| 28 | F | 305 | LUT | C12-C13-C14-C15 |
| 28 | F2 | 305 | LUT | C12-C13-C14-C15 |
| 32 | 5 | 625 | NEX | C28-C29-C30-C31 |
| 32 | 6 | 625 | NEX | C28-C29-C30-C31 |
| 32 | 52 | 625 | NEX | C28-C29-C30-C31 |
| 32 | 62 | 625 | NEX | C28-C29-C30-C31 |
| 27 | 82 | 629 | LMG | C15-C16-C17-C18 |
| 27 | 8 | 629 | LMG | C15-C16-C17-C18 |
| 21 | B | 818 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 826 | CLA | C2B-C3B-CAB-CBB |
| 21 | K | 206 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | 1 | 616 | CLA | C2B-C3B-CAB-CBB |
| 21 | 8 | 608 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z | 616 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 616 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 621 | CLA | C2B-C3B-CAB-CBB |
| 21 | 6 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 835 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 818 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 826 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 840 | CLA | C2B-C3B-CAB-CBB |
| 21 | K2 | 206 | CLA | C2B-C3B-CAB-CBB |
| 21 | 12 | 612 | CLA | C2B-C3B-CAB-CBB |
| 21 | 12 | 616 | CLA | C2B-C3B-CAB-CBB |
| 21 | 82 | 608 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z2 | 609 | CLA | C2B-C3B-CAB-CBB |
| 21 | Z2 | 616 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 613 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 616 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 617 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 621 | CLA | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 62 | 614 | CLA | C2B-C3B-CAB-CBB |
| 24 | A | 848 | BCR | C5-C6-C7-C8 |
| 24 | B | 847 | BCR | C23-C24-C25-C26 |
| 24 | B | 848 | BCR | C5-C6-C7-C8 |
| 24 | L | 205 | BCR | C23-C24-C25-C26 |
| 24 | 6 | 623 | BCR | C23-C24-C25-C26 |
| 24 | A2 | 848 | BCR | C5-C6-C7-C8 |
| 24 | B2 | 847 | BCR | C23-C24-C25-C26 |
| 24 | B2 | 848 | BCR | C5-C6-C7-C8 |
| 24 | L2 | 205 | BCR | C23-C24-C25-C26 |
| 24 | 62 | 623 | BCR | C23-C24-C25-C26 |
| 28 | 1 | 617 | LUT | C5-C6-C7-C8 |
| 28 | 3 | 621 | LUT | C5-C6-C7-C8 |
| 28 | 3 | 622 | LUT | C5-C6-C7-C8 |
| 28 | 7 | 621 | LUT | C1-C6-C7-C8 |
| 28 | 8 | 617 | LUT | C5-C6-C7-C8 |
| 28 | Z | 617 | LUT | C5-C6-C7-C8 |
| 28 | 4 | 619 | LUT | C1-C6-C7-C8 |
| 28 | 5 | 620 | LUT | C5-C6-C7-C8 |
| 28 | 6 | 621 | LUT | C5-C6-C7-C8 |
| 28 | 9 | 616 | LUT | C5-C6-C7-C8 |
| 28 | 12 | 617 | LUT | C5-C6-C7-C8 |
| 28 | 32 | 621 | LUT | C5-C6-C7-C8 |
| 28 | 32 | 622 | LUT | C5-C6-C7-C8 |
| 28 | 72 | 621 | LUT | C1-C6-C7-C8 |
| 28 | 82 | 617 | LUT | C5-C6-C7-C8 |
| 28 | Z2 | 617 | LUT | C5-C6-C7-C8 |
| 28 | 42 | 619 | LUT | C1-C6-C7-C8 |
| 28 | 52 | 620 | LUT | C5-C6-C7-C8 |
| 28 | 62 | 621 | LUT | C5-C6-C7-C8 |
| 28 | 92 | 616 | LUT | C5-C6-C7-C8 |
| 21 | 4 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | K2 | 206 | CLA | CAA-CBA-CGA-O1A |
| 21 | 42 | 612 | CLA | CAA-CBA-CGA-O2A |
| 30 | 7 | 606 | CHL | CAA-CBA-CGA-O2A |
| 30 | 72 | 606 | CHL | CAA-CBA-CGA-O2A |
| 21 | B | 804 | CLA | CAA-CBA-CGA-O1A |
| 21 | K | 206 | CLA | CAA-CBA-CGA-O1A |
| 21 | 9 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 804 | CLA | CAA-CBA-CGA-O1A |
| 21 | 82 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 823 | CLA | C4-C3-C5-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 836 | CLA | C4-C3-C5-C6 |
| 21 | F | 301 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 604 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 823 | CLA | C4-C3-C5-C6 |
| 21 | F2 | 301 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 604 | CLA | C4-C3-C5-C6 |
| 30 | 8 | 606 | CHL | C4-C3-C5-C6 |
| 30 | 82 | 606 | CHL | C4-C3-C5-C6 |
| 23 | 4 | 622 | LHG | O6-C4-C5-C6 |
| 23 | 42 | 622 | LHG | O6-C4-C5-C6 |
| 21 | 8 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 4 | 603 | CLA | C2-C3-C5-C6 |
| 21 | 82 | 613 | CLA | C2-C3-C5-C6 |
| 21 | 42 | 603 | CLA | C2-C3-C5-C6 |
| 21 | A | 824 | CLA | CAA-CBA-CGA-O2A |
| 21 | 5 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | 52 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | 92 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 823 | CLA | C11-C12-C13-C15 |
| 21 | B | 808 | CLA | C12-C13-C15-C16 |
| 21 | B | 809 | CLA | C6-C7-C8-C10 |
| 21 | B | 832 | CLA | C11-C12-C13-C15 |
| 21 | G | 203 | CLA | C6-C7-C8-C10 |
| 21 | 1 | 613 | CLA | C11-C12-C13-C15 |
| 21 | 4 | 611 | CLA | C6-C7-C8-C10 |
| 21 | 5 | 601 | CLA | C6-C7-C8-C10 |
| 21 | A2 | 823 | CLA | C11-C12-C13-C15 |
| 21 | B2 | 808 | CLA | C12-C13-C15-C16 |
| 21 | B2 | 809 | CLA | C6-C7-C8-C10 |
| 21 | B2 | 832 | CLA | C11-C12-C13-C15 |
| 21 | G2 | 203 | CLA | C6-C7-C8-C10 |
| 21 | 12 | 613 | CLA | C11-C12-C13-C15 |
| 21 | 42 | 611 | CLA | C6-C7-C8-C10 |
| 21 | 52 | 601 | CLA | C6-C7-C8-C10 |
| 23 | 9 | 622 | LHG | O7-C5-C6-O8 |
| 23 | 92 | 622 | LHG | O7-C5-C6-O8 |
| 27 | B | 852 | LMG | O1-C7-C8-O7 |
| 27 | B2 | 852 | LMG | O1-C7-C8-O7 |
| 29 | B2 | 850 | DGD | O1G-C1G-C2G-O2G |
| 26 | 1 | 621 | LMU | C3'-C4'-O1B-C1B |
| 21 | 8 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | A2 | 824 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | A2 | 827 | CLA | C13-C15-C16-C17 |
| 21 | 6 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | 62 | 612 | CLA | CAA-CBA-CGA-O2A |
| 26 | 12 | 621 | LMU | C3'-C4'-O1B-C1B |
| 21 | A | 825 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 824 | CLA | CAA-CBA-CGA-O1A |
| 21 | A2 | 824 | CLA | CAA-CBA-CGA-O1A |
| 21 | 52 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 841 | CLA | C4-C3-C5-C6 |
| 21 | 8 | 614 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 841 | CLA | C4-C3-C5-C6 |
| 21 | 82 | 614 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 609 | CLA | C4-C3-C5-C6 |
| 21 | A | 827 | CLA | C13-C15-C16-C17 |
| 21 | B | 811 | CLA | C2-C3-C5-C6 |
| 21 | Z | 604 | CLA | C2-C3-C5-C6 |
| 21 | 4 | 611 | CLA | C2-C3-C5-C6 |
| 21 | 5 | 603 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 811 | CLA | C2-C3-C5-C6 |
| 21 | Z2 | 604 | CLA | C2-C3-C5-C6 |
| 21 | 42 | 611 | CLA | C2-C3-C5-C6 |
| 21 | 52 | 603 | CLA | C2-C3-C5-C6 |
| 23 | 3 | 623 | LHG | C28-C29-C30-C31 |
| 21 | 32 | 609 | CLA | C4C-C3C-CAC-CBC |
| 21 | 1 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | 12 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 840 | CLA | C11-C10-C8-C9 |
| 21 | L | 203 | CLA | C14-C13-C15-C16 |
| 21 | 3 | 615 | CLA | C11-C10-C8-C9 |
| 21 | 8 | 610 | CLA | C11-C12-C13-C14 |
| 21 | A2 | 840 | CLA | C11-C10-C8-C9 |
| 21 | 32 | 615 | CLA | C11-C10-C8-C9 |
| 21 | 82 | 610 | CLA | C11-C12-C13-C14 |
| 21 | B2 | 834 | CLA | C8-C10-C11-C12 |
| 21 | 3 | 609 | CLA | C4C-C3C-CAC-CBC |
| 30 | 5 | 607 | CHL | CAA-CBA-CGA-O1A |
| 21 | B | 834 | CLA | C8-C10-C11-C12 |
| 23 | A2 | 846 | LHG | C11-C12-C13-C14 |
| 23 | 32 | 623 | LHG | C28-C29-C30-C31 |
| 21 | B | 804 | CLA | CAA-CBA-CGA-O2A |
| 21 | 5 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 804 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 7 | 606 | CHL | CAA-CBA-CGA-O1A |
| 30 | 72 | 606 | CHL | CAA-CBA-CGA-O1A |
| 21 | A2 | 825 | CLA | C2C-C3C-CAC-CBC |
| 23 | A | 846 | LHG | C11-C12-C13-C14 |
| 26 | 62 | 631 | LMU | C3-C4-C5-C6 |
| 21 | A | 814 | CLA | C4-C3-C5-C6 |
| 21 | B | 811 | CLA | C4-C3-C5-C6 |
| 21 | Z | 604 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 609 | CLA | C4-C3-C5-C6 |
| 21 | 6 | 611 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 814 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 811 | CLA | C4-C3-C5-C6 |
| 21 | Z2 | 604 | CLA | C4-C3-C5-C6 |
| 21 | 62 | 611 | CLA | C4-C3-C5-C6 |
| 21 | 92 | 614 | CLA | CAA-CBA-CGA-O1A |
| 23 | 9 | 622 | LHG | C5-C4-O6-P |
| 23 | 92 | 622 | LHG | C5-C4-O6-P |
| 21 | 5 | 610 | CLA | C2-C3-C5-C6 |
| 21 | 52 | 610 | CLA | C2-C3-C5-C6 |
| 21 | 9 | 614 | CLA | CAA-CBA-CGA-O1A |
| 26 | 6 | 631 | LMU | C3-C4-C5-C6 |
| 27 | B | 852 | LMG | O1-C7-C8-C9 |
| 27 | B2 | 852 | LMG | O1-C7-C8-C9 |
| 30 | Z | 606 | CHL | CAA-CBA-CGA-O1A |
| 30 | Z2 | 606 | CHL | CAA-CBA-CGA-O1A |
| 26 | 1 | 621 | LMU | C2B-C1B-O1B-C4' |
| 26 | 12 | 621 | LMU | C2B-C1B-O1B-C4' |
| 30 | 52 | 607 | CHL | CAA-CBA-CGA-O1A |
| 21 | 3 | 615 | CLA | C4-C3-C5-C6 |
| 21 | 32 | 615 | CLA | C4-C3-C5-C6 |
| 30 | Z | 601 | CHL | C4-C3-C5-C6 |
| 30 | Z2 | 601 | CHL | C4-C3-C5-C6 |
| 32 | 6 | 625 | NEX | C9-C10-C11-C12 |
| 21 | 4 | 613 | CLA | CAA-CBA-CGA-O2A |
| 21 | 42 | 613 | CLA | CAA-CBA-CGA-O2A |
| 27 | 82 | 629 | LMG | C21-C22-C23-C24 |
| 21 | A | 809 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 820 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 1 | 616 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 608 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z | 609 | CLA | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | Z | 616 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 809 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 820 | CLA | C4B-C3B-CAB-CBB |
| 21 | 12 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 12 | 616 | CLA | C4B-C3B-CAB-CBB |
| 21 | 82 | 608 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z2 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z2 | 616 | CLA | C4B-C3B-CAB-CBB |
| 21 | 62 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | K | 206 | CLA | CAA-CBA-CGA-O2A |
| 21 | K2 | 206 | CLA | CAA-CBA-CGA-O2A |
| 30 | Z | 606 | CHL | CAA-CBA-CGA-O2A |
| 30 | Z2 | 606 | CHL | CAA-CBA-CGA-O2A |
| 29 | B | 850 | DGD | O1B-C1B-C2B-C3B |
| 27 | 7 | 626 | LMG | C14-C15-C16-C17 |
| 27 | 8 | 629 | LMG | C21-C22-C23-C24 |
| 26 | K | 208 | LMU | C5-C6-C7-C8 |
| 26 | K2 | 208 | LMU | C5-C6-C7-C8 |
| 27 | 72 | 626 | LMG | C14-C15-C16-C17 |
| 30 | 4 | 608 | CHL | CHA-CBD-CGD-O1D |
| 30 | 5 | 606 | CHL | CHA-CBD-CGD-O1D |
| 30 | 5 | 606 | CHL | CHA-CBD-CGD-O2D |
| 30 | 6 | 606 | CHL | CHA-CBD-CGD-O1D |
| 30 | 6 | 606 | CHL | CHA-CBD-CGD-O2D |
| 30 | 6 | 607 | CHL | CHA-CBD-CGD-O1D |
| 30 | 6 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 42 | 608 | CHL | CHA-CBD-CGD-O1D |
| 30 | 52 | 606 | CHL | CHA-CBD-CGD-O1D |
| 30 | 52 | 606 | CHL | CHA-CBD-CGD-O2D |
| 30 | 62 | 606 | CHL | CHA-CBD-CGD-O1D |
| 30 | 62 | 606 | CHL | CHA-CBD-CGD-O2D |
| 30 | 62 | 607 | CHL | CHA-CBD-CGD-O1D |
| 30 | 62 | 607 | CHL | CHA-CBD-CGD-O2D |
| 30 | 92 | 607 | CHL | CHA-CBD-CGD-O1D |
| 21 | 5 | 616 | CLA | C4-C3-C5-C6 |
| 21 | 6 | 609 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 616 | CLA | C4-C3-C5-C6 |
| 21 | 62 | 609 | CLA | C4-C3-C5-C6 |
| 23 | 4 | 623 | LHG | O7-C5-C6-O8 |
| 23 | 42 | 623 | LHG | O7-C5-C6-O8 |
| 27 | 7 | 626 | LMG | O7-C8-C9-O8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | 9 | 620 | LMG | O1-C7-C8-O7 |
| 27 | 72 | 626 | LMG | O7-C8-C9-O8 |
| 27 | 92 | 620 | LMG | O1-C7-C8-O7 |
| 21 | 6 | 611 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 836 | CLA | C2-C3-C5-C6 |
| 21 | 62 | 611 | CLA | C2-C3-C5-C6 |
| 21 | B | 817 | CLA | C11-C10-C8-C7 |
| 21 | B2 | 817 | CLA | C11-C10-C8-C7 |
| 29 | B2 | 850 | DGD | C9B-CAB-CBB-CCB |
| 21 | Z | 612 | CLA | CAA-CBA-CGA-O1A |
| 32 | 62 | 625 | NEX | C9-C10-C11-C12 |
| 21 | A | 826 | CLA | C11-C10-C8-C9 |
| 21 | A | 839 | CLA | C11-C12-C13-C14 |
| 21 | A | 843 | CLA | C11-C12-C13-C14 |
| 21 | B | 841 | CLA | C11-C10-C8-C9 |
| 21 | A2 | 826 | CLA | C11-C10-C8-C9 |
| 21 | A2 | 839 | CLA | C11-C12-C13-C14 |
| 21 | A2 | 843 | CLA | C11-C12-C13-C14 |
| 21 | B2 | 841 | CLA | C11-C10-C8-C9 |
| 21 | L2 | 203 | CLA | C14-C13-C15-C16 |
| 27 | 4 | 624 | LMG | C8-C7-O1-C1 |
| 27 | 42 | 624 | LMG | C8-C7-O1-C1 |
| 21 | 5 | 621 | CLA | C2A-CAA-CBA-CGA |
| 21 | 52 | 621 | CLA | C2A-CAA-CBA-CGA |
| 30 | 92 | 607 | CHL | C2-C1-O2A-CGA |
| 21 | Z2 | 612 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 814 | CLA | C2-C3-C5-C6 |
| 21 | A2 | 814 | CLA | C2-C3-C5-C6 |
| 26 | 1 | 621 | LMU | C5'-C4'-O1B-C1B |
| 26 | 12 | 621 | LMU | C5'-C4'-O1B-C1B |
| 21 | B | 817 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 817 | CLA | CAA-CBA-CGA-O2A |
| 27 | 8 | 626 | LMG | O8-C28-C29-C30 |
| 27 | 82 | 626 | LMG | O8-C28-C29-C30 |
| 30 | Z | 607 | CHL | O2A-C1-C2-C3 |
| 30 | Z2 | 607 | CHL | O2A-C1-C2-C3 |
| 21 | B | 809 | CLA | C3-C5-C6-C7 |
| 21 | B2 | 809 | CLA | C3-C5-C6-C7 |
| 21 | B | 836 | CLA | C2-C3-C5-C6 |
| 23 | 4 | 622 | LHG | O6-C4-C5-O7 |
| 23 | 42 | 622 | LHG | O6-C4-C5-O7 |
| 27 | J | 103 | LMG | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | J2 | 103 | LMG | C22-C23-C24-C25 |
| 23 | 82 | 620 | LHG | C12-C13-C14-C15 |
| 23 | 8 | 620 | LHG | C12-C13-C14-C15 |
| 27 | 1 | 624 | LMG | C31-C32-C33-C34 |
| 27 | 12 | 624 | LMG | C31-C32-C33-C34 |
| 30 | 32 | 608 | CHL | C4-C3-C5-C6 |
| 21 | A2 | 807 | CLA | CAA-CBA-CGA-O2A |
| 26 | A | 865 | LMU | C5-C6-C7-C8 |
| 26 | A2 | 865 | LMU | C5-C6-C7-C8 |
| 21 | B | 811 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 811 | CLA | CAA-CBA-CGA-O2A |
| 21 | 52 | 604 | CLA | CAA-CBA-CGA-O2A |
| 23 | A | 846 | LHG | O8-C23-C24-C25 |
| 21 | A | 813 | CLA | C6-C7-C8-C9 |
| 21 | A2 | 813 | CLA | C6-C7-C8-C9 |
| 21 | A | 807 | CLA | CAA-CBA-CGA-O2A |
| 21 | 1 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 5 | 616 | CLA | CAA-CBA-CGA-O2A |
| 21 | 12 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 52 | 616 | CLA | CAA-CBA-CGA-O2A |
| 23 | A2 | 846 | LHG | O8-C23-C24-C25 |
| 27 | A | 859 | LMG | C13-C14-C15-C16 |
| 27 | A2 | 859 | LMG | C13-C14-C15-C16 |
| 23 | 72 | 625 | LHG | C10-C11-C12-C13 |
| 30 | 3 | 608 | CHL | C4-C3-C5-C6 |
| 21 | 5 | 604 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 810 | CLA | C11-C10-C8-C7 |
| 21 | A | 820 | CLA | C11-C12-C13-C15 |
| 21 | A | 839 | CLA | C11-C12-C13-C15 |
| 21 | A | 843 | CLA | C11-C10-C8-C7 |
| 21 | 3 | 615 | CLA | C11-C10-C8-C7 |
| 21 | 7 | 611 | CLA | C11-C12-C13-C15 |
| 21 | 8 | 610 | CLA | C11-C12-C13-C15 |
| 21 | 5 | 603 | CLA | C12-C13-C15-C16 |
| 21 | A2 | 810 | CLA | C11-C10-C8-C7 |
| 21 | A2 | 820 | CLA | C11-C12-C13-C15 |
| 21 | A2 | 839 | CLA | C11-C12-C13-C15 |
| 21 | A2 | 843 | CLA | C11-C10-C8-C7 |
| 21 | 32 | 615 | CLA | C11-C10-C8-C7 |
| 21 | 72 | 611 | CLA | C11-C12-C13-C15 |
| 21 | 82 | 610 | CLA | C11-C12-C13-C15 |
| 21 | 52 | 603 | CLA | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | B | 842 | PQN | C16-C17-C18-C20 |
| 30 | 5 | 607 | CHL | C6-C7-C8-C10 |
| 30 | 5 | 607 | CHL | C11-C10-C8-C7 |
| 30 | 52 | 607 | CHL | C6-C7-C8-C10 |
| 30 | 52 | 607 | CHL | C11-C10-C8-C7 |
| 23 | 7 | 625 | LHG | C10-C11-C12-C13 |
| 21 | 32 | 604 | CLA | C3-C5-C6-C7 |
| 21 | A | 809 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 824 | CLA | C2B-C3B-CAB-CBB |
| 21 | A | 835 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 802 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 807 | CLA | C2B-C3B-CAB-CBB |
| 21 | B | 820 | CLA | C2B-C3B-CAB-CBB |
| 21 | L | 203 | CLA | C2B-C3B-CAB-CBB |
| 21 | 8 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 5 | 617 | CLA | C2B-C3B-CAB-CBB |
| 21 | 9 | 603 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 809 | CLA | C2B-C3B-CAB-CBB |
| 21 | A2 | 824 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 802 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 807 | CLA | C2B-C3B-CAB-CBB |
| 21 | B2 | 820 | CLA | C2B-C3B-CAB-CBB |
| 21 | L2 | 203 | CLA | C2B-C3B-CAB-CBB |
| 21 | 82 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 611 | CLA | C2B-C3B-CAB-CBB |
| 21 | 52 | 614 | CLA | C2B-C3B-CAB-CBB |
| 21 | 92 | 603 | CLA | C2B-C3B-CAB-CBB |
| 24 | G | 205 | BCR | C1-C6-C7-C8 |
| 24 | L | 205 | BCR | C23-C24-C25-C30 |
| 24 | L | 201 | BCR | C5-C6-C7-C8 |
| 24 | K | 207 | BCR | C1-C6-C7-C8 |
| 24 | K | 207 | BCR | C5-C6-C7-C8 |
| 24 | 3 | 718 | BCR | C23-C24-C25-C26 |
| 24 | G2 | 205 | BCR | C1-C6-C7-C8 |
| 24 | L2 | 205 | BCR | C23-C24-C25-C30 |
| 24 | L2 | 201 | BCR | C5-C6-C7-C8 |
| 24 | K2 | 207 | BCR | C1-C6-C7-C8 |
| 24 | K2 | 207 | BCR | C5-C6-C7-C8 |
| 24 | 32 | 718 | BCR | C23-C24-C25-C26 |
| 28 | 7 | 621 | LUT | C5-C6-C7-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 28 | 72 | 621 | LUT | C5-C6-C7-C8 |
| 21 | B | 834 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 812 | CLA | C2-C1-O2A-CGA |
| 21 | A2 | 812 | CLA | C2-C1-O2A-CGA |
| 21 | 3 | 604 | CLA | C3-C5-C6-C7 |
| 21 | B | 814 | CLA | CAA-CBA-CGA-O2A |
| 21 | 4 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 814 | CLA | CAA-CBA-CGA-O2A |
| 20 | A2 | 801 | CL0 | C5-C6-C7-C8 |
| 27 | J | 104 | LMG | O7-C10-C11-C12 |
| 27 | J2 | 104 | LMG | O7-C10-C11-C12 |
| 20 | A | 801 | CL0 | C5-C6-C7-C8 |
| 21 | 52 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 834 | CLA | CAA-CBA-CGA-O2A |
| 27 | 9 | 620 | LMG | O7-C10-C11-C12 |
| 27 | 92 | 620 | LMG | O7-C10-C11-C12 |
| 26 | 1 | 625 | LMU | C2-C3-C4-C5 |
| 27 | 7 | 626 | LMG | O10-C28-C29-C30 |
| 23 | 42 | 622 | LHG | O8-C23-C24-C25 |
| 26 | 12 | 625 | LMU | C2-C3-C4-C5 |
| 27 | 72 | 626 | LMG | O10-C28-C29-C30 |
| 23 | 4 | 622 | LHG | O8-C23-C24-C25 |
| 27 | 1 | 624 | LMG | O7-C10-C11-C12 |
| 27 | 12 | 624 | LMG | O7-C10-C11-C12 |
| 21 | 5 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 827 | CLA | C8-C10-C11-C12 |
| 30 | 9 | 607 | CHL | C2A-CAA-CBA-CGA |
| 21 | B2 | 827 | CLA | C8-C10-C11-C12 |
| 21 | G2 | 204 | CLA | CAA-CBA-CGA-O2A |
| 21 | 42 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 806 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 806 | CLA | C14-C13-C15-C16 |
| 30 | 6 | 607 | CHL | C14-C13-C15-C16 |
| 30 | 72 | 601 | CHL | C11-C10-C8-C9 |
| 30 | 62 | 607 | CHL | C14-C13-C15-C16 |
| 21 | G | 204 | CLA | CAA-CBA-CGA-O2A |
| 21 | 8 | 604 | CLA | CAA-CBA-CGA-O2A |
| 21 | Z | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 72 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 82 | 604 | CLA | CAA-CBA-CGA-O2A |
| 23 | 3 | 721 | LHG | O7-C7-C8-C9 |
| 23 | 32 | 721 | LHG | O7-C7-C8-C9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | Z2 | 601 | CHL | C5-C6-C7-C8 |
| 21 | A | 807 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 824 | CLA | C4B-C3B-CAB-CBB |
| 21 | A | 843 | CLA | C4B-C3B-CAB-CBB |
| 21 | B | 807 | CLA | C4B-C3B-CAB-CBB |
| 21 | 7 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 8 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | Z | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 5 | 603 | CLA | C1A-C2A-CAA-CBA |
| 21 | 5 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 6 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 9 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 807 | CLA | C4B-C3B-CAB-CBB |
| 21 | A2 | 824 | CLA | C4B-C3B-CAB-CBB |
| 21 | B2 | 807 | CLA | C4B-C3B-CAB-CBB |
| 21 | 32 | 607 | CLA | C4B-C3B-CAB-CBB |
| 21 | 72 | 609 | CLA | C4B-C3B-CAB-CBB |
| 21 | 82 | 614 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z2 | 611 | CLA | C1A-C2A-CAA-CBA |
| 21 | Z2 | 612 | CLA | C4B-C3B-CAB-CBB |
| 21 | 52 | 603 | CLA | C1A-C2A-CAA-CBA |
| 21 | 52 | 611 | CLA | C4B-C3B-CAB-CBB |
| 21 | 62 | 613 | CLA | C4B-C3B-CAB-CBB |
| 21 | 92 | 603 | CLA | C4B-C3B-CAB-CBB |
| 21 | Z | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | Z | 616 | CLA | C3-C5-C6-C7 |
| 21 | Z2 | 616 | CLA | C3-C5-C6-C7 |
| 21 | A | 803 | CLA | C4-C3-C5-C6 |
| 21 | A2 | 803 | CLA | C4-C3-C5-C6 |
| 21 | 6 | 603 | CLA | C13-C15-C16-C17 |
| 21 | 62 | 603 | CLA | C13-C15-C16-C17 |
| 30 | Z | 601 | CHL | C5-C6-C7-C8 |
| 26 | 1 | 625 | LMU | O5'-C1'-O1'-C1 |
| 26 | 9 | 624 | LMU | O5'-C1'-O1'-C1 |
| 26 | 12 | 625 | LMU | O5'-C1'-O1'-C1 |
| 26 | 92 | 624 | LMU | O5'-C1'-O1'-C1 |
| 21 | 7 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | A2 | 826 | CLA | CAA-CBA-CGA-O2A |
| 21 | 52 | 621 | CLA | CAA-CBA-CGA-O2A |
| 27 | 1 | 628 | LMG | O8-C28-C29-C30 |
| 27 | 12 | 628 | LMG | O8-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | B | 852 | LMG | C12-C13-C14-C15 |
| 21 | 5 | 616 | CLA | C2-C3-C5-C6 |
| 23 | 1 | 620 | LHG | O7-C5-C6-O8 |
| 23 | 12 | 620 | LHG | O7-C5-C6-O8 |
| 27 | 1 | 624 | LMG | O1-C7-C8-O7 |
| 27 | 12 | 624 | LMG | O1-C7-C8-O7 |
| 32 | 62 | 625 | NEX | C13-C14-C15-C35 |
| 21 | Z2 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | 8 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | 5 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 82 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | Z2 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 52 | 603 | CLA | CAA-CBA-CGA-O2A |
| 27 | B2 | 852 | LMG | C12-C13-C14-C15 |
| 21 | 3 | 613 | CLA | C10-C11-C12-C13 |
| 23 | 7 | 625 | LHG | O6-C4-C5-C6 |
| 21 | 5 | 621 | CLA | CAA-CBA-CGA-O2A |
| 23 | 1 | 620 | LHG | C11-C10-C9-C8 |
| 26 | 82 | 627 | LMU | C4-C5-C6-C7 |
| 21 | A | 810 | CLA | C8-C10-C11-C12 |
| 21 | A2 | 810 | CLA | C8-C10-C11-C12 |
| 21 | 32 | 613 | CLA | C10-C11-C12-C13 |
| 21 | B | 824 | CLA | C4-C3-C5-C6 |
| 21 | B2 | 824 | CLA | C4-C3-C5-C6 |
| 23 | 12 | 620 | LHG | C11-C10-C9-C8 |
| 21 | A | 825 | CLA | C2-C1-O2A-CGA |
| 21 | A | 843 | CLA | C2-C1-O2A-CGA |
| 21 | B | 811 | CLA | C2-C1-O2A-CGA |
| 21 | B | 836 | CLA | C2-C1-O2A-CGA |
| 21 | Z | 609 | CLA | C2-C1-O2A-CGA |
| 21 | 5 | 616 | CLA | C2-C1-O2A-CGA |
| 21 | A2 | 825 | CLA | C2-C1-O2A-CGA |
| 21 | B2 | 811 | CLA | C2-C1-O2A-CGA |
| 21 | B2 | 836 | CLA | C2-C1-O2A-CGA |
| 21 | Z2 | 609 | CLA | C2-C1-O2A-CGA |
| 21 | 52 | 616 | CLA | C2-C1-O2A-CGA |
| 30 | 8 | 607 | CHL | C2-C1-O2A-CGA |
| 30 | 9 | 607 | CHL | C2-C1-O2A-CGA |
| 30 | 82 | 607 | CHL | C2-C1-O2A-CGA |
| 21 | A | 826 | CLA | CAA-CBA-CGA-O2A |
| 21 | F | 304 | CLA | CAA-CBA-CGA-O2A |
| 21 | F2 | 304 | CLA | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 42 | 603 | CLA | CAA-CBA-CGA-O2A |
| 27 | J | 104 | LMG | O8-C28-C29-C30 |
| 27 | 82 | 629 | LMG | O8-C28-C29-C30 |
| 26 | 8 | 627 | LMU | C4-C5-C6-C7 |
| 21 | A | 840 | CLA | C6-C7-C8-C10 |
| 21 | A | 841 | CLA | C11-C10-C8-C7 |
| 21 | B | 822 | CLA | C6-C7-C8-C10 |
| 21 | L | 203 | CLA | C12-C13-C15-C16 |
| 21 | A2 | 840 | CLA | C6-C7-C8-C10 |
| 21 | A2 | 841 | CLA | C11-C10-C8-C7 |
| 21 | B2 | 822 | CLA | C6-C7-C8-C10 |
| 21 | L2 | 203 | CLA | C12-C13-C15-C16 |
| 22 | A | 844 | PQN | C21-C22-C23-C25 |
| 22 | A2 | 844 | PQN | C21-C22-C23-C25 |
| 22 | B2 | 842 | PQN | C16-C17-C18-C20 |
| 30 | 1 | 601 | CHL | C6-C7-C8-C10 |
| 30 | 1 | 601 | CHL | C11-C10-C8-C7 |
| 30 | 12 | 601 | CHL | C6-C7-C8-C10 |
| 30 | 12 | 601 | CHL | C11-C10-C8-C7 |
| 21 | B | 841 | CLA | C2-C3-C5-C6 |
| 21 | B2 | 841 | CLA | C2-C3-C5-C6 |
| 23 | 9 | 622 | LHG | C26-C27-C28-C29 |
| 21 | B | 824 | CLA | O2A-C1-C2-C3 |
| 21 | B2 | 824 | CLA | O2A-C1-C2-C3 |
| 29 | B2 | 850 | DGD | C3G-C2G-O2G-C1B |
| 30 | 6 | 607 | CHL | O2A-C1-C2-C3 |
| 30 | 62 | 607 | CHL | O2A-C1-C2-C3 |
| 21 | 3 | 617 | CLA | C2C-C3C-CAC-CBC |
| 21 | A2 | 825 | CLA | C4C-C3C-CAC-CBC |
| 29 | B2 | 850 | DGD | C7B-C8B-C9B-CAB |
| 27 | 8 | 629 | LMG | O8-C28-C29-C30 |
| 27 | J2 | 104 | LMG | O8-C28-C29-C30 |
| 23 | 92 | 622 | LHG | C26-C27-C28-C29 |
| 27 | A | 859 | LMG | C29-C30-C31-C32 |
| 21 | A | 818 | CLA | C2A-CAA-CBA-CGA |
| 21 | A2 | 818 | CLA | C2A-CAA-CBA-CGA |
| 23 | 9 | 622 | LHG | C29-C30-C31-C32 |
| 27 | A2 | 859 | LMG | C29-C30-C31-C32 |
| 21 | 5 | 604 | CLA | CAA-CBA-CGA-O1A |
| 21 | 52 | 604 | CLA | CAA-CBA-CGA-O1A |
| 27 | J2 | 104 | LMG | O9-C10-C11-C12 |
| 21 | A | 825 | CLA | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 23 | 92 | 622 | LHG | C29-C30-C31-C32 |
| 21 | 3 | 609 | CLA | C2C-C3C-CAC-CBC |
| 21 | A | 836 | CLA | C3A-C2A-CAA-CBA |
| 21 | F | 304 | CLA | C3A-C2A-CAA-CBA |
| 21 | 3 | 615 | CLA | C3A-C2A-CAA-CBA |
| 21 | 8 | 614 | CLA | C3A-C2A-CAA-CBA |
| 21 | 4 | 613 | CLA | C3A-C2A-CAA-CBA |
| 21 | 4 | 614 | CLA | C3A-C2A-CAA-CBA |
| 21 | 4 | 614 | CLA | C4-C3-C5-C6 |
| 21 | 5 | 603 | CLA | C3A-C2A-CAA-CBA |
| 21 | 5 | 604 | CLA | C3A-C2A-CAA-CBA |
| 21 | 9 | 611 | CLA | C3A-C2A-CAA-CBA |
| 21 | A2 | 836 | CLA | C3A-C2A-CAA-CBA |
| 21 | F2 | 304 | CLA | C3A-C2A-CAA-CBA |
| 21 | 32 | 615 | CLA | C3A-C2A-CAA-CBA |
| 21 | 82 | 614 | CLA | C3A-C2A-CAA-CBA |
| 21 | 42 | 613 | CLA | C3A-C2A-CAA-CBA |
| 21 | 42 | 614 | CLA | C3A-C2A-CAA-CBA |
| 21 | 42 | 614 | CLA | C4-C3-C5-C6 |
| 21 | 52 | 603 | CLA | C3A-C2A-CAA-CBA |
| 21 | 52 | 604 | CLA | C3A-C2A-CAA-CBA |
| 21 | 92 | 611 | CLA | C3A-C2A-CAA-CBA |
| 21 | B | 814 | CLA | CAA-CBA-CGA-O1A |
| 21 | B2 | 814 | CLA | CAA-CBA-CGA-O1A |
| 21 | B | 806 | CLA | CAA-CBA-CGA-O2A |
| 27 | A2 | 860 | LMG | O8-C28-C29-C30 |
| 21 | 52 | 616 | CLA | C2-C3-C5-C6 |
| 21 | 32 | 617 | CLA | C2C-C3C-CAC-CBC |
| 27 | A | 859 | LMG | C30-C31-C32-C33 |
| 23 | A | 846 | LHG | O10-C23-C24-C25 |
| 23 | 42 | 622 | LHG | O10-C23-C24-C25 |
| 27 | J | 104 | LMG | O9-C10-C11-C12 |
| 21 | A | 813 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 809 | CLA | CAA-CBA-CGA-O2A |
| 21 | 4 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 806 | CLA | CAA-CBA-CGA-O2A |
| 27 | A | 860 | LMG | O8-C28-C29-C30 |
| 21 | 5 | 614 | CLA | CAA-CBA-CGA-O1A |
| 23 | 4 | 622 | LHG | O10-C23-C24-C25 |
| 23 | A2 | 846 | LHG | O10-C23-C24-C25 |
| 27 | J2 | 104 | LMG | O10-C28-C29-C30 |
| 21 | 32 | 609 | CLA | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 92 | 613 | CLA | CBA-CGA-O2A-C1 |
| 21 | 52 | 614 | CLA | CAA-CBA-CGA-O1A |
| 21 | A | 816 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 816 | CLA | C14-C13-C15-C16 |
| 21 | A2 | 813 | CLA | CAA-CBA-CGA-O2A |
| 21 | 12 | 603 | CLA | CAA-CBA-CGA-O1A |
| 27 | A2 | 859 | LMG | C30-C31-C32-C33 |
| 32 | 6 | 625 | NEX | C13-C14-C15-C35 |
| 21 | B | 811 | CLA | CAA-CBA-CGA-O1A |
| 21 | B2 | 811 | CLA | CAA-CBA-CGA-O1A |
| 21 | 9 | 613 | CLA | CBA-CGA-O2A-C1 |
| 21 | 3 | 615 | CLA | C2-C3-C5-C6 |
| 21 | B | 802 | CLA | C8-C10-C11-C12 |
| 21 | B2 | 802 | CLA | C8-C10-C11-C12 |
| 28 | 5 | 626 | LUT | C21-C26-C27-C28 |
| 28 | 52 | 626 | LUT | C21-C26-C27-C28 |
| 21 | 1 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | 5 | 621 | CLA | CAA-CBA-CGA-O1A |
| 21 | 82 | 614 | CLA | CAA-CBA-CGA-O1A |
| 27 | J | 104 | LMG | O10-C28-C29-C30 |
| 21 | 8 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | 8 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | B2 | 809 | CLA | CAA-CBA-CGA-O2A |
| 21 | 82 | 603 | CLA | CAA-CBA-CGA-O2A |
| 21 | A | 826 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 614 | CLA | CAA-CBA-CGA-O1A |
| 21 | 4 | 614 | CLA | CAA-CBA-CGA-O1A |
| 21 | 52 | 621 | CLA | CAA-CBA-CGA-O1A |
| 23 | 3 | 721 | LHG | O9-C7-C8-C9 |
| 27 | J | 103 | LMG | C8-C7-O1-C1 |
| 27 | 8 | 629 | LMG | C8-C7-O1-C1 |
| 27 | J2 | 103 | LMG | C8-C7-O1-C1 |
| 27 | 82 | 629 | LMG | C8-C7-O1-C1 |
| 23 | Z | 620 | LHG | C5-C6-O8-C23 |
| 21 | A | 807 | CLA | CAA-CBA-CGA-O1A |
| 21 | G | 204 | CLA | CAA-CBA-CGA-O1A |
| 21 | 7 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | A2 | 807 | CLA | CAA-CBA-CGA-O1A |
| 21 | A2 | 826 | CLA | CAA-CBA-CGA-O1A |
| 21 | G2 | 204 | CLA | CAA-CBA-CGA-O1A |
| 21 | 42 | 614 | CLA | CAA-CBA-CGA-O1A |
| 27 | 9 | 620 | LMG | O9-C10-C11-C12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 27 | 92 | 620 | LMG | O9-C10-C11-C12 |
| 21 | 82 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | B | 813 | CLA | C8-C10-C11-C12 |
| 21 | B2 | 813 | CLA | C8-C10-C11-C12 |
| 21 | 3 | 617 | CLA | C4C-C3C-CAC-CBC |
| 23 | 8 | 620 | LHG | C4-C5-C6-O8 |
| 23 | 9 | 622 | LHG | C4-C5-C6-O8 |
| 23 | 82 | 620 | LHG | C4-C5-C6-O8 |
| 23 | 92 | 622 | LHG | C4-C5-C6-O8 |
| 27 | A | 859 | LMG | C7-C8-C9-O8 |
| 27 | A2 | 859 | LMG | C7-C8-C9-O8 |
| 21 | L | 204 | CLA | CAA-CBA-CGA-O2A |
| 21 | 32 | 617 | CLA | C4C-C3C-CAC-CBC |
| 21 | F | 304 | CLA | CAA-CBA-CGA-O1A |
| 21 | 8 | 604 | CLA | CAA-CBA-CGA-O1A |
| 21 | 5 | 616 | CLA | CAA-CBA-CGA-O1A |
| 21 | A2 | 813 | CLA | CAA-CBA-CGA-O1A |
| 21 | F2 | 304 | CLA | CAA-CBA-CGA-O1A |
| 21 | 72 | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | 82 | 604 | CLA | CAA-CBA-CGA-O1A |
| 21 | 52 | 616 | CLA | CAA-CBA-CGA-O1A |
| 23 | 32 | 721 | LHG | O9-C7-C8-C9 |
| 21 | B | 809 | CLA | C8-C10-C11-C12 |
| 21 | 4 | 610 | CLA | C5-C6-C7-C8 |
| 21 | B2 | 809 | CLA | C8-C10-C11-C12 |
| 21 | 42 | 610 | CLA | C5-C6-C7-C8 |
| 21 | 72 | 612 | CLA | CAA-CBA-CGA-O2A |
| 21 | 32 | 615 | CLA | C2-C3-C5-C6 |
| 21 | L2 | 204 | CLA | CAA-CBA-CGA-O2A |
| 27 | 1 | 624 | LMG | O9-C10-C11-C12 |
| 27 | 3 | 722 | LMG | O10-C28-C29-C30 |
| 27 | 12 | 624 | LMG | O9-C10-C11-C12 |
| 21 | A | 805 | CLA | CAD-CBD-CGD-O2D |
| 21 | A | 823 | CLA | CAD-CBD-CGD-O2D |
| 21 | A | 826 | CLA | CAD-CBD-CGD-O2D |
| 21 | A | 842 | CLA | CAD-CBD-CGD-O2D |
| 21 | B | 839 | CLA | CAD-CBD-CGD-O2D |
| 21 | 1 | 608 | CLA | CAD-CBD-CGD-O2D |
| 21 | 1 | 612 | CLA | CAD-CBD-CGD-O2D |
| 21 | 4 | 604 | CLA | CAD-CBD-CGD-O2D |
| 21 | 4 | 614 | CLA | CAD-CBD-CGD-O2D |
| 21 | 5 | 621 | CLA | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | 6 | 603 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 805 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 810 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 823 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 826 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 830 | CLA | CAD-CBD-CGD-O2D |
| 21 | A2 | 842 | CLA | CAD-CBD-CGD-O2D |
| 21 | B2 | 839 | CLA | CAD-CBD-CGD-O2D |
| 21 | 12 | 608 | CLA | CAD-CBD-CGD-O2D |
| 21 | 12 | 612 | CLA | CAD-CBD-CGD-O2D |
| 21 | 42 | 604 | CLA | CAD-CBD-CGD-O2D |
| 21 | 42 | 614 | CLA | CAD-CBD-CGD-O2D |
| 21 | 52 | 621 | CLA | CAD-CBD-CGD-O2D |
| 21 | 62 | 603 | CLA | CAD-CBD-CGD-O2D |
| 21 | 12 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | 62 | 603 | CLA | CAA-CBA-CGA-O2A |
| 23 | 6 | 619 | LHG | O7-C7-C8-C9 |
| 23 | 62 | 619 | LHG | O7-C7-C8-C9 |
| 21 | F | 303 | CLA | CAA-CBA-CGA-O2A |
| 23 | Z2 | 620 | LHG | C5-C6-O8-C23 |
| 21 | A | 813 | CLA | CAA-CBA-CGA-O1A |
| 23 | 72 | 625 | LHG | O6-C4-C5-C6 |
| 21 | Z2 | 611 | CLA | C4C-C3C-CAC-CBC |
| 23 | B | 851 | LHG | C25-C26-C27-C28 |
| 21 | A2 | 843 | CLA | C2-C1-O2A-CGA |
| 30 | 4 | 608 | CHL | C2-C1-O2A-CGA |
| 30 | 42 | 608 | CHL | C2-C1-O2A-CGA |
| 23 | 4 | 622 | LHG | C16-C17-C18-C19 |
| 27 | 32 | 722 | LMG | O10-C28-C29-C30 |
| 21 | A2 | 814 | CLA | CAA-CBA-CGA-O2A |
| 23 | 3 | 623 | LHG | C24-C25-C26-C27 |
| 23 | B2 | 851 | LHG | C25-C26-C27-C28 |
| 23 | 32 | 623 | LHG | C24-C25-C26-C27 |
| 23 | 42 | 622 | LHG | C16-C17-C18-C19 |
| 21 | A | 814 | CLA | CAA-CBA-CGA-O2A |
| 21 | 1 | 614 | CLA | CAA-CBA-CGA-O2A |
| 21 | 7 | 613 | CLA | CAA-CBA-CGA-O2A |
| 21 | 6 | 603 | CLA | CAA-CBA-CGA-O2A |
| 23 | 8 | 620 | LHG | O7-C7-C8-C9 |
| 23 | 82 | 620 | LHG | O7-C7-C8-C9 |
| 27 | 32 | 722 | LMG | O7-C10-C11-C12 |
| 30 | 6 | 601 | CHL | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 30 | 62 | 601 | CHL | CAA-CBA-CGA-O2A |
| 21 | L | 204 | CLA | CAA-CBA-CGA-O1A |
| 21 | B2 | 835 | CLA | CAA-CBA-CGA-O2A |
| 30 | 7 | 607 | CHL | CAA-CBA-CGA-O2A |
| 30 | 72 | 607 | CHL | CAA-CBA-CGA-O2A |
| 27 | 3 | 722 | LMG | O9-C10-C11-C12 |
| 21 | Z | 611 | CLA | C4C-C3C-CAC-CBC |
| 21 | A | 829 | CLA | CAA-CBA-CGA-O2A |
| 21 | 3 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | 32 | 611 | CLA | CAA-CBA-CGA-O2A |
| 21 | F2 | 303 | CLA | CAA-CBA-CGA-O2A |
| 21 | L2 | 204 | CLA | CAA-CBA-CGA-O1A |
| 21 | Z | 603 | CLA | CAA-CBA-CGA-O1A |
| 21 | Z2 | 603 | CLA | CAA-CBA-CGA-O1A |
| 23 | 6 | 619 | LHG | O9-C7-C8-C9 |
| 27 | 1 | 628 | LMG | O10-C28-C29-C30 |
| 27 | 12 | 628 | LMG | O10-C28-C29-C30 |
| 26 | A | 864 | LMU | C5-C6-C7-C8 |

All (2) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 32 | 52 | 625 | NEX | C1-C2-C3-C4-C5-C6 |
| 32 | 5 | 625 | NEX | C1-C2-C3-C4-C5-C6 |

300 monomers are involved in 403 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | L | 201 | BCR | 1 | 0 |
| 21 | B | 802 | CLA | 2 | 0 |
| 23 | 42 | 623 | LHG | 1 | 0 |
| 27 | A | 860 | LMG | 1 | 0 |
| 30 | 72 | 601 | CHL | 2 | 0 |
| 21 | Z | 616 | CLA | 2 | 0 |
| 30 | 6 | 606 | CHL | 1 | 0 |
| 21 | 1 | 613 | CLA | 1 | 0 |
| 21 | B | 823 | CLA | 1 | 0 |
| 28 | F | 305 | LUT | 3 | 0 |
| 21 | A2 | 809 | CLA | 2 | 0 |
| 21 | A | 831 | CLA | 2 | 0 |
| 21 | B | 821 | CLA | 1 | 0 |
| 30 | 82 | 601 | CHL | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | 52 | 617 | CLA | 1 | 0 |
| 24 | B | 845 | BCR | 3 | 0 |
| 21 | K2 | 201 | CLA | 2 | 0 |
| 24 | 3 | 620 | BCR | 1 | 0 |
| 21 | A2 | 811 | CLA | 2 | 0 |
| 21 | B2 | 834 | CLA | 1 | 0 |
| 24 | A | 849 | BCR | 2 | 0 |
| 21 | B | 841 | CLA | 2 | 0 |
| 31 | 72 | 622 | XAT | 1 | 0 |
| 21 | 82 | 613 | CLA | 1 | 0 |
| 24 | B2 | 847 | BCR | 1 | 0 |
| 26 | A2 | 858 | LMU | 1 | 0 |
| 21 | 4 | 609 | CLA | 1 | 0 |
| 24 | B | 844 | BCR | 3 | 0 |
| 21 | B | 833 | CLA | 1 | 0 |
| 30 | Z | 601 | CHL | 1 | 0 |
| 24 | B | 843 | BCR | 2 | 0 |
| 28 | 7 | 624 | LUT | 4 | 0 |
| 21 | 32 | 602 | CLA | 1 | 0 |
| 21 | 3 | 609 | CLA | 1 | 0 |
| 21 | 52 | 602 | CLA | 1 | 0 |
| 23 | 5 | 623 | LHG | 1 | 0 |
| 28 | Z | 617 | LUT | 2 | 0 |
| 21 | B2 | 814 | CLA | 1 | 0 |
| 21 | A2 | 813 | CLA | 2 | 0 |
| 26 | 72 | 628 | LMU | 1 | 0 |
| 21 | B | 837 | CLA | 2 | 0 |
| 21 | 8 | 612 | CLA | 1 | 0 |
| 24 | 9 | 623 | BCR | 1 | 0 |
| 28 | 32 | 622 | LUT | 2 | 0 |
| 26 | Z2 | 622 | LMU | 1 | 0 |
| 21 | 72 | 608 | CLA | 1 | 0 |
| 30 | 62 | 601 | CHL | 3 | 0 |
| 21 | B2 | 832 | CLA | 1 | 0 |
| 24 | 8 | 619 | BCR | 2 | 0 |
| 30 | 8 | 606 | CHL | 1 | 0 |
| 28 | 6 | 621 | LUT | 1 | 0 |
| 24 | A | 852 | BCR | 4 | 0 |
| 24 | A2 | 852 | BCR | 2 | 0 |
| 27 | 8 | 626 | LMG | 1 | 0 |
| 21 | B2 | 823 | CLA | 1 | 0 |
| 21 | 72 | 609 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | 62 | 608 | CHL | 2 | 0 |
| 23 | 12 | 620 | LHG | 1 | 0 |
| 21 | A | 822 | CLA | 1 | 0 |
| 21 | 5 | 621 | CLA | 3 | 0 |
| 24 | 42 | 621 | BCR | 1 | 0 |
| 21 | A | 803 | CLA | 1 | 0 |
| 21 | 82 | 604 | CLA | 1 | 0 |
| 27 | J2 | 104 | LMG | 1 | 0 |
| 21 | B | 817 | CLA | 1 | 0 |
| 24 | A | 848 | BCR | 3 | 0 |
| 26 | 7 | 628 | LMU | 1 | 0 |
| 24 | K2 | 207 | BCR | 2 | 0 |
| 28 | 92 | 616 | LUT | 1 | 0 |
| 21 | 7 | 608 | CLA | 1 | 0 |
| 29 | B2 | 850 | DGD | 1 | 0 |
| 24 | 82 | 619 | BCR | 2 | 0 |
| 21 | B | 834 | CLA | 1 | 0 |
| 23 | 52 | 623 | LHG | 1 | 0 |
| 30 | 42 | 607 | CHL | 1 | 0 |
| 21 | A2 | 804 | CLA | 1 | 0 |
| 21 | Z2 | 611 | CLA | 1 | 0 |
| 24 | 32 | 719 | BCR | 4 | 0 |
| 21 | F | 304 | CLA | 1 | 0 |
| 26 | A | 863 | LMU | 2 | 0 |
| 26 | Z | 622 | LMU | 1 | 0 |
| 21 | B2 | 817 | CLA | 1 | 0 |
| 21 | 7 | 609 | CLA | 1 | 0 |
| 21 | 3 | 611 | CLA | 1 | 0 |
| 24 | B2 | 844 | BCR | 2 | 0 |
| 24 | 62 | 623 | BCR | 1 | 0 |
| 21 | 42 | 610 | CLA | 1 | 0 |
| 30 | 4 | 606 | CHL | 2 | 0 |
| 26 | 9 | 624 | LMU | 1 | 0 |
| 30 | 4 | 607 | CHL | 1 | 0 |
| 21 | 52 | 610 | CLA | 1 | 0 |
| 21 | B2 | 826 | CLA | 1 | 0 |
| 24 | 3 | 718 | BCR | 1 | 0 |
| 24 | 6 | 623 | BCR | 2 | 0 |
| 21 | A2 | 835 | CLA | 1 | 0 |
| 21 | A | 840 | CLA | 1 | 0 |
| 28 | 1 | 617 | LUT | 2 | 0 |
| 21 | 6 | 602 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | 3 | 602 | CLA | 1 | 0 |
| 30 | 62 | 606 | CHL | 1 | 0 |
| 24 | L | 205 | BCR | 4 | 0 |
| 27 | A2 | 860 | LMG | 1 | 0 |
| 21 | B | 816 | CLA | 2 | 0 |
| 21 | 72 | 620 | CLA | 1 | 0 |
| 30 | 3 | 608 | CHL | 2 | 0 |
| 28 | F2 | 305 | LUT | 2 | 0 |
| 23 | 72 | 625 | LHG | 1 | 0 |
| 30 | 6 | 608 | CHL | 2 | 0 |
| 21 | B | 835 | CLA | 1 | 0 |
| 21 | 4 | 614 | CLA | 1 | 0 |
| 24 | I | 172 | BCR | 1 | 0 |
| 21 | A | 813 | CLA | 3 | 0 |
| 21 | Z2 | 603 | CLA | 3 | 0 |
| 21 | 9 | 614 | CLA | 1 | 0 |
| 21 | F2 | 304 | CLA | 1 | 0 |
| 21 | A2 | 812 | CLA | 1 | 0 |
| 21 | 72 | 610 | CLA | 3 | 0 |
| 21 | 5 | 603 | CLA | 3 | 0 |
| 21 | B2 | 806 | CLA | 1 | 0 |
| 21 | 12 | 603 | CLA | 3 | 0 |
| 21 | Z | 610 | CLA | 1 | 0 |
| 24 | L2 | 205 | BCR | 4 | 0 |
| 24 | A2 | 850 | BCR | 3 | 0 |
| 32 | 62 | 625 | NEX | 1 | 0 |
| 21 | 82 | 603 | CLA | 1 | 0 |
| 30 | 62 | 607 | CHL | 1 | 0 |
| 23 | 32 | 623 | LHG | 1 | 0 |
| 28 | 42 | 619 | LUT | 1 | 0 |
| 21 | 32 | 603 | CLA | 2 | 0 |
| 21 | B2 | 829 | CLA | 6 | 0 |
| 21 | A | 804 | CLA | 1 | 0 |
| 21 | 7 | 620 | CLA | 1 | 0 |
| 30 | 82 | 606 | CHL | 1 | 0 |
| 30 | 7 | 601 | CHL | 3 | 0 |
| 24 | K | 207 | BCR | 2 | 0 |
| 24 | B2 | 801 | BCR | 3 | 0 |
| 21 | 32 | 609 | CLA | 1 | 0 |
| 28 | 9 | 616 | LUT | 1 | 0 |
| 26 | A | 858 | LMU | 2 | 0 |
| 21 | Z2 | 616 | CLA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | 8 | 603 | CLA | 1 | 0 |
| 28 | 62 | 621 | LUT | 1 | 0 |
| 21 | B2 | 841 | CLA | 2 | 0 |
| 21 | B2 | 822 | CLA | 1 | 0 |
| 21 | Z | 608 | CLA | 1 | 0 |
| 21 | 7 | 610 | CLA | 3 | 0 |
| 21 | B2 | 836 | CLA | 1 | 0 |
| 21 | B2 | 802 | CLA | 3 | 0 |
| 21 | 32 | 611 | CLA | 1 | 0 |
| 21 | K | 201 | CLA | 2 | 0 |
| 21 | A2 | 840 | CLA | 1 | 0 |
| 21 | B2 | 821 | CLA | 1 | 0 |
| 24 | A2 | 848 | BCR | 2 | 0 |
| 31 | 6 | 624 | XAT | 1 | 0 |
| 28 | 9 | 617 | LUT | 2 | 0 |
| 28 | 92 | 617 | LUT | 2 | 0 |
| 31 | 1 | 618 | XAT | 1 | 0 |
| 21 | 62 | 603 | CLA | 1 | 0 |
| 21 | B2 | 827 | CLA | 1 | 0 |
| 21 | B | 839 | CLA | 1 | 0 |
| 21 | 8 | 604 | CLA | 1 | 0 |
| 21 | 3 | 603 | CLA | 2 | 0 |
| 21 | 12 | 613 | CLA | 1 | 0 |
| 21 | 92 | 614 | CLA | 1 | 0 |
| 30 | 1 | 601 | CHL | 1 | 0 |
| 24 | K2 | 202 | BCR | 4 | 0 |
| 27 | 92 | 620 | LMG | 1 | 0 |
| 21 | B2 | 835 | CLA | 1 | 0 |
| 21 | 52 | 603 | CLA | 3 | 0 |
| 24 | B | 847 | BCR | 1 | 0 |
| 21 | A | 829 | CLA | 3 | 0 |
| 21 | 32 | 607 | CLA | 1 | 0 |
| 21 | 3 | 615 | CLA | 5 | 0 |
| 21 | Z2 | 608 | CLA | 1 | 0 |
| 21 | A2 | 820 | CLA | 1 | 0 |
| 21 | 5 | 616 | CLA | 3 | 0 |
| 30 | 5 | 608 | CHL | 1 | 0 |
| 21 | 42 | 613 | CLA | 3 | 0 |
| 24 | 92 | 623 | BCR | 2 | 0 |
| 21 | B | 808 | CLA | 1 | 0 |
| 21 | A | 854 | CLA | 2 | 0 |
| 21 | A2 | 806 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 24 | J2 | 102 | BCR | 1 | 0 |
| 30 | 52 | 608 | CHL | 1 | 0 |
| 24 | A2 | 849 | BCR | 2 | 0 |
| 24 | A2 | 851 | BCR | 1 | 0 |
| 21 | J | 101 | CLA | 1 | 0 |
| 26 | 42 | 625 | LMU | 1 | 0 |
| 21 | 4 | 613 | CLA | 2 | 0 |
| 21 | A2 | 832 | CLA | 1 | 0 |
| 26 | 4 | 625 | LMU | 1 | 0 |
| 26 | A | 857 | LMU | 1 | 0 |
| 27 | 3 | 722 | LMG | 1 | 0 |
| 27 | J2 | 103 | LMG | 1 | 0 |
| 21 | B | 814 | CLA | 1 | 0 |
| 21 | A | 817 | CLA | 1 | 0 |
| 21 | A | 835 | CLA | 1 | 0 |
| 27 | J | 103 | LMG | 1 | 0 |
| 21 | A | 833 | CLA | 3 | 0 |
| 21 | A2 | 818 | CLA | 1 | 0 |
| 27 | B2 | 854 | LMG | 1 | 0 |
| 32 | 6 | 625 | NEX | 1 | 0 |
| 28 | A | 856 | LUT | 1 | 0 |
| 21 | 62 | 602 | CLA | 1 | 0 |
| 21 | A2 | 830 | CLA | 1 | 0 |
| 21 | A2 | 803 | CLA | 1 | 0 |
| 21 | A2 | 810 | CLA | 1 | 0 |
| 30 | 8 | 601 | CHL | 1 | 0 |
| 23 | 4 | 623 | LHG | 1 | 0 |
| 26 | 8 | 627 | LMU | 1 | 0 |
| 21 | 5 | 602 | CLA | 1 | 0 |
| 30 | 6 | 607 | CHL | 1 | 0 |
| 24 | G2 | 205 | BCR | 2 | 0 |
| 24 | L2 | 201 | BCR | 1 | 0 |
| 21 | A2 | 829 | CLA | 2 | 0 |
| 21 | B | 840 | CLA | 2 | 0 |
| 24 | B | 848 | BCR | 1 | 0 |
| 23 | 7 | 625 | LHG | 1 | 0 |
| 24 | I2 | 172 | BCR | 1 | 0 |
| 24 | B2 | 848 | BCR | 1 | 0 |
| 21 | 3 | 607 | CLA | 1 | 0 |
| 24 | J | 102 | BCR | 1 | 0 |
| 28 | 52 | 620 | LUT | 3 | 0 |
| 29 | B | 850 | DGD | 1 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | A | 811 | CLA | 3 | 0 |
| 30 | Z2 | 601 | CHL | 1 | 0 |
| 30 | 42 | 601 | CHL | 1 | 0 |
| 21 | B | 826 | CLA | 1 | 0 |
| 28 | 72 | 624 | LUT | 4 | 0 |
| 21 | Z2 | 610 | CLA | 1 | 0 |
| 21 | B2 | 816 | CLA | 2 | 0 |
| 27 | 32 | 722 | LMG | 1 | 0 |
| 21 | B | 822 | CLA | 1 | 0 |
| 31 | 12 | 618 | XAT | 1 | 0 |
| 21 | B2 | 839 | CLA | 1 | 0 |
| 28 | Z2 | 617 | LUT | 2 | 0 |
| 26 | A | 862 | LMU | 2 | 0 |
| 28 | 82 | 617 | LUT | 1 | 0 |
| 26 | 92 | 624 | LMU | 1 | 0 |
| 24 | A | 851 | BCR | 3 | 0 |
| 24 | K | 202 | BCR | 3 | 0 |
| 27 | J | 104 | LMG | 1 | 0 |
| 21 | A | 802 | CLA | 2 | 0 |
| 21 | A | 818 | CLA | 1 | 0 |
| 21 | Z | 603 | CLA | 2 | 0 |
| 28 | 4 | 619 | LUT | 1 | 0 |
| 21 | A2 | 833 | CLA | 3 | 0 |
| 24 | B | 801 | BCR | 1 | 0 |
| 24 | B2 | 845 | BCR | 2 | 0 |
| 21 | 12 | 602 | CLA | 1 | 0 |
| 21 | Z2 | 613 | CLA | 1 | 0 |
| 21 | A | 812 | CLA | 1 | 0 |
| 28 | A2 | 856 | LUT | 2 | 0 |
| 21 | B | 827 | CLA | 1 | 0 |
| 21 | 8 | 613 | CLA | 1 | 0 |
| 21 | J2 | 101 | CLA | 1 | 0 |
| 21 | A | 810 | CLA | 2 | 0 |
| 31 | 62 | 624 | XAT | 1 | 0 |
| 21 | B2 | 840 | CLA | 3 | 0 |
| 28 | 12 | 617 | LUT | 2 | 0 |
| 26 | B | 853 | LMU | 3 | 0 |
| 24 | B2 | 843 | BCR | 2 | 0 |
| 21 | A | 809 | CLA | 2 | 0 |
| 23 | Z2 | 620 | LHG | 1 | 0 |
| 21 | 52 | 621 | CLA | 2 | 0 |
| 21 | 3 | 610 | CLA | 2 | 0 |

*Continued on next page...*

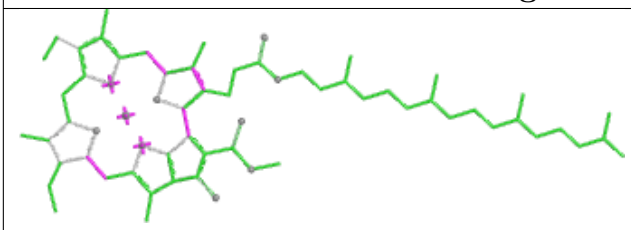
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 30 | 32 | 608 | CHL | 3 | 0 |
| 27 | B | 854 | LMG | 1 | 0 |
| 24 | A | 850 | BCR | 1 | 0 |
| 30 | 6 | 601 | CHL | 3 | 0 |
| 21 | A2 | 843 | CLA | 1 | 0 |
| 21 | Z | 613 | CLA | 1 | 0 |
| 21 | 32 | 610 | CLA | 3 | 0 |
| 27 | 9 | 620 | LMG | 1 | 0 |
| 21 | 1 | 603 | CLA | 3 | 0 |
| 21 | B2 | 837 | CLA | 1 | 0 |
| 21 | 42 | 614 | CLA | 1 | 0 |
| 21 | A2 | 831 | CLA | 1 | 0 |
| 21 | 52 | 616 | CLA | 2 | 0 |
| 28 | 5 | 620 | LUT | 3 | 0 |
| 21 | L | 203 | CLA | 1 | 0 |
| 21 | B | 829 | CLA | 6 | 0 |
| 21 | B2 | 808 | CLA | 1 | 0 |
| 21 | 1 | 602 | CLA | 1 | 0 |
| 21 | A2 | 817 | CLA | 1 | 0 |
| 24 | 3 | 719 | BCR | 5 | 0 |
| 30 | 4 | 601 | CHL | 1 | 0 |
| 21 | A2 | 854 | CLA | 3 | 0 |
| 23 | 3 | 623 | LHG | 1 | 0 |
| 21 | A2 | 802 | CLA | 2 | 0 |
| 21 | 32 | 615 | CLA | 6 | 0 |
| 21 | 6 | 603 | CLA | 1 | 0 |
| 28 | 3 | 622 | LUT | 2 | 0 |
| 21 | B | 806 | CLA | 1 | 0 |
| 21 | A2 | 822 | CLA | 1 | 0 |
| 26 | B2 | 853 | LMU | 2 | 0 |
| 21 | A | 843 | CLA | 1 | 0 |
| 23 | 1 | 620 | LHG | 1 | 0 |
| 26 | A2 | 857 | LMU | 1 | 0 |
| 21 | B | 836 | CLA | 1 | 0 |

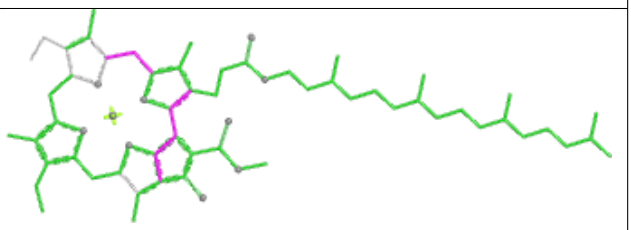
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

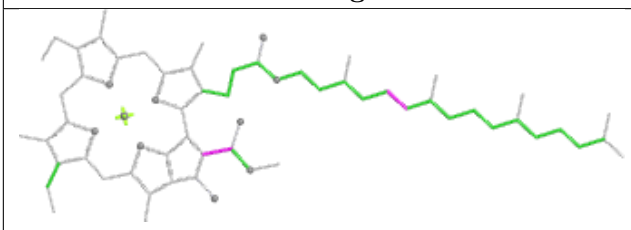
**Ligand CL0 A2 801**



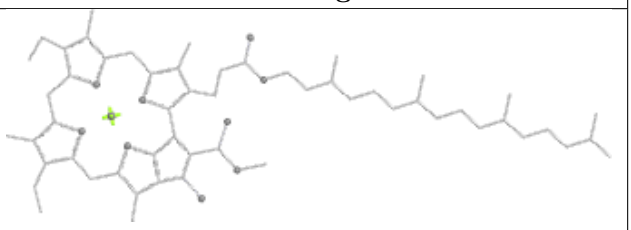
**Bond lengths**



**Bond angles**

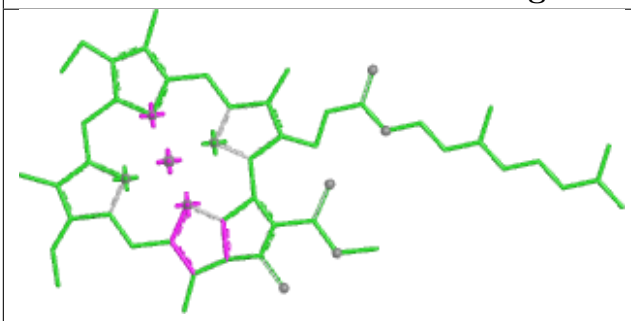


**Torsions**

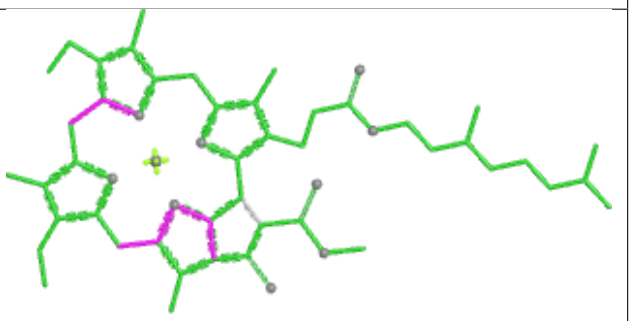


**Rings**

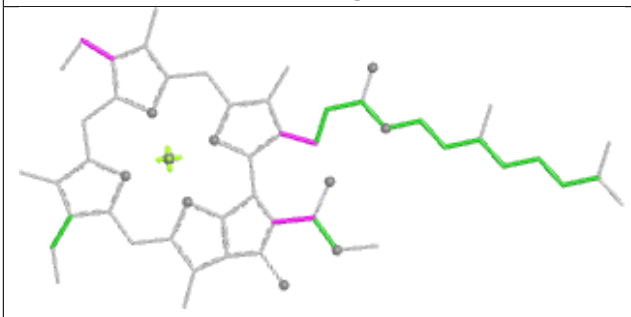
**Ligand CLA 9 603**



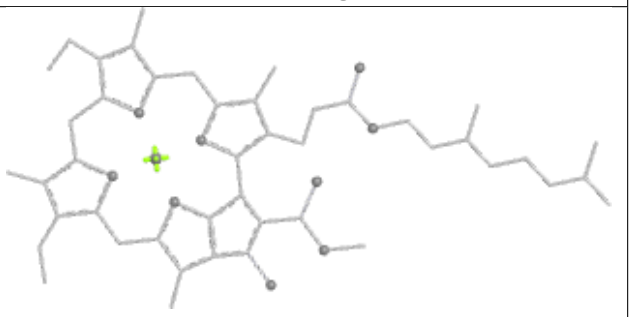
**Bond lengths**



**Bond angles**

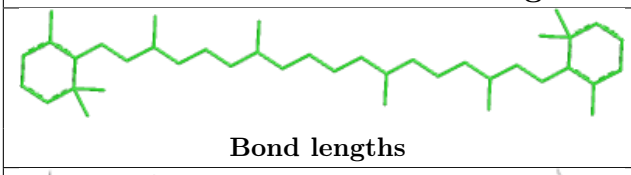


**Torsions**

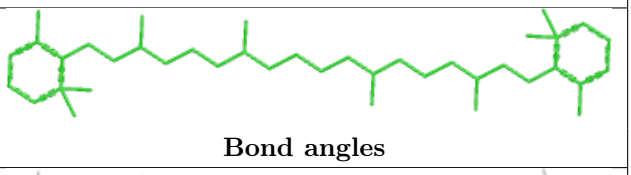


**Rings**

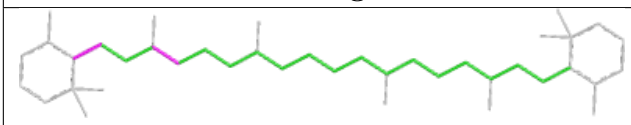
## Ligand BCR L 201



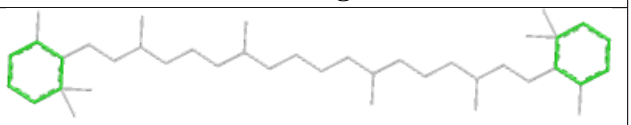
Bond lengths



Bond angles

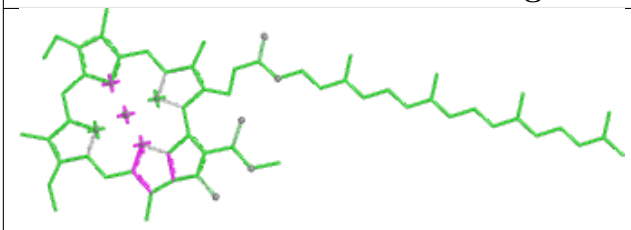


Torsions

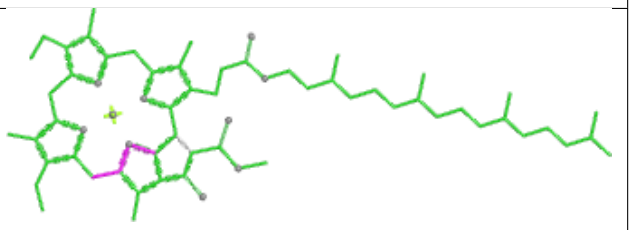


Rings

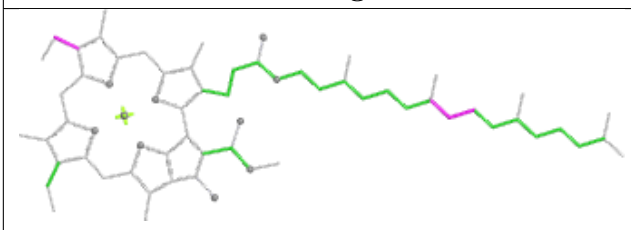
## Ligand CLA B 802



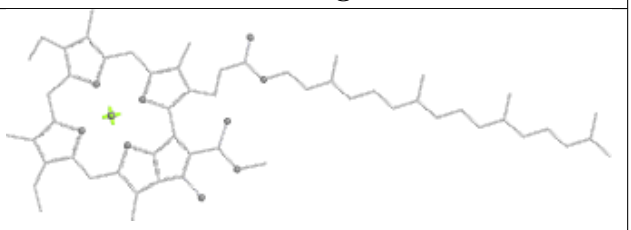
Bond lengths



Bond angles

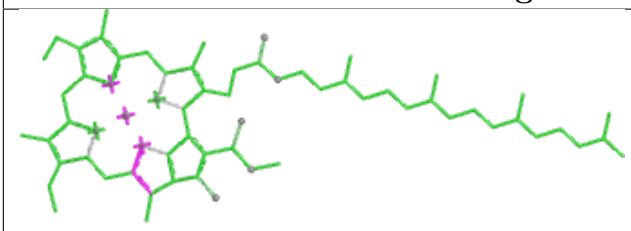


Torsions

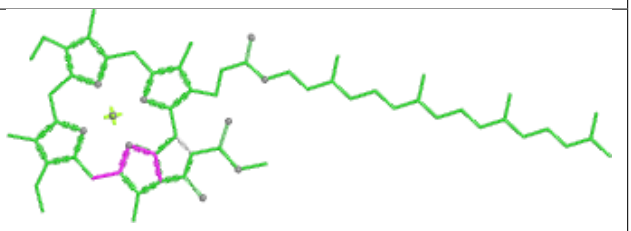


Rings

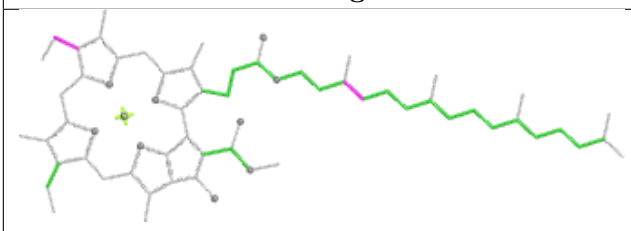
## Ligand CLA B2 828



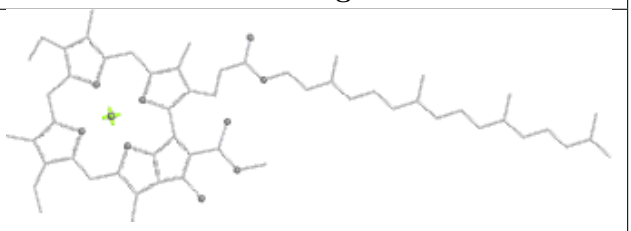
Bond lengths



Bond angles

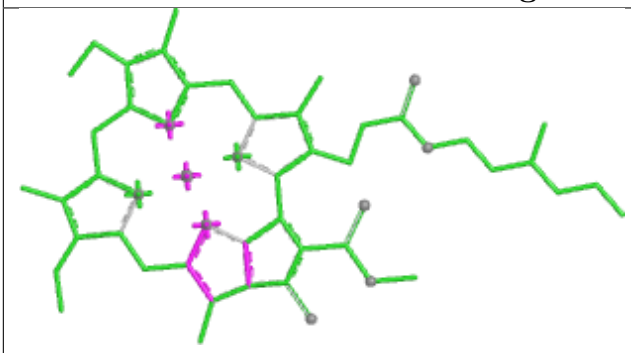


Torsions

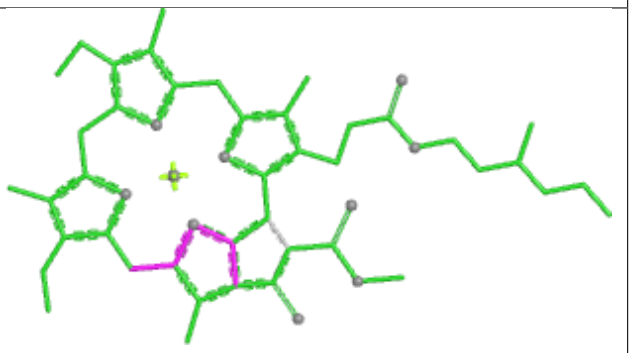


Rings

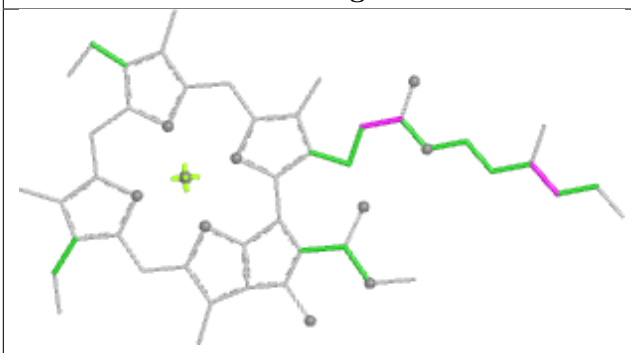
## Ligand CLA 72 603



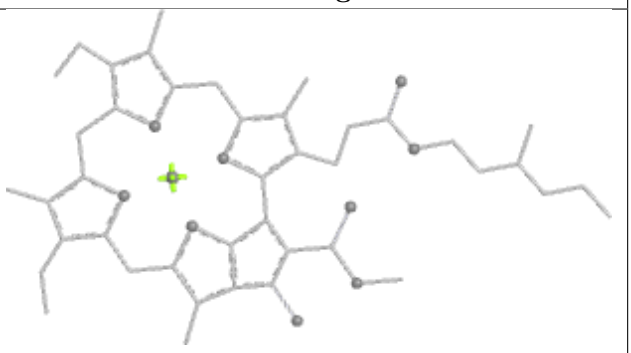
Bond lengths



Bond angles

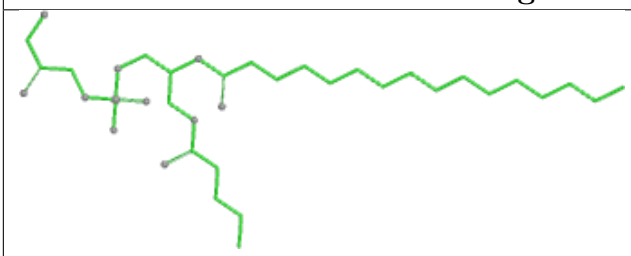


Torsions

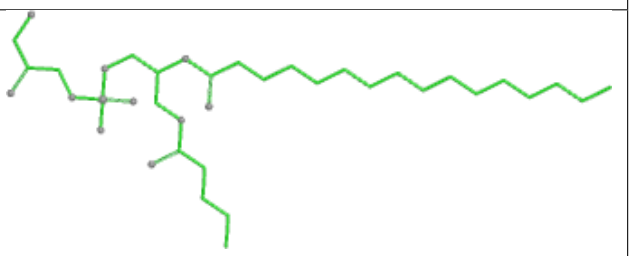


Rings

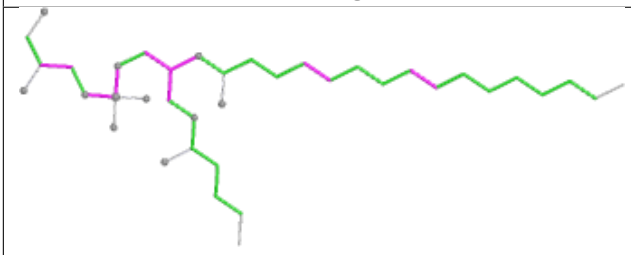
## Ligand LHG 42 623



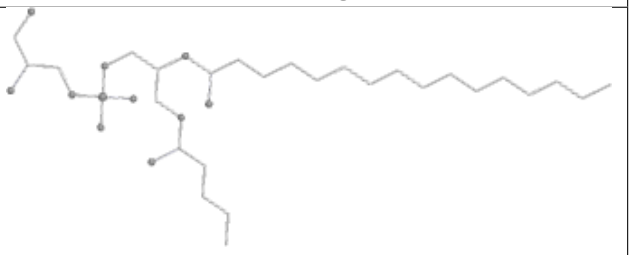
Bond lengths



Bond angles

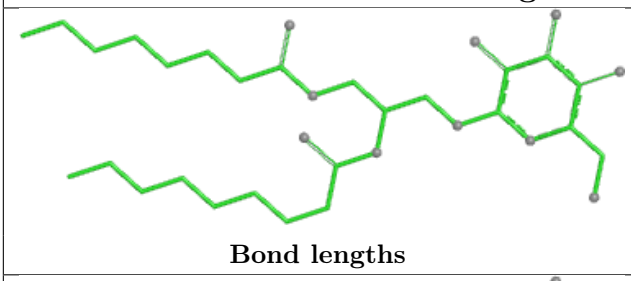


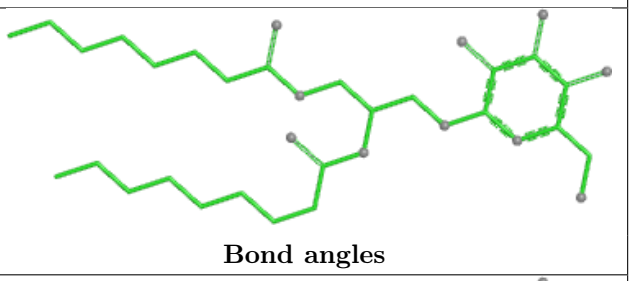
Torsions

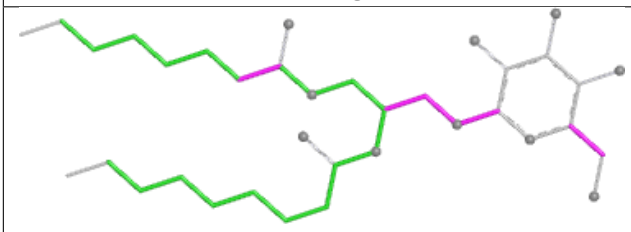


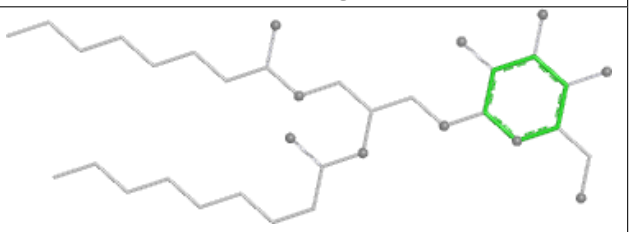
Rings

## Ligand LMG A 860

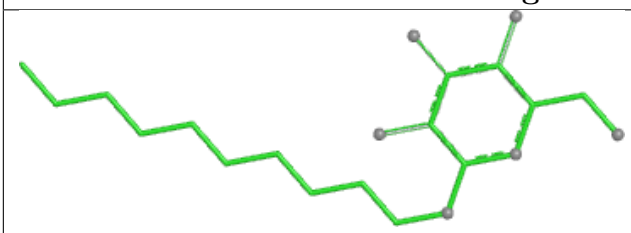

Bond lengths

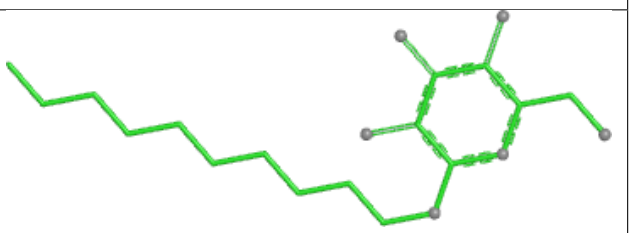

Bond angles

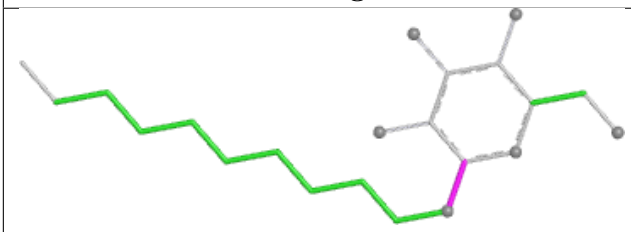

Torsions

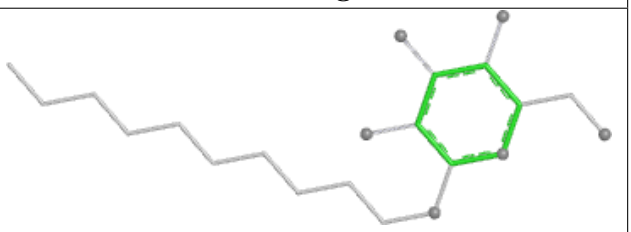

Rings

## Ligand LMU Z 621

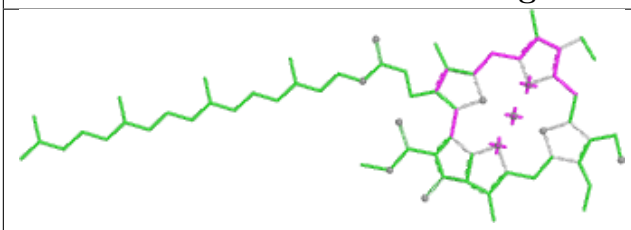

Bond lengths

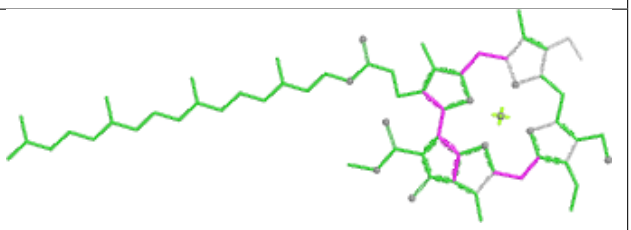

Bond angles

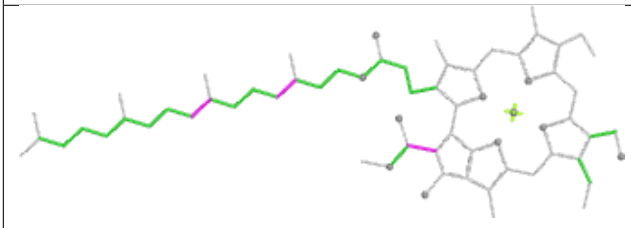

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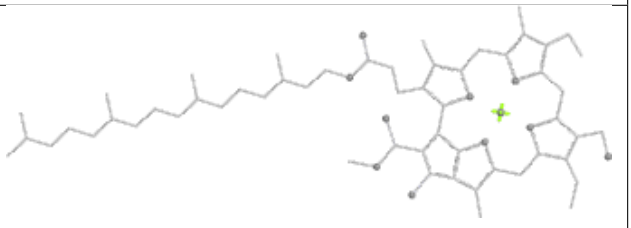

Rings

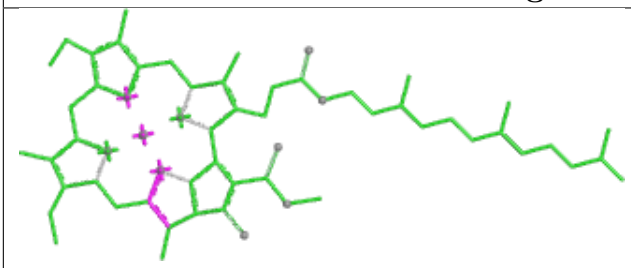
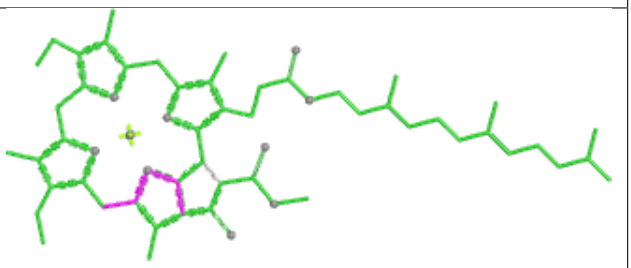
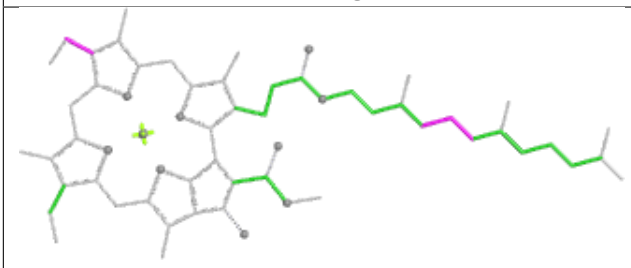
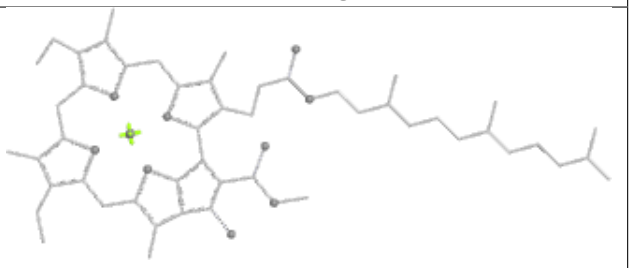
## Ligand CHL 72 601

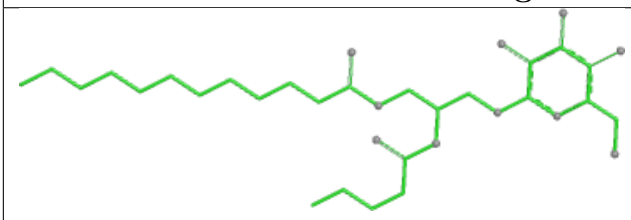
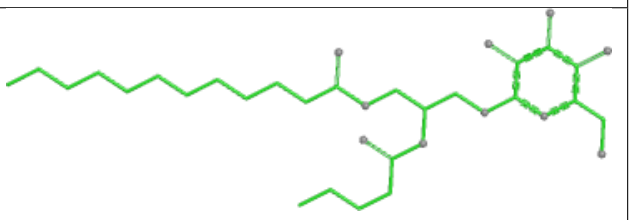
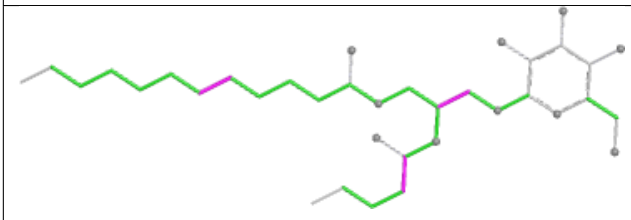
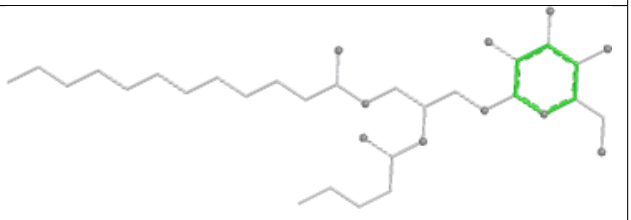

Bond lengths


Bond angles

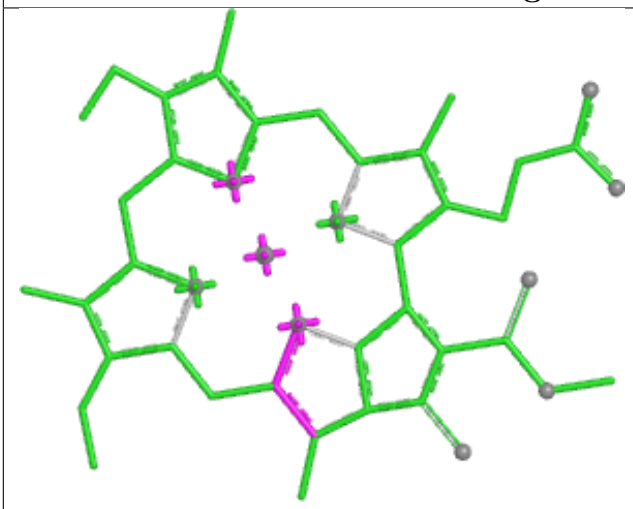

Torsions


Rings

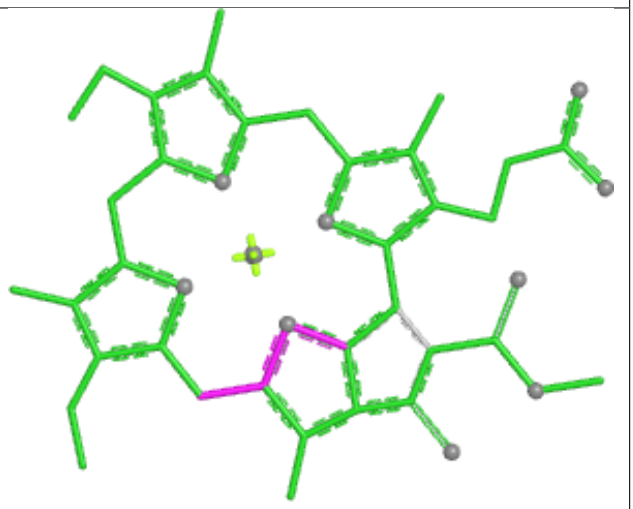
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|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand LMG 12 624 | |
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|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

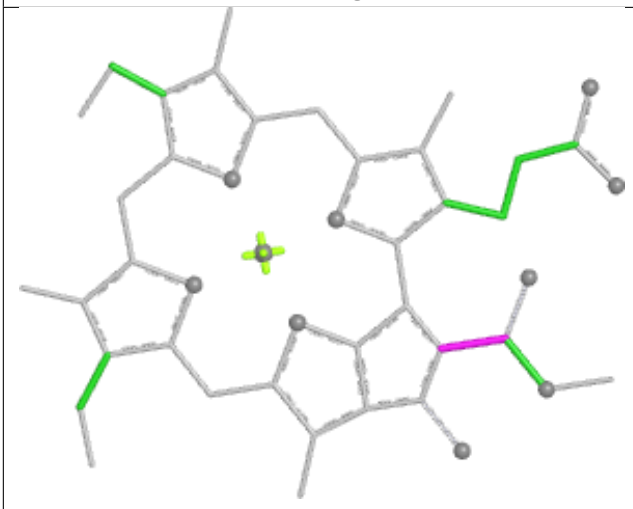
**Ligand CLA A 845**



**Bond lengths**



**Bond angles**

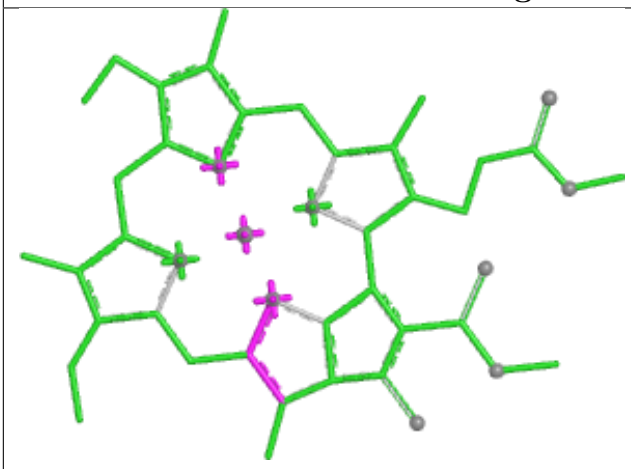


**Torsions**

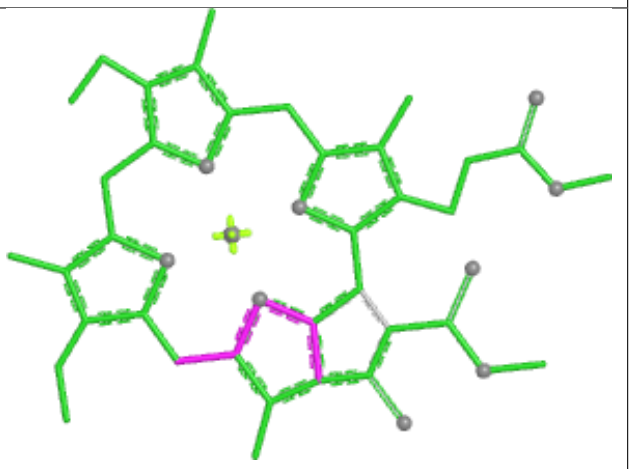


**Rings**

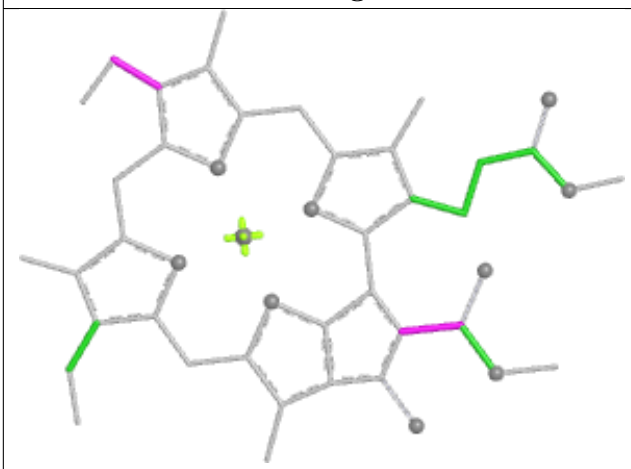
**Ligand CLA K2 204**



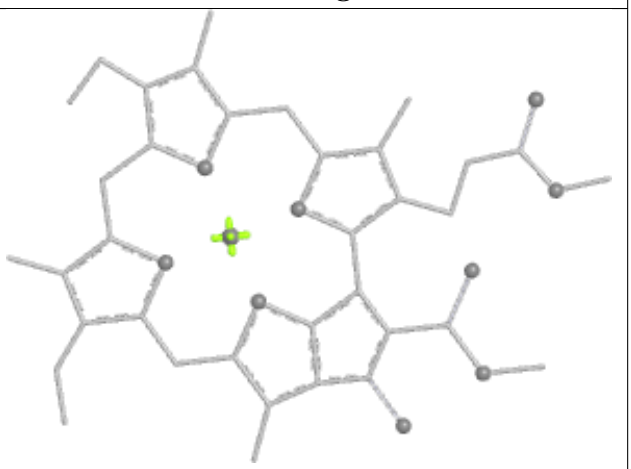
Bond lengths



Bond angles

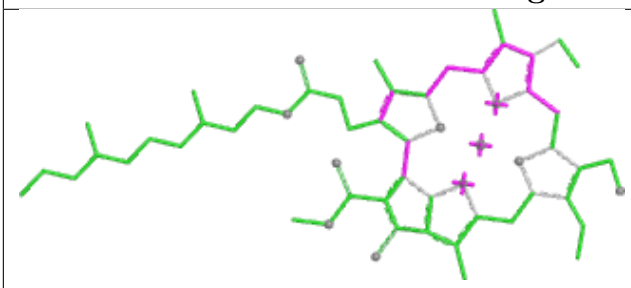


Torsions

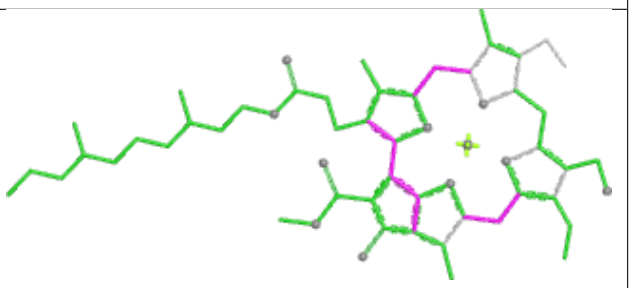


Rings

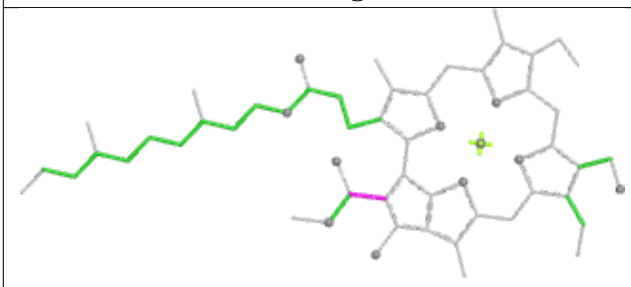
**Ligand CHL 6 606**



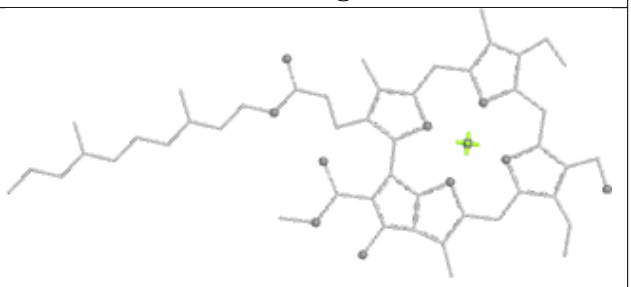
Bond lengths



Bond angles

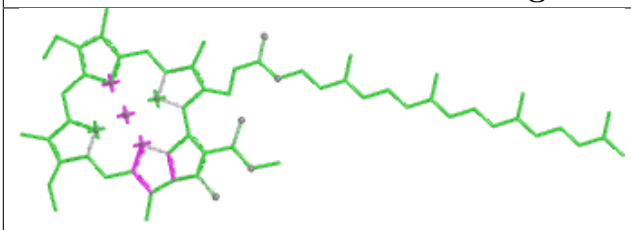


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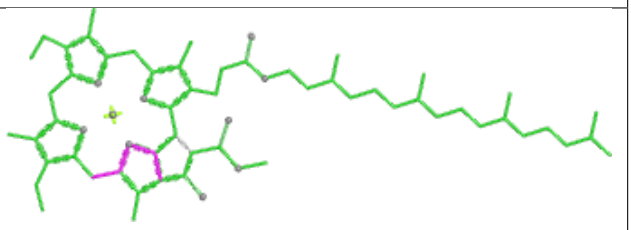


Rings

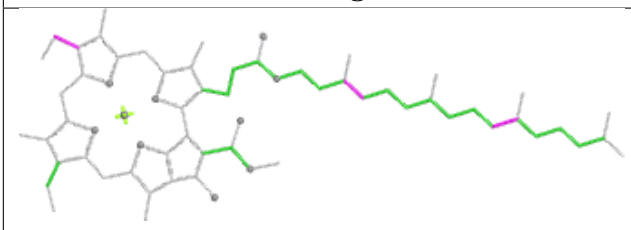
## Ligand CLA 1 613



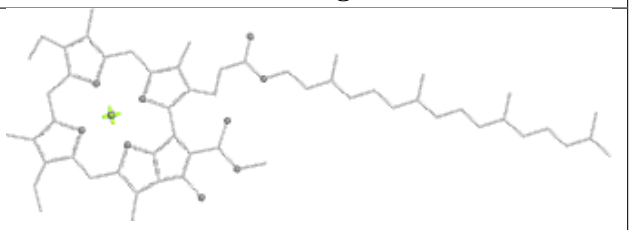
Bond lengths



Bond angles

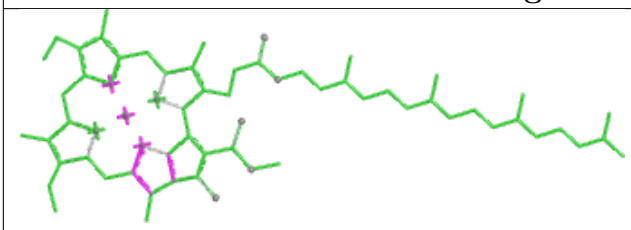


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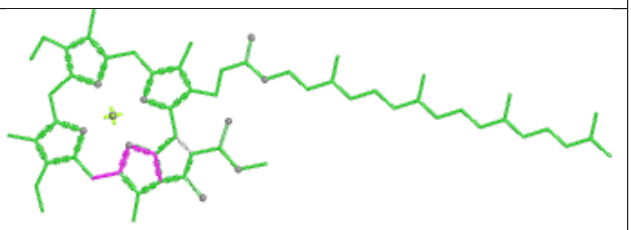


Rings

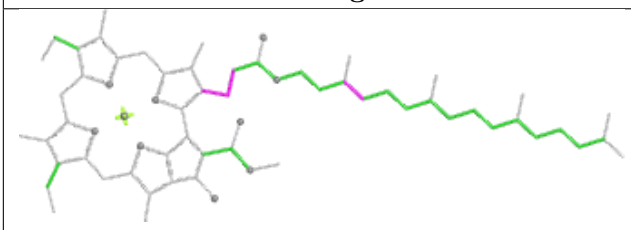
## Ligand CLA B 823



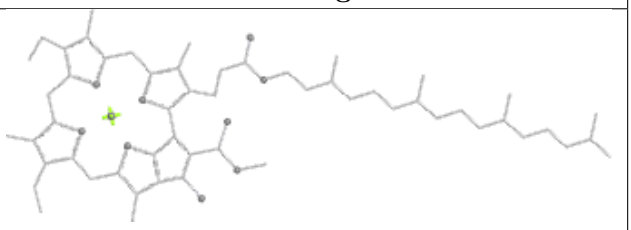
Bond lengths



Bond angles



Torsions



Rings

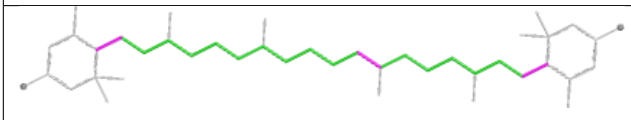
## Ligand LUT F 305



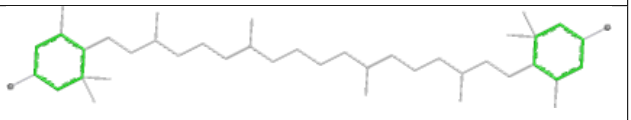
Bond lengths



Bond angles

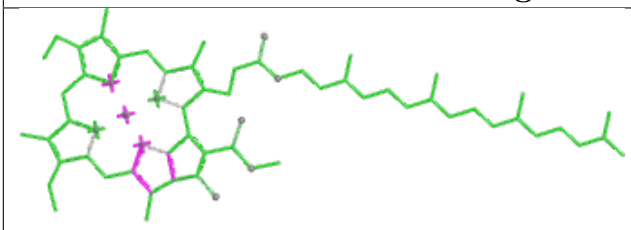


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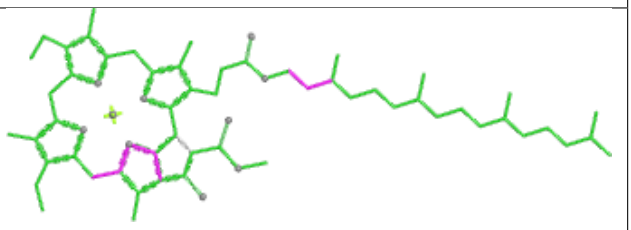


Rings

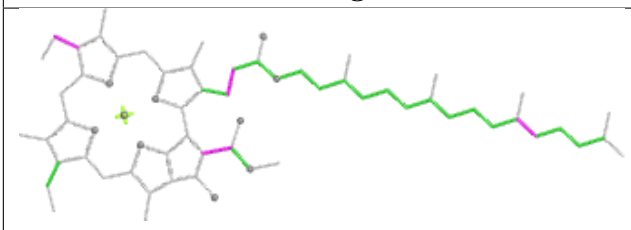
**Ligand CLA A2 809**



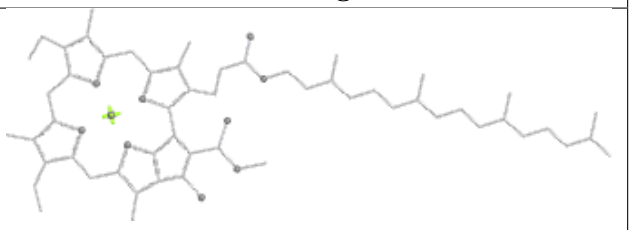
Bond lengths



Bond angles

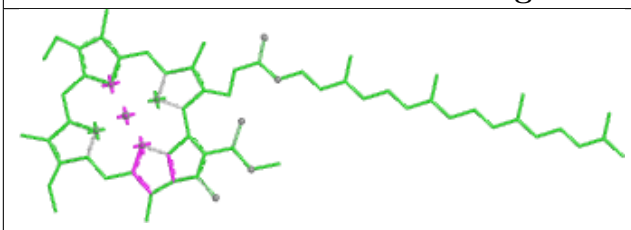


Torsions

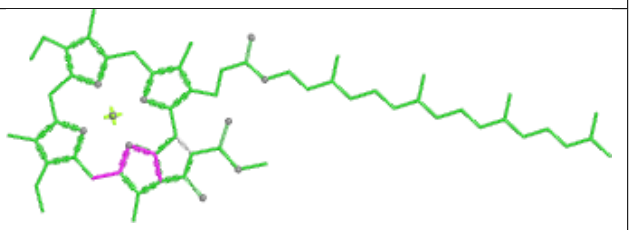


Rings

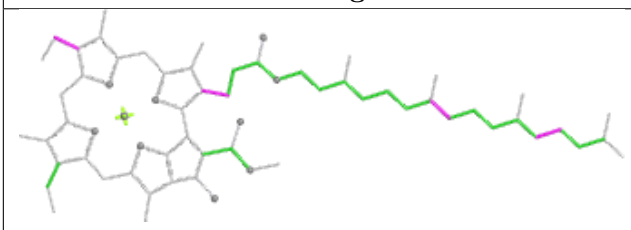
**Ligand CLA A2 834**



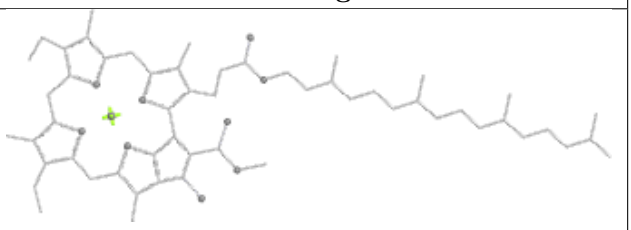
Bond lengths



Bond angles

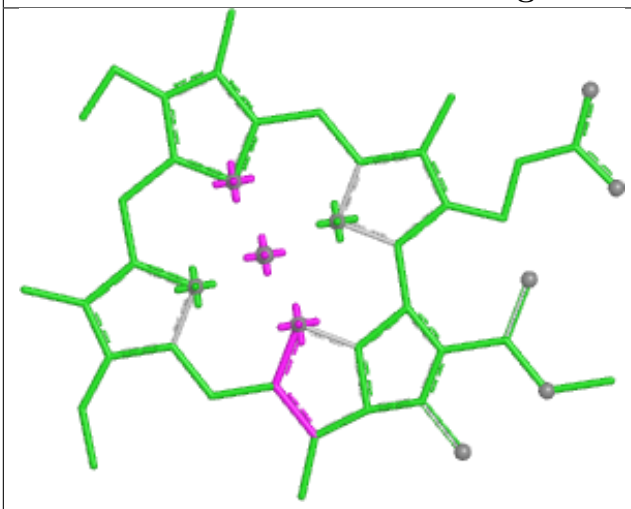


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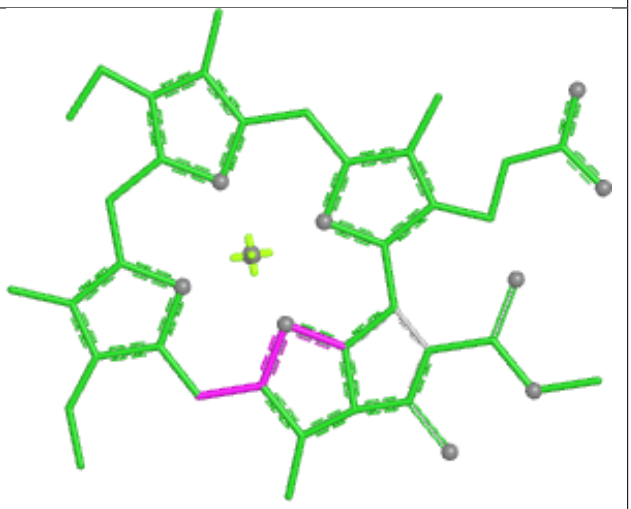


Rings

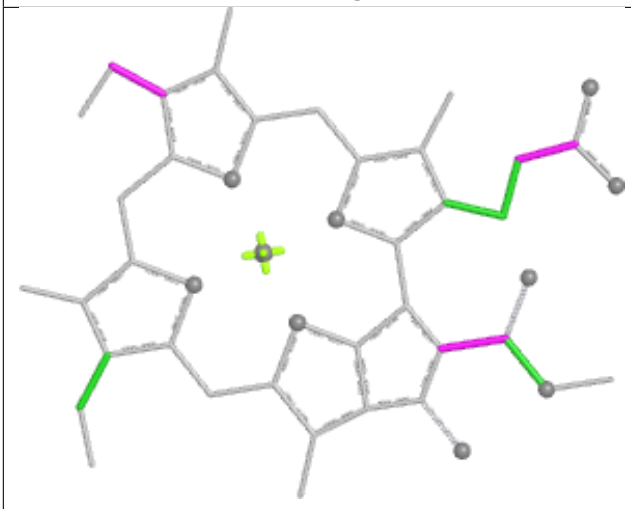
**Ligand CLA Z2 612**



**Bond lengths**



**Bond angles**

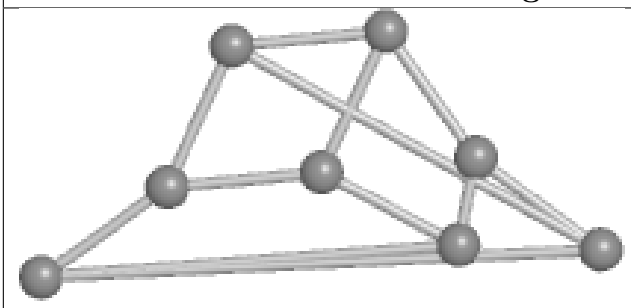


**Torsions**

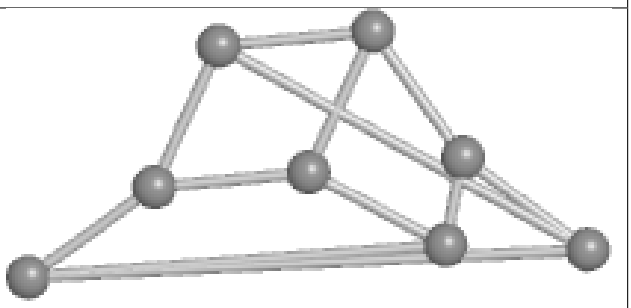


**Rings**

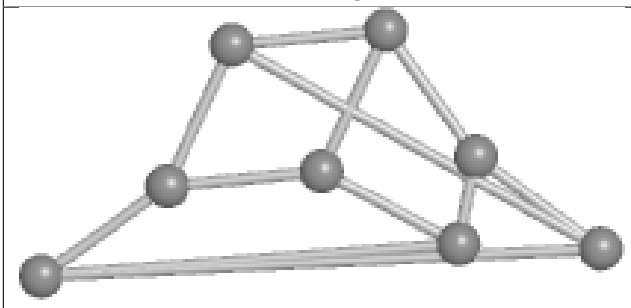
**Ligand SF4 C2 102**



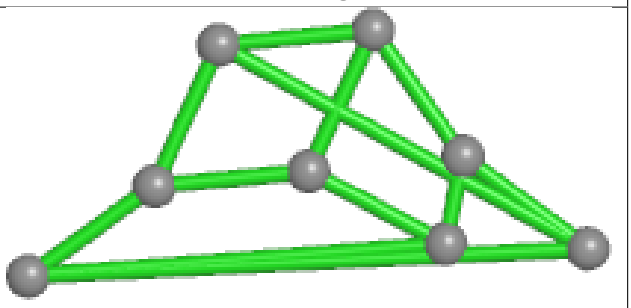
Bond lengths



Bond angles

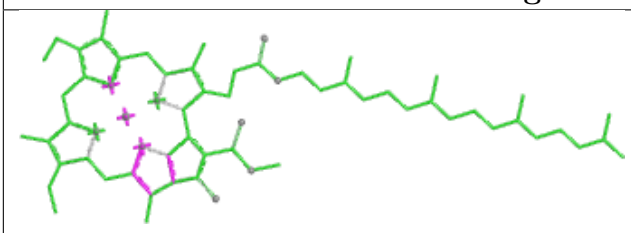


Torsions

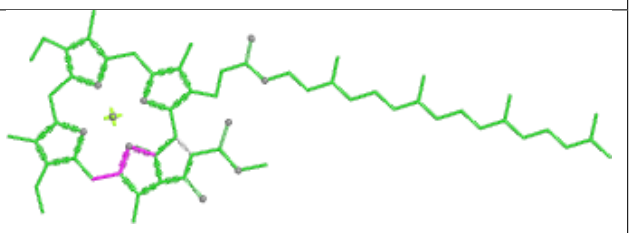


Rings

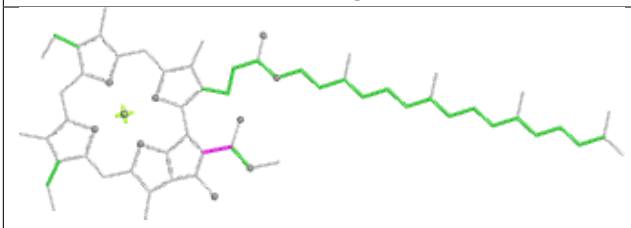
**Ligand CLA A 831**



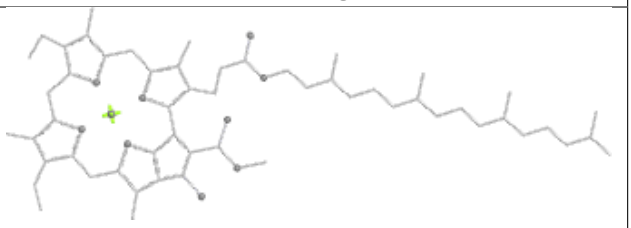
Bond lengths



Bond angles

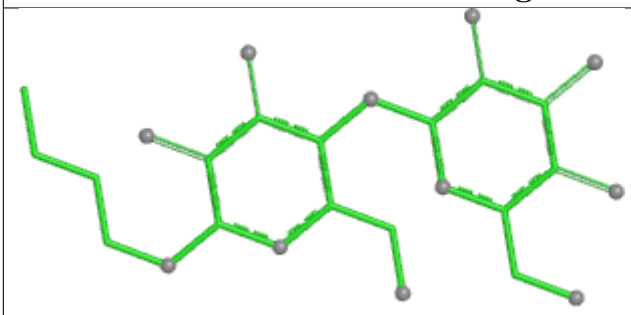


Torsions

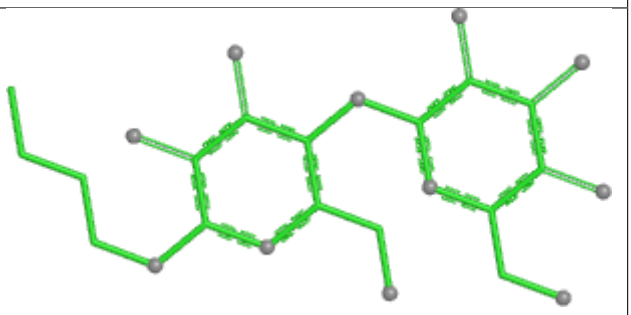


Rings

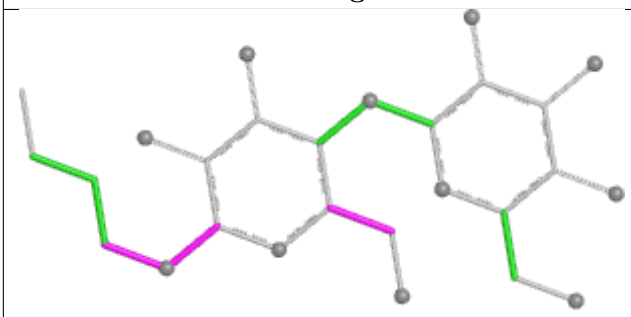
## Ligand LMU 72 629



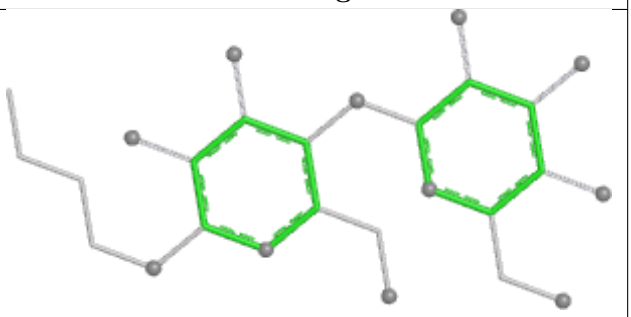
Bond lengths



Bond angles

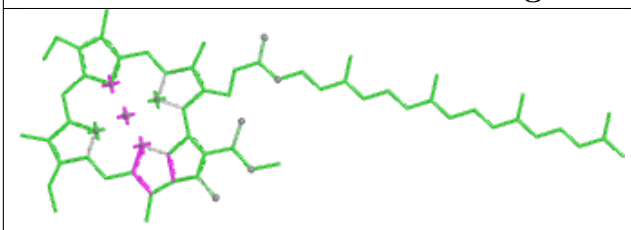


Torsions

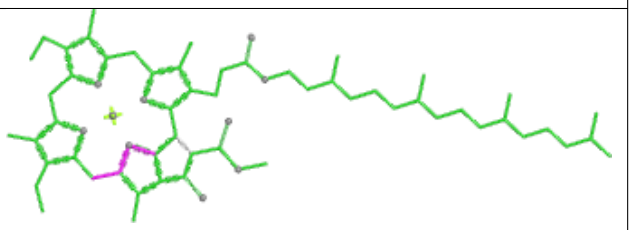


Rings

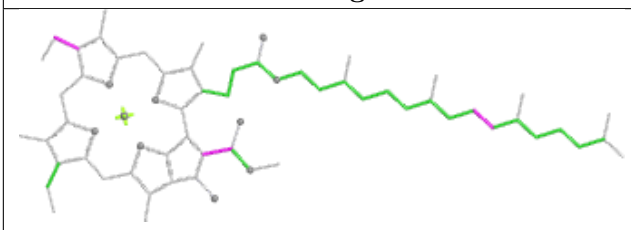
## Ligand CLA B 821



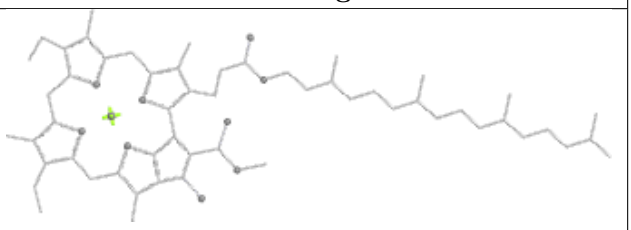
Bond lengths



Bond angles

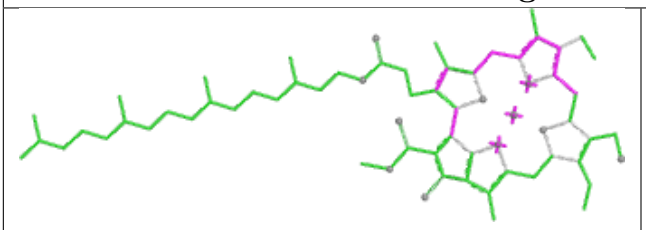


Torsions

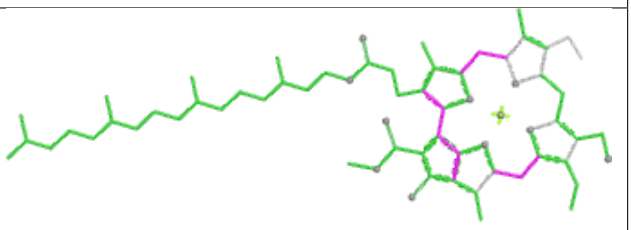


Rings

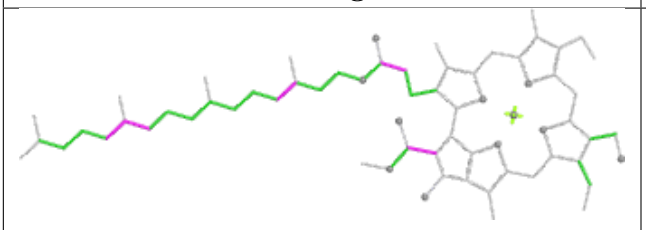
**Ligand CHL 82 601**



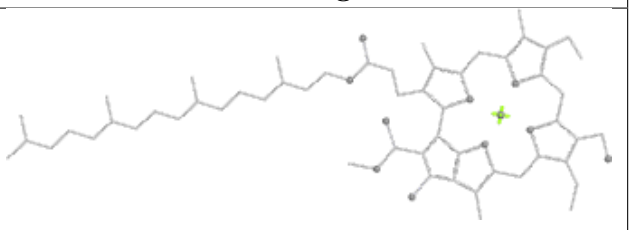
Bond lengths



Bond angles

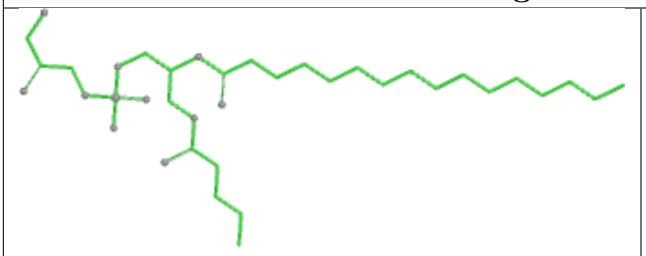


Torsions

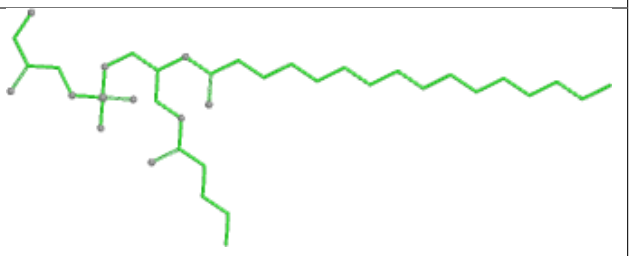


Rings

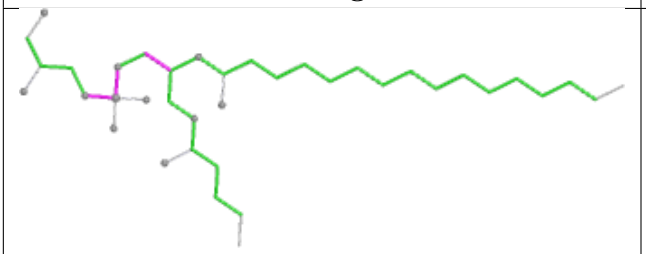
**Ligand LHG A2 847**



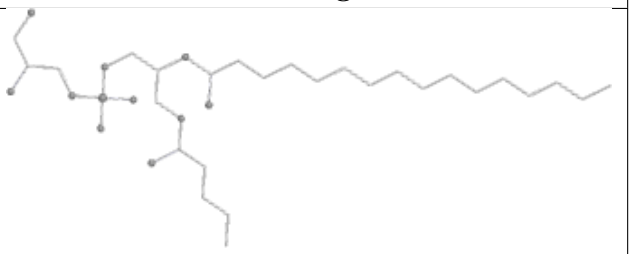
Bond lengths



Bond angles

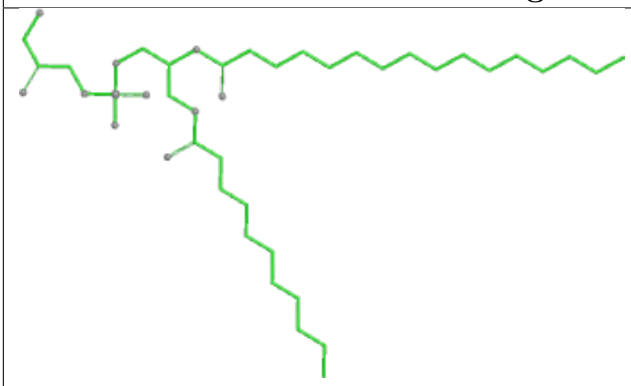


Torsions

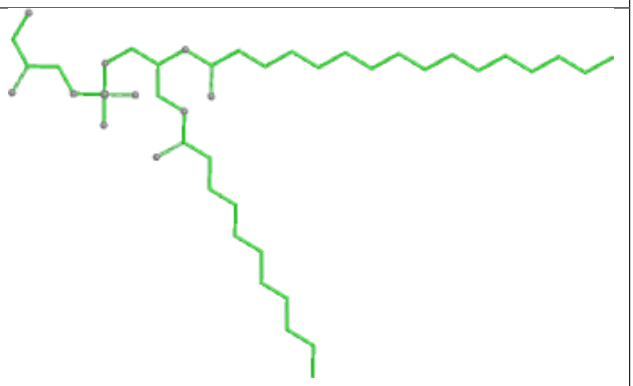


Rings

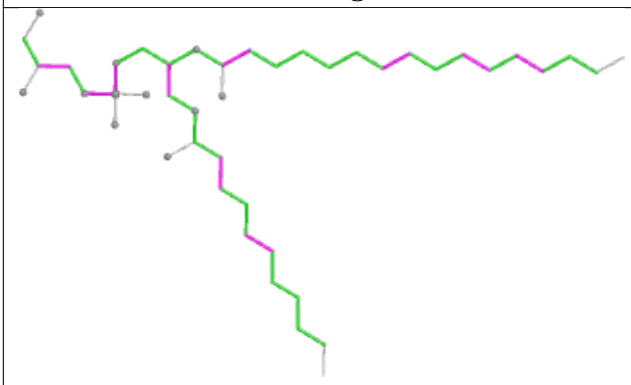
## Ligand LHG 8 620



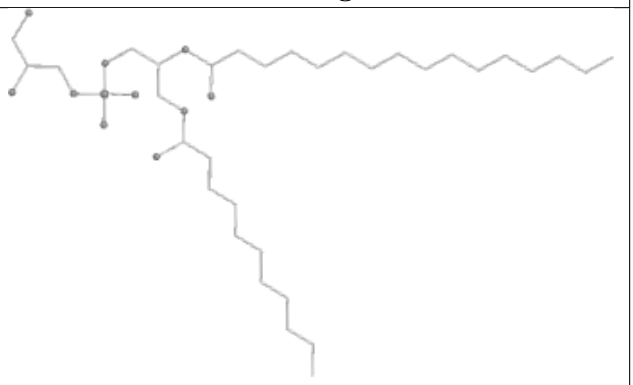
Bond lengths



Bond angles

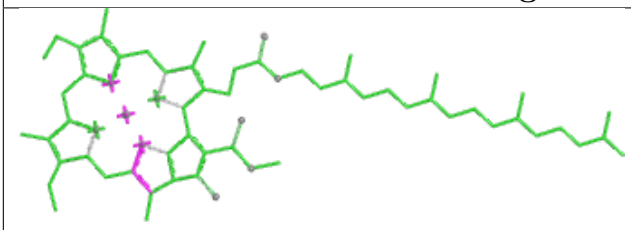


Torsions

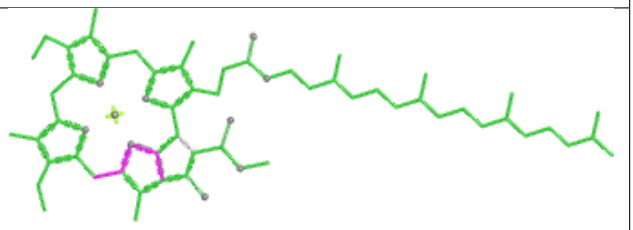


Rings

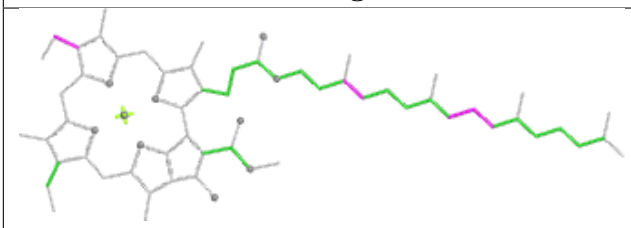
## Ligand CLA 52 617



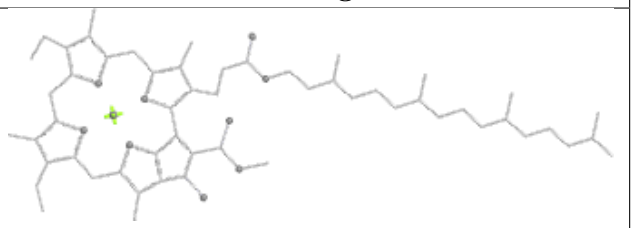
Bond lengths



Bond angles

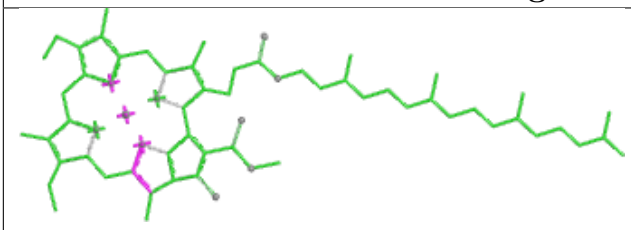


Torsions

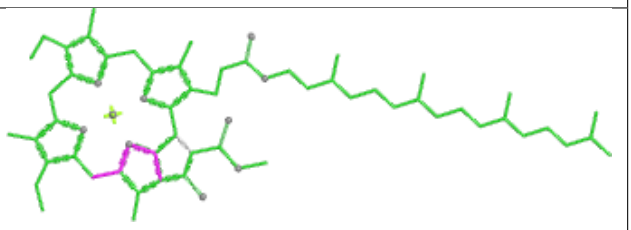


Rings

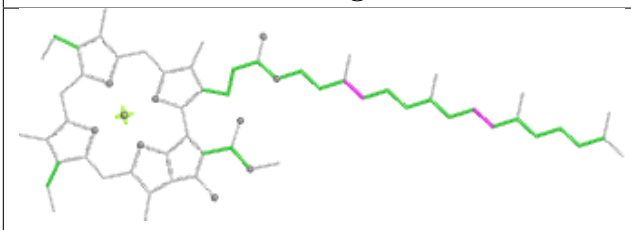
## Ligand CLA 5 609



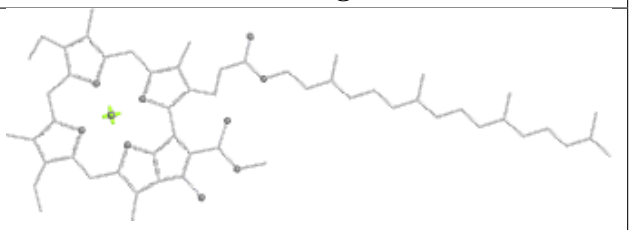
Bond lengths



Bond angles

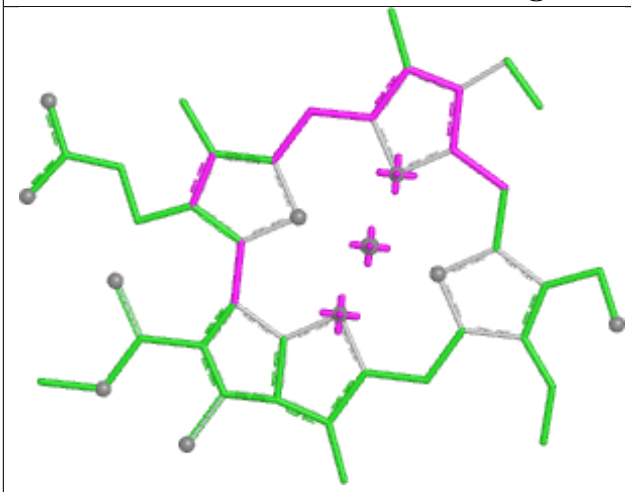


Torsions

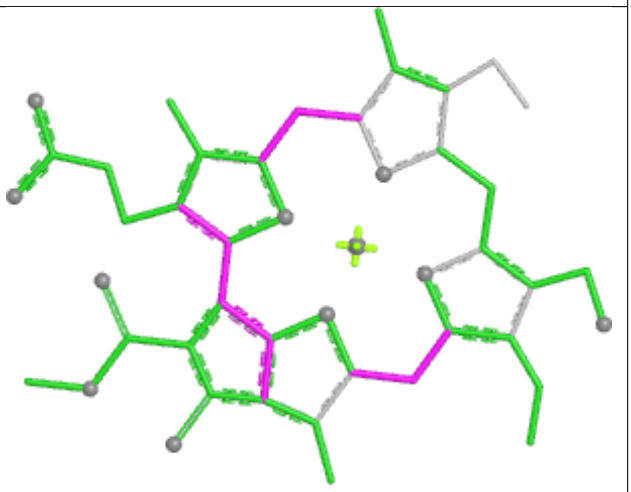


Rings

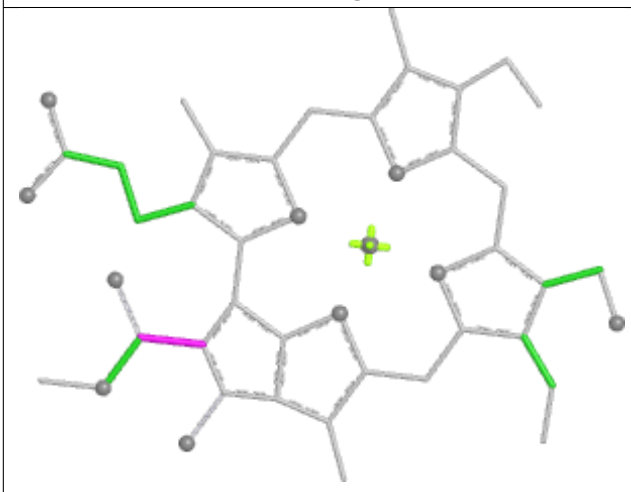
## Ligand CHL 5 606



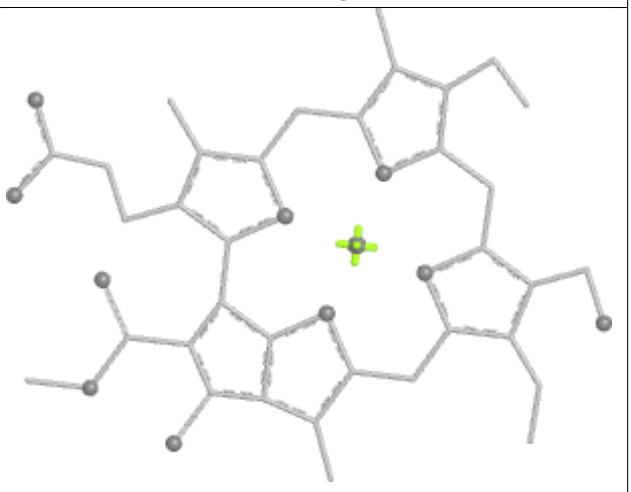
Bond lengths



Bond angles

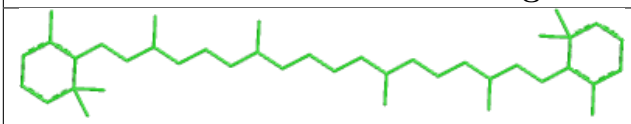


Torsions

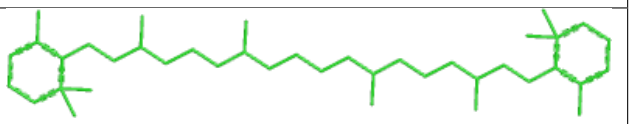


Rings

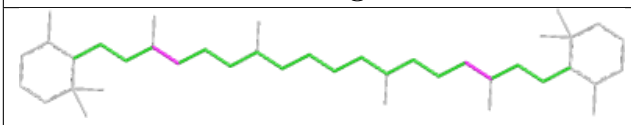
## Ligand BCR B 845



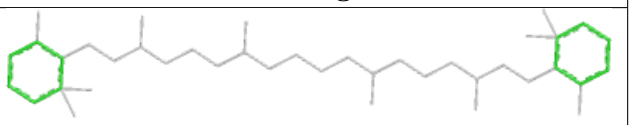
Bond lengths



Bond angles

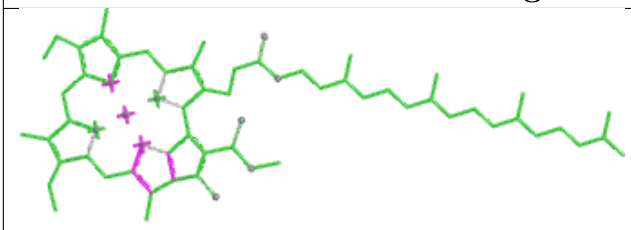


Torsions

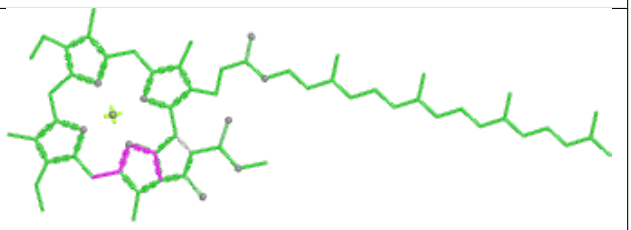


Rings

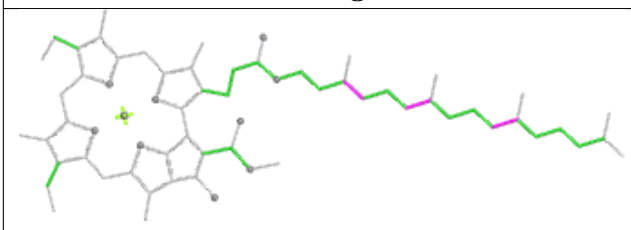
## Ligand CLA A 820



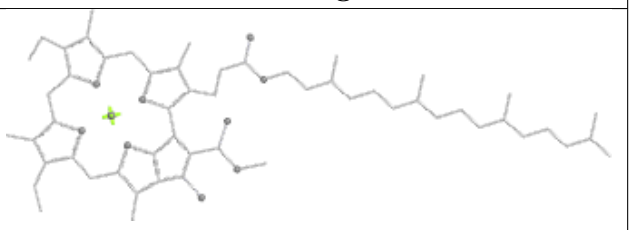
Bond lengths



Bond angles

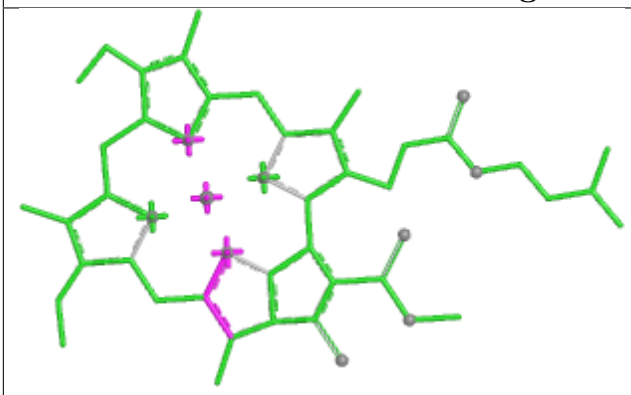


Torsions

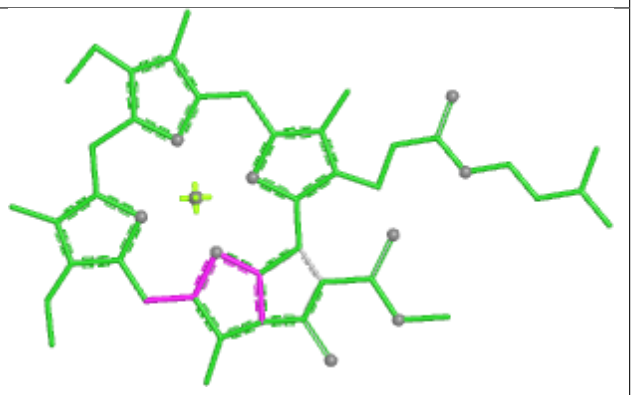


Rings

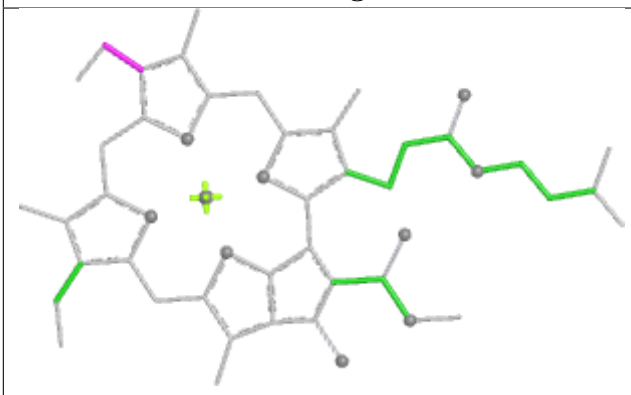
## Ligand CLA 62 614



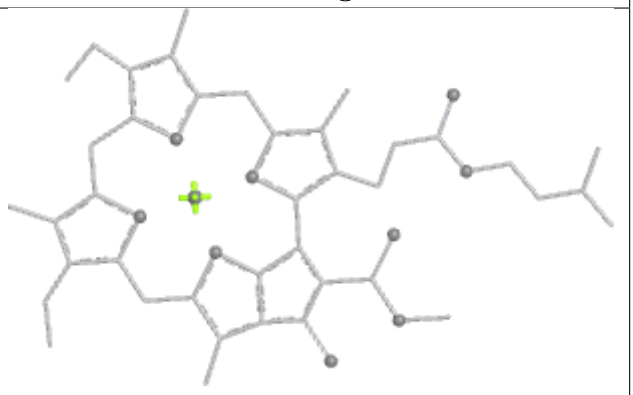
Bond lengths



Bond angles

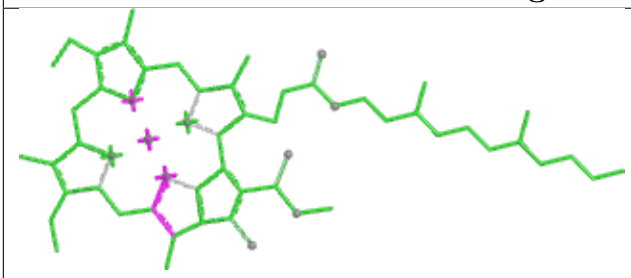


Torsions

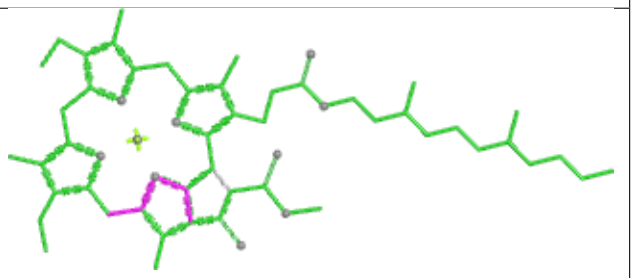


Rings

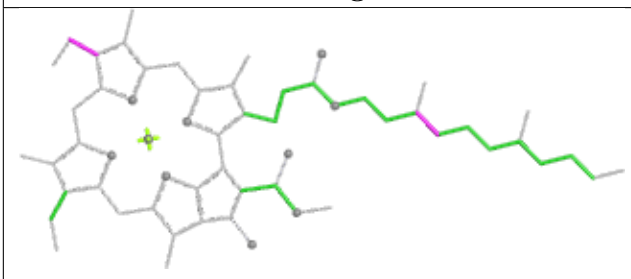
## Ligand CLA 6 611



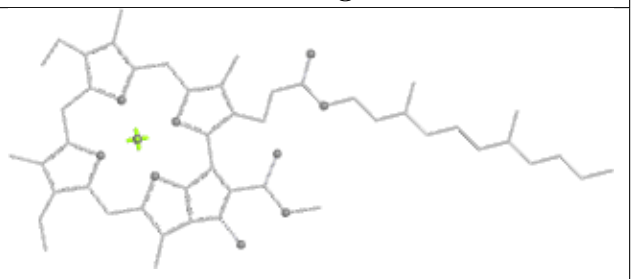
Bond lengths



Bond angles

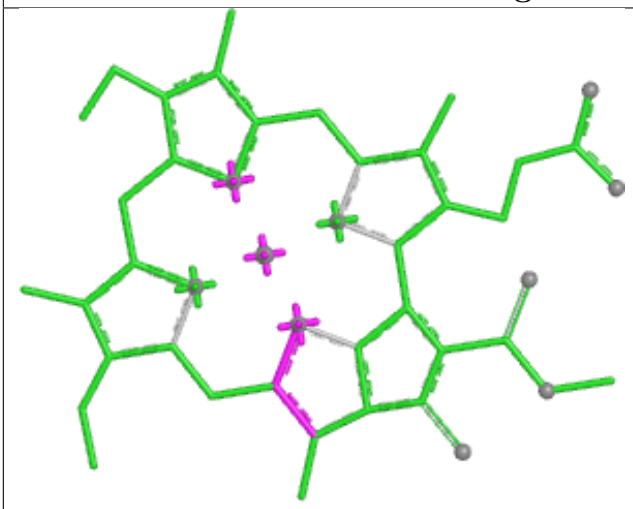


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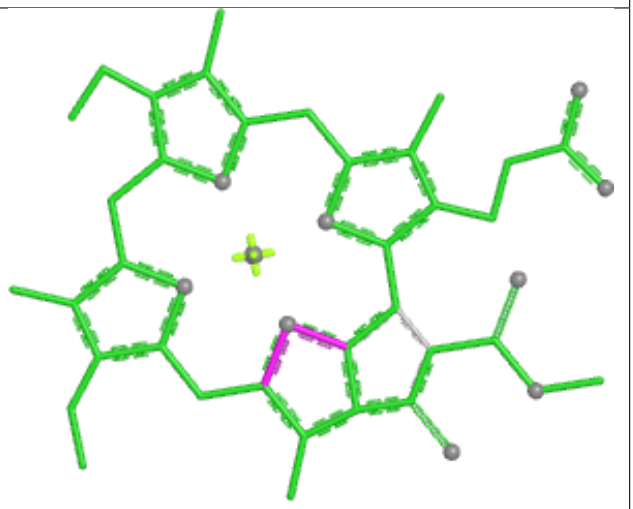


Rings

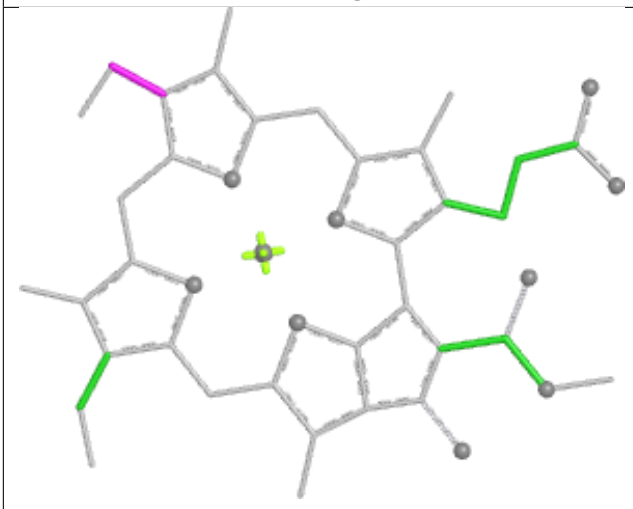
## Ligand CLA K2 201



Bond lengths



Bond angles

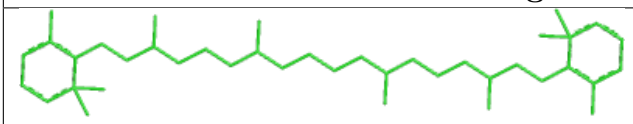


Torsions

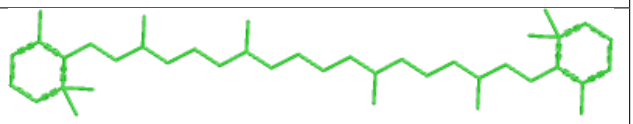


Rings

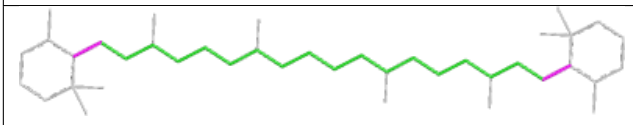
## Ligand BCR 3 620



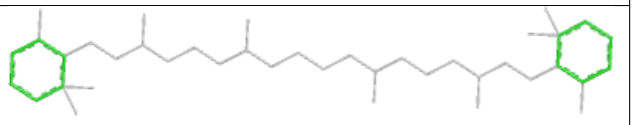
Bond lengths



Bond angles

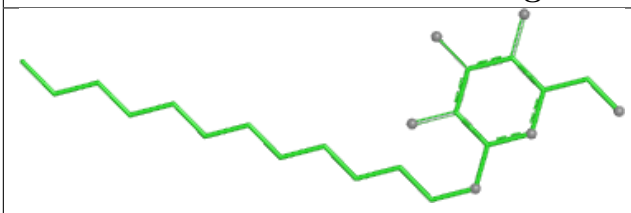


Torsions

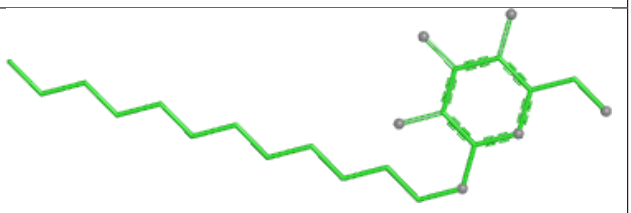


Rings

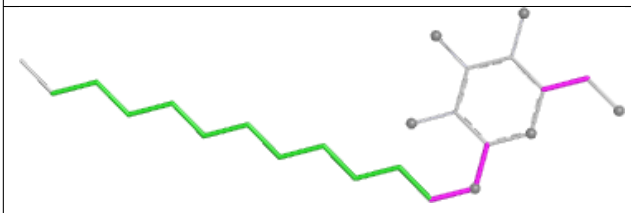
## Ligand LMU 8 628



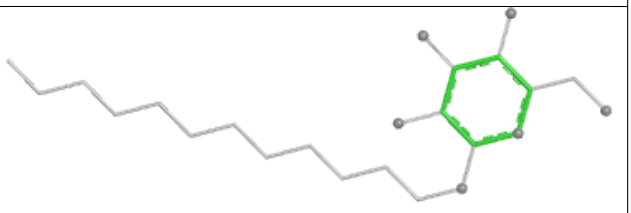
Bond lengths



Bond angles

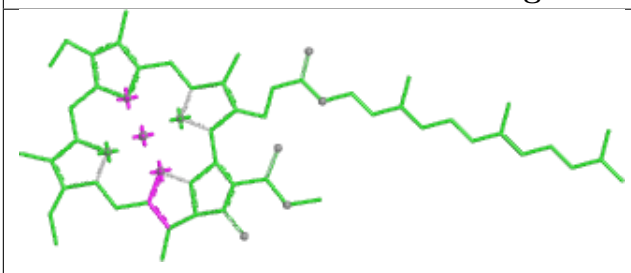


Torsions

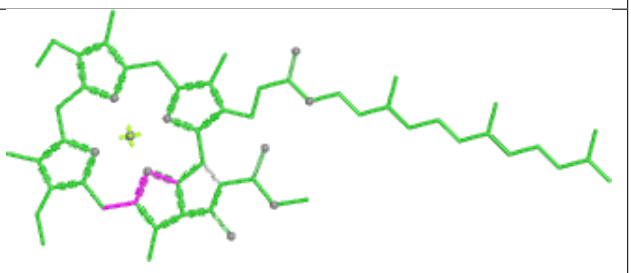


Rings

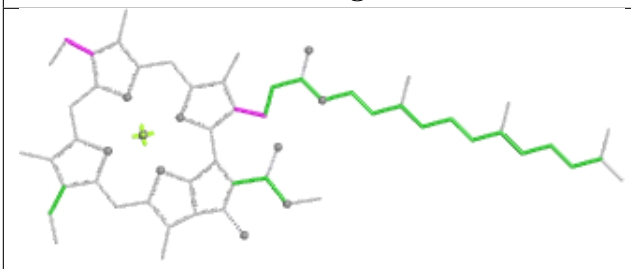
## Ligand CLA A 819



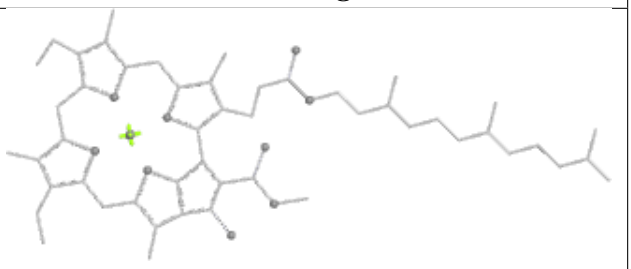
Bond lengths



Bond angles

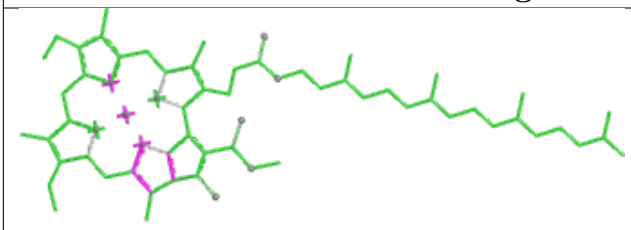


Torsions

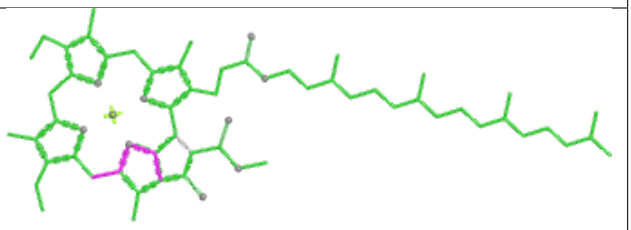


Rings

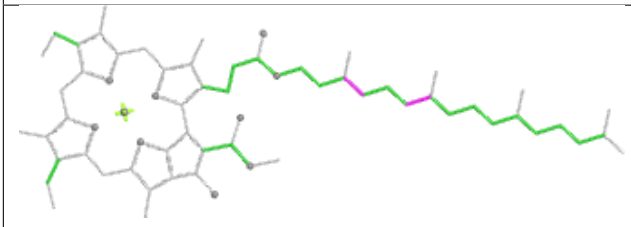
## Ligand CLA A2 811



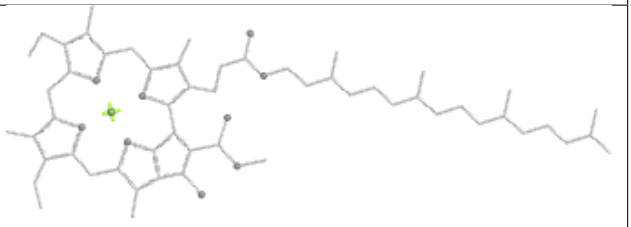
Bond lengths



Bond angles

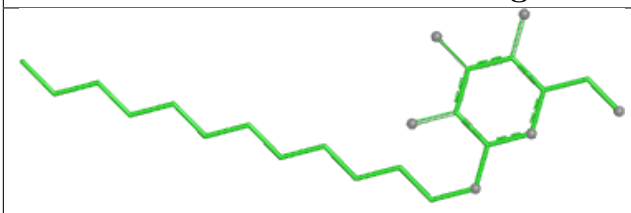


Torsions

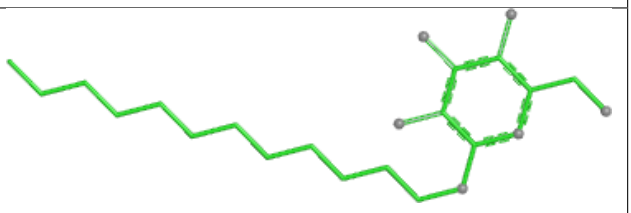


Rings

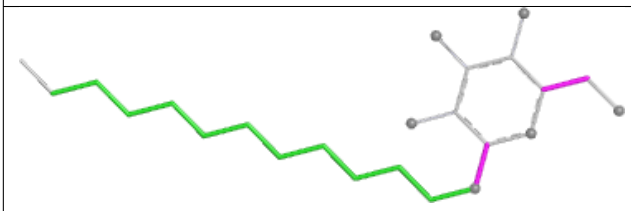
## Ligand LMU A2 861



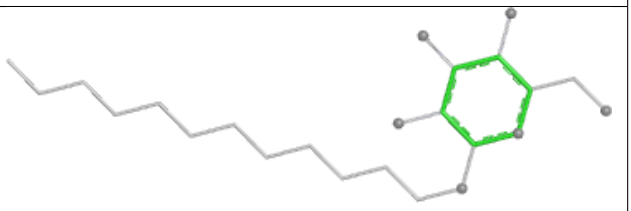
Bond lengths



Bond angles

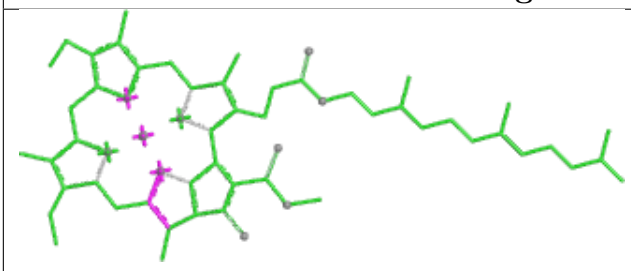


Torsions

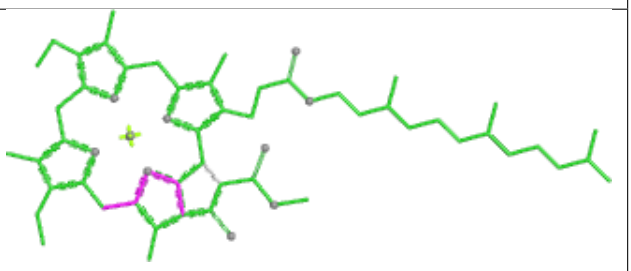


Rings

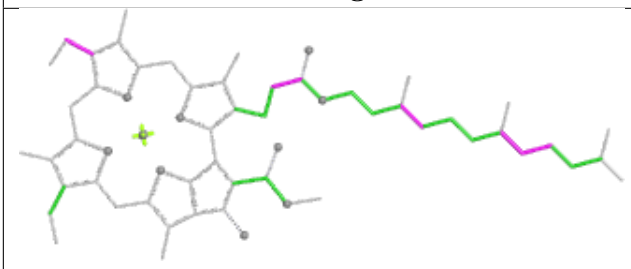
## Ligand CLA B2 834



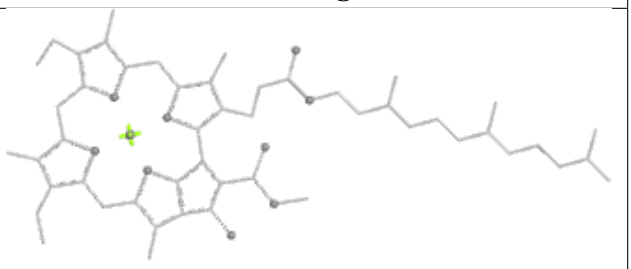
Bond lengths



Bond angles

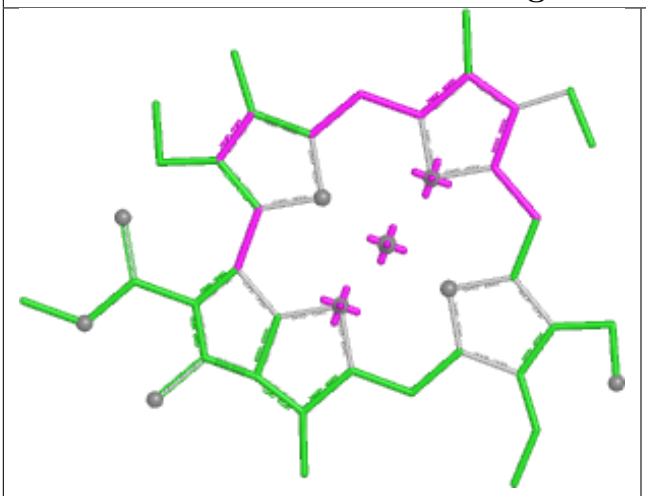


Torsions

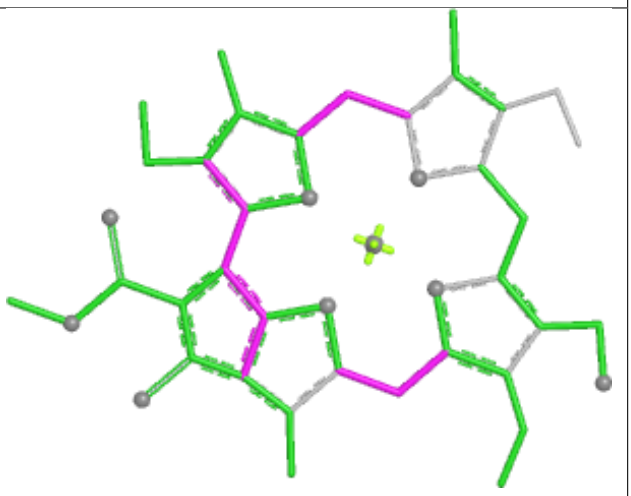


Rings

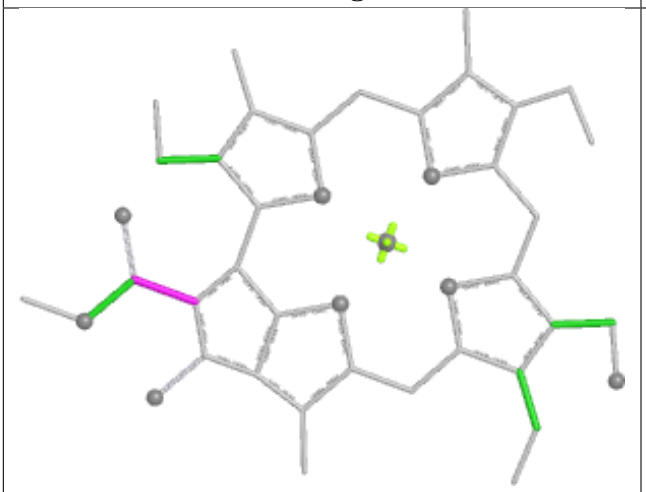
## Ligand CHL 5 618



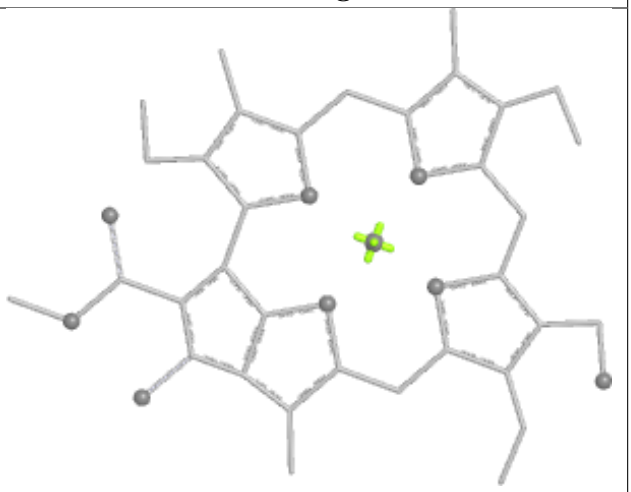
Bond lengths



Bond angles

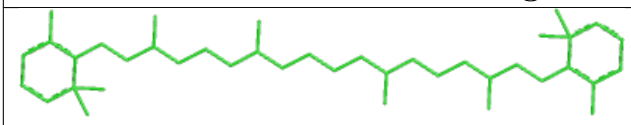


Torsions

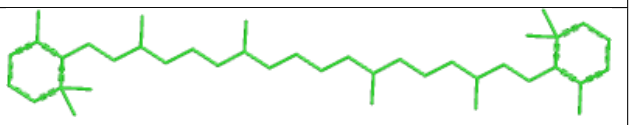


Rings

## Ligand BCR A 849



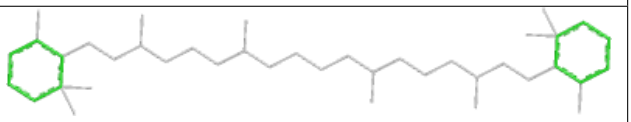
Bond lengths



Bond angles

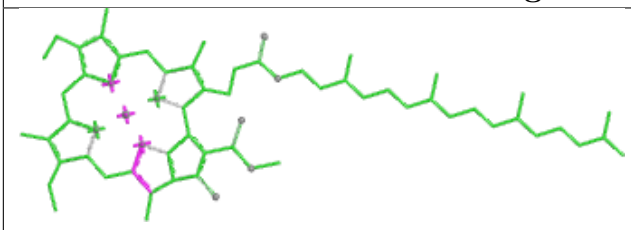


Torsions

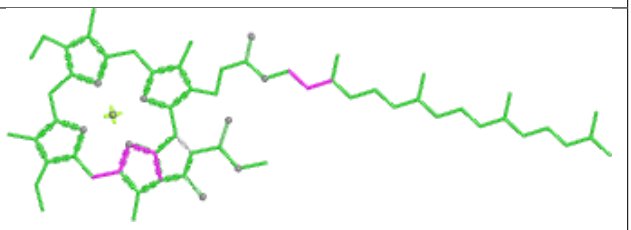


Rings

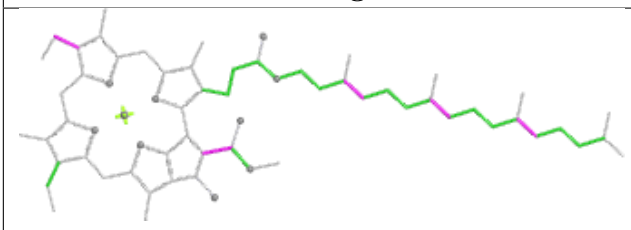
## Ligand CLA B 841



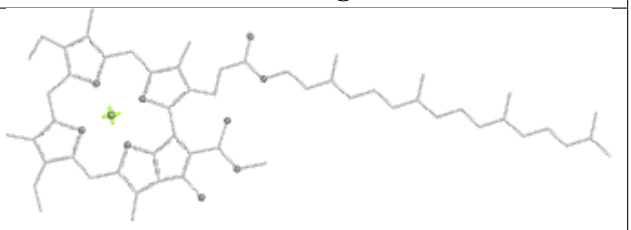
Bond lengths



Bond angles

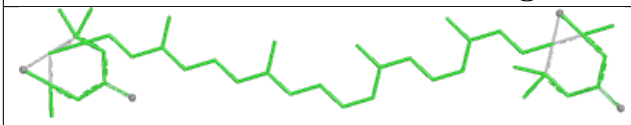


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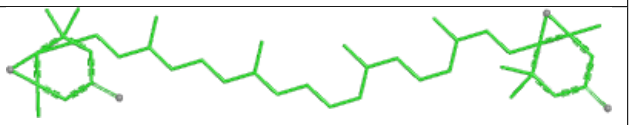


Rings

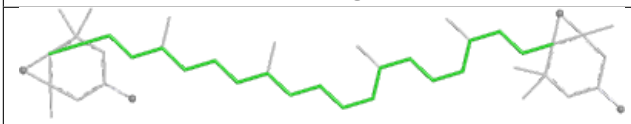
## Ligand XAT 72 622



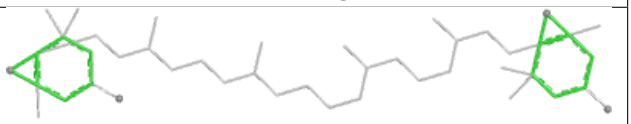
Bond lengths



Bond angles

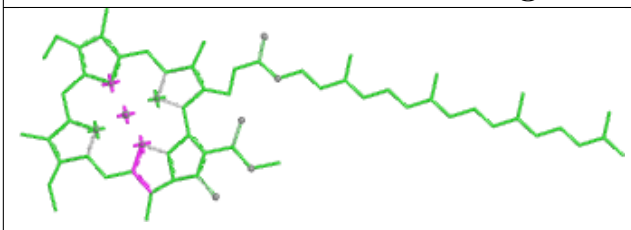


Torsions

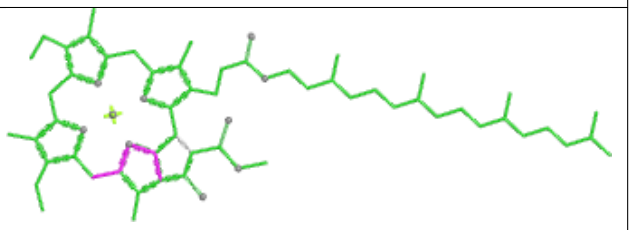


Rings

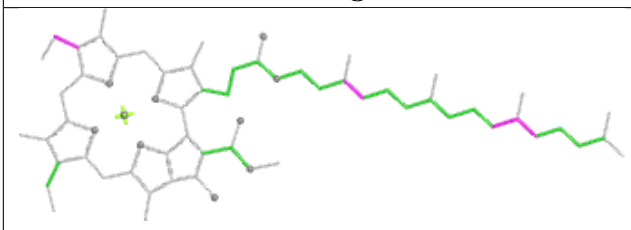
## Ligand CLA 82 613



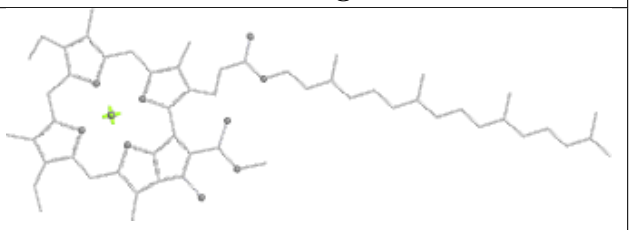
Bond lengths



Bond angles

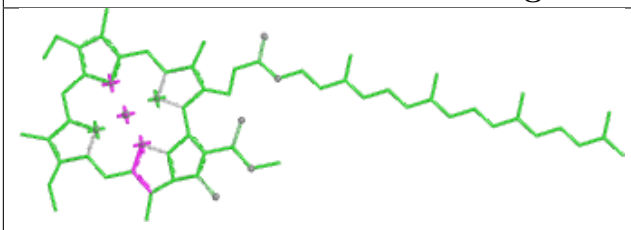


Torsions

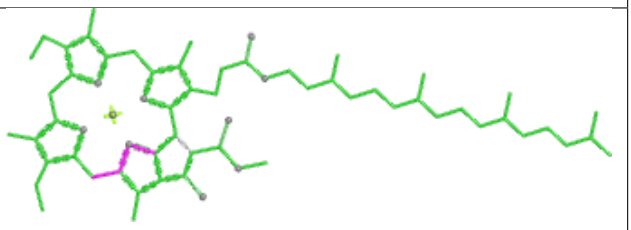


Rings

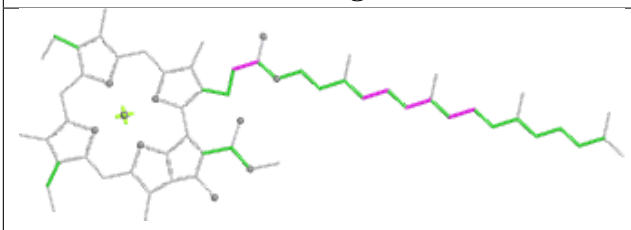
## Ligand CLA B 809



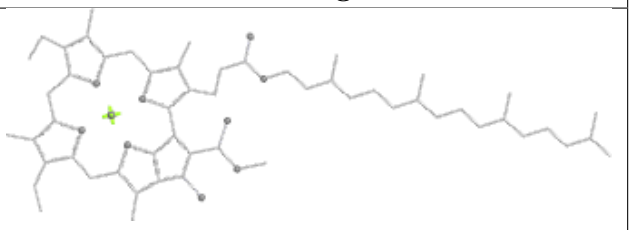
Bond lengths



Bond angles

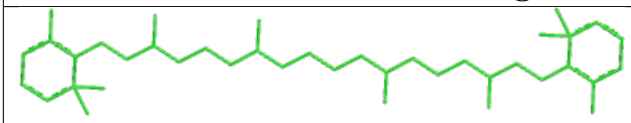


Torsions

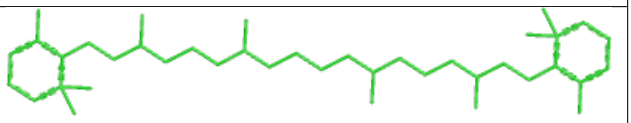


Rings

## Ligand BCR B2 847



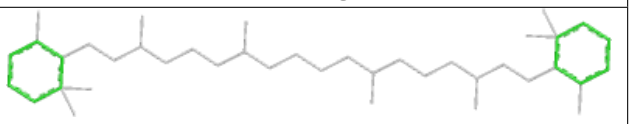
Bond lengths



Bond angles

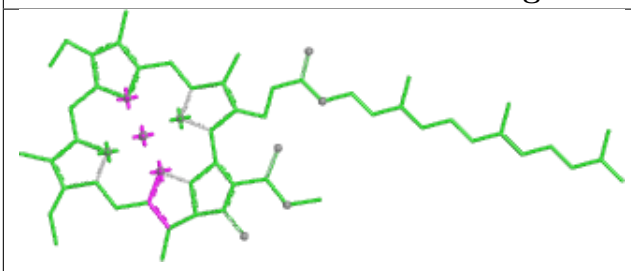


Torsions

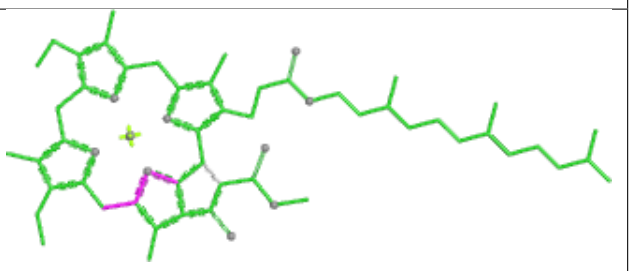


Rings

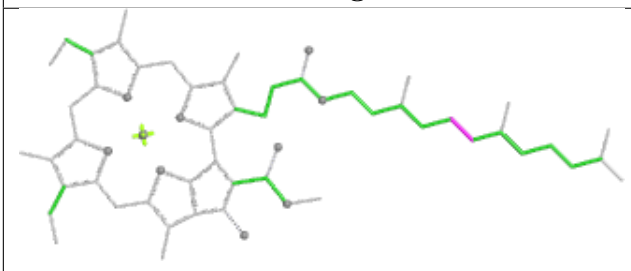
## Ligand CLA K 203



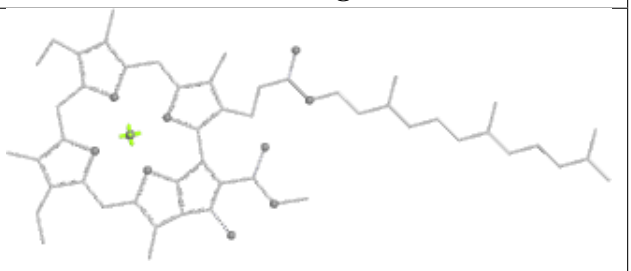
Bond lengths



Bond angles

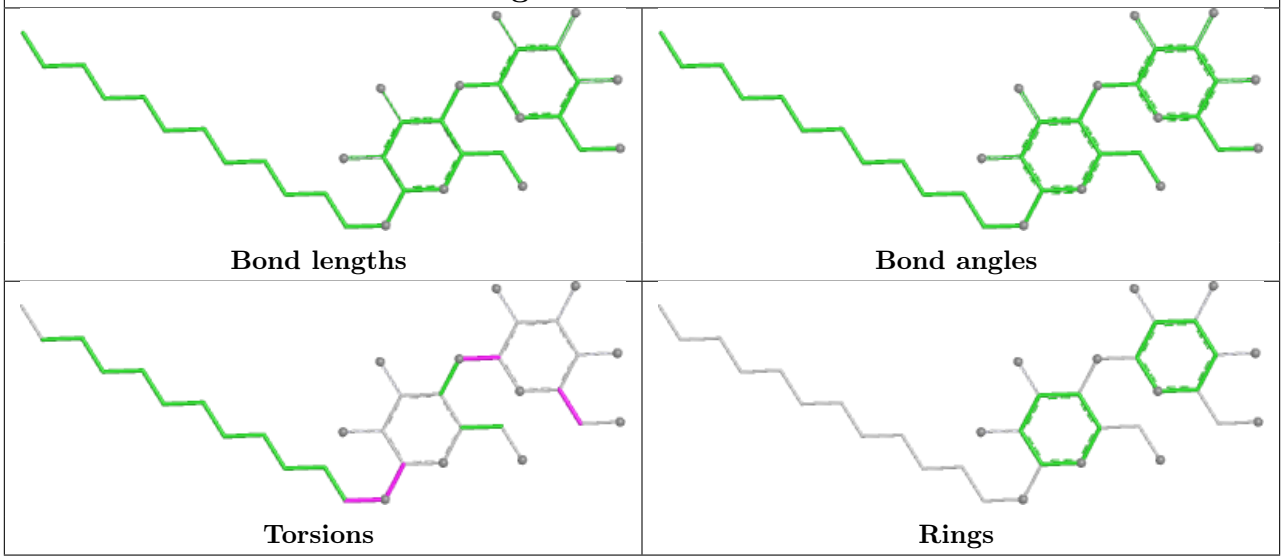


Torsions

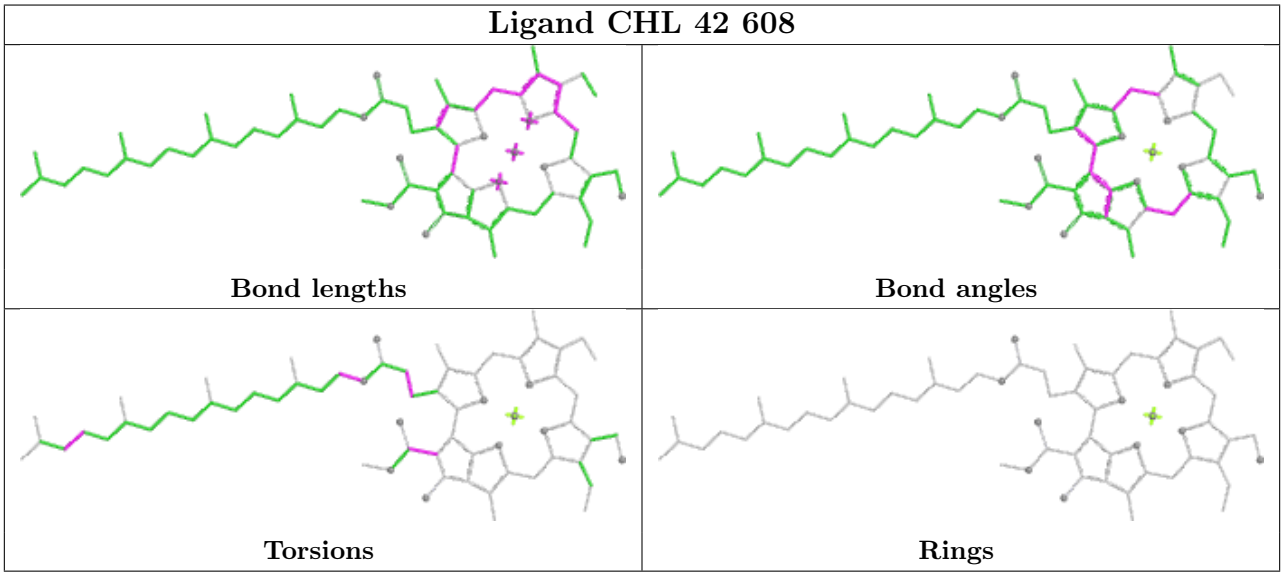


Rings

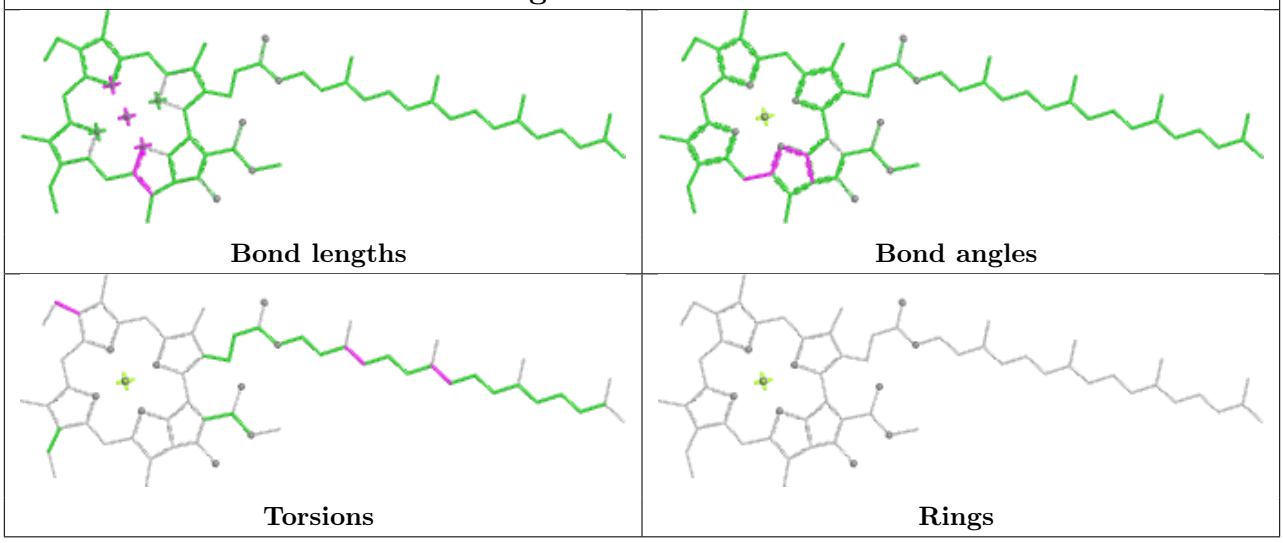
## Ligand LMU A2 858



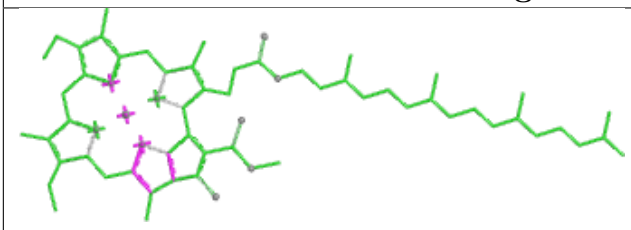

## Ligand CHL 42 608



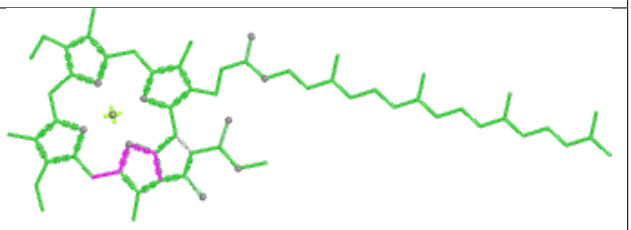

## Ligand CLA 6 613



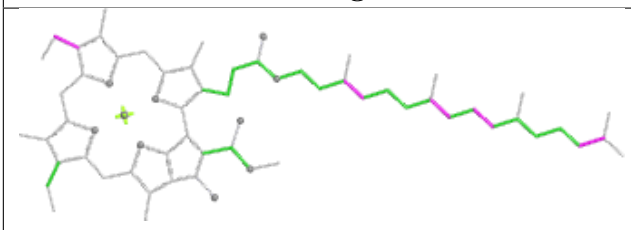
**Ligand CLA A2 841**



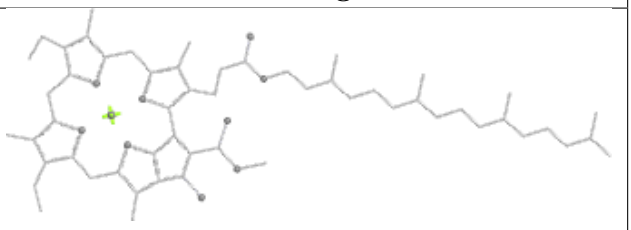
Bond lengths



Bond angles

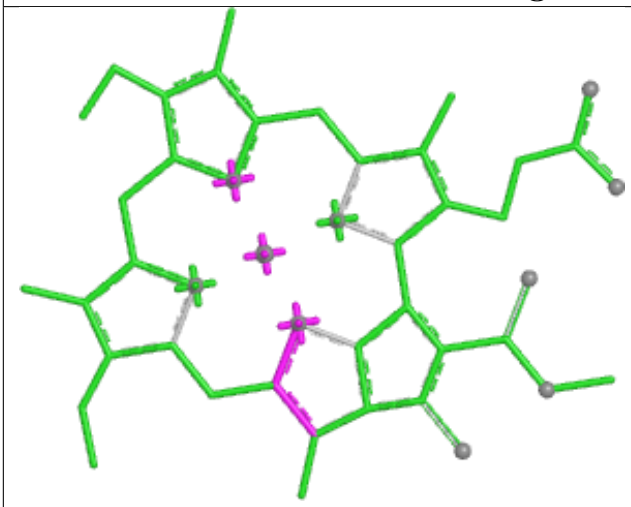


Torsions

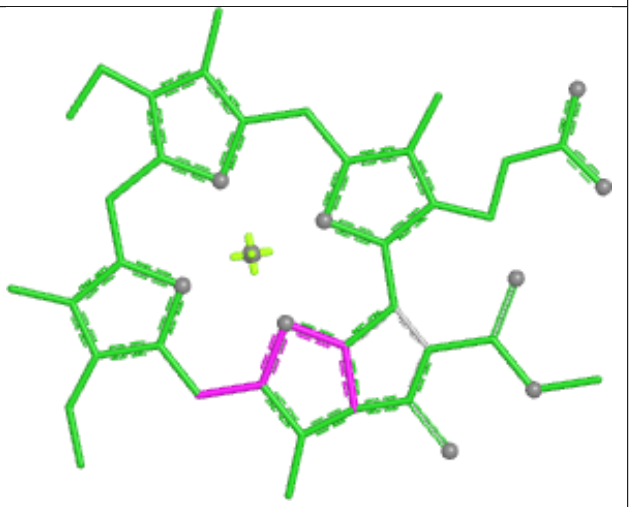


Rings

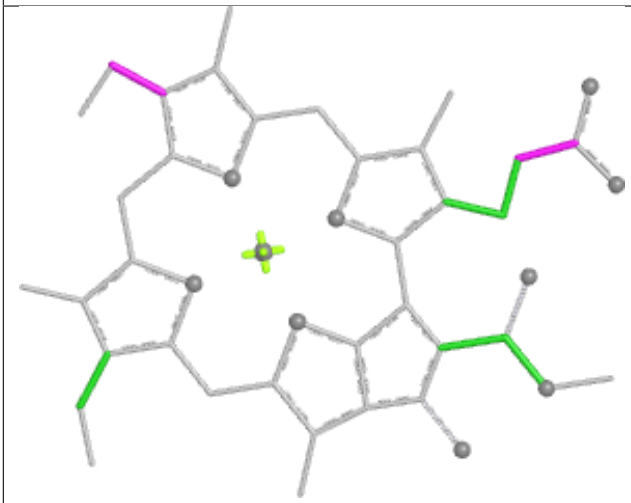
**Ligand CLA 5 614**



Bond lengths



Bond angles

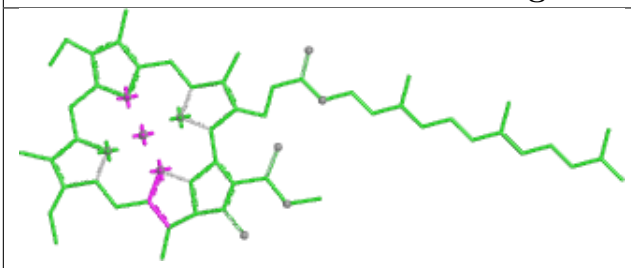


Torsions

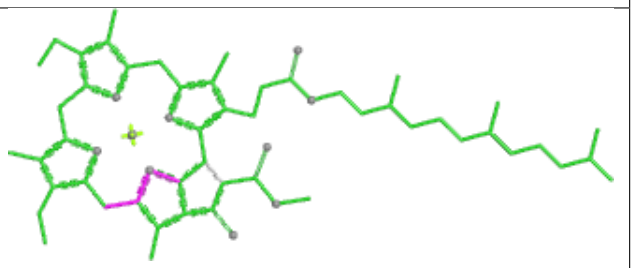


Rings

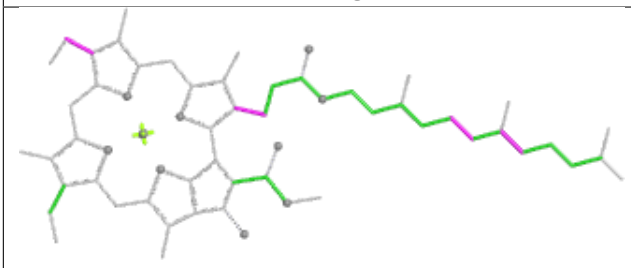
## Ligand CLA 4 609



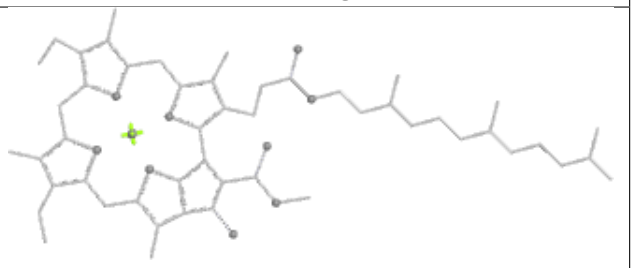
Bond lengths



Bond angles

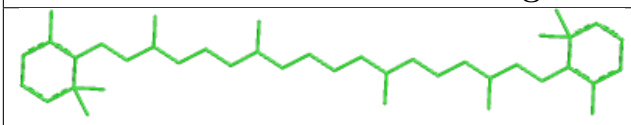


Torsions

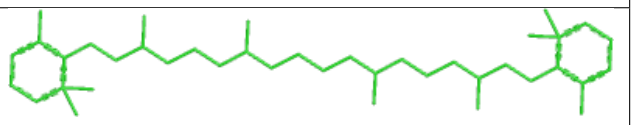


Rings

## Ligand BCR B 844



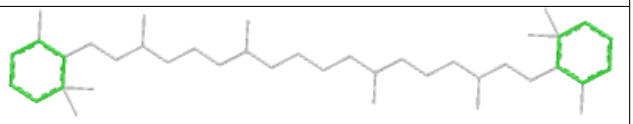
Bond lengths



Bond angles

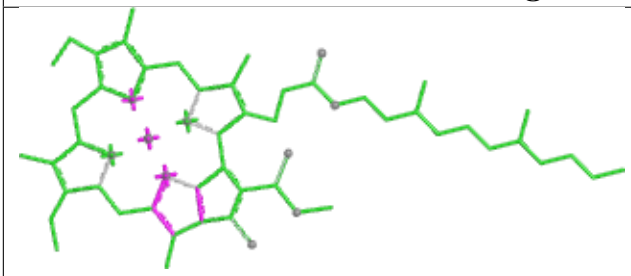


Torsions

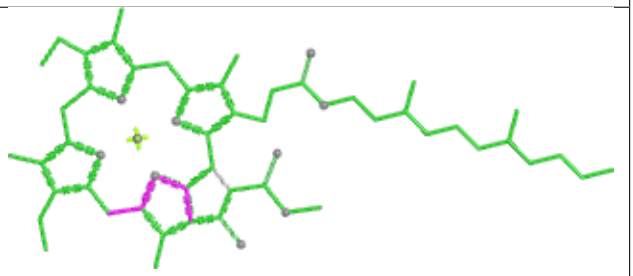


Rings

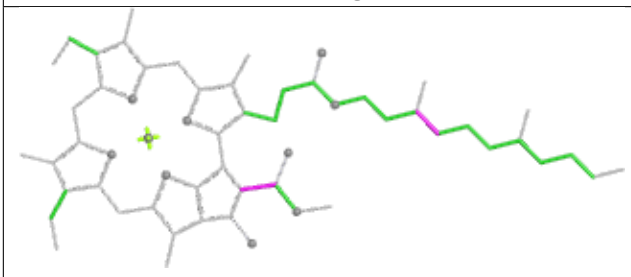
## Ligand CLA B 833



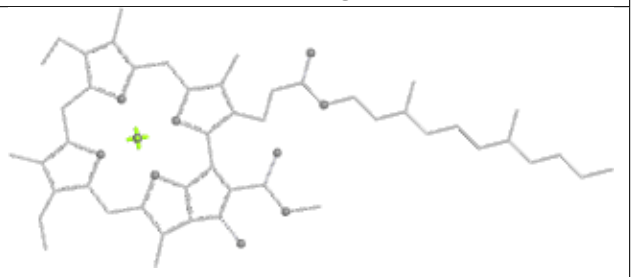
Bond lengths



Bond angles

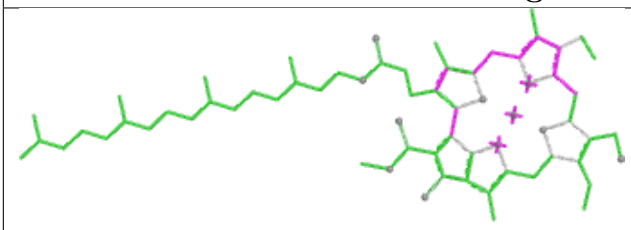


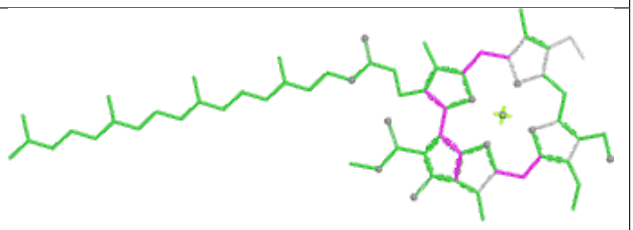
Torsions

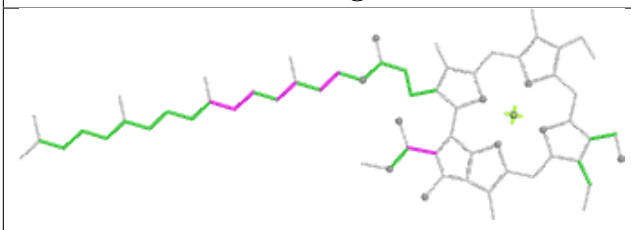


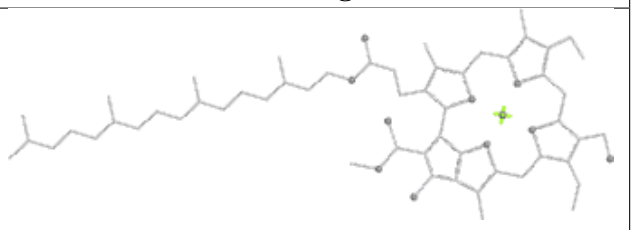
Rings

## Ligand CHL Z 601

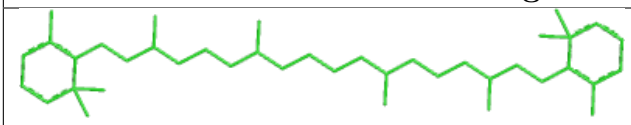

Bond lengths

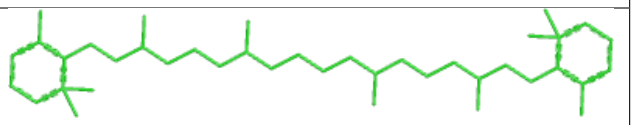

Bond angles

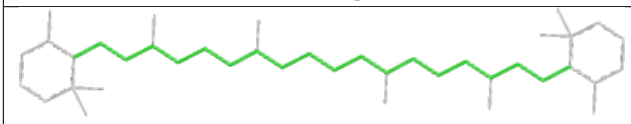

Torsions

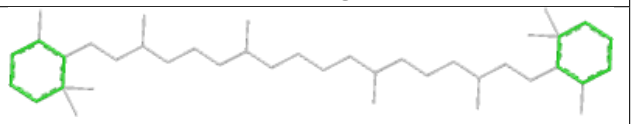

Rings

## Ligand BCR B 843

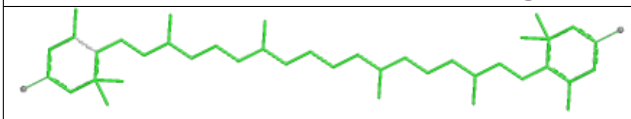

Bond lengths

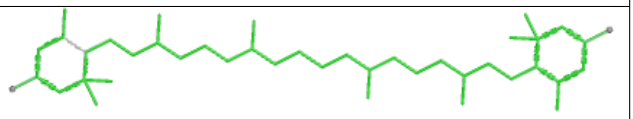

Bond angles

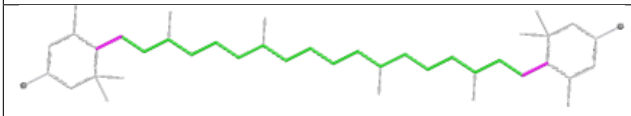

Torsions

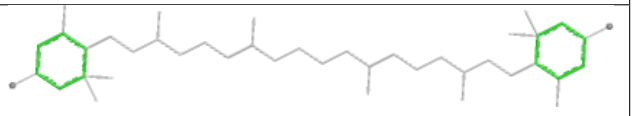

Rings

## Ligand LUT 52 626

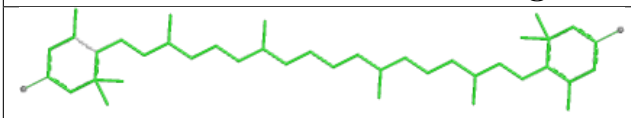

Bond lengths

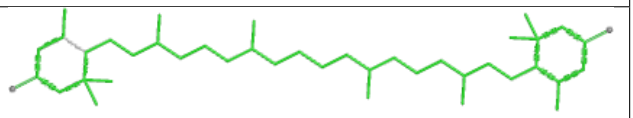

Bond angles

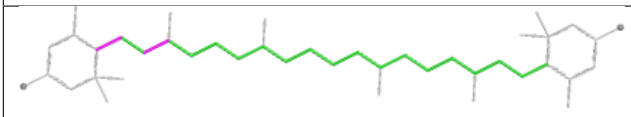

Torsions

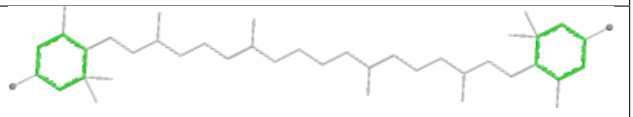

Rings

## Ligand LUT 7 624

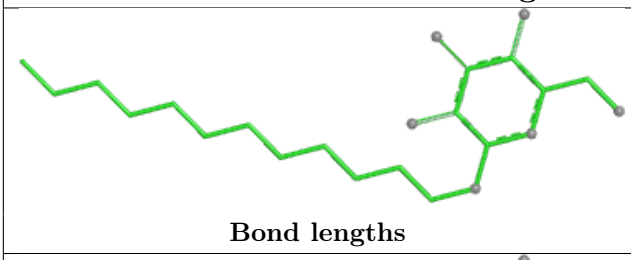

Bond lengths


Bond angles

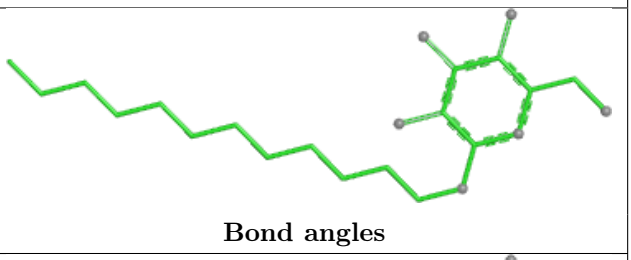

Torsions


Rings

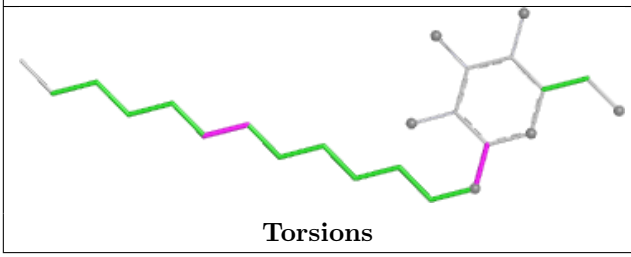
## Ligand LMU K 208



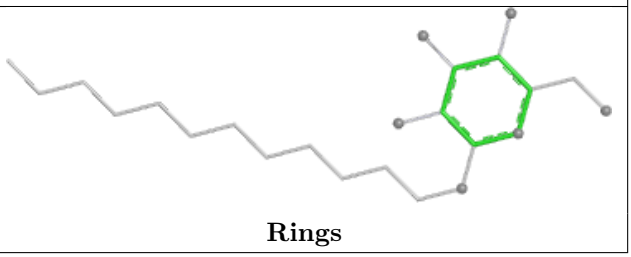
Bond lengths



Bond angles

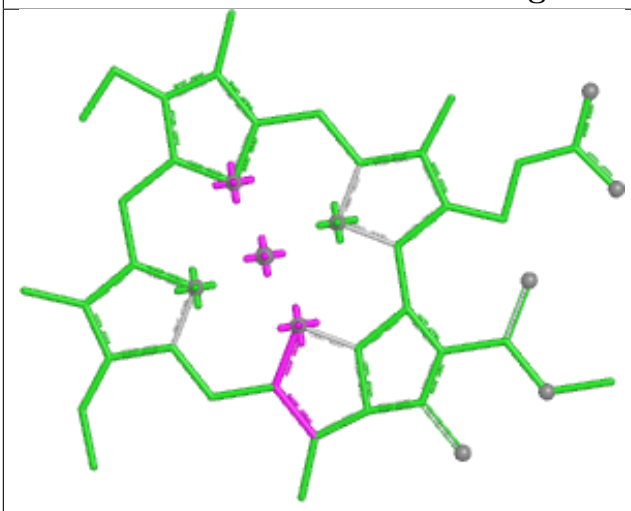


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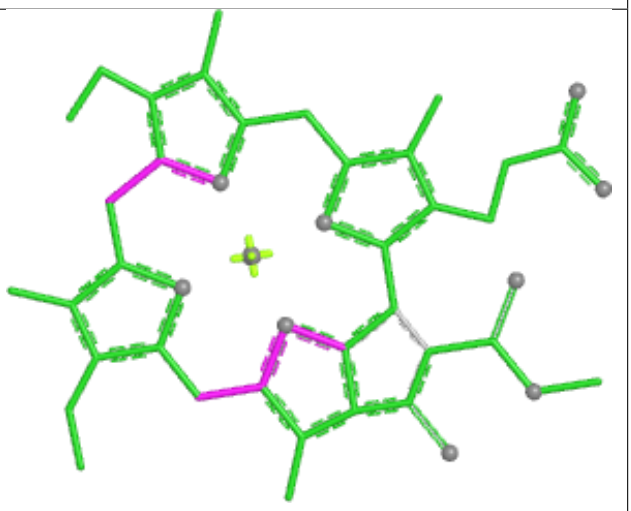


Rings

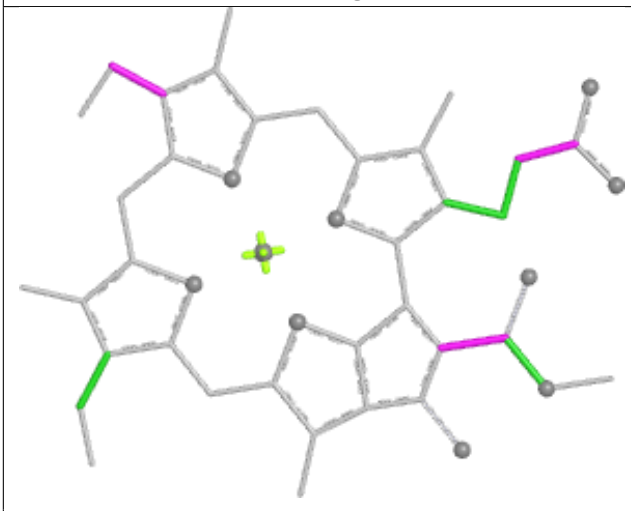
## Ligand CLA 1 612



Bond lengths



Bond angles

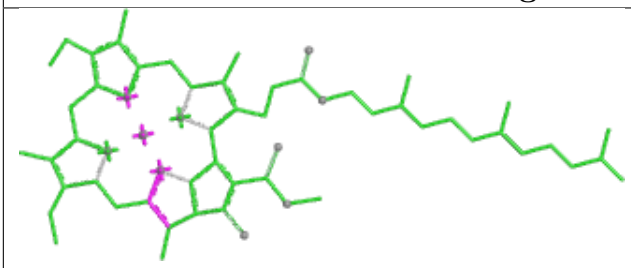


Torsions

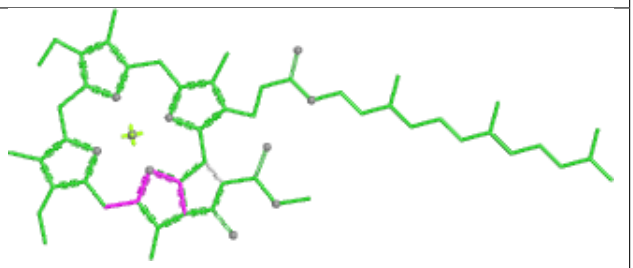


Rings

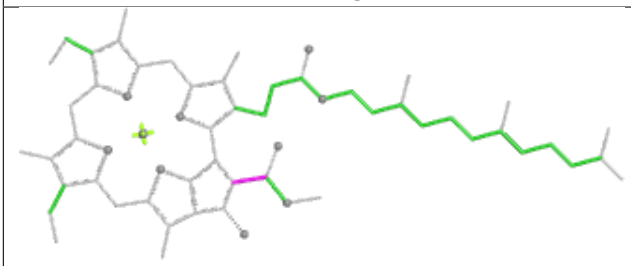
**Ligand CLA 32 602**



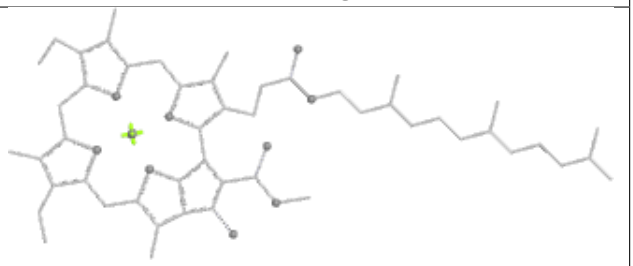
Bond lengths



Bond angles

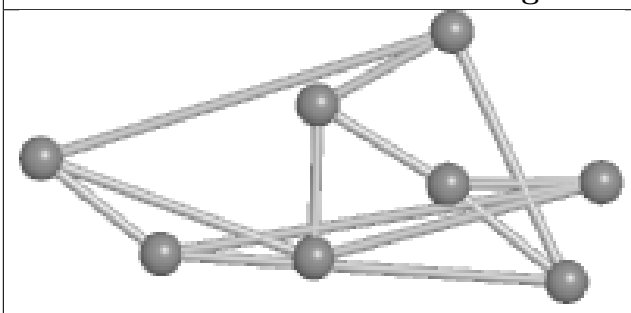


Torsions

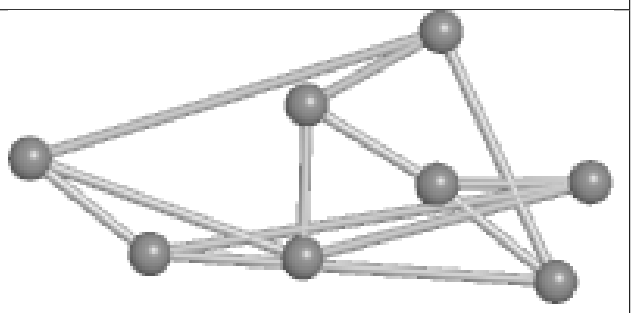


Rings

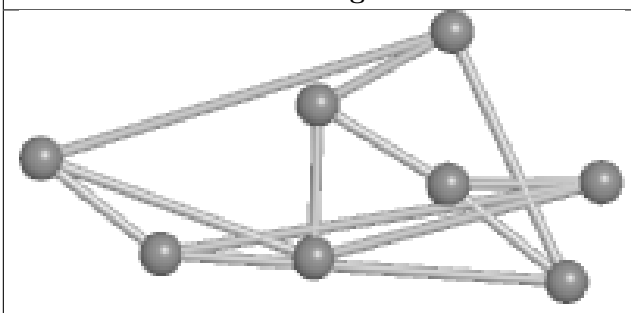
**Ligand SF4 A2 853**



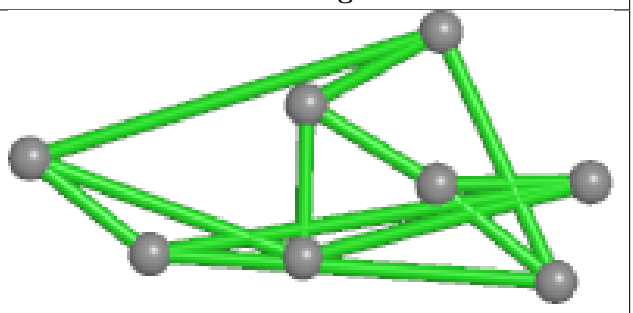
Bond lengths



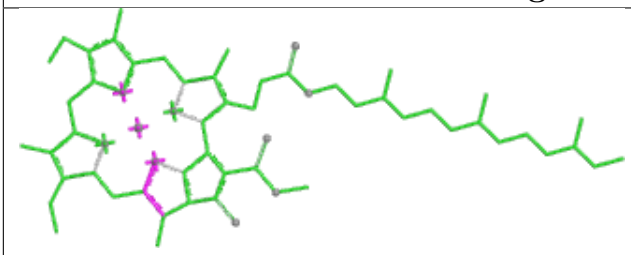
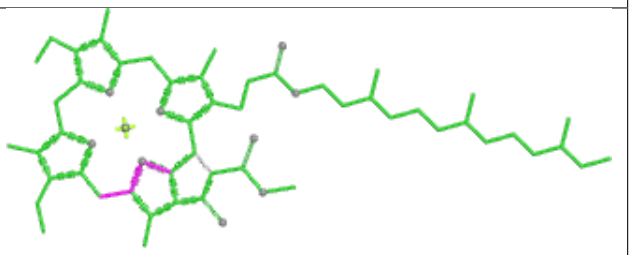
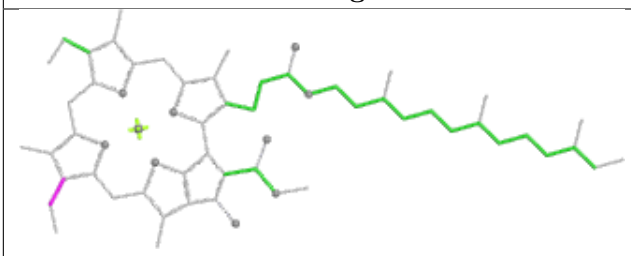
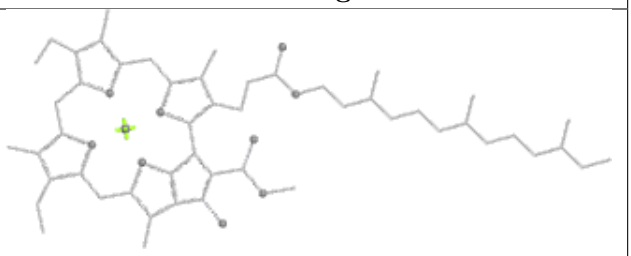
Bond angles

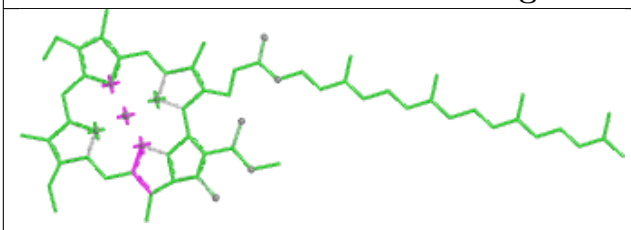
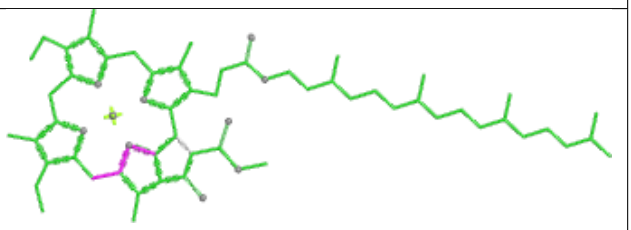
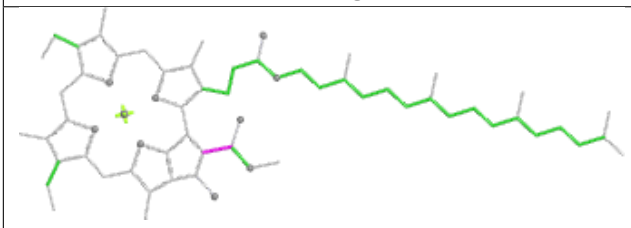
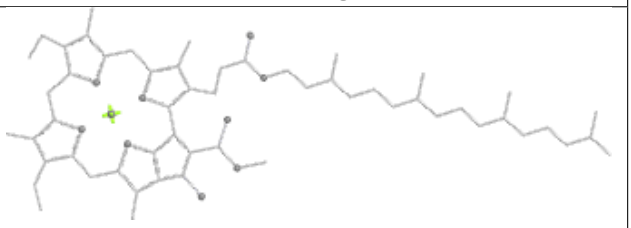


Torsions

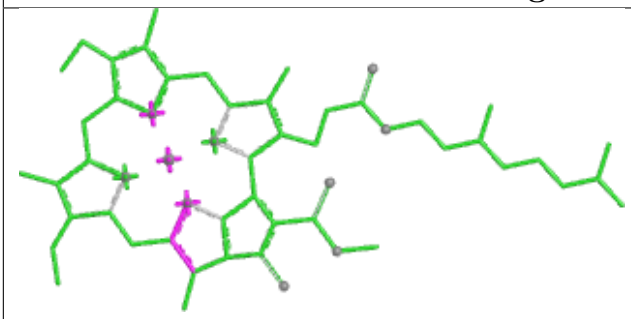


Rings

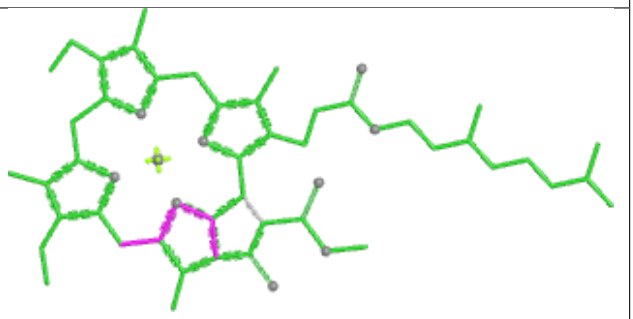
| Ligand CLA 3 609 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 52 602 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

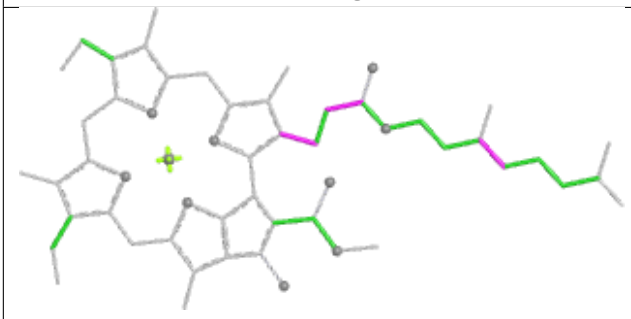
**Ligand CLA 5 604**



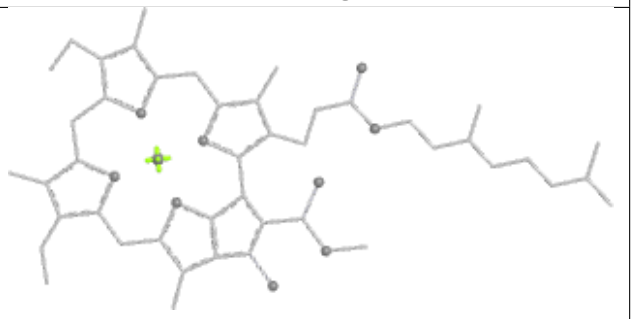
Bond lengths



Bond angles

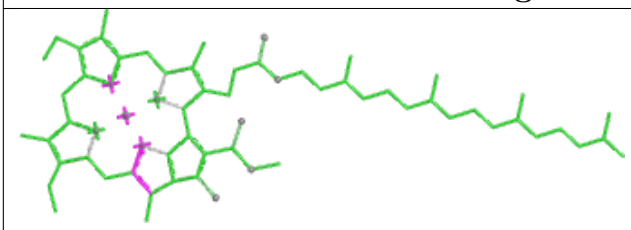


Torsions

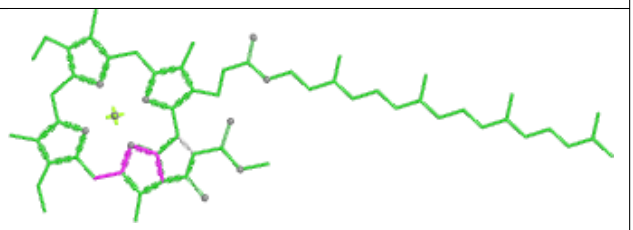


Rings

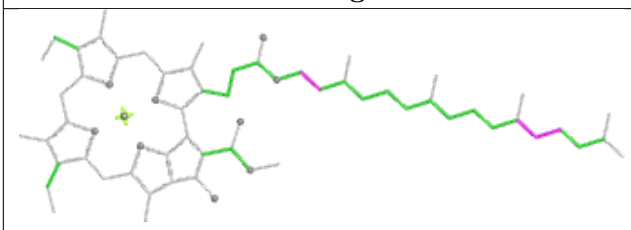
**Ligand CLA A2 816**



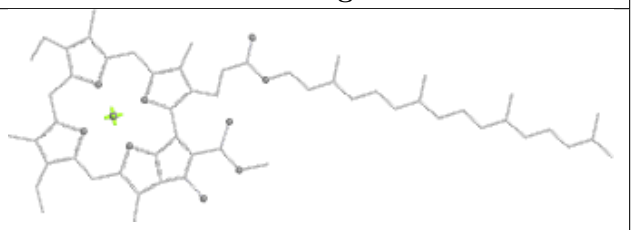
Bond lengths



Bond angles

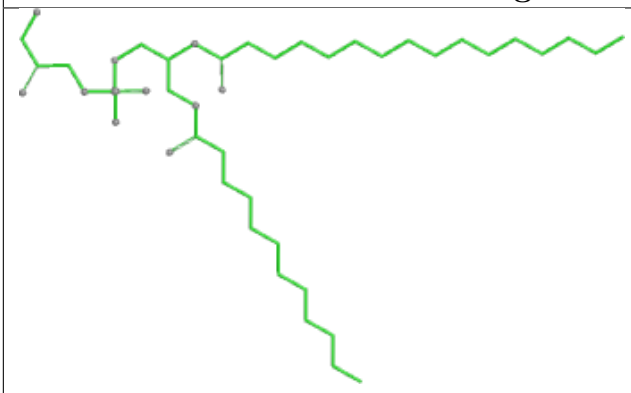


Torsions

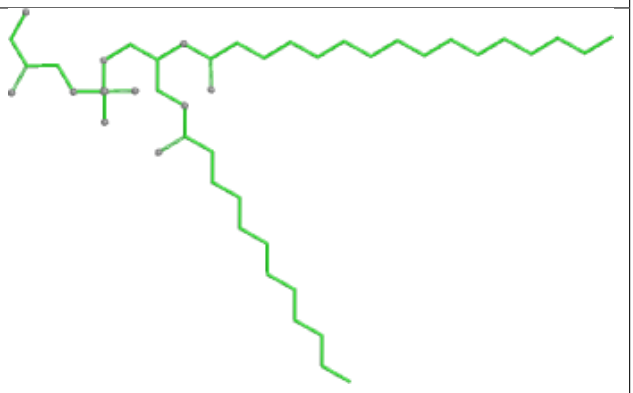


Rings

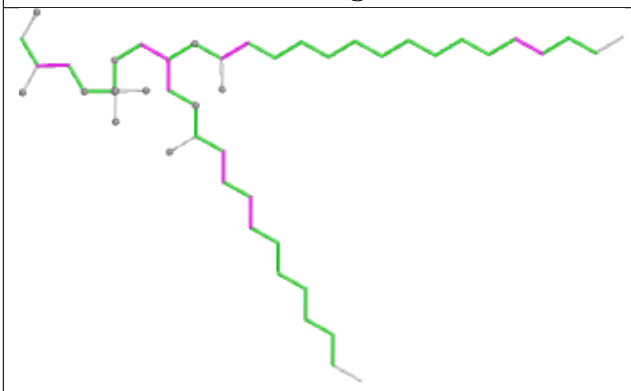
## Ligand LHG B2 851



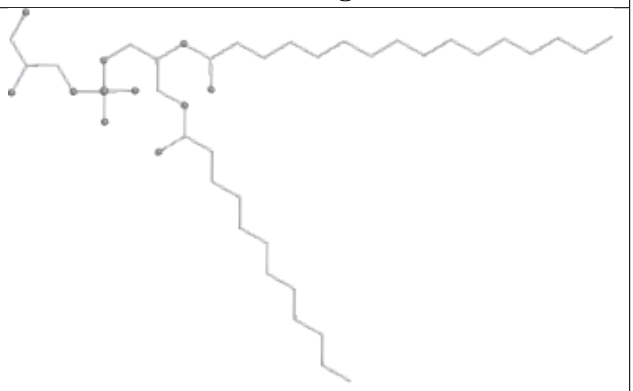
Bond lengths



Bond angles

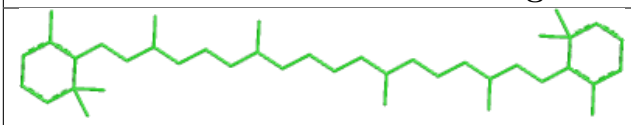


Torsions

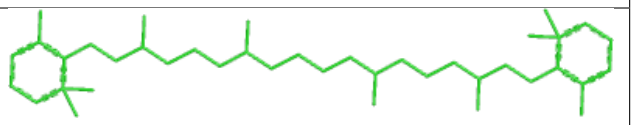


Rings

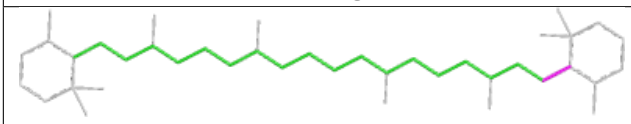
## Ligand BCR 5 622



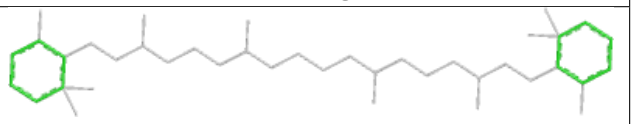
Bond lengths



Bond angles

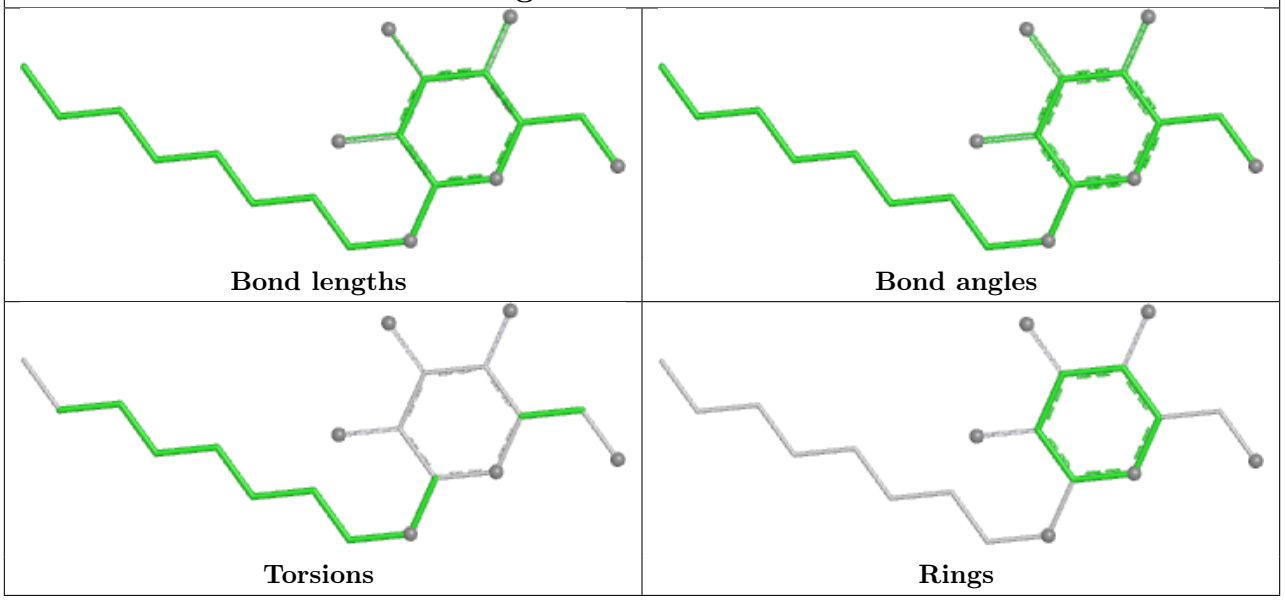


Torsions

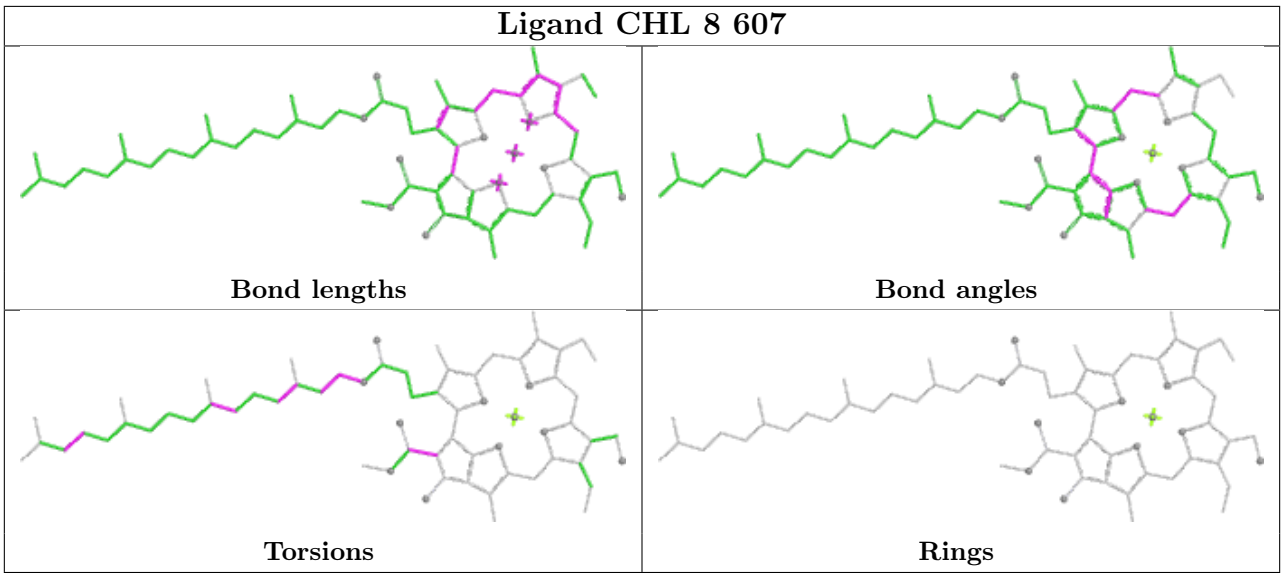


Rings

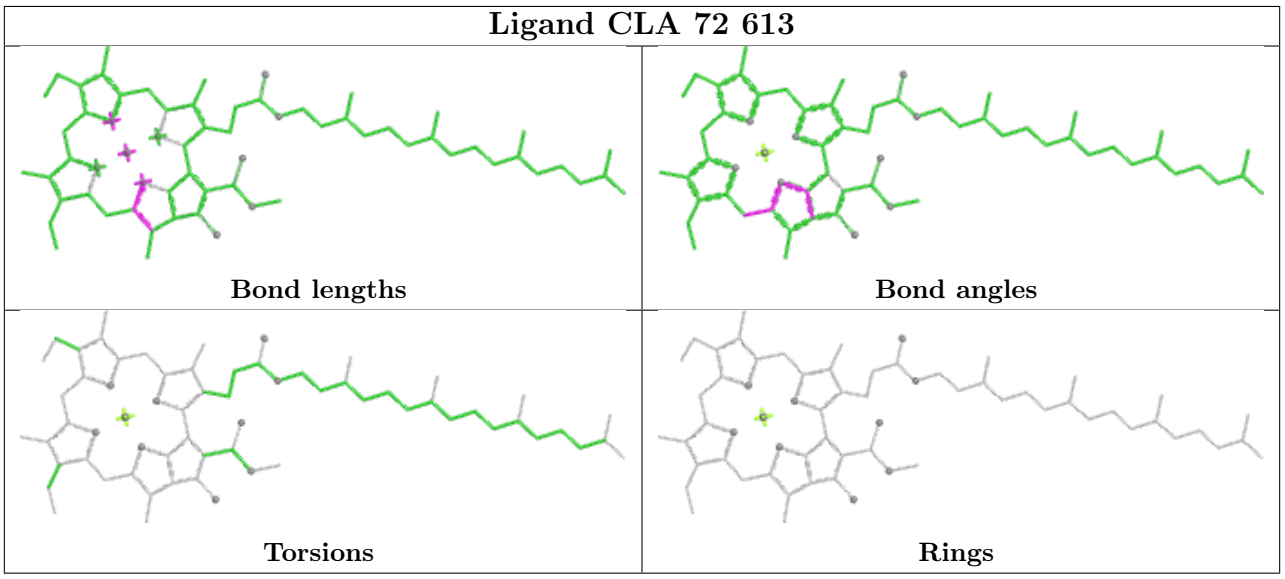
## Ligand LMU 42 626



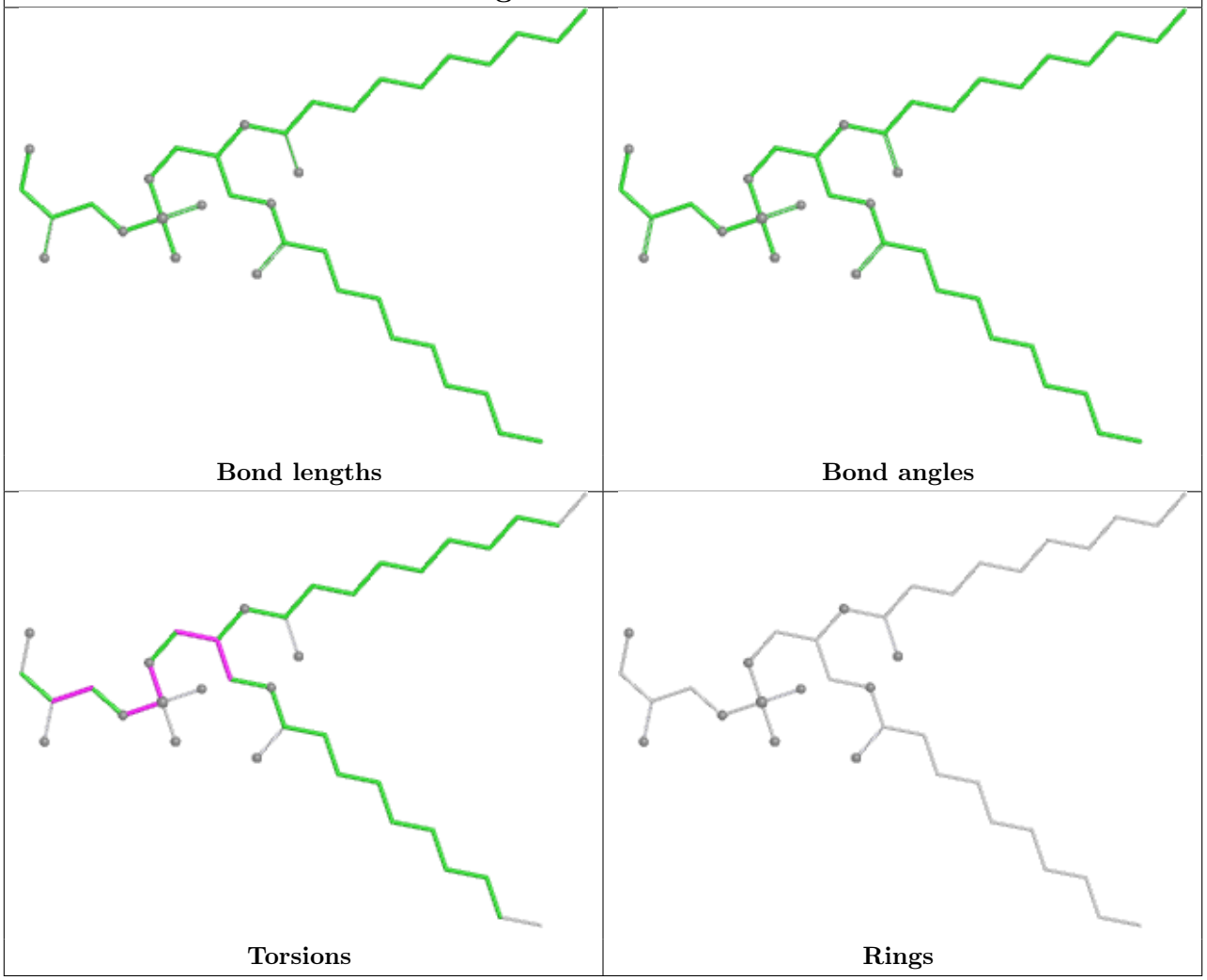

## Ligand CHL 8 607



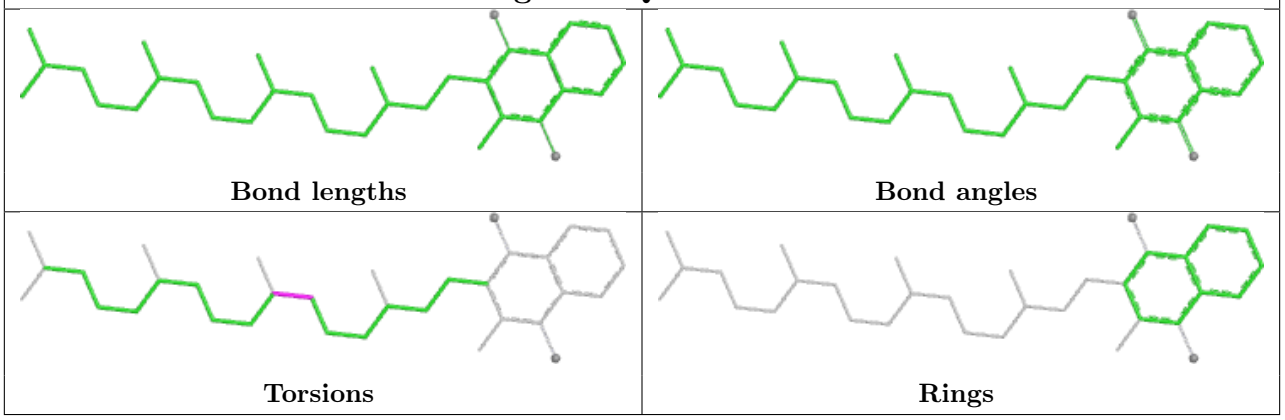

## Ligand CLA 72 613



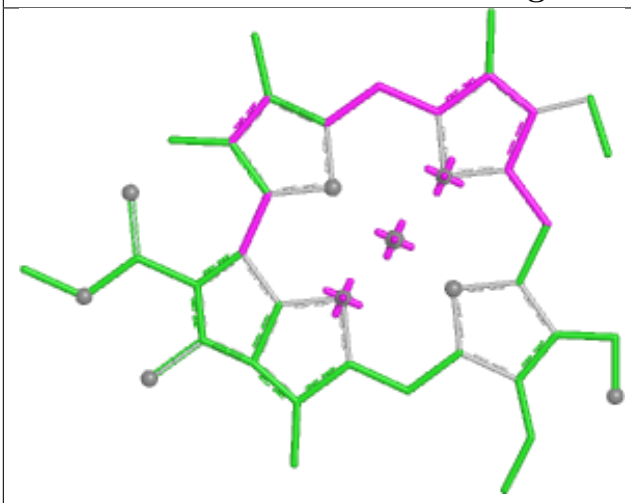
**Ligand LHG 5 623**




**Ligand PQN B2 842**



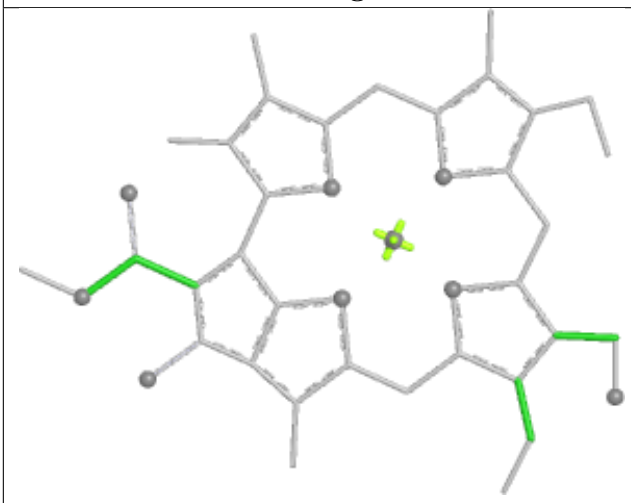
**Ligand CHL 9 606**



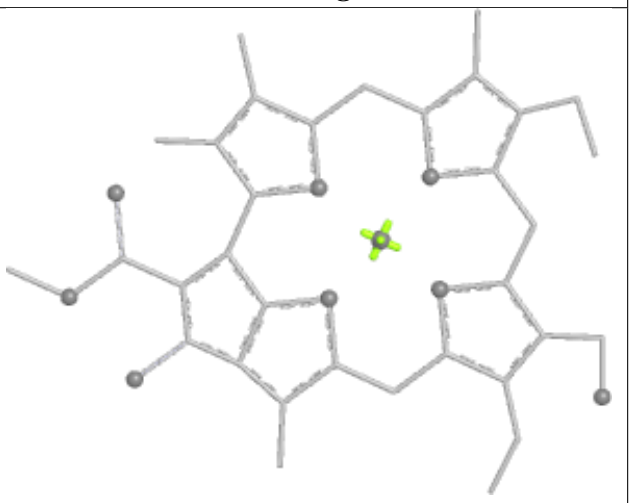
**Bond lengths**



**Bond angles**

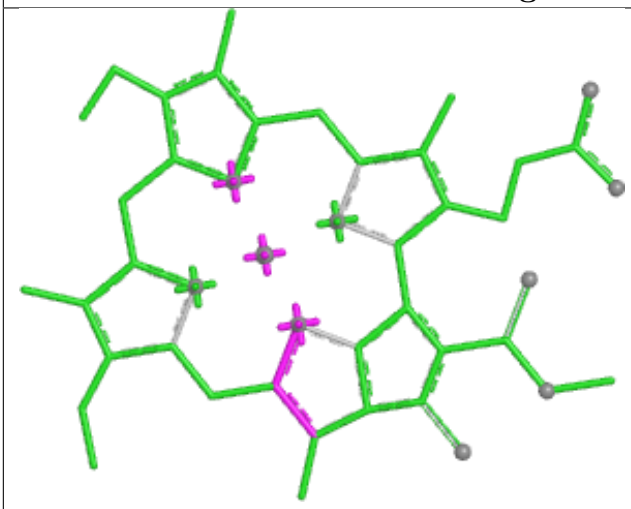


**Torsions**

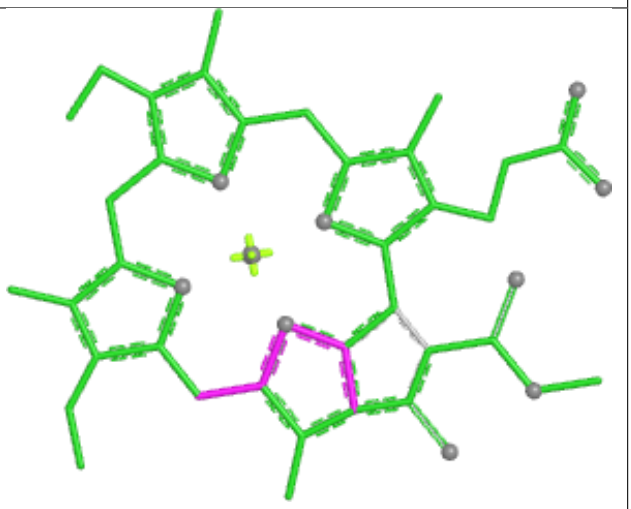


**Rings**

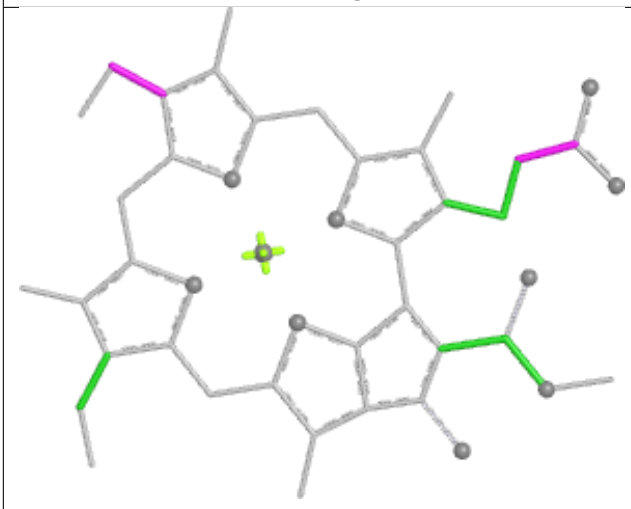
## Ligand CLA 52 614



Bond lengths



Bond angles

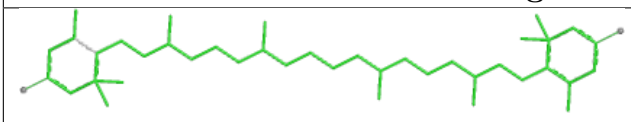


Torsions

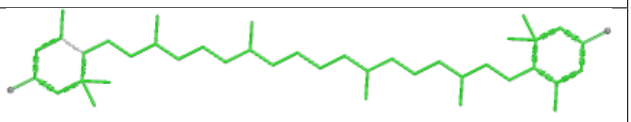


Rings

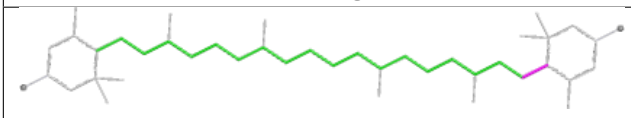
## Ligand LUT Z 617



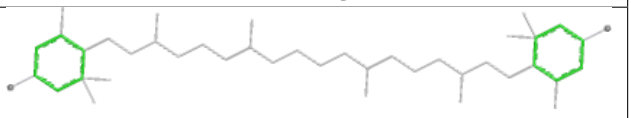
Bond lengths



Bond angles

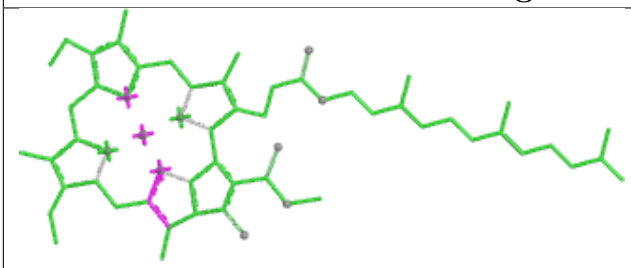


Torsions

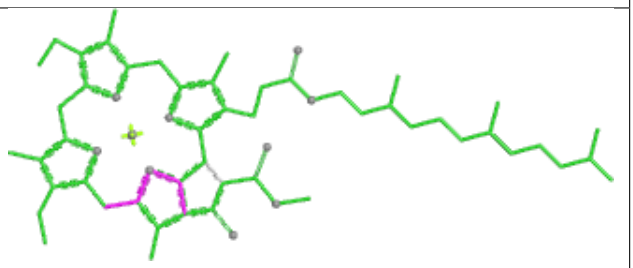


Rings

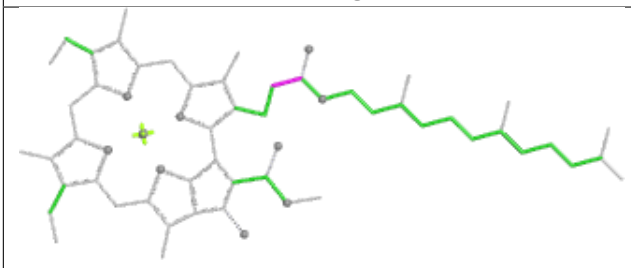
**Ligand CLA B2 814**



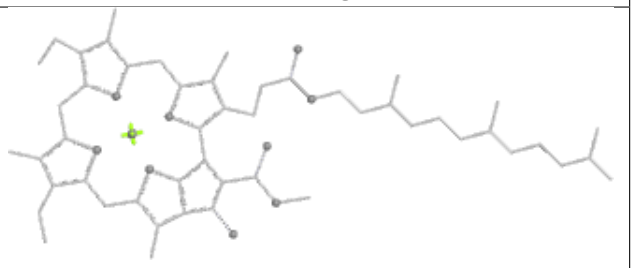
Bond lengths



Bond angles

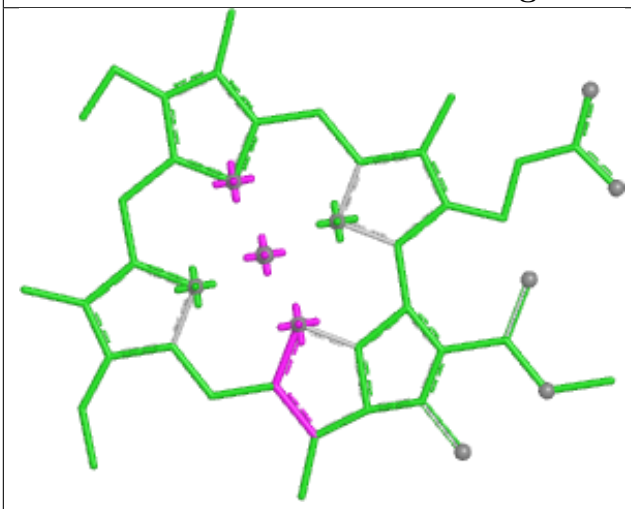


Torsions

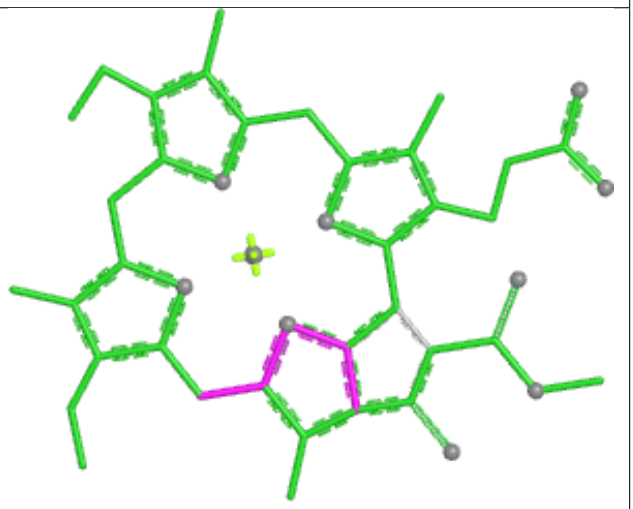


Rings

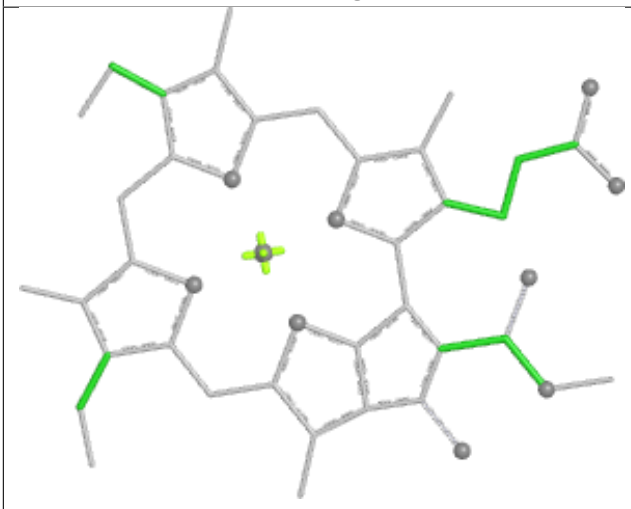
**Ligand CLA 42 616**



Bond lengths



Bond angles

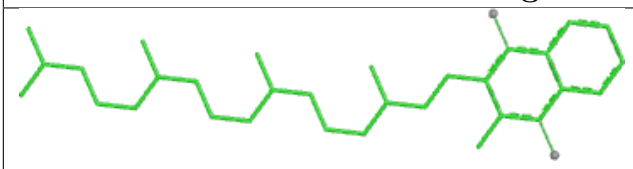


Torsions

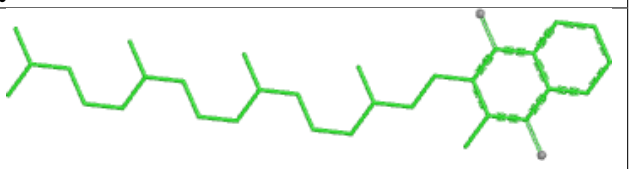


Rings

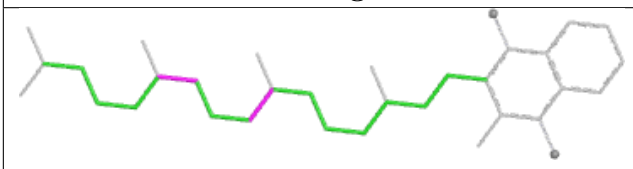
## Ligand PQN A 844



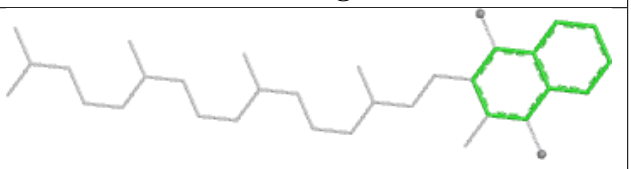
Bond lengths



Bond angles

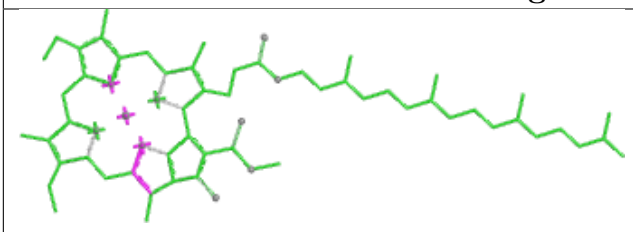


Torsions

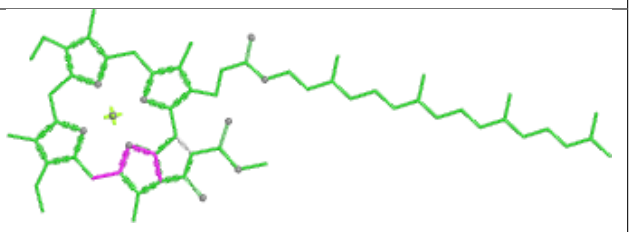


Rings

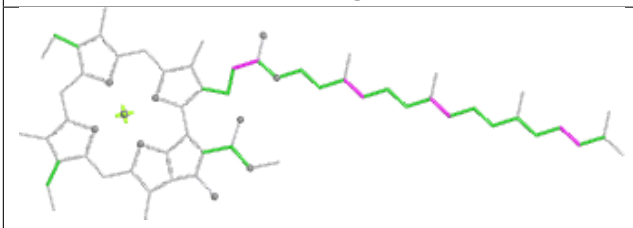
## Ligand CLA 1 609



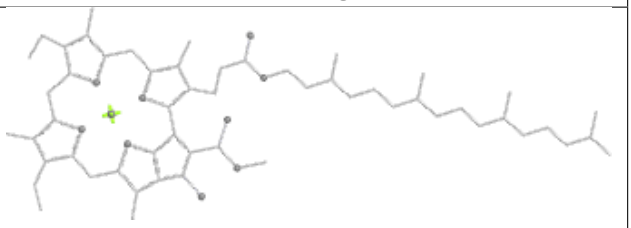
Bond lengths



Bond angles

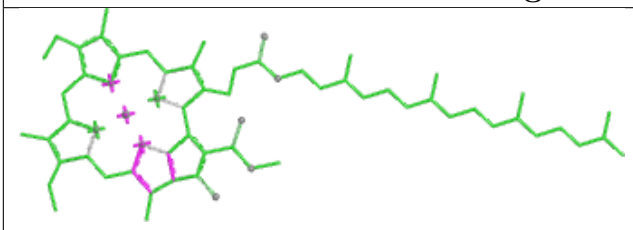


Torsions

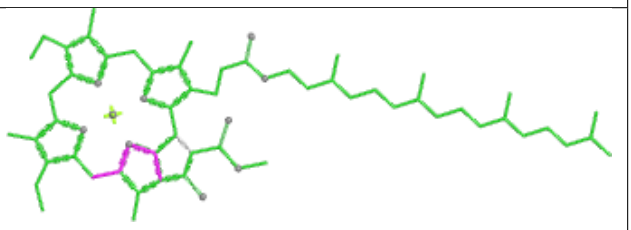


Rings

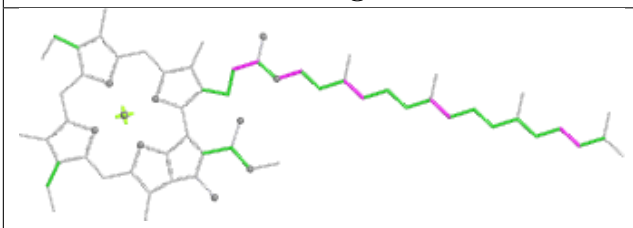
## Ligand CLA B 811



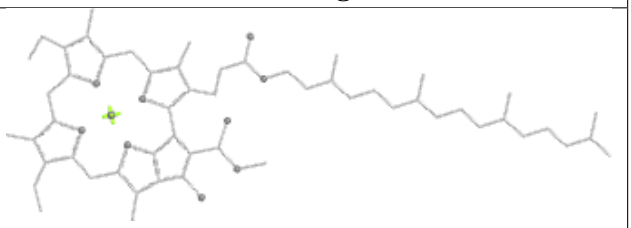
Bond lengths



Bond angles

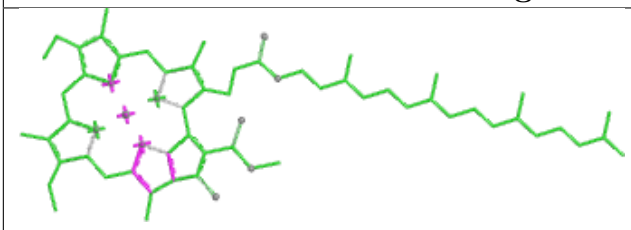


Torsions

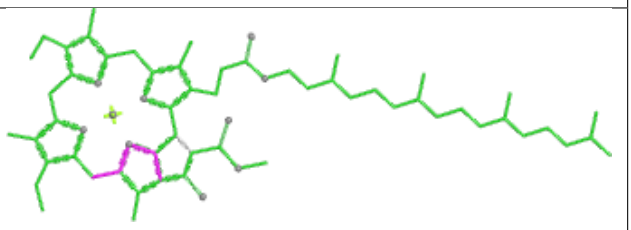


Rings

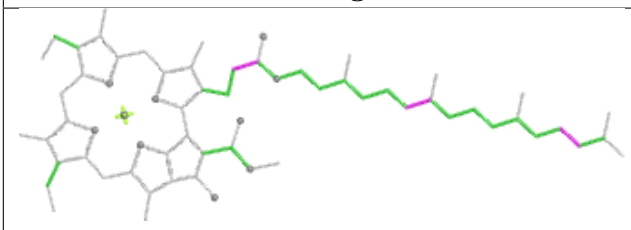
## Ligand CLA A2 813



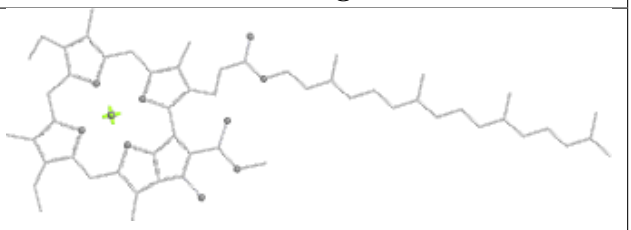
Bond lengths



Bond angles

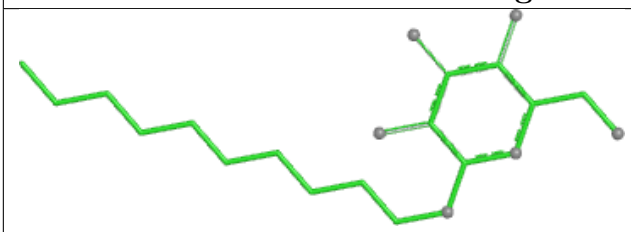


Torsions

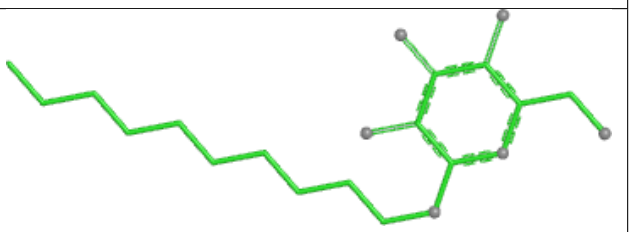


Rings

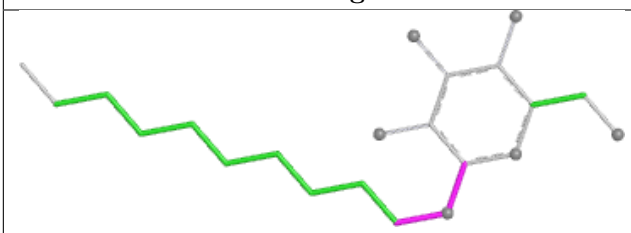
## Ligand LMU 72 628



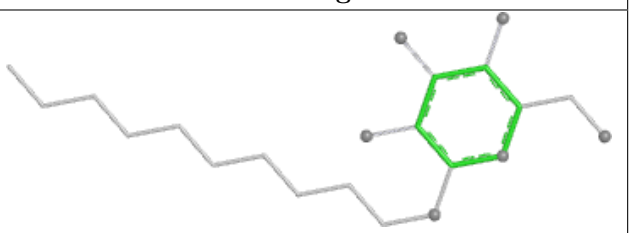
Bond lengths



Bond angles

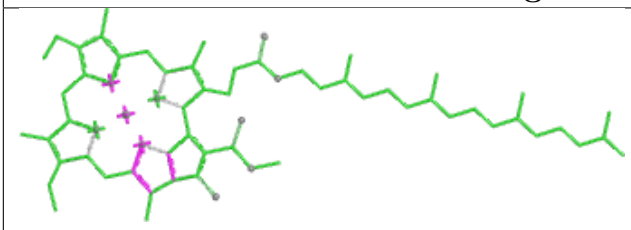


Torsions

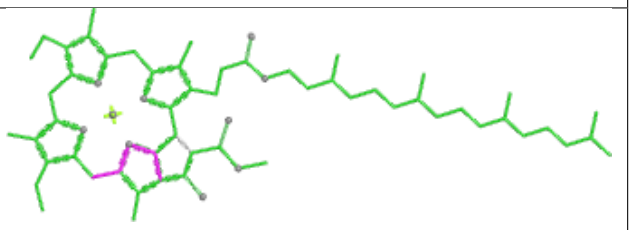


Rings

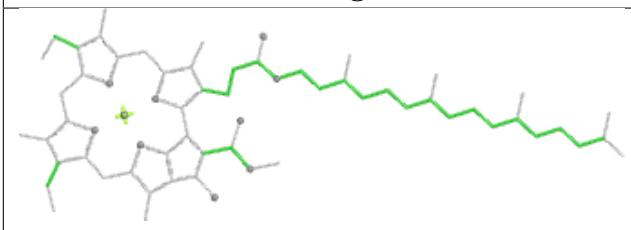
## Ligand CLA B 837



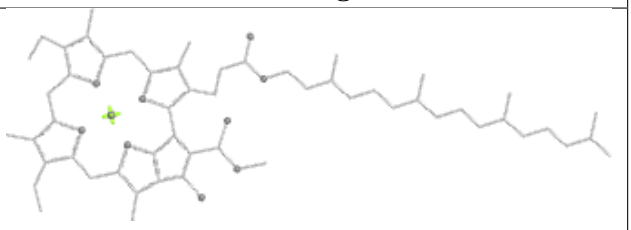
Bond lengths



Bond angles

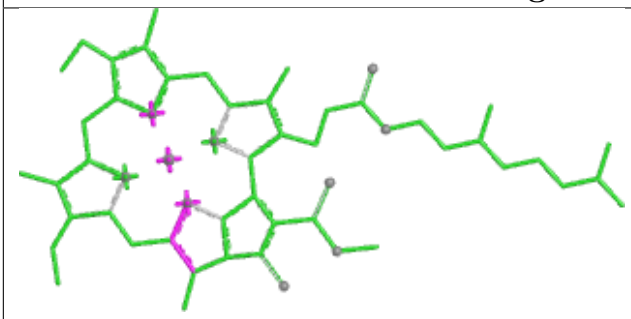


Torsions

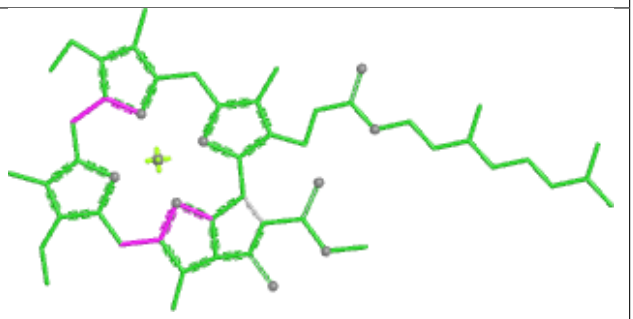


Rings

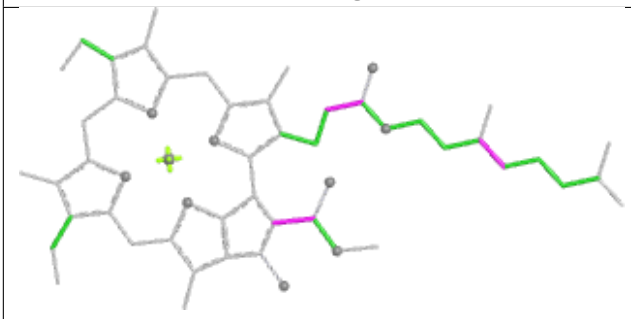
**Ligand CLA 8 612**



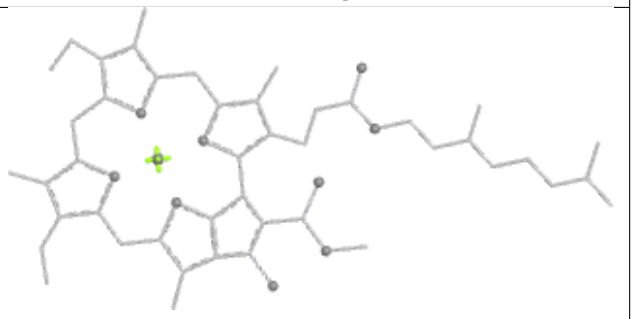
**Bond lengths**



**Bond angles**

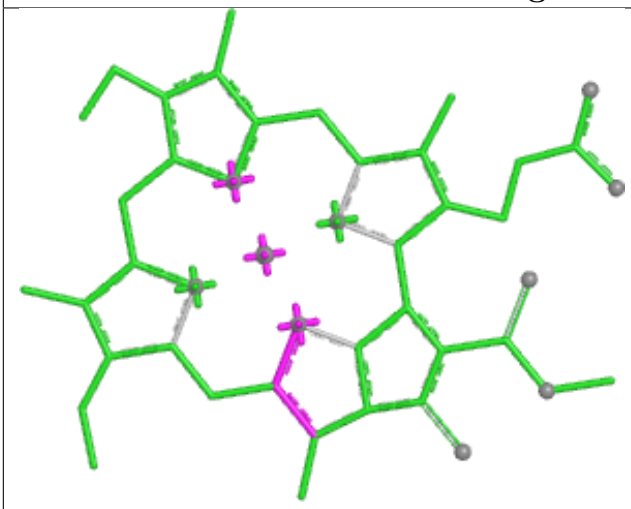


**Torsions**

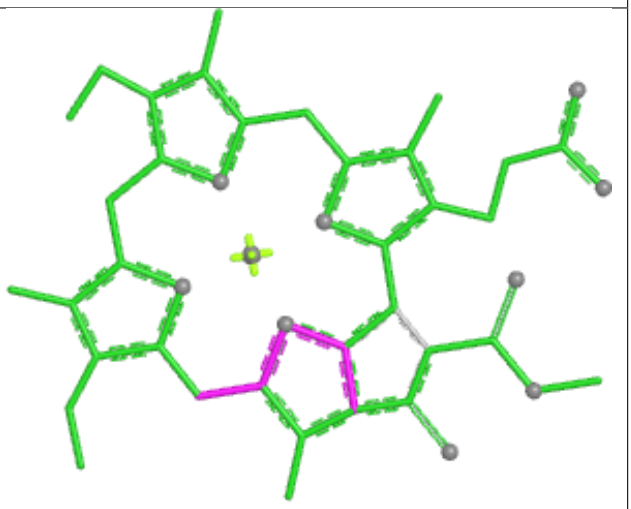


**Rings**

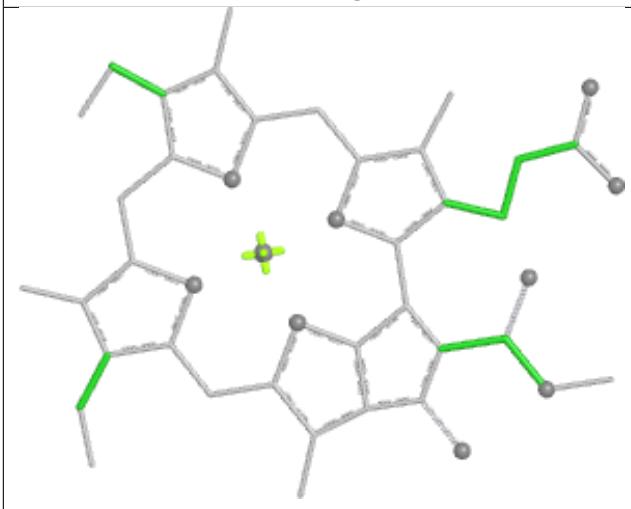
**Ligand CLA 4 616**



**Bond lengths**



**Bond angles**

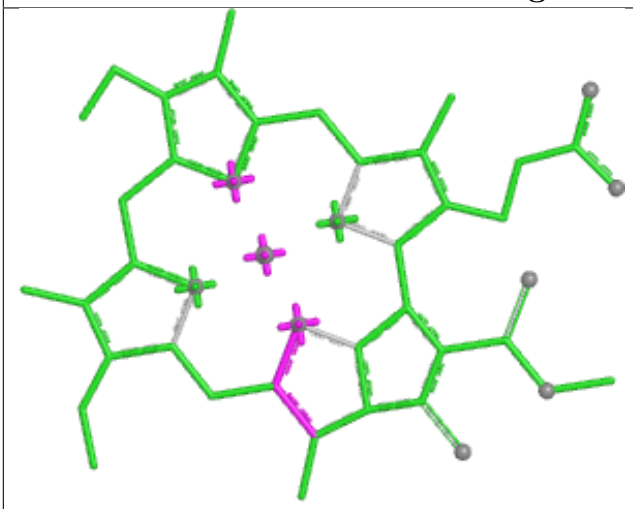


**Torsions**

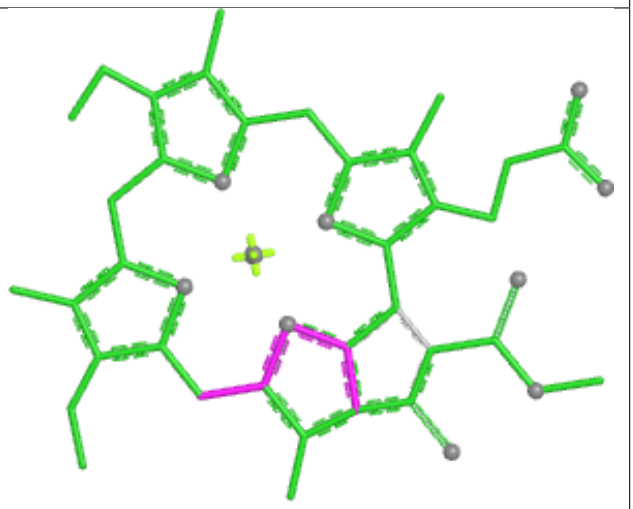


**Rings**

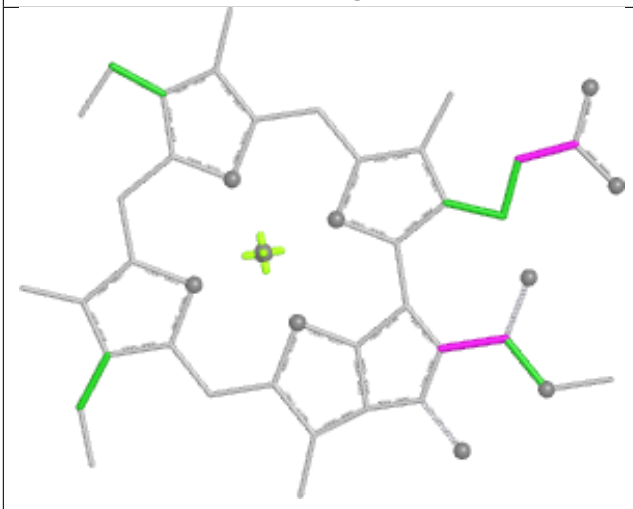
## Ligand CLA 4 612



Bond lengths



Bond angles

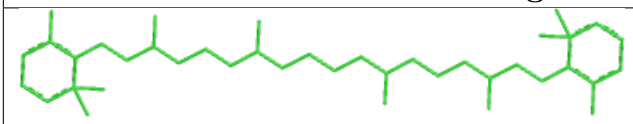


Torsions

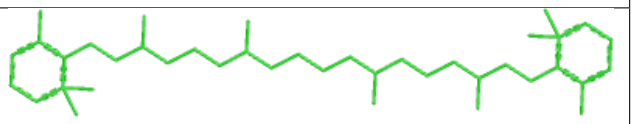


Rings

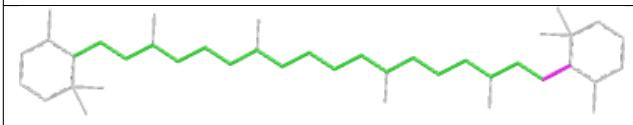
## Ligand BCR 9 623



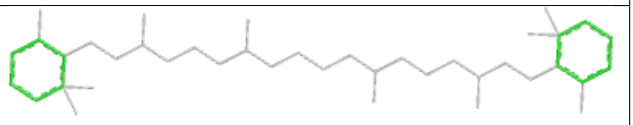
Bond lengths



Bond angles

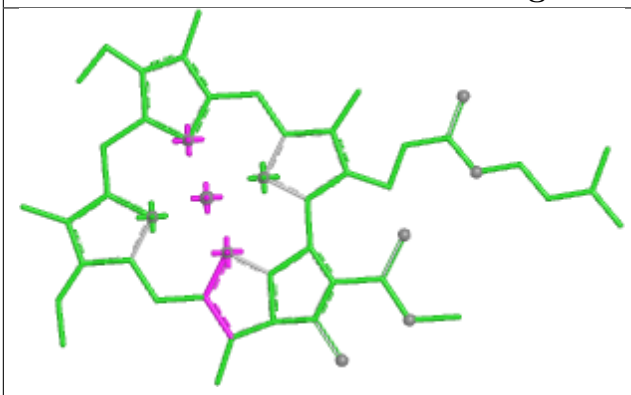


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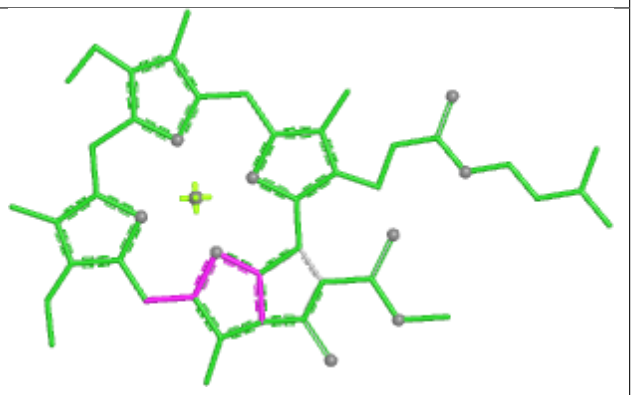


Rings

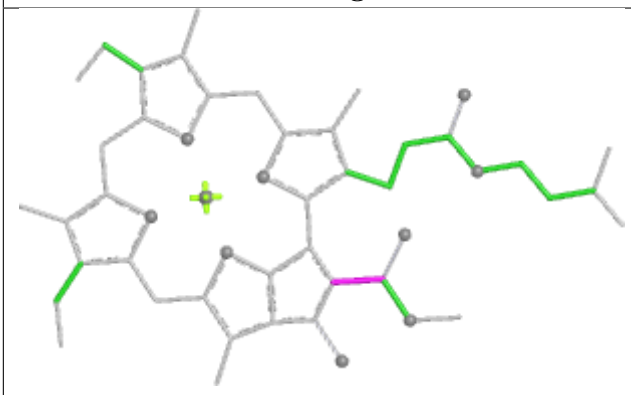
## Ligand CLA 4 604



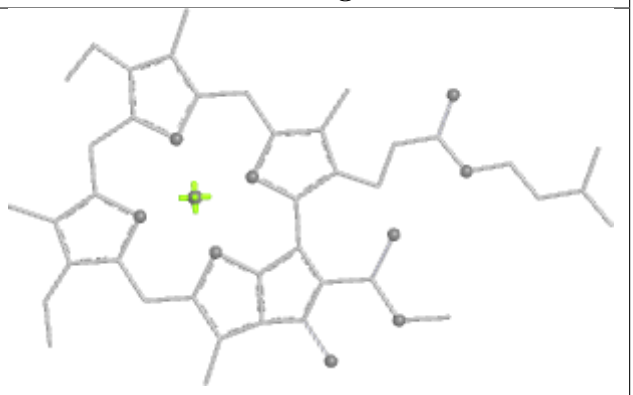
Bond lengths



Bond angles



Torsions

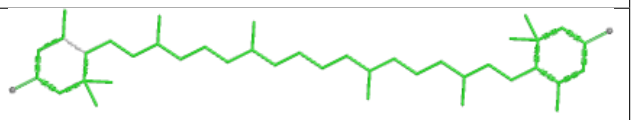


Rings

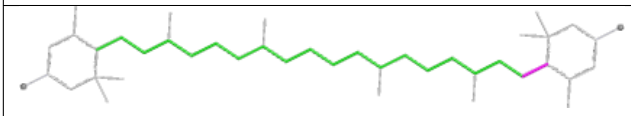
## Ligand LUT 32 622



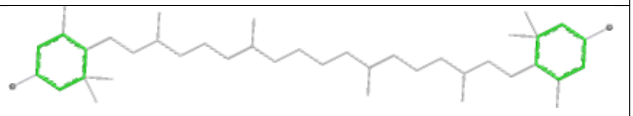
Bond lengths



Bond angles

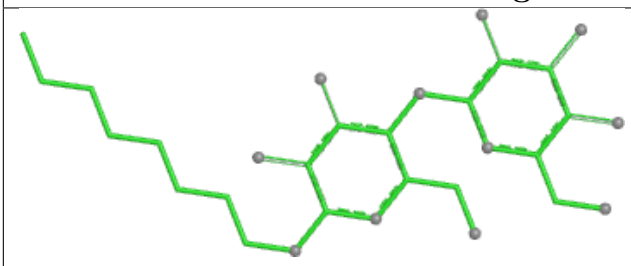


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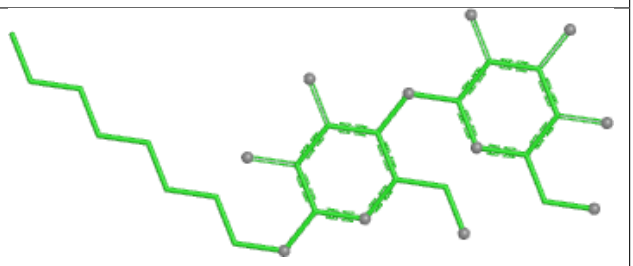


Rings

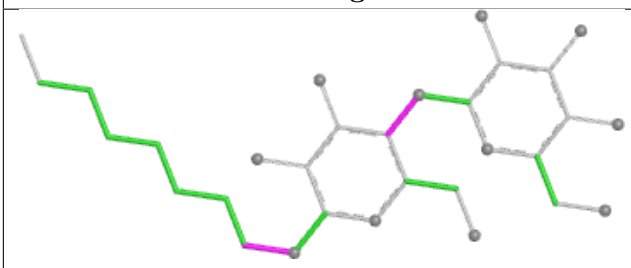
## Ligand LMU Z2 622



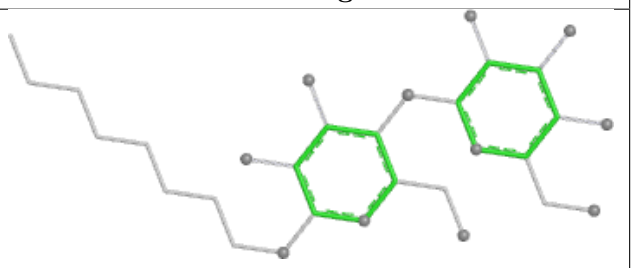
Bond lengths



Bond angles

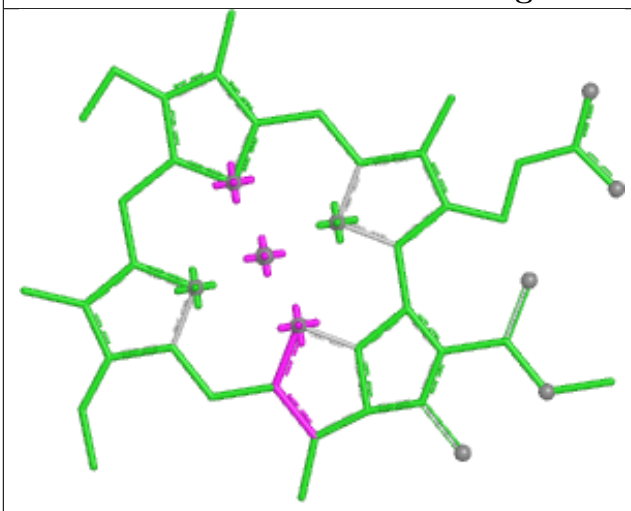


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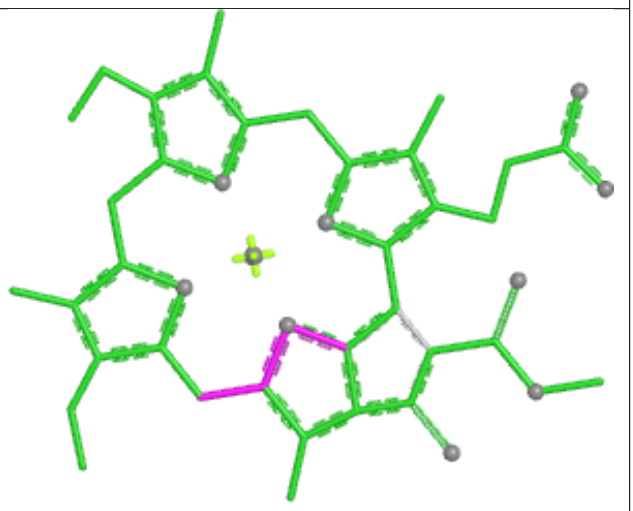


Rings

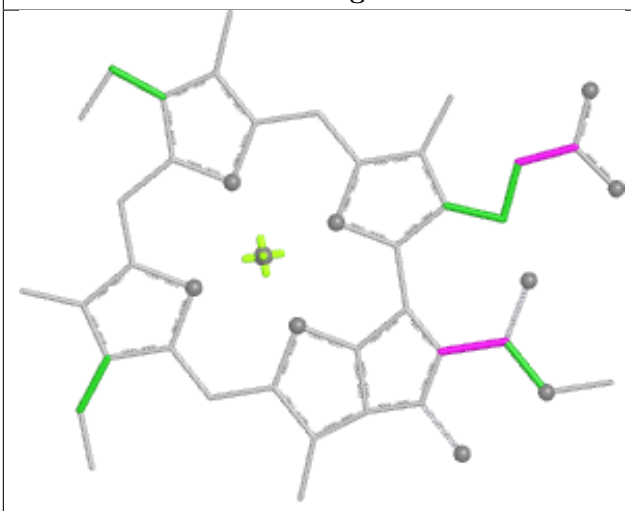
## Ligand CLA B2 804



Bond lengths



Bond angles

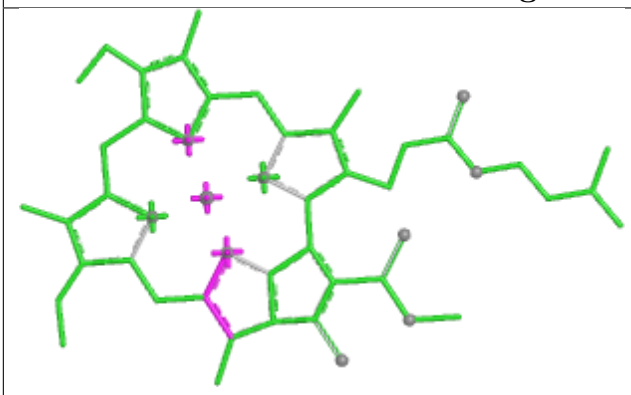


Torsions

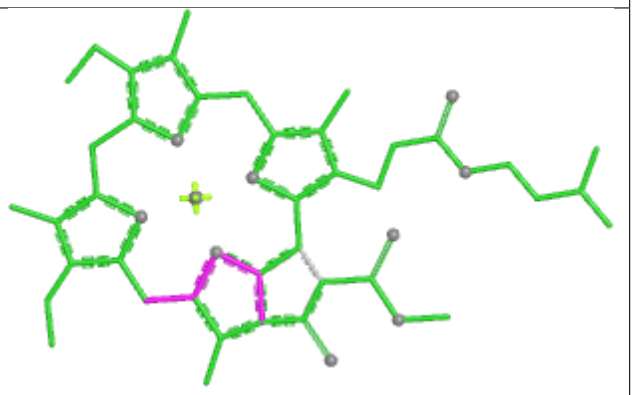


Rings

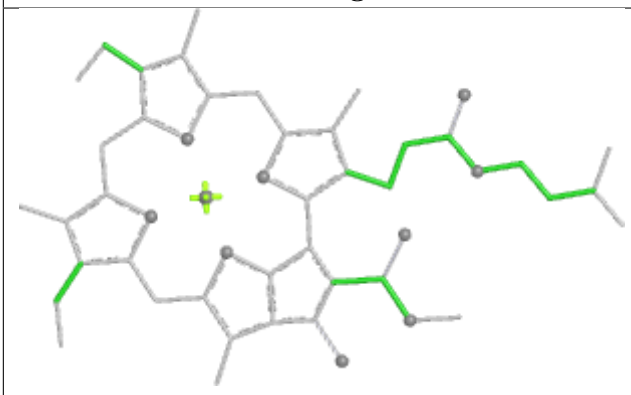
## Ligand CLA 72 608



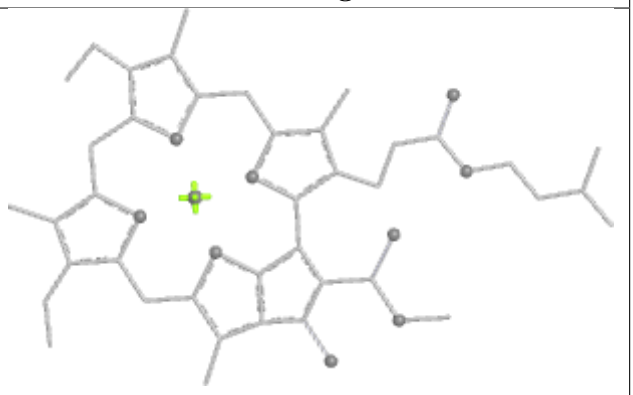
Bond lengths



Bond angles

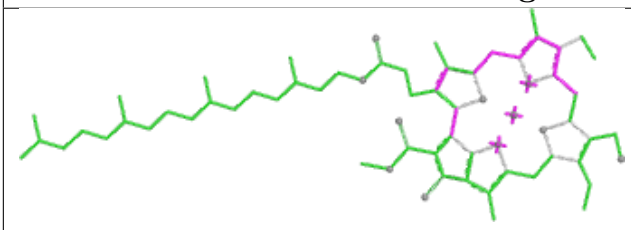


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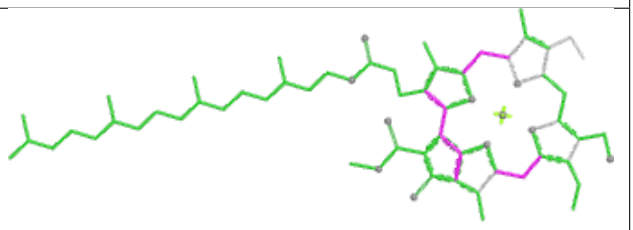


Rings

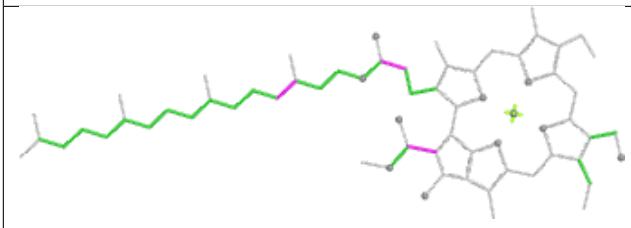
## Ligand CHL 62 601



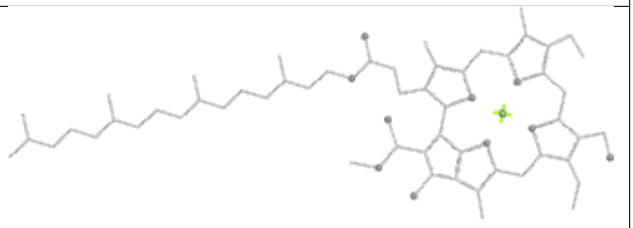
Bond lengths



Bond angles

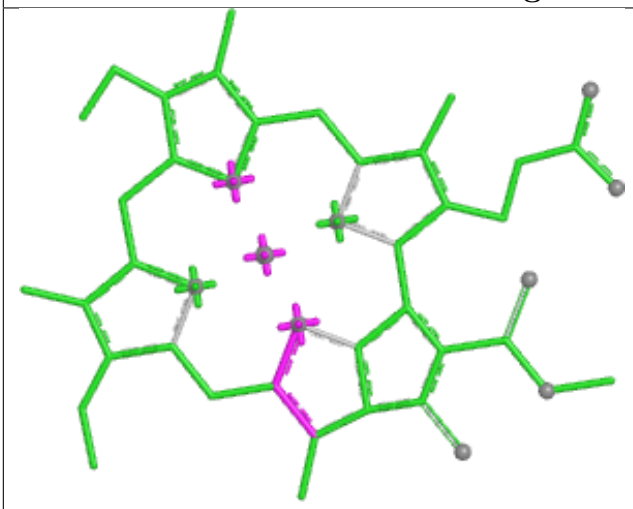


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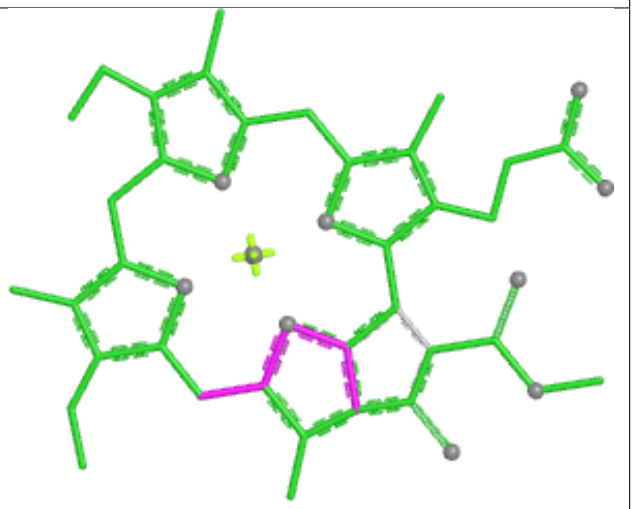


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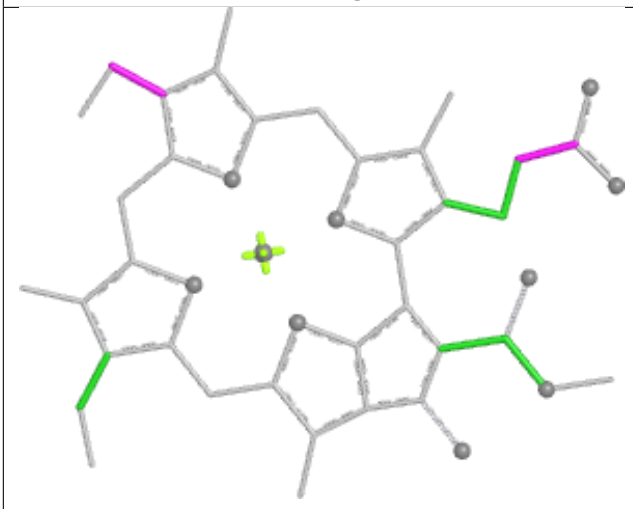
## Ligand CLA A 824



Bond lengths



Bond angles

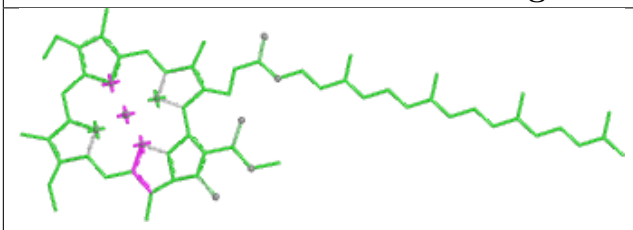


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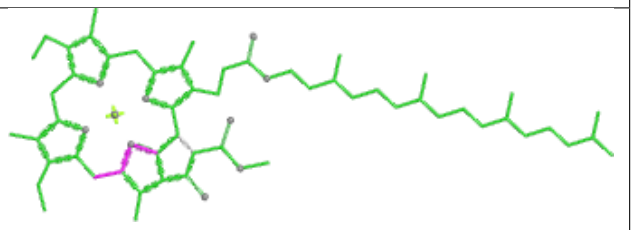


Rings

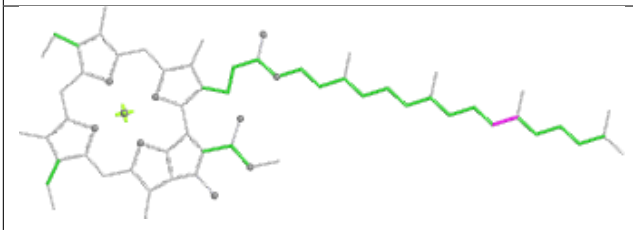
## Ligand CLA 8 610



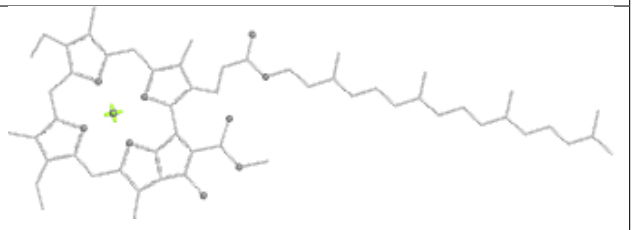
Bond lengths



Bond angles

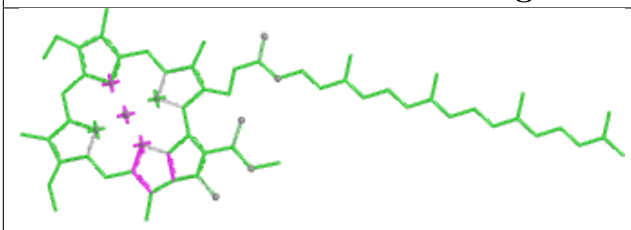


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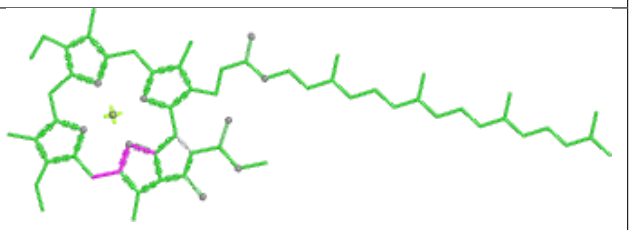


Rings

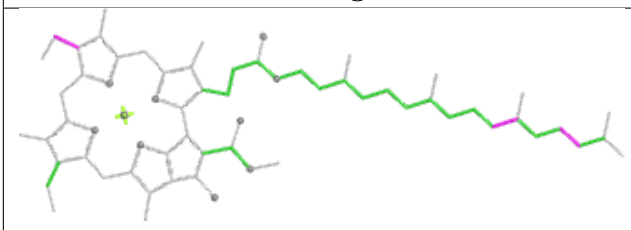
## Ligand CLA B2 832



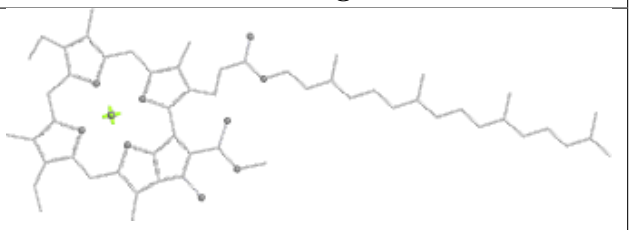
Bond lengths



Bond angles

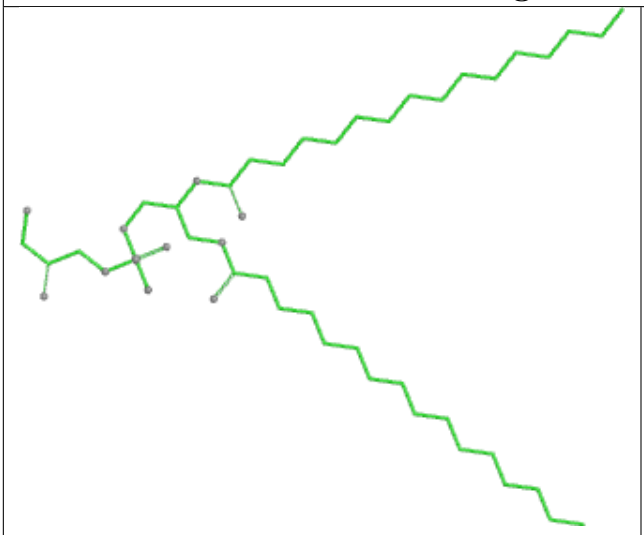


Torsions

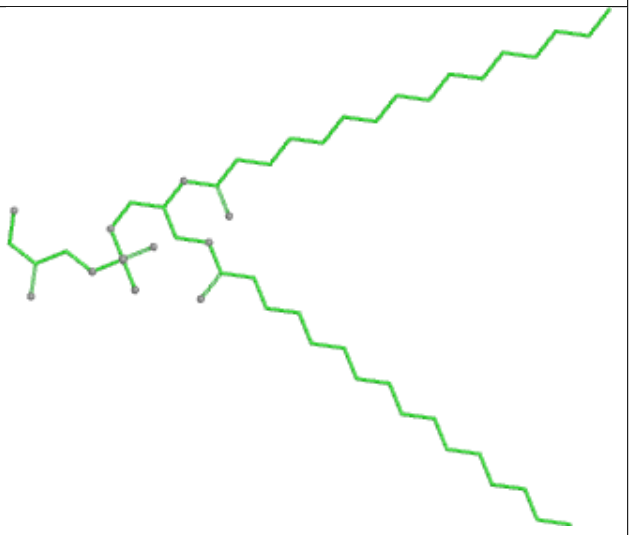


Rings

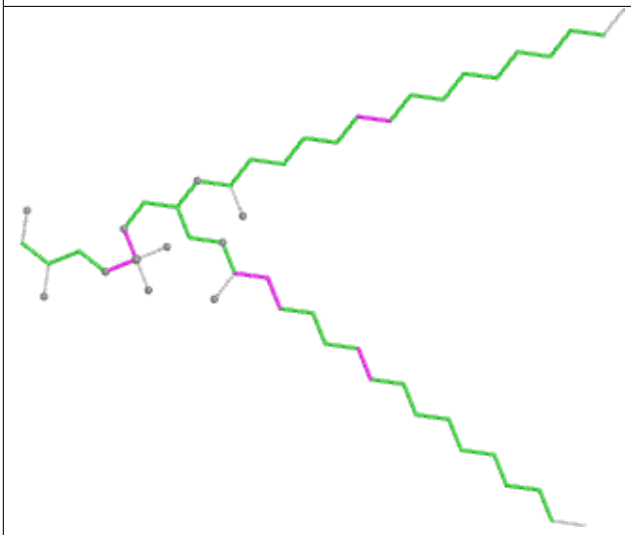
## Ligand LHG A2 846



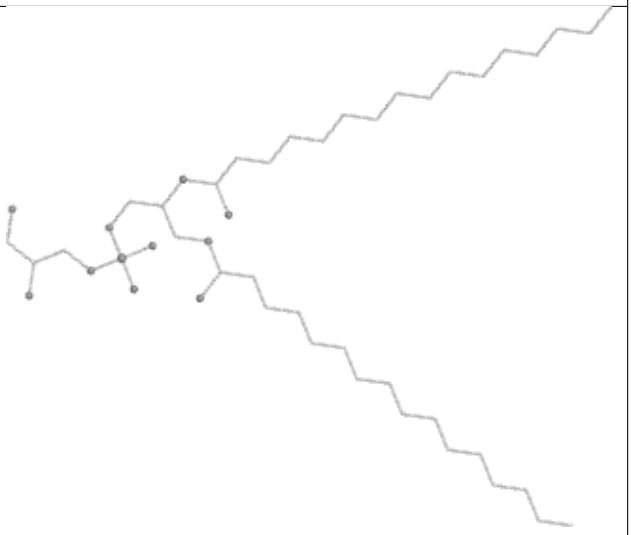
Bond lengths



Bond angles

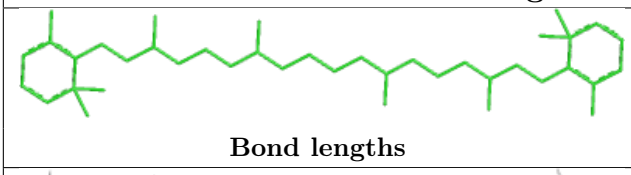


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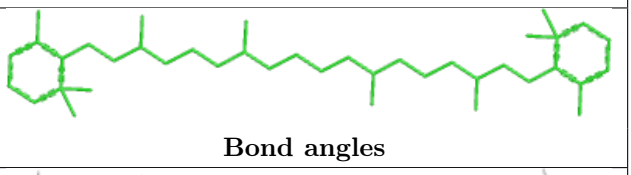


Rings

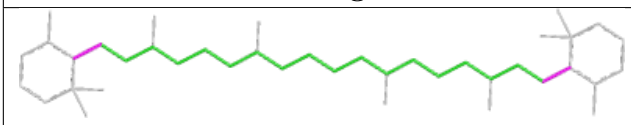
## Ligand BCR 8 619



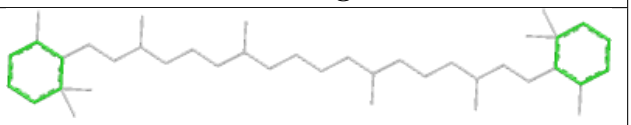
Bond lengths



Bond angles

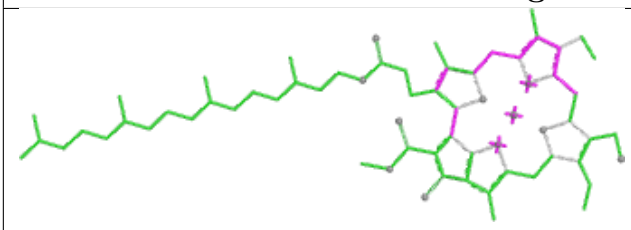


Torsions

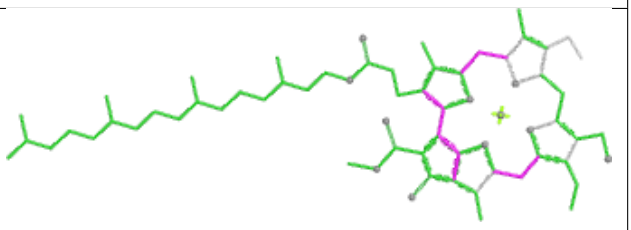


Rings

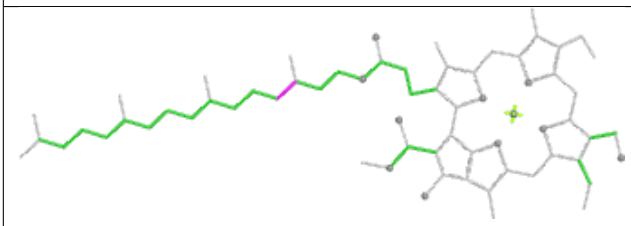
## Ligand CHL 8 606



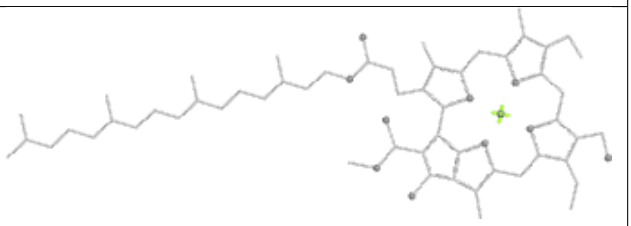
Bond lengths



Bond angles

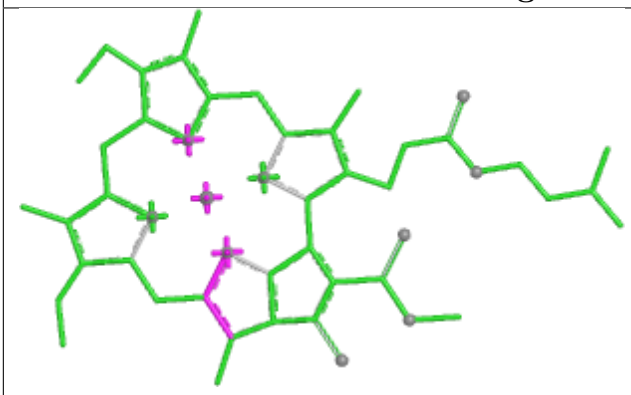


Torsions

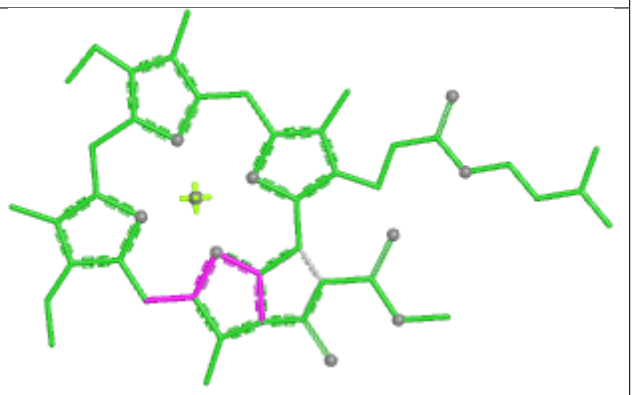


Rings

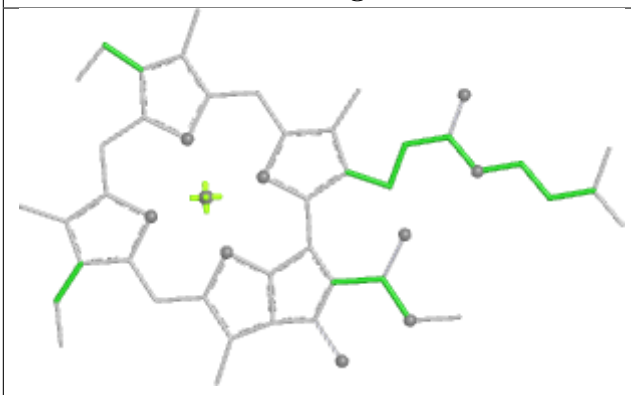
## Ligand CLA Z2 614



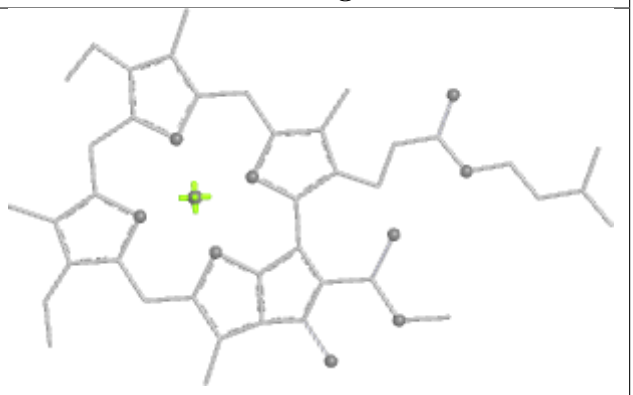
Bond lengths



Bond angles



Torsions

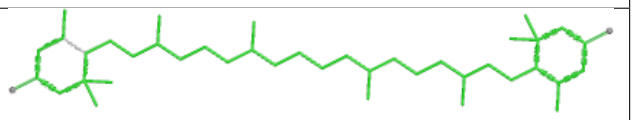


Rings

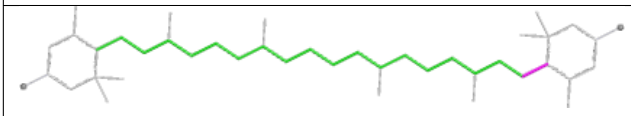
## Ligand LUT 6 621



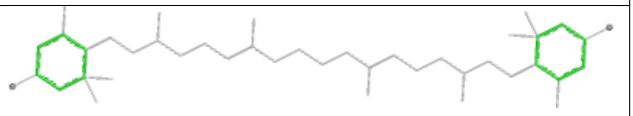
Bond lengths



Bond angles

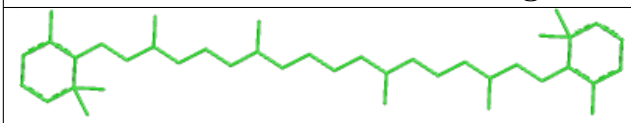


Torsions

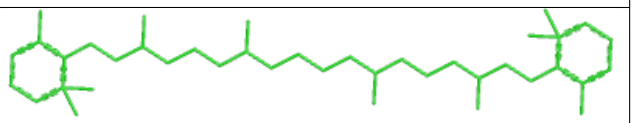


Rings

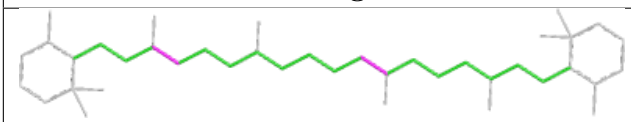
## Ligand BCR A 852



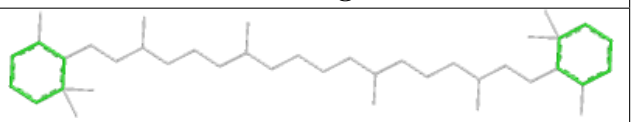
Bond lengths



Bond angles

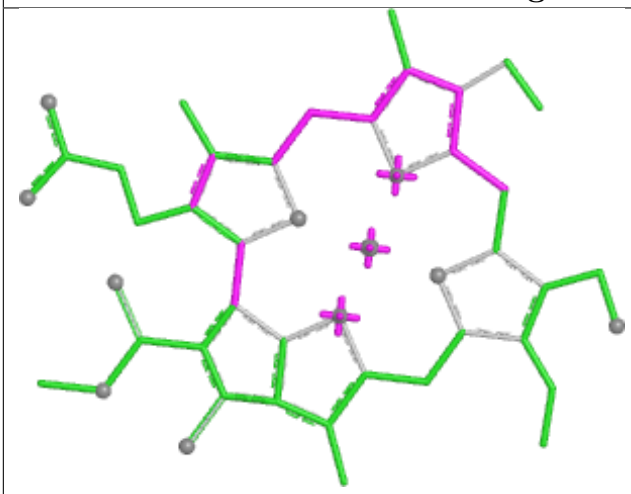


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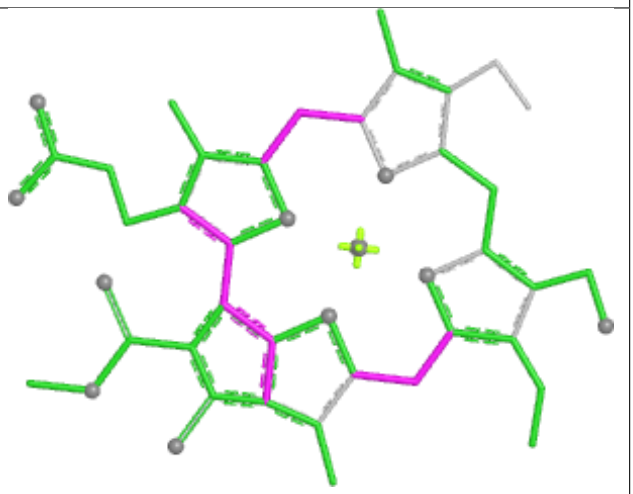


Rings

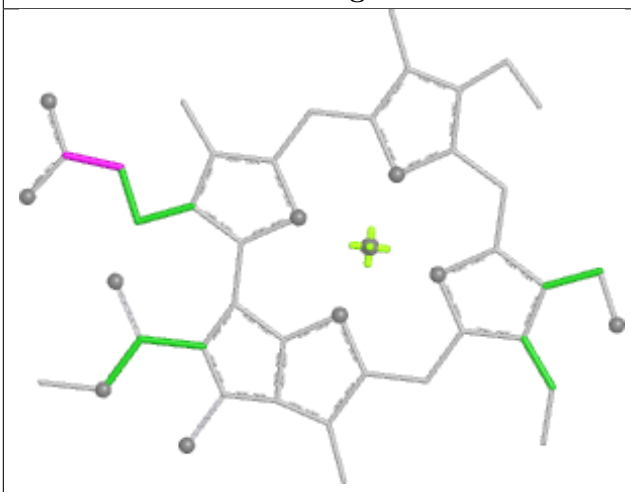
## Ligand CHL 7 607



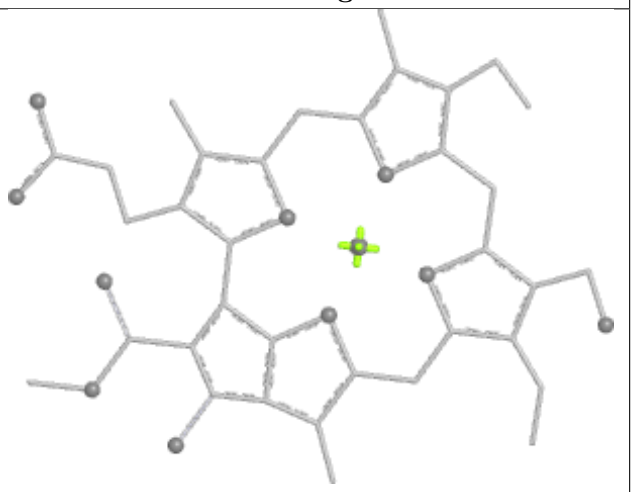
Bond lengths



Bond angles

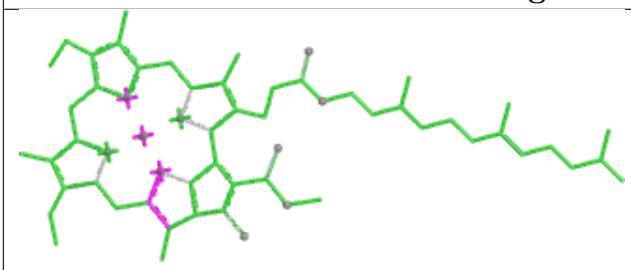


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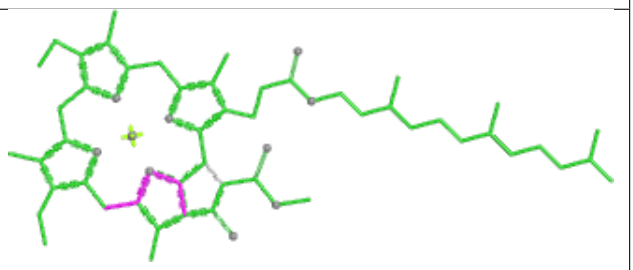


Rings

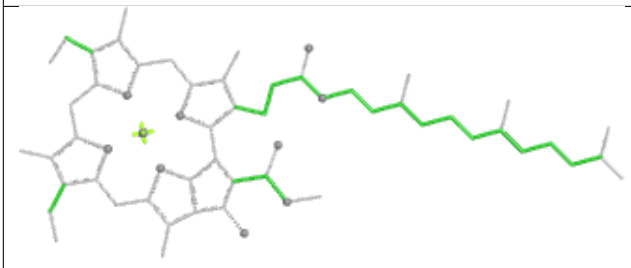
## Ligand CLA 6 610



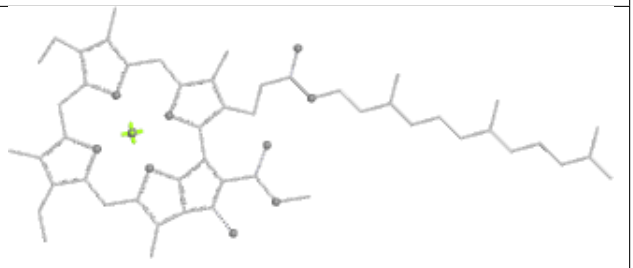
Bond lengths



Bond angles

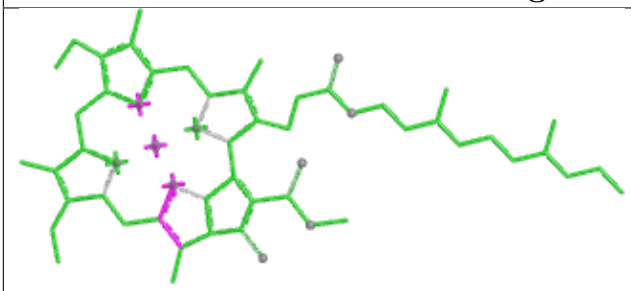


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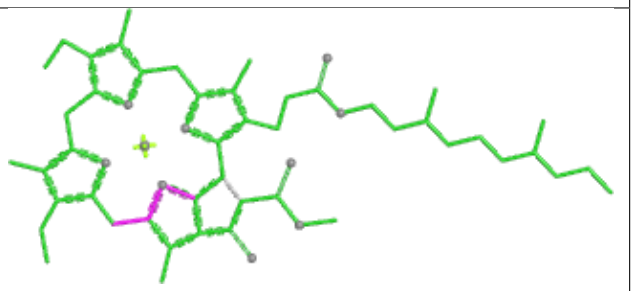


Rings

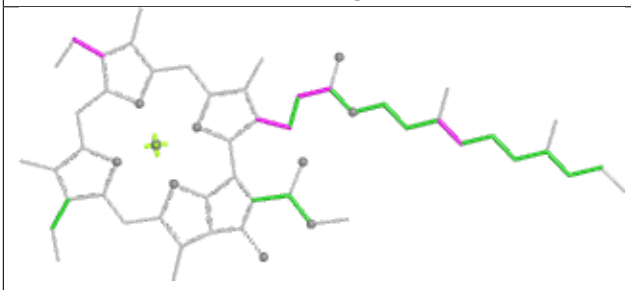
## Ligand CLA 8 614



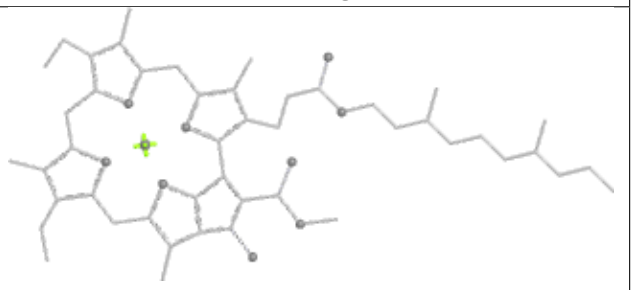
Bond lengths



Bond angles

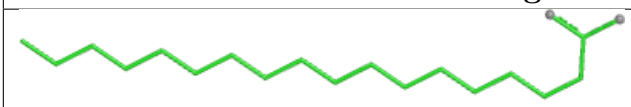


Torsions

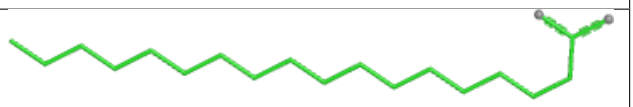


Rings

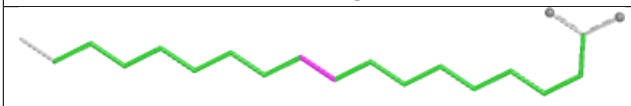
## Ligand LMG 6 633



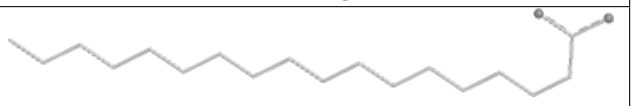
Bond lengths



Bond angles

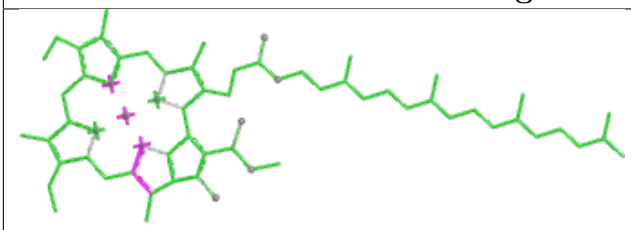


Torsions

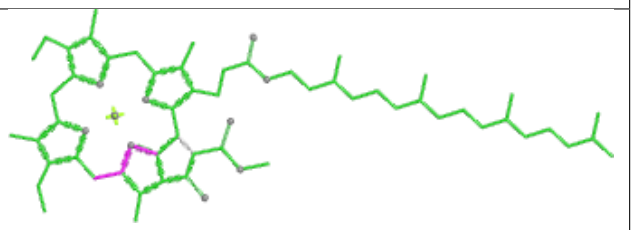


Rings

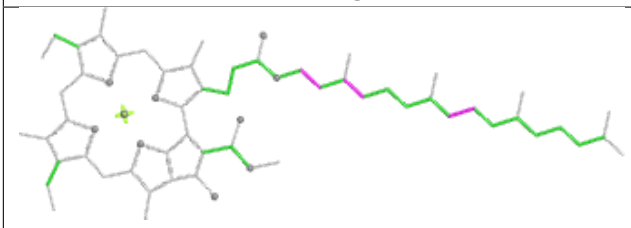
## Ligand CLA B2 824



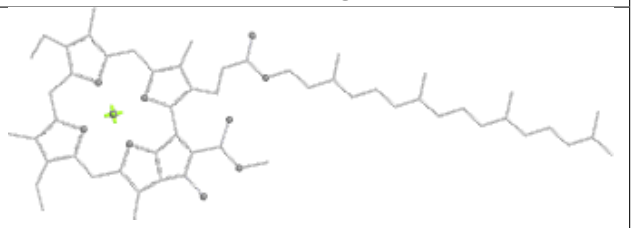
Bond lengths



Bond angles

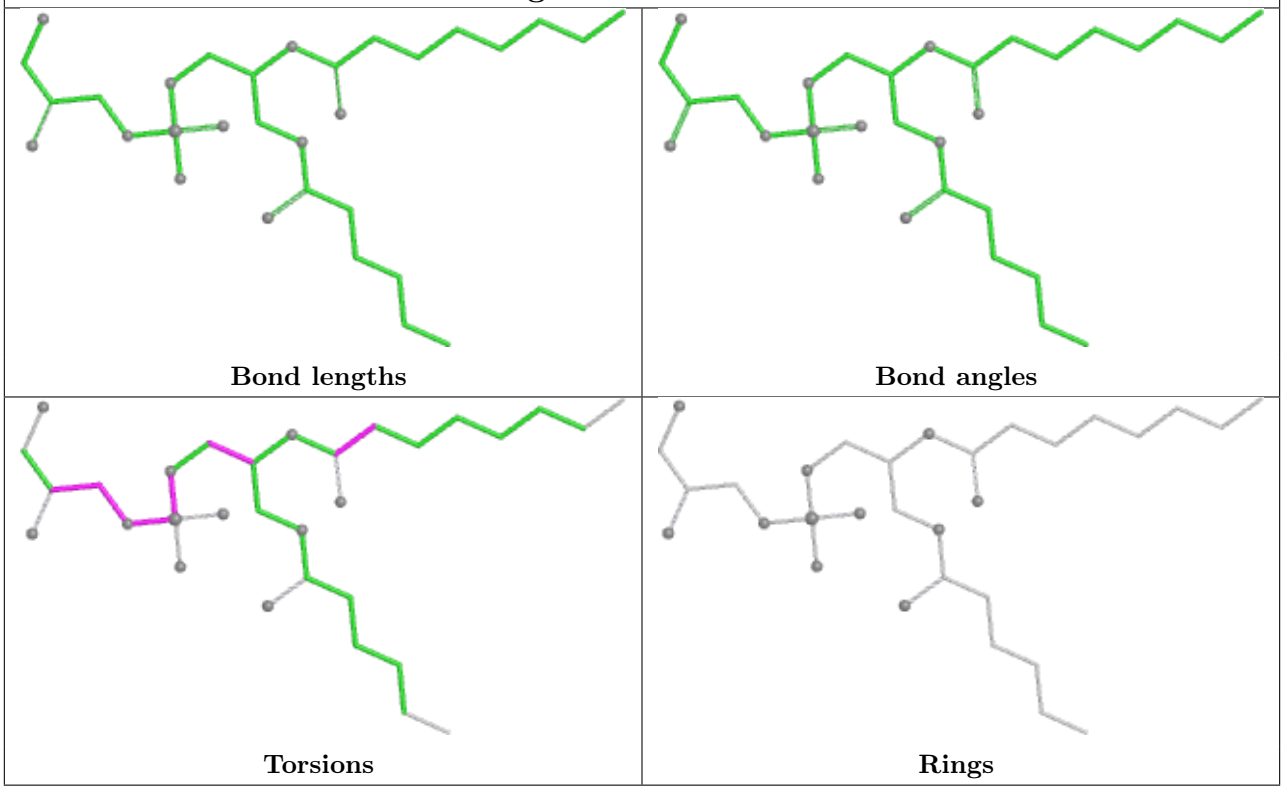


Torsions

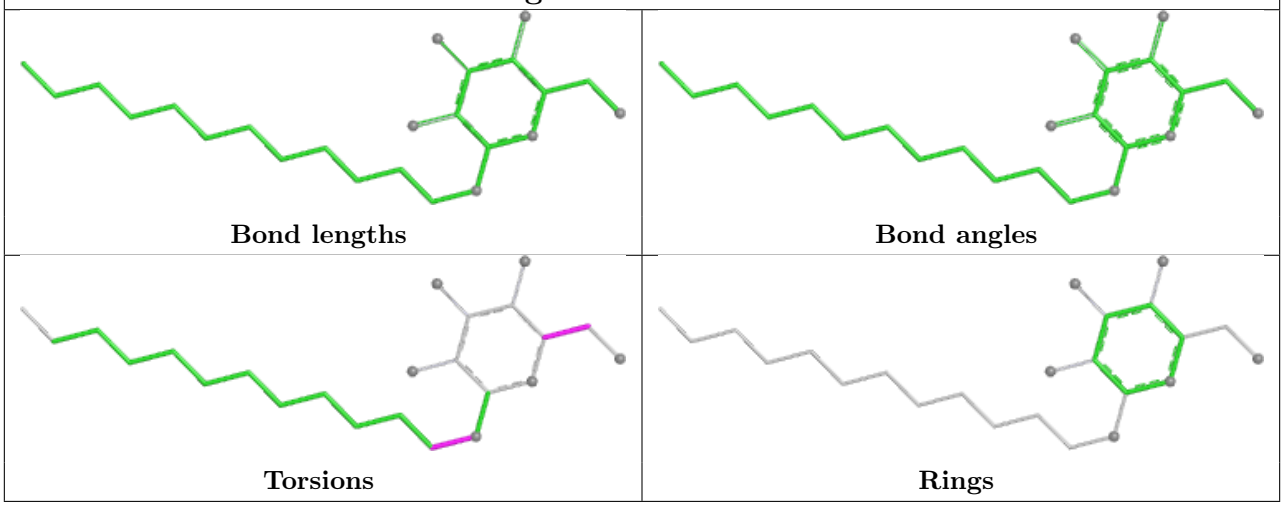


Rings

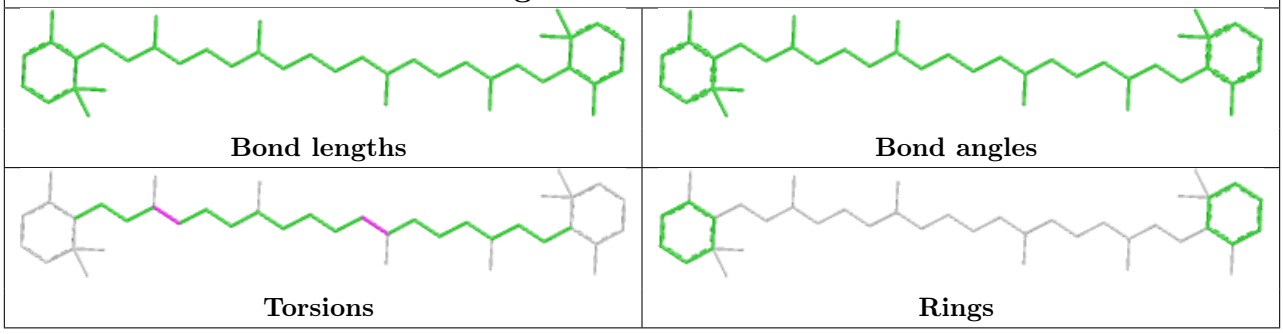
## Ligand LHG 3 721



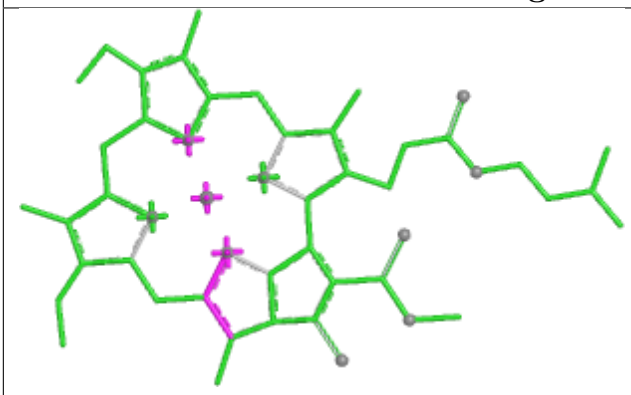

## Ligand LMU 8 625



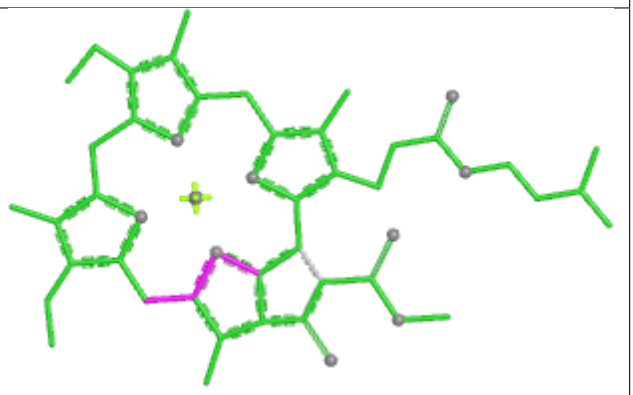

## Ligand BCR A2 852



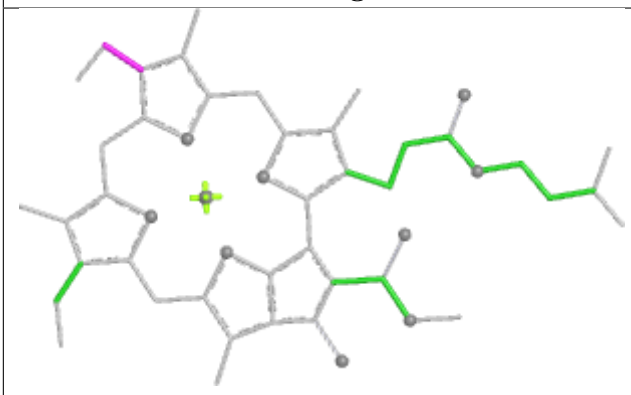
## Ligand CLA 8 608



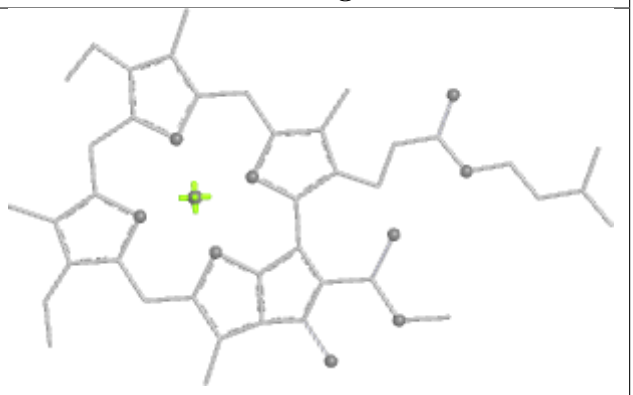
Bond lengths



Bond angles

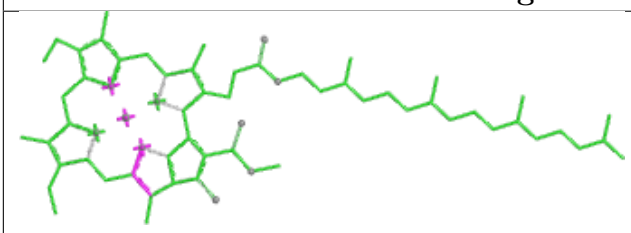


Torsions

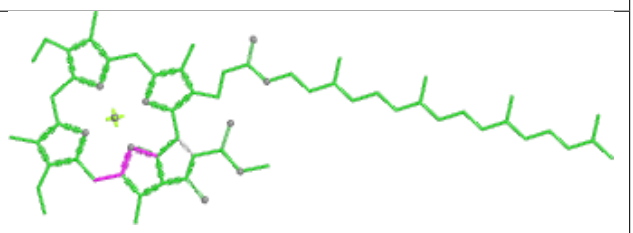


Rings

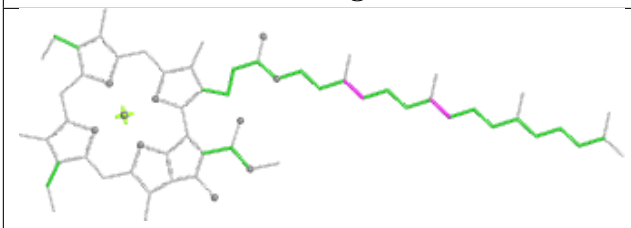
## Ligand CLA F2 301



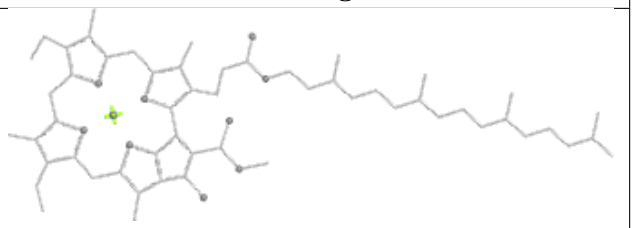
Bond lengths



Bond angles

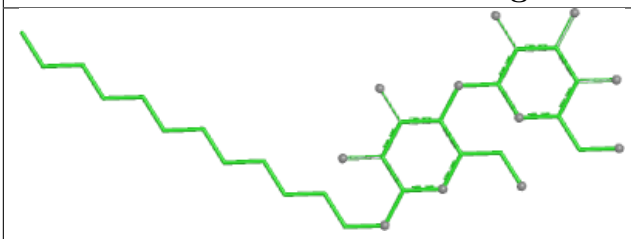


Torsions

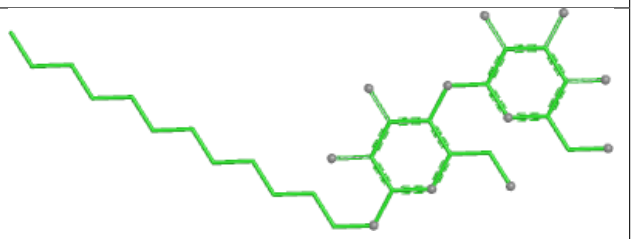


Rings

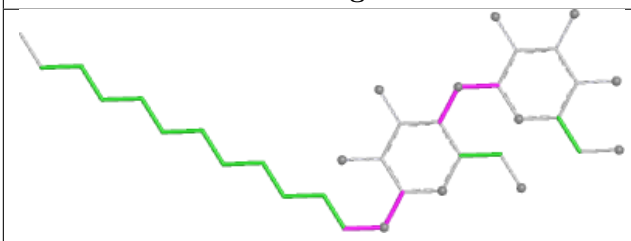
## Ligand LMU A2 863



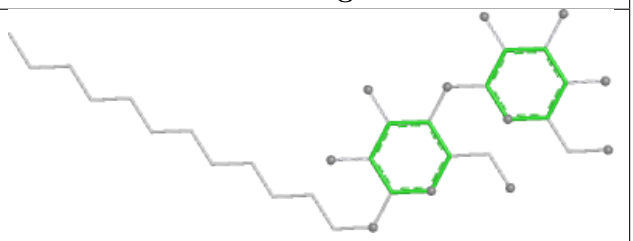
Bond lengths



Bond angles

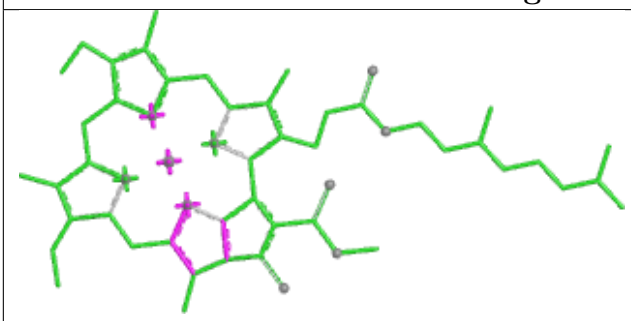


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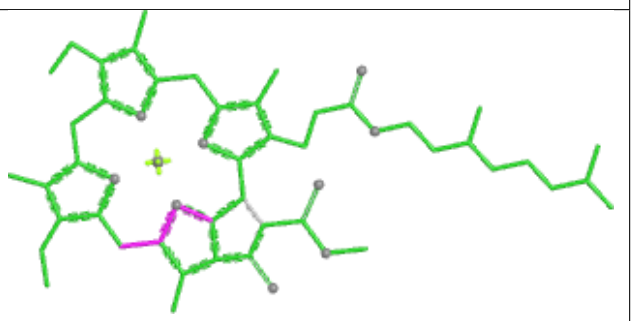


Rings

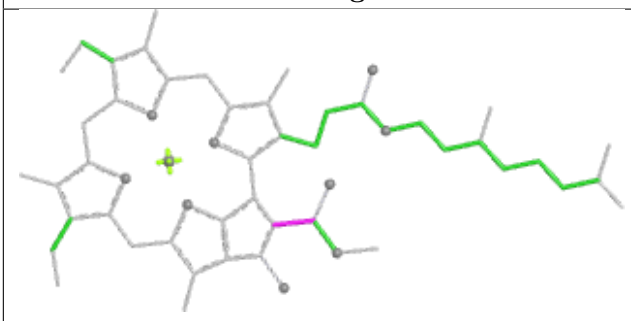
## Ligand CLA A 805



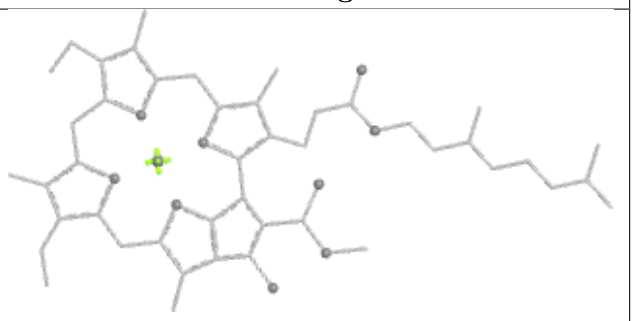
Bond lengths



Bond angles

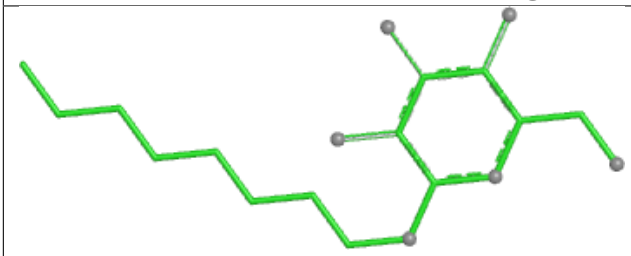


Torsions

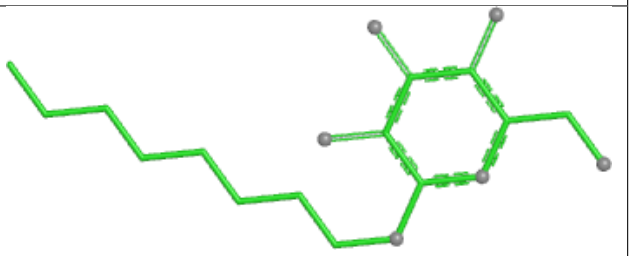


Rings

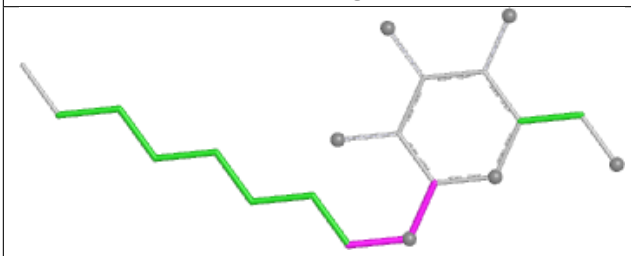
## Ligand LMU 6 632



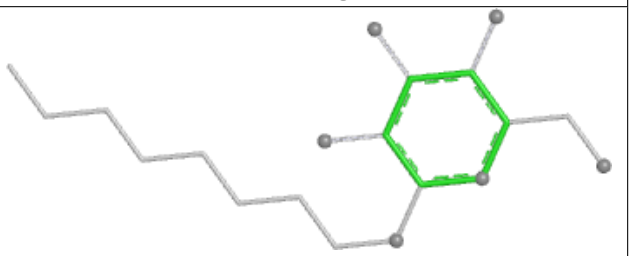
Bond lengths



Bond angles

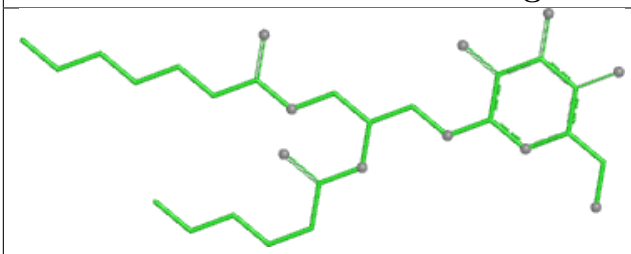


Torsions

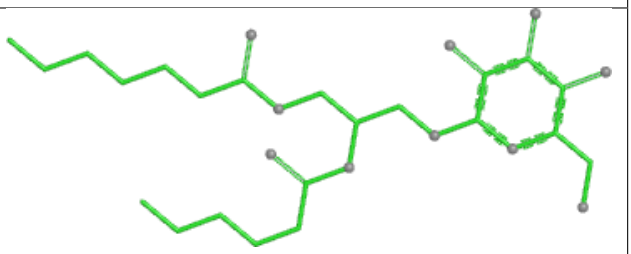


Rings

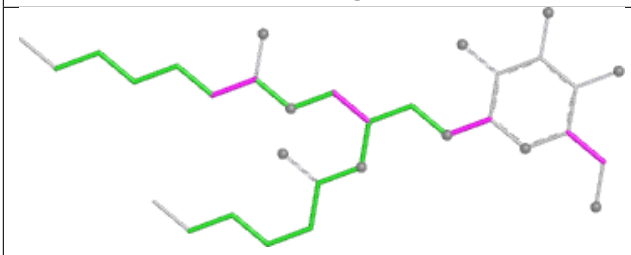
## Ligand LMG 8 626



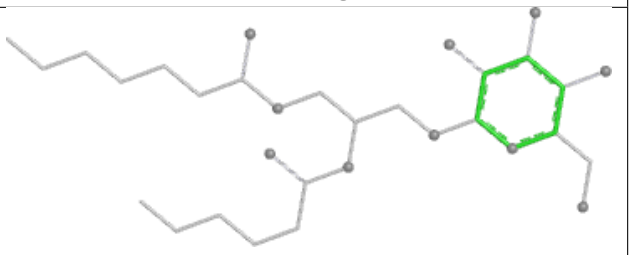
Bond lengths



Bond angles

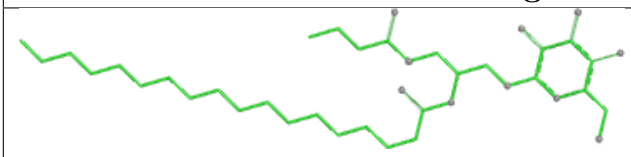


Torsions

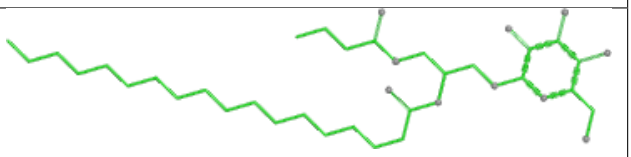


Rings

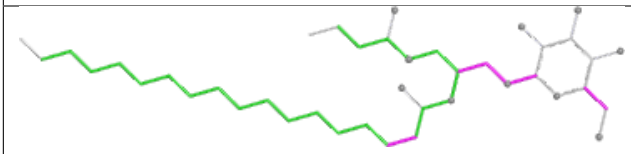
## Ligand LMG 4 624



Bond lengths



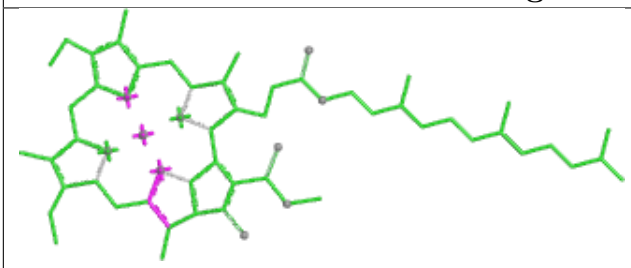
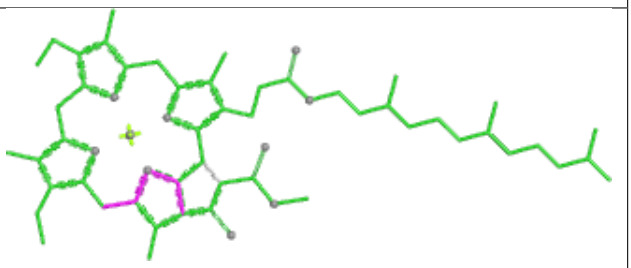
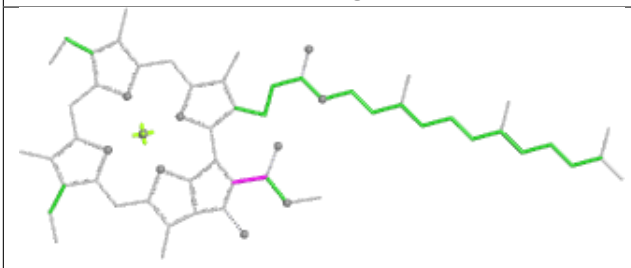
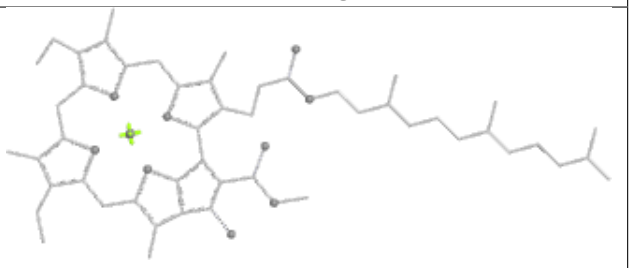
Bond angles

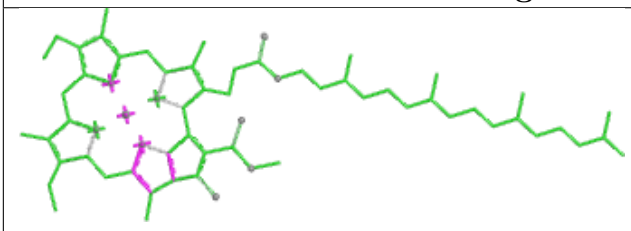
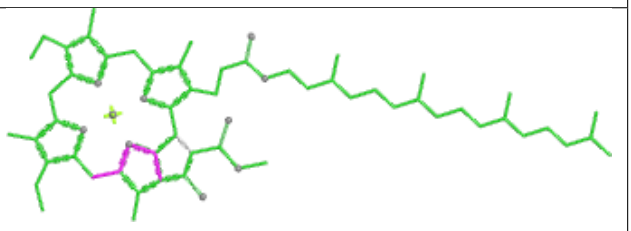
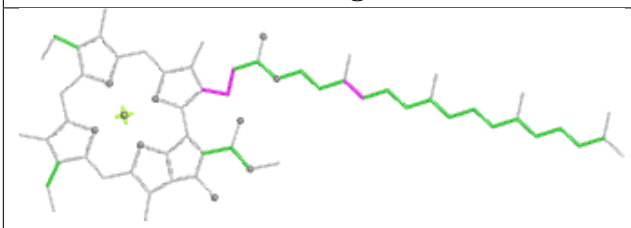
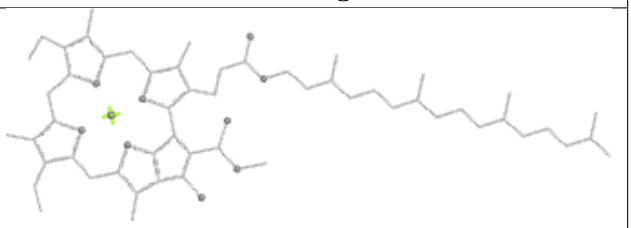


Torsions

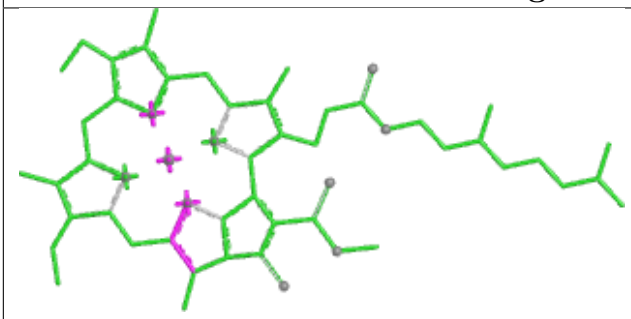


Rings

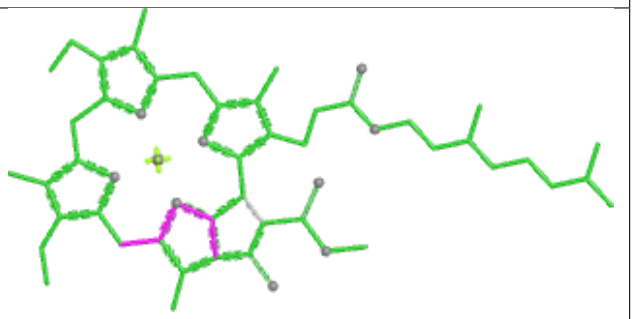
| Ligand CLA Z 602 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA B2 823 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

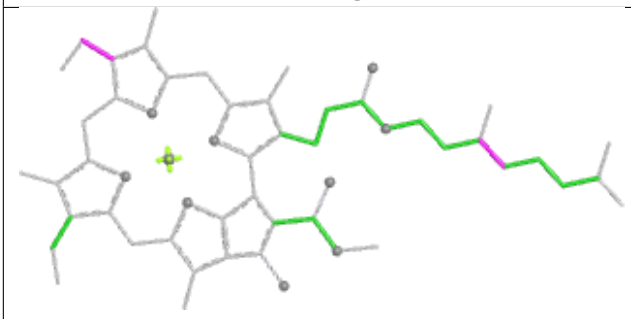
**Ligand CLA 5 611**



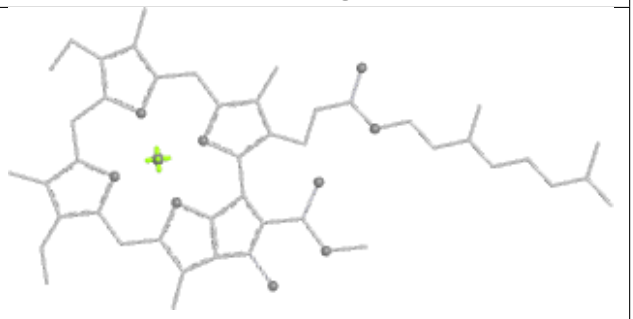
**Bond lengths**



**Bond angles**

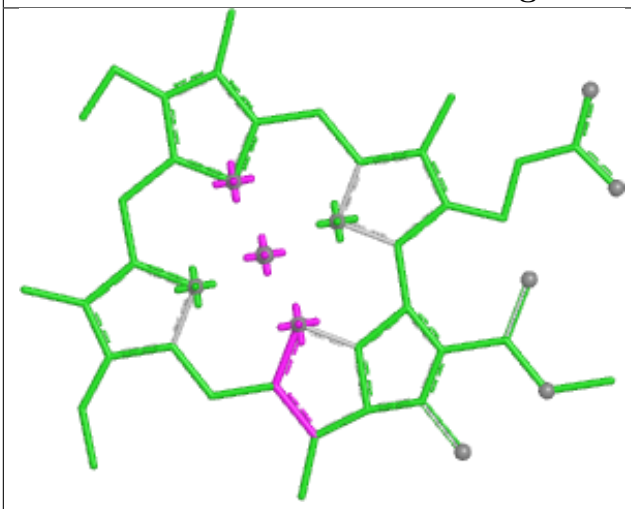


**Torsions**

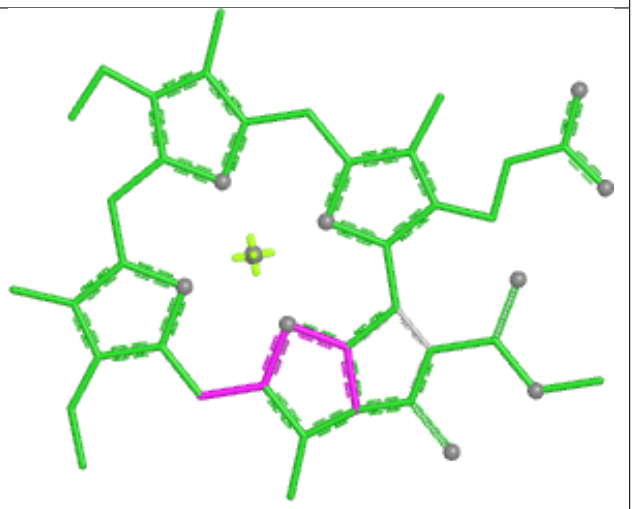


**Rings**

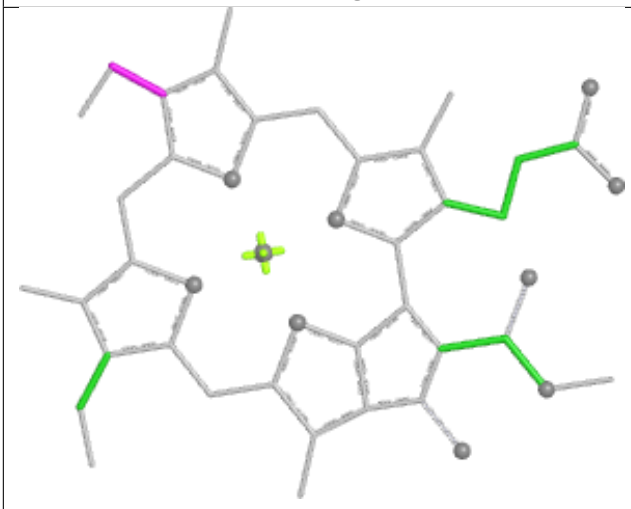
## Ligand CLA 72 609



Bond lengths



Bond angles

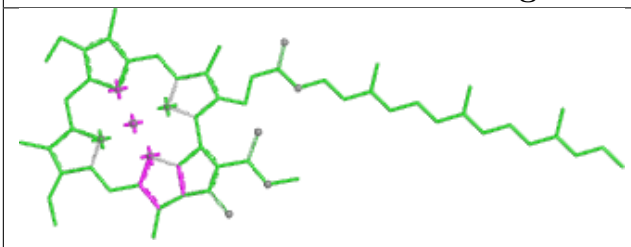


Torsions

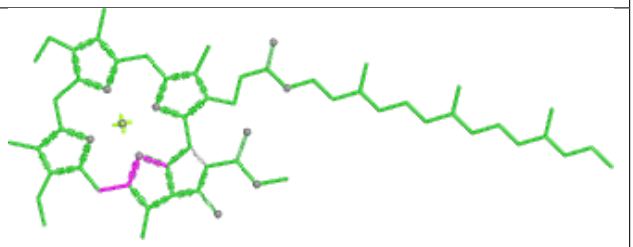


Rings

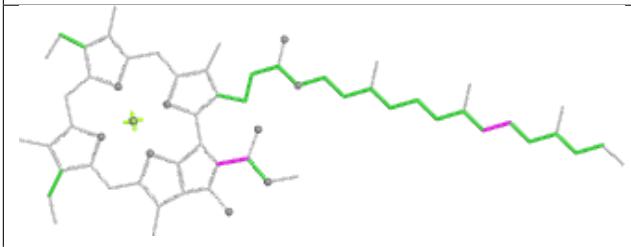
## Ligand CLA 82 602



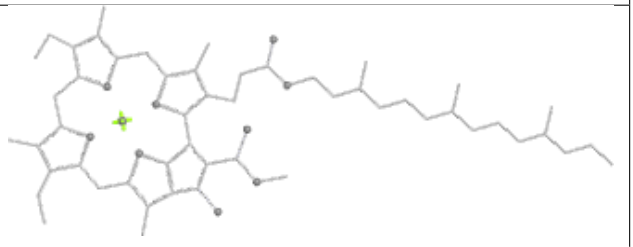
Bond lengths



Bond angles

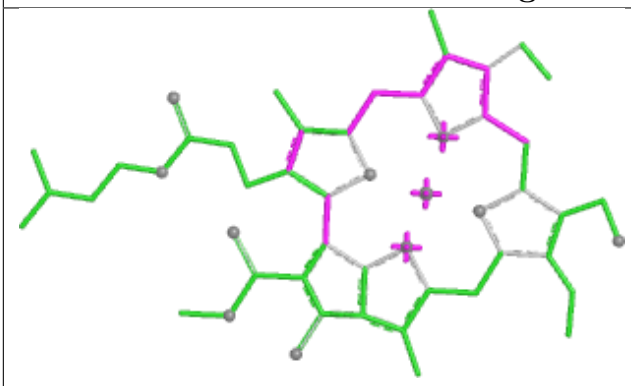


Torsions

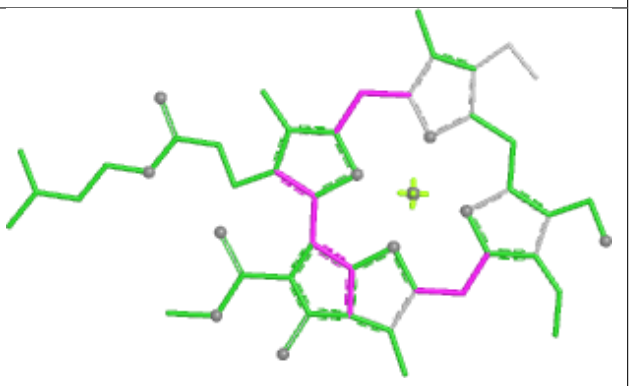


Rings

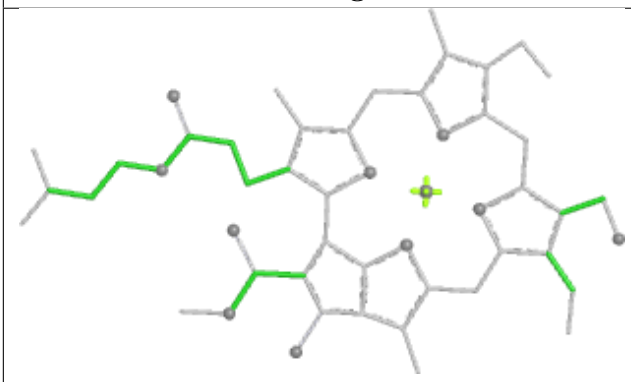
**Ligand CHL 62 608**



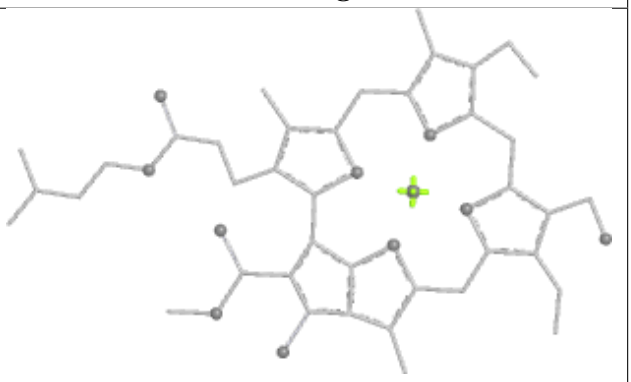
**Bond lengths**



**Bond angles**

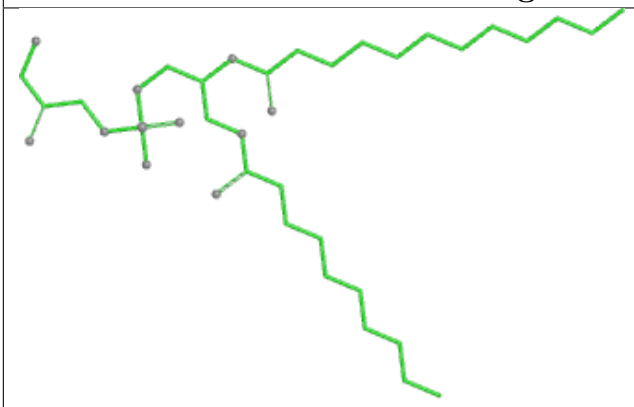


**Torsions**

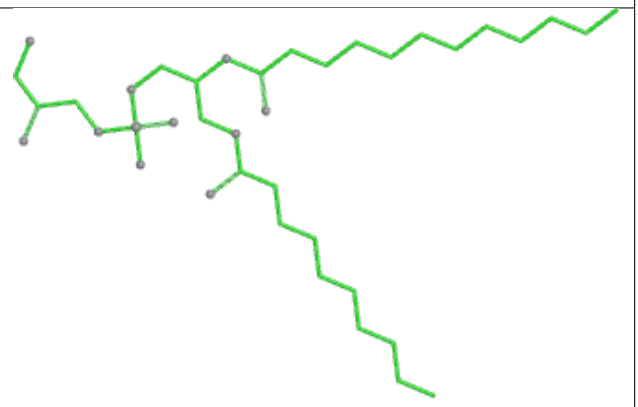


**Rings**

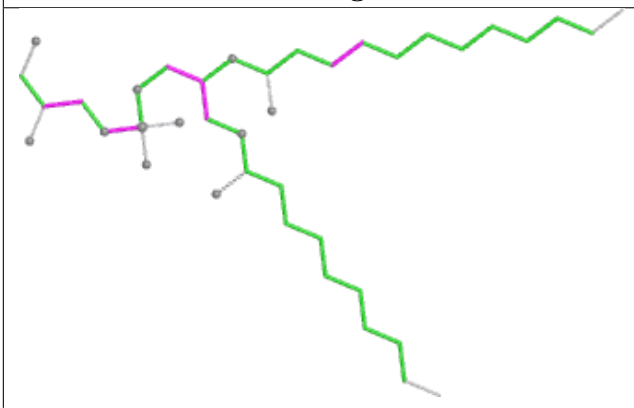
**Ligand LHG 12 620**



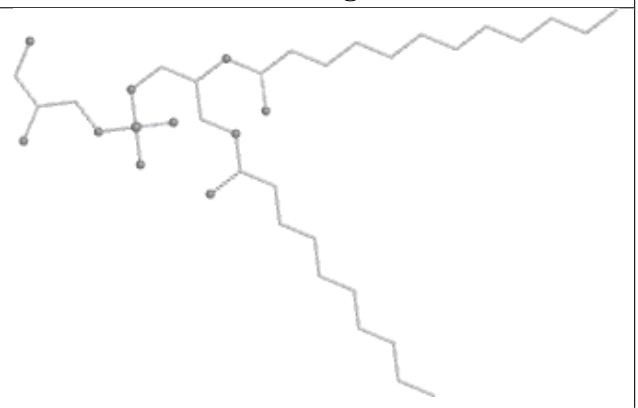
**Bond lengths**



**Bond angles**

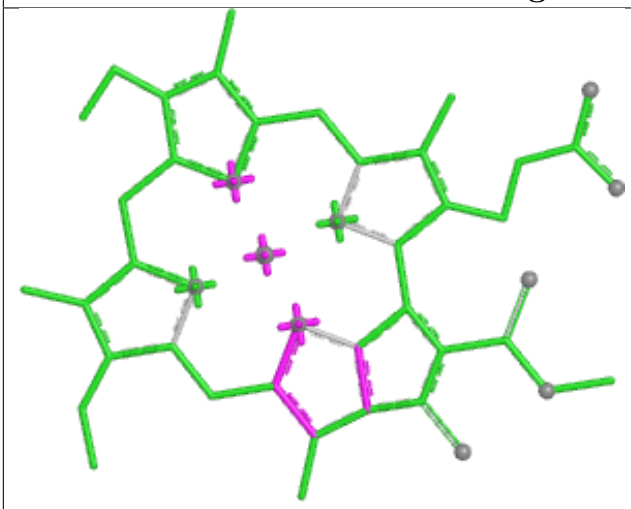


**Torsions**

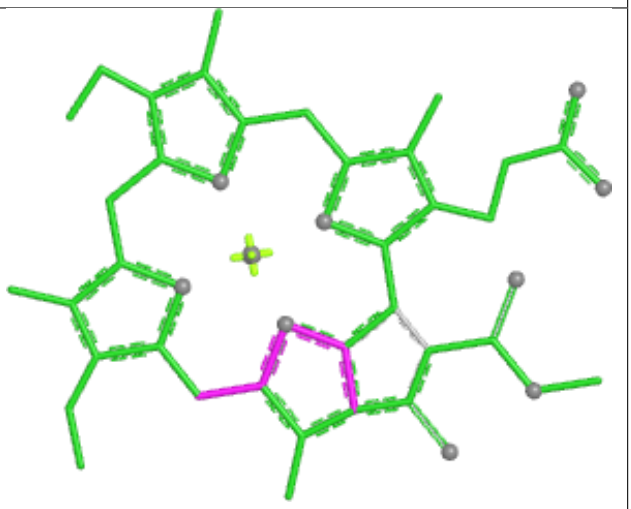


**Rings**

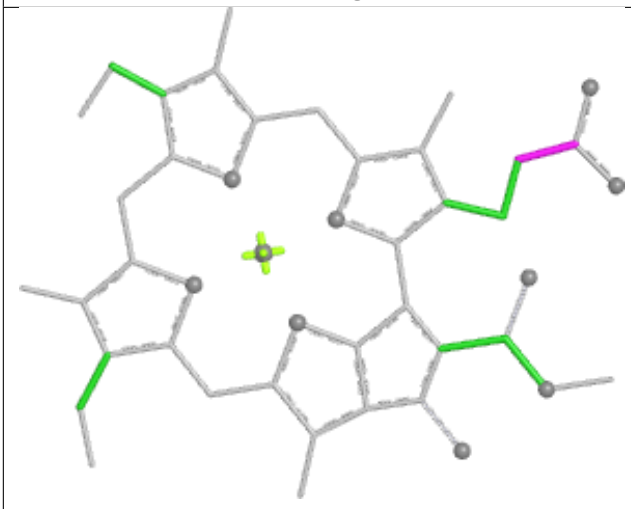
**Ligand CLA 8 611**



**Bond lengths**



**Bond angles**

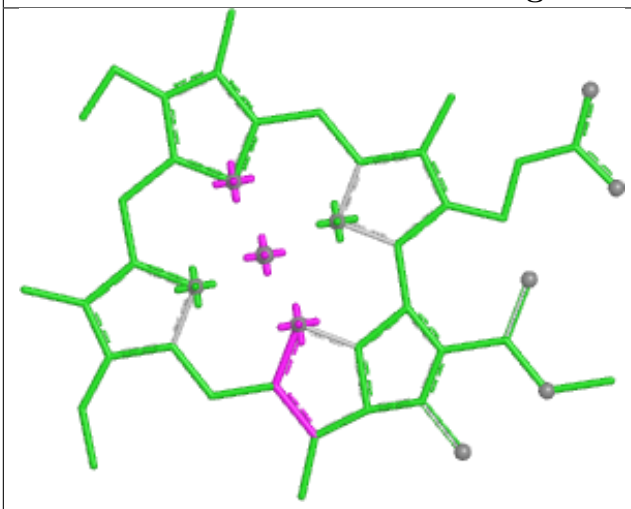


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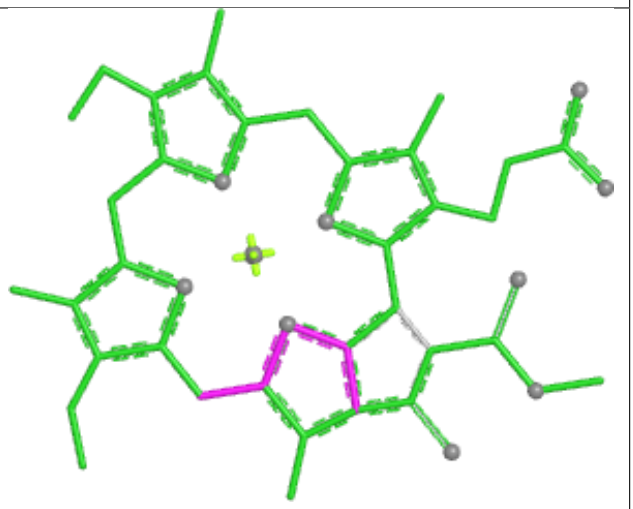


**Rings**

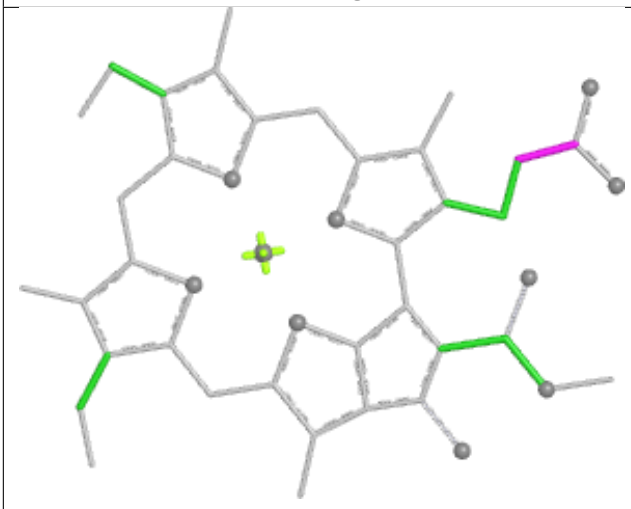
## Ligand CLA L 204



Bond lengths



Bond angles

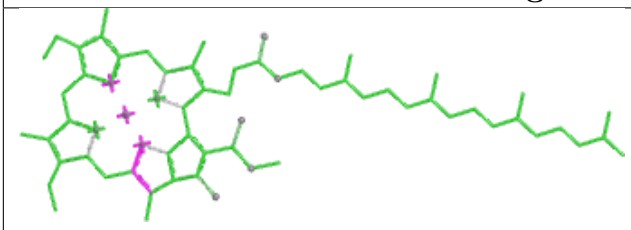


Torsions

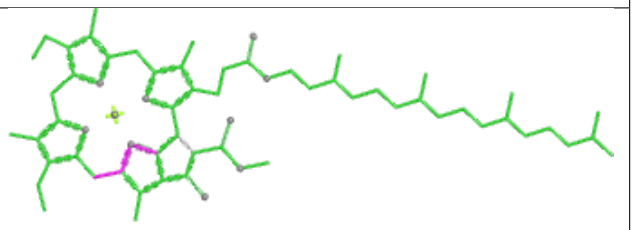


Rings

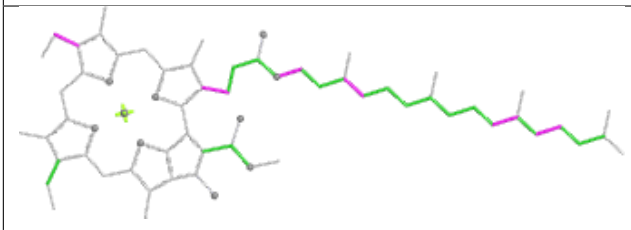
## Ligand CLA Z 609



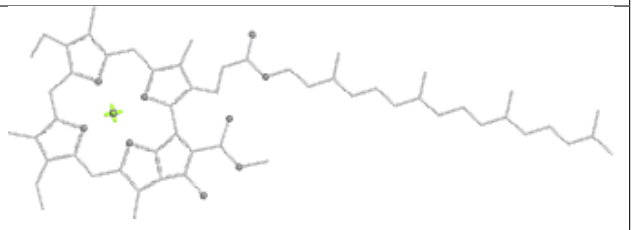
Bond lengths



Bond angles

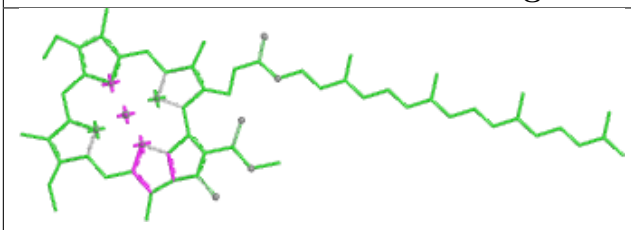


Torsions

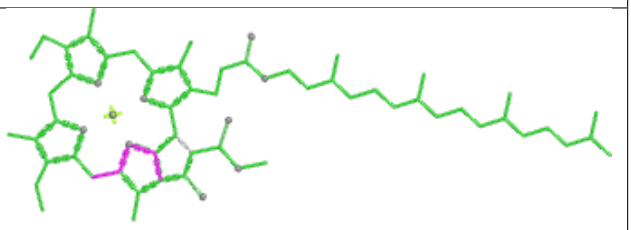


Rings

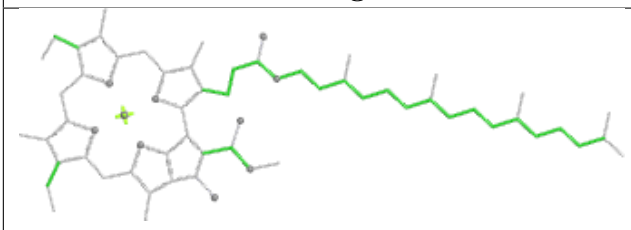
**Ligand CLA A 822**



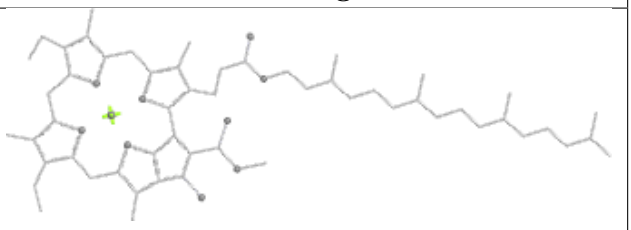
Bond lengths



Bond angles

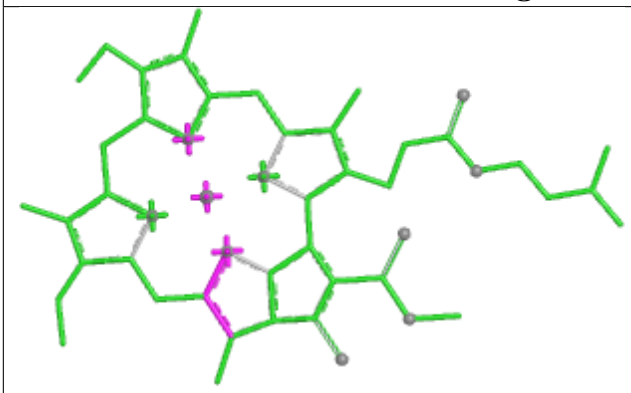


Torsions

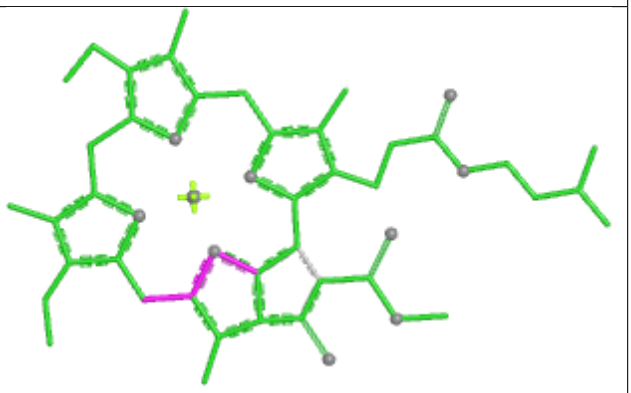


Rings

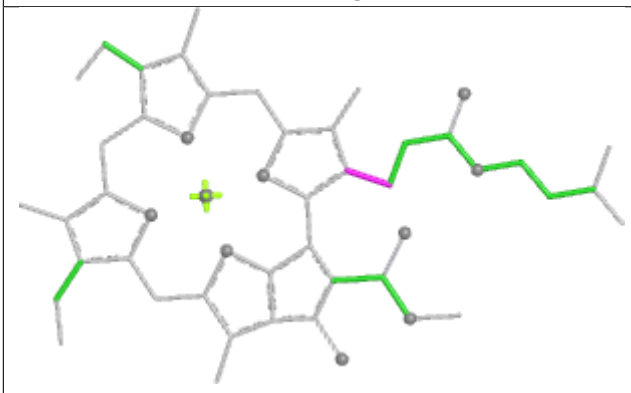
**Ligand CLA B2 838**



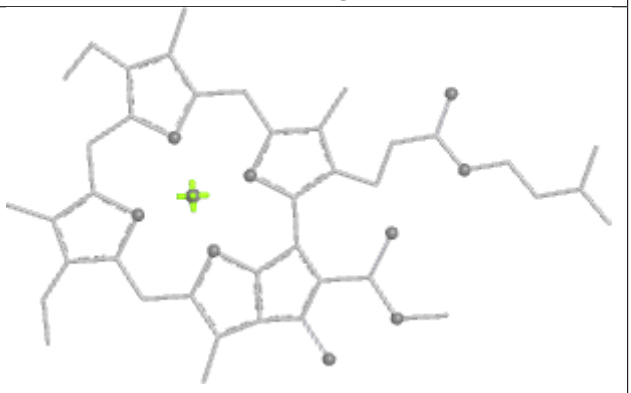
Bond lengths



Bond angles

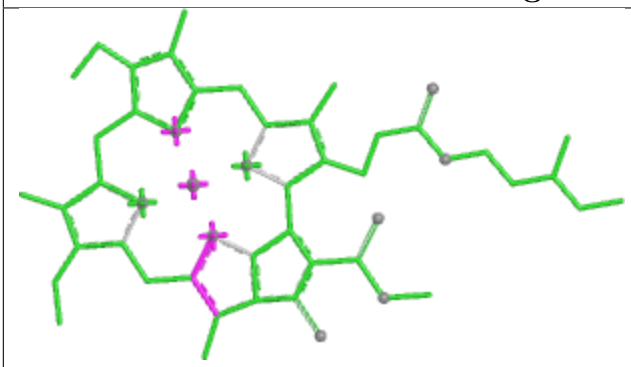


Torsions

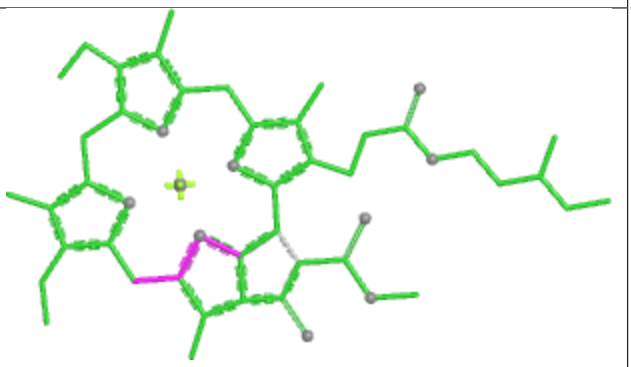


Rings

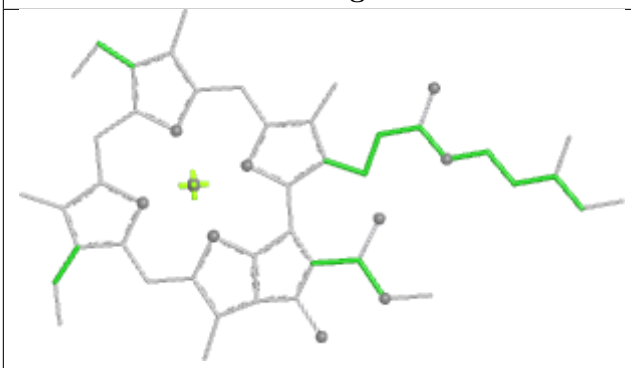
## Ligand CLA A 838



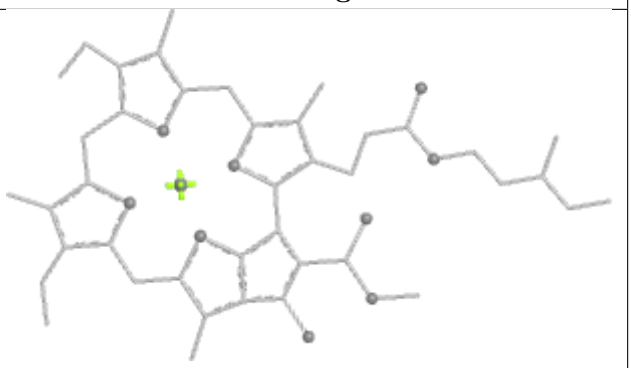
Bond lengths



Bond angles

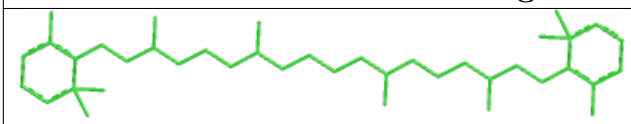


Torsions

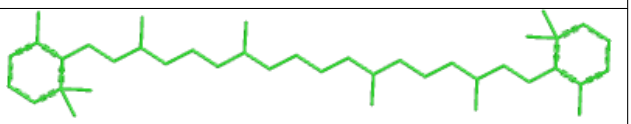


Rings

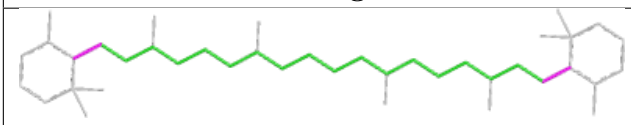
## Ligand BCR 32 620



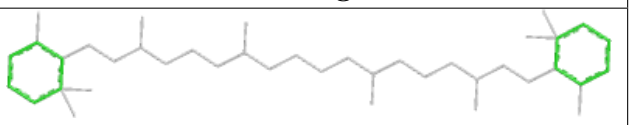
Bond lengths



Bond angles

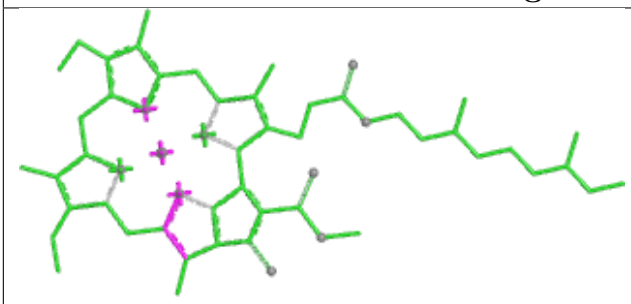


Torsions

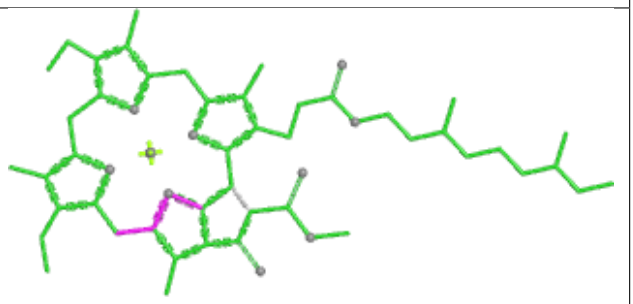


Rings

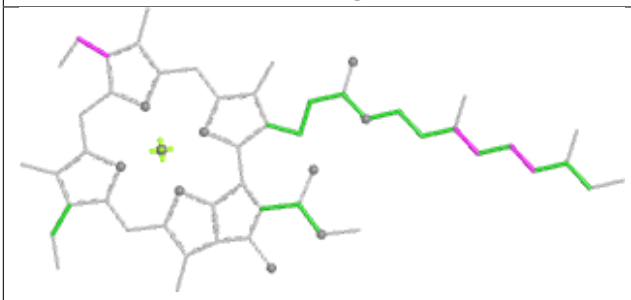
## Ligand CLA B 820



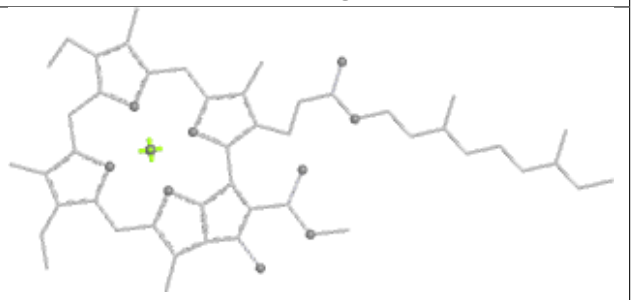
Bond lengths



Bond angles

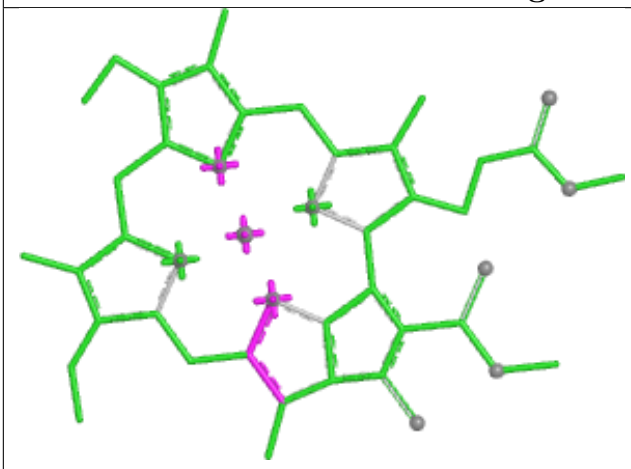


Torsions

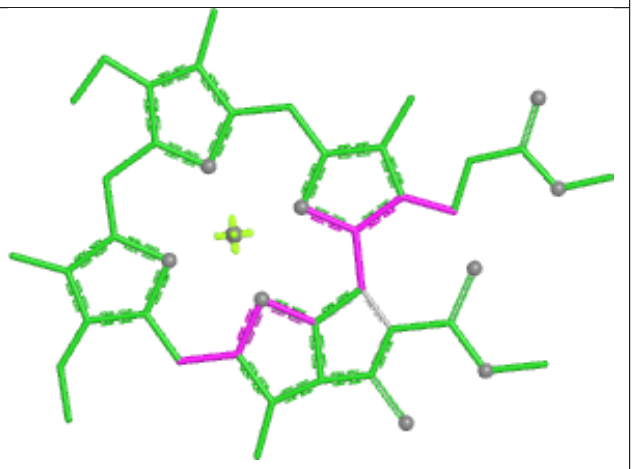


Rings

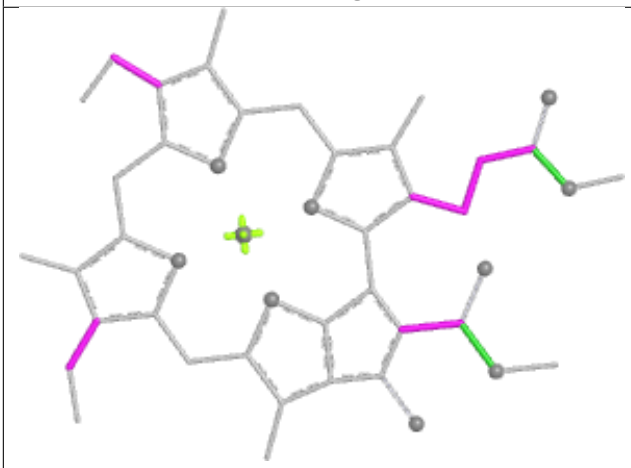
## Ligand CLA 5 621



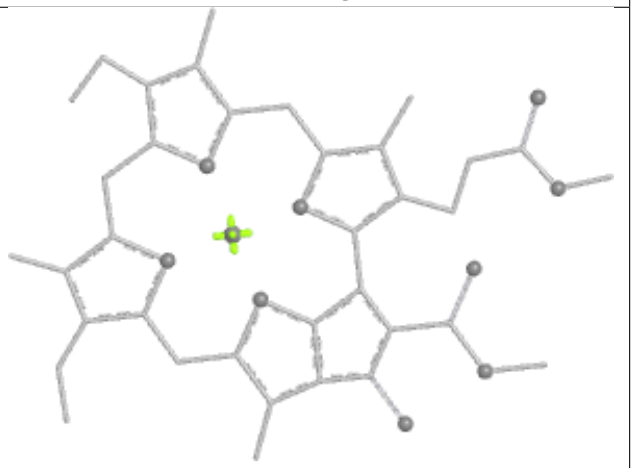
Bond lengths



Bond angles

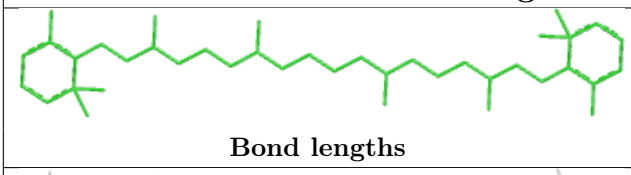


Torsions

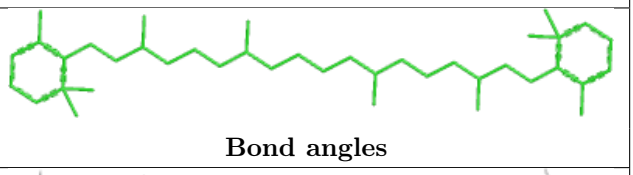


Rings

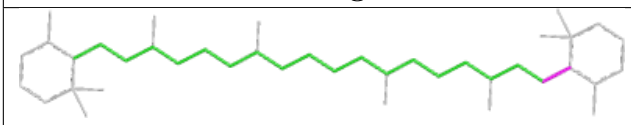
## Ligand BCR 42 621



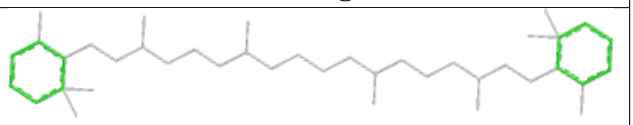
Bond lengths



Bond angles

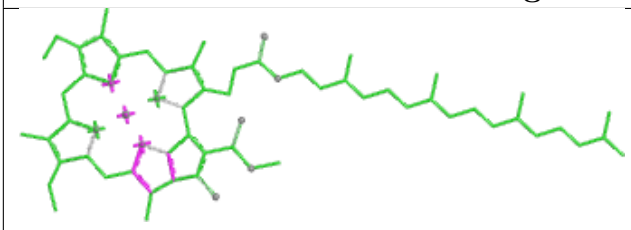


Torsions

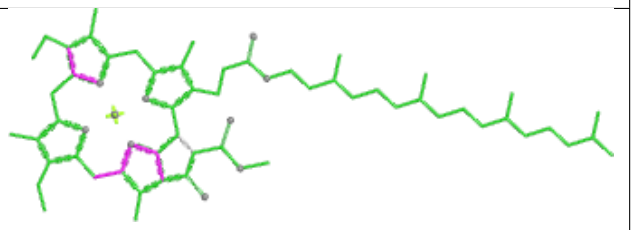


Rings

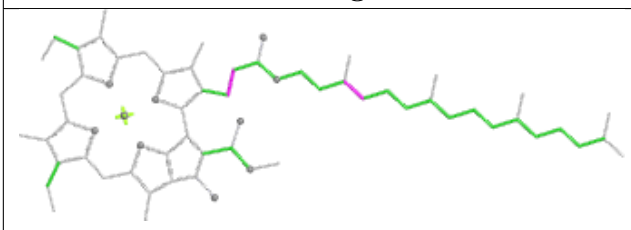
## Ligand CLA A 803



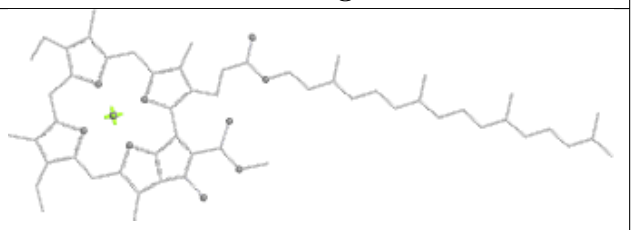
Bond lengths



Bond angles

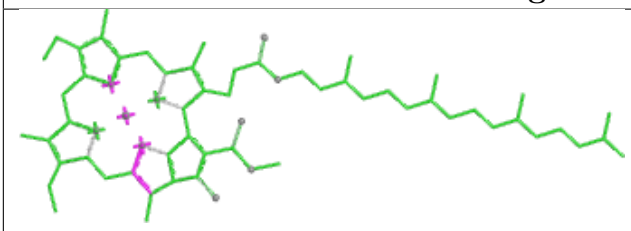


Torsions

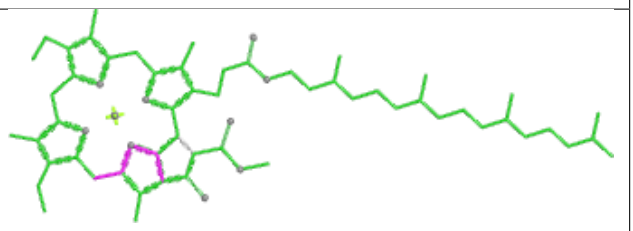


Rings

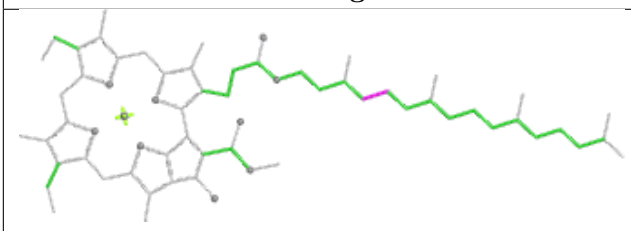
## Ligand CLA 3 604



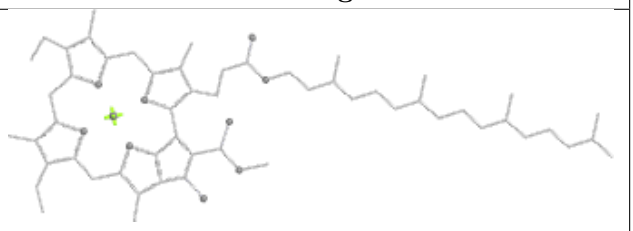
Bond lengths



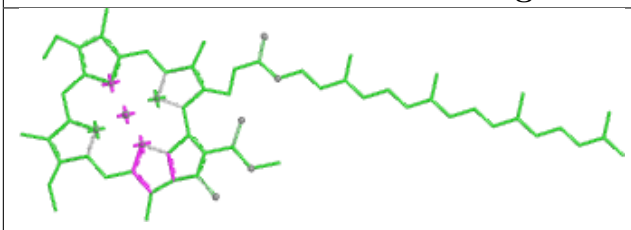
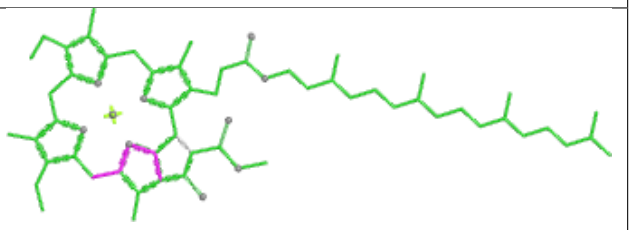
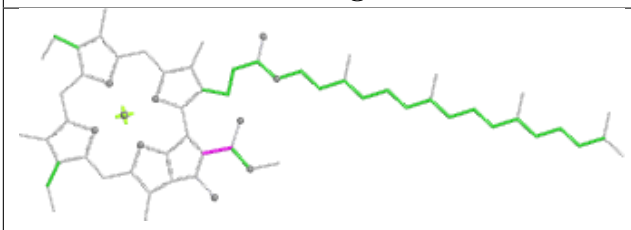
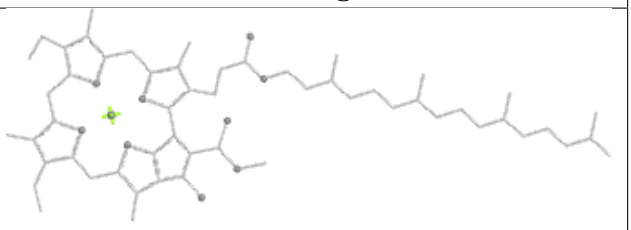
Bond angles

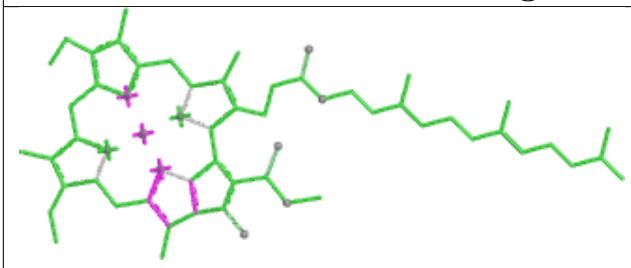
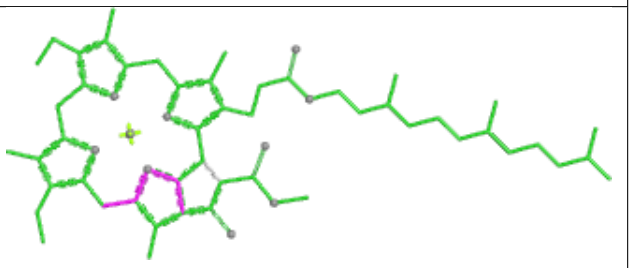
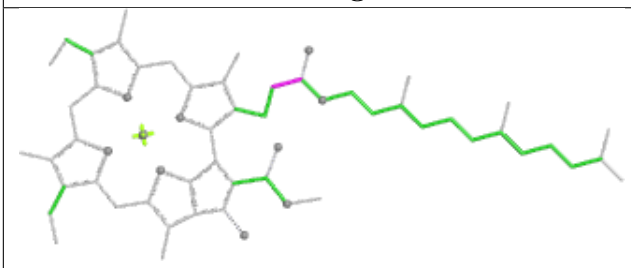
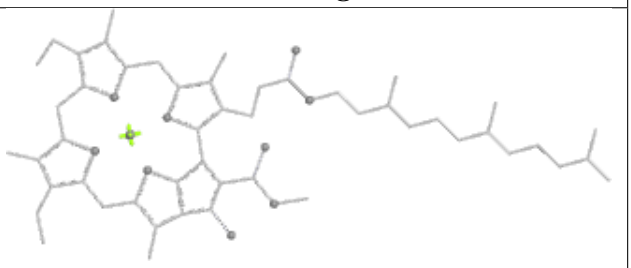


Torsions

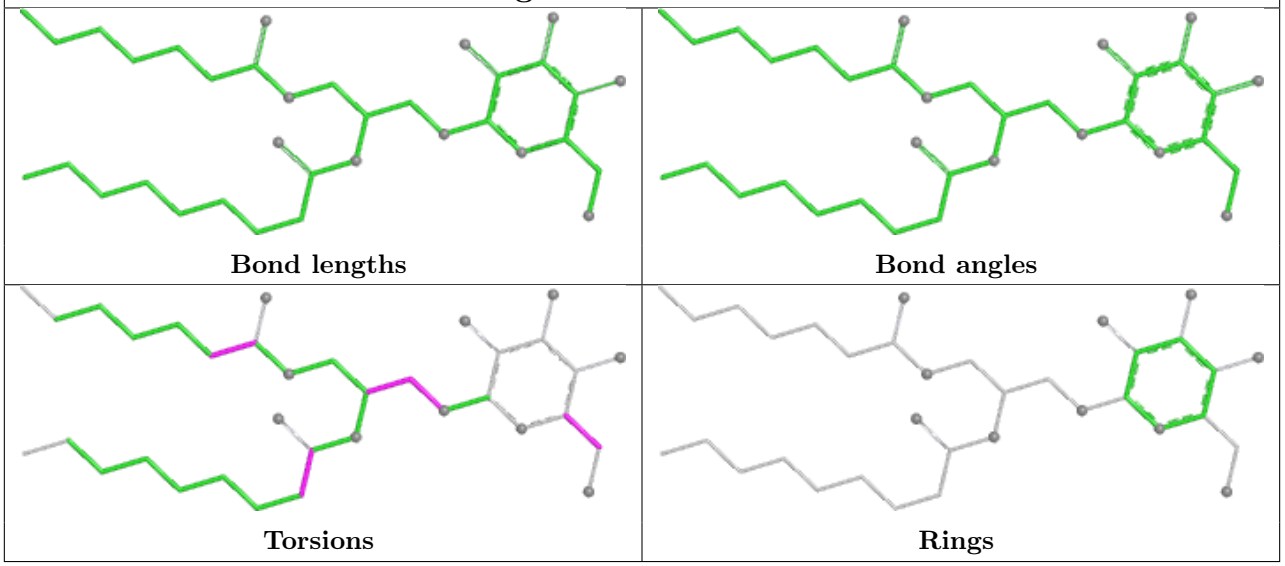


Rings

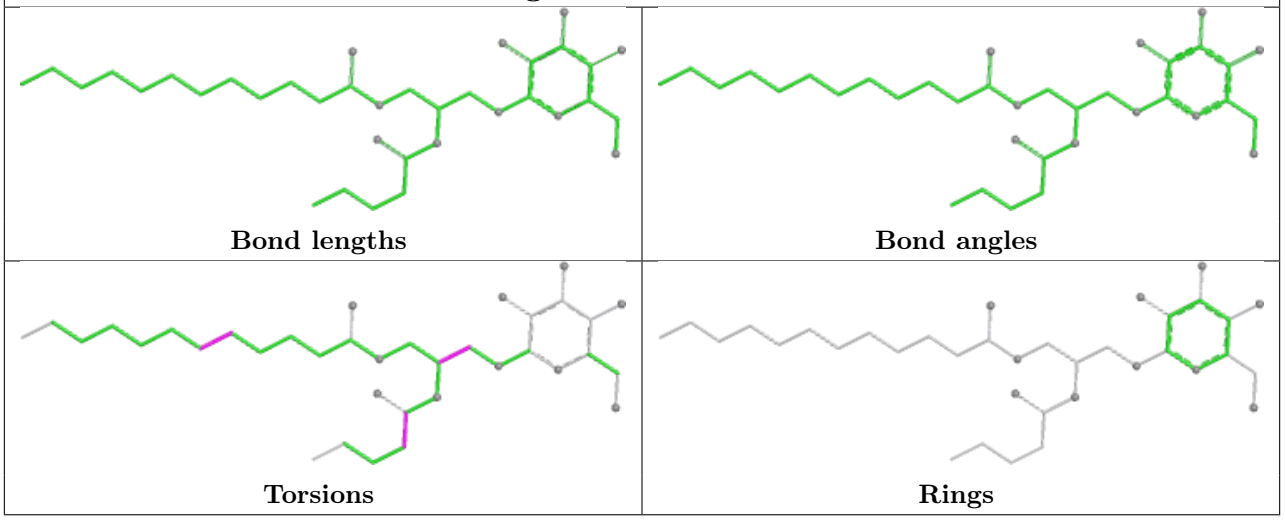
| Ligand CLA B2 825 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 82 604 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

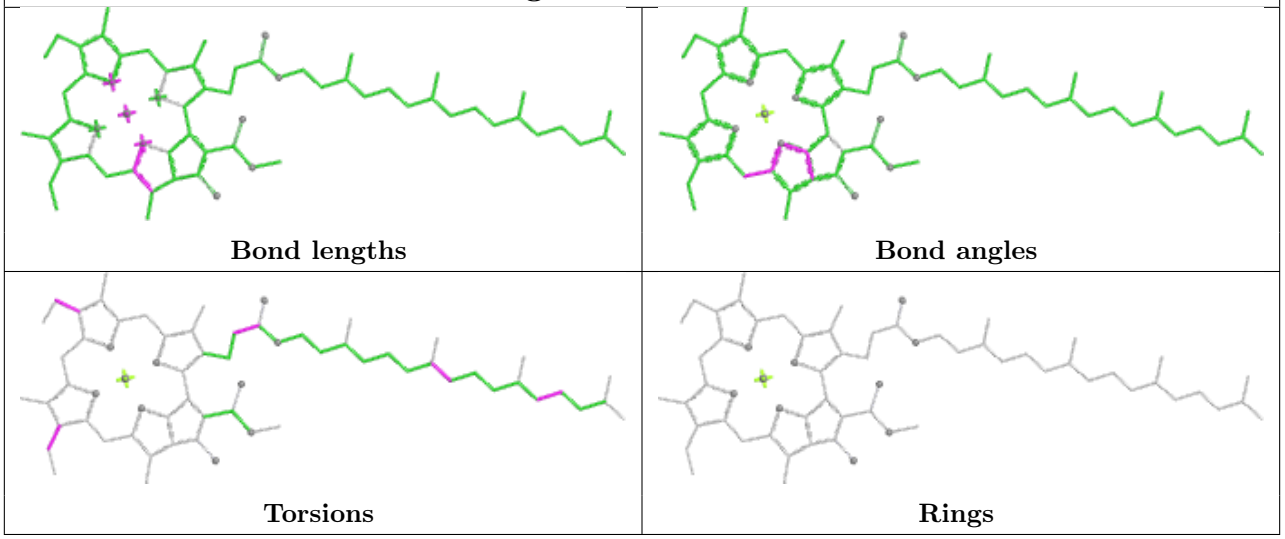
## Ligand LMG J2 104



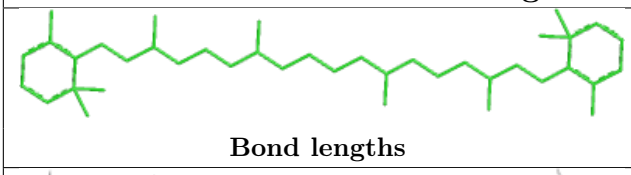

## Ligand LMG 1 624



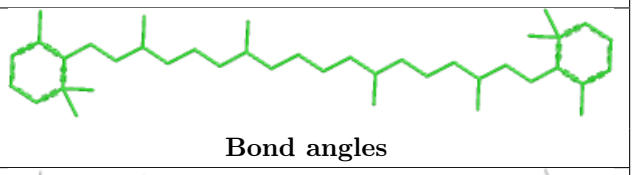

## Ligand CLA B 817



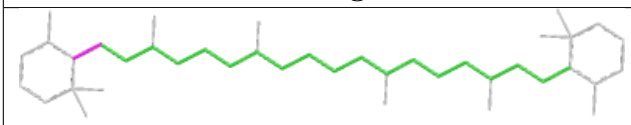
## Ligand BCR A 848



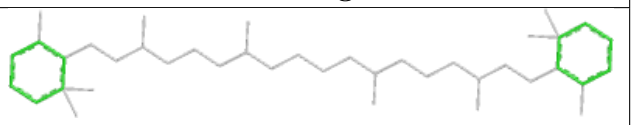
Bond lengths



Bond angles

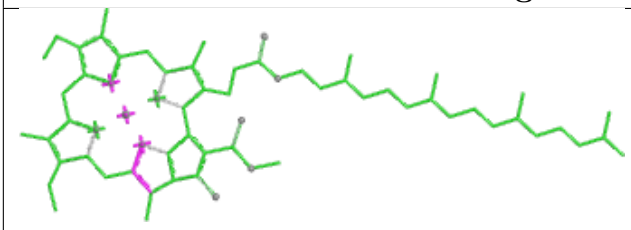


Torsions

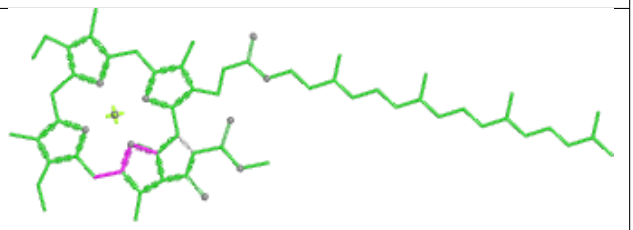


Rings

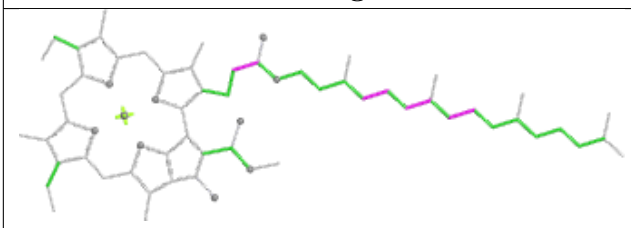
## Ligand CLA B2 809



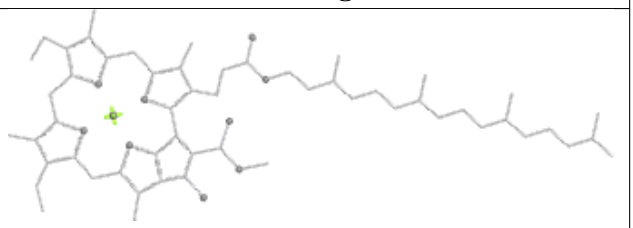
Bond lengths



Bond angles

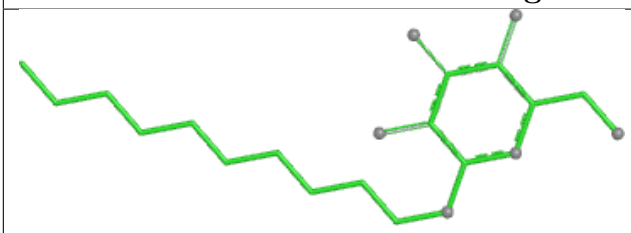


Torsions

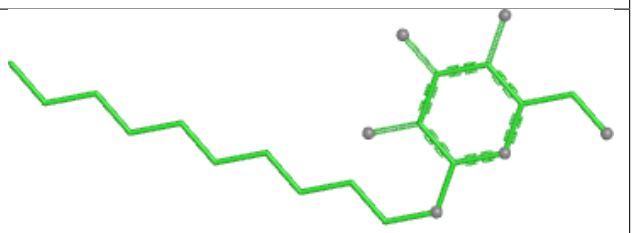


Rings

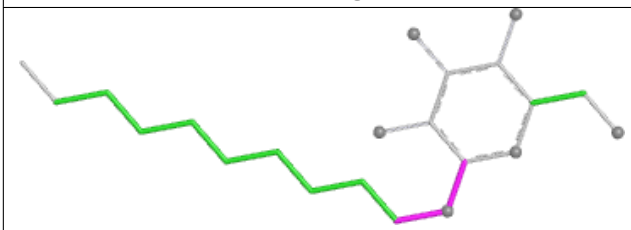
## Ligand LMU 7 628



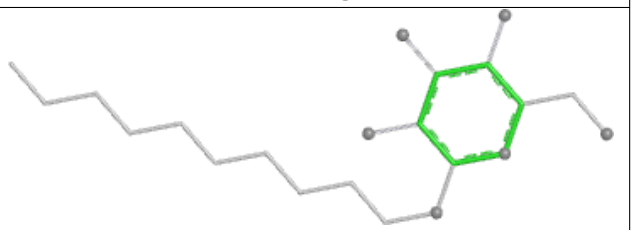
Bond lengths



Bond angles

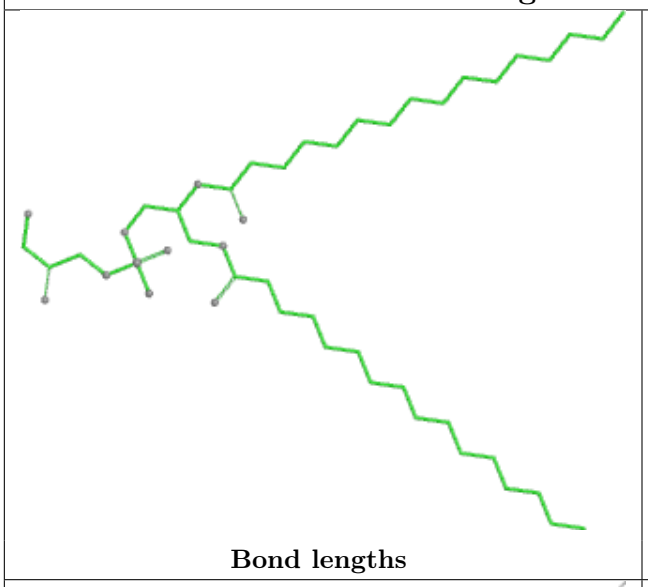


Torsions

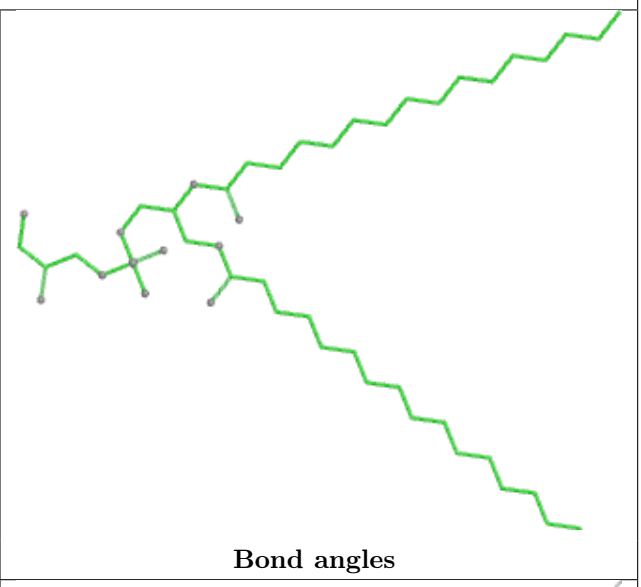


Rings

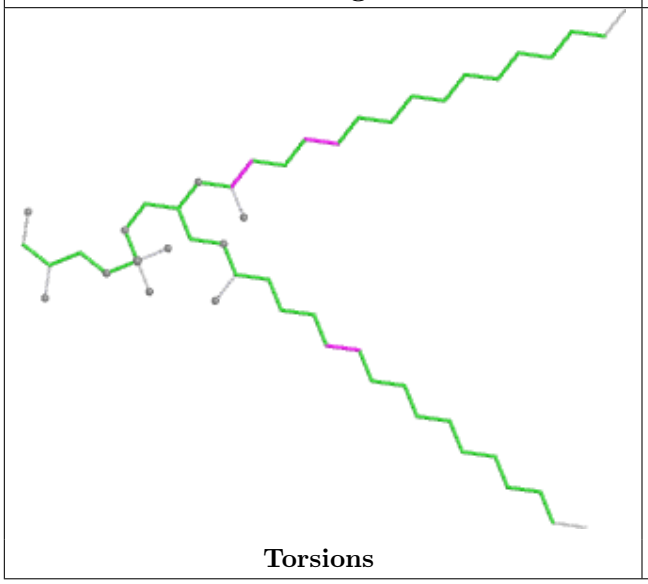
## Ligand LHG 62 619



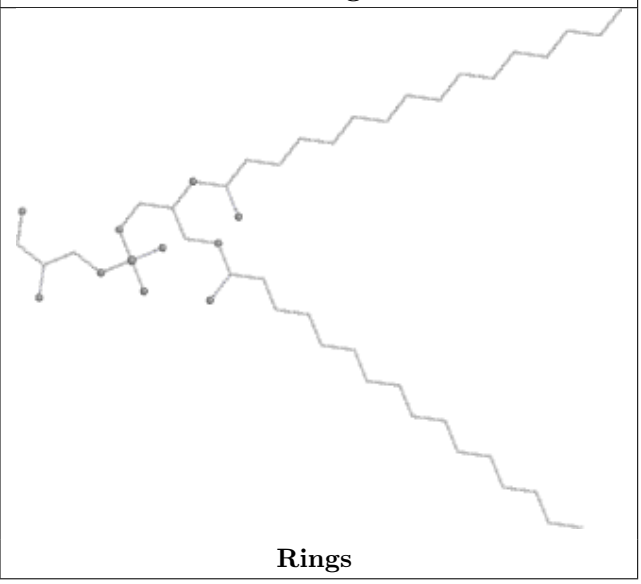
Bond lengths



Bond angles



Torsions



Rings

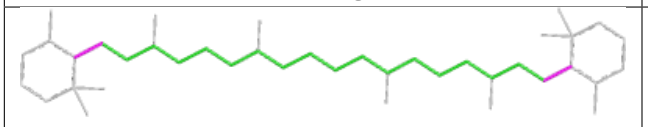
## Ligand BCR K2 207



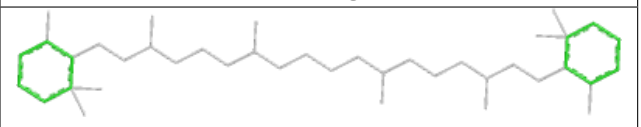
Bond lengths



Bond angles

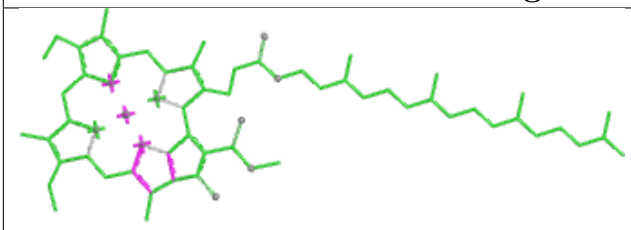


Torsions

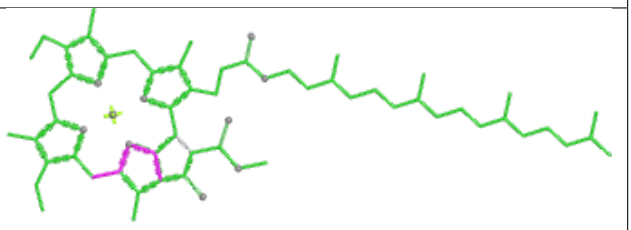


Rings

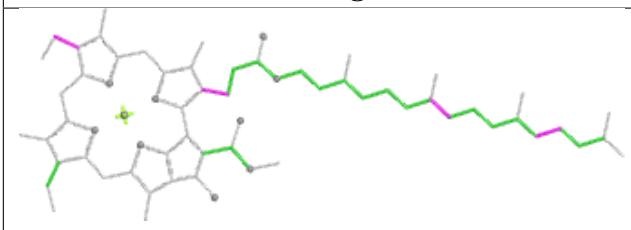
## Ligand CLA A 834



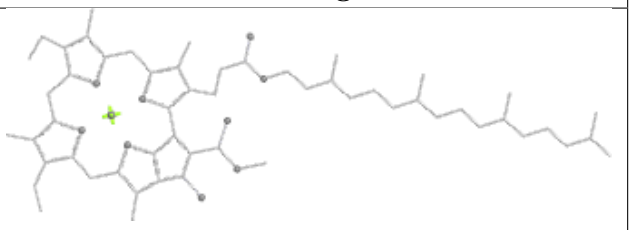
Bond lengths



Bond angles

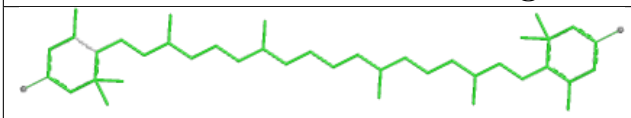


Torsions

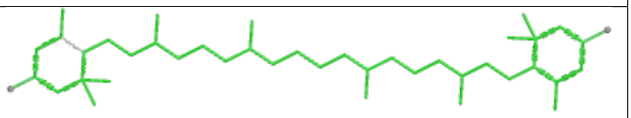


Rings

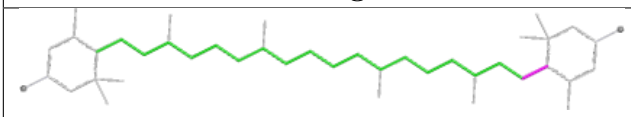
## Ligand LUT 92 616



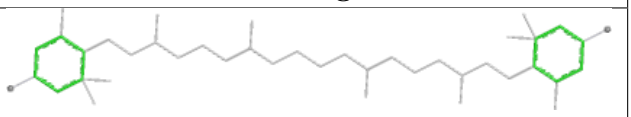
Bond lengths



Bond angles

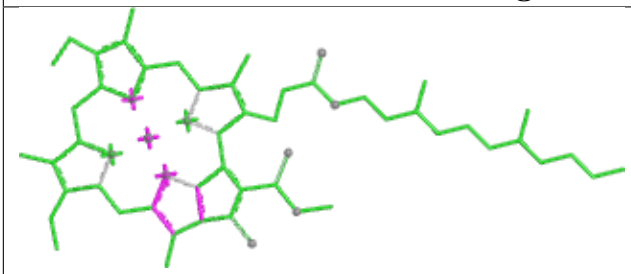


Torsions

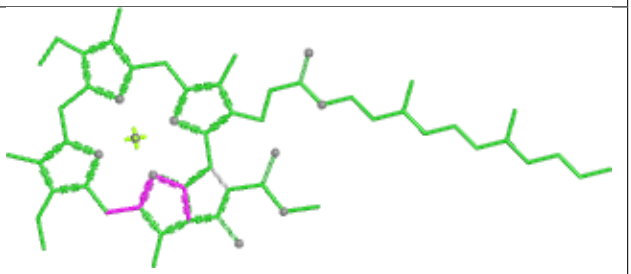


Rings

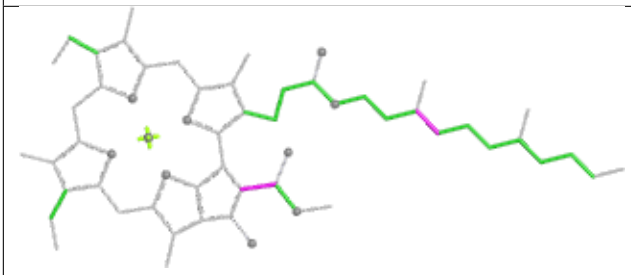
## Ligand CLA B2 833



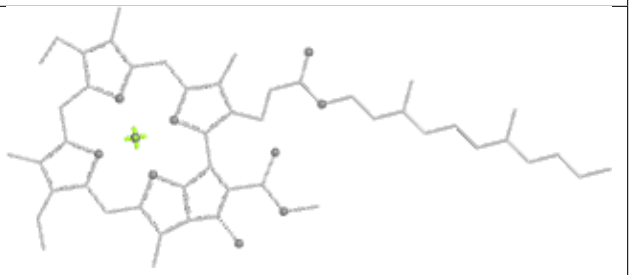
Bond lengths



Bond angles

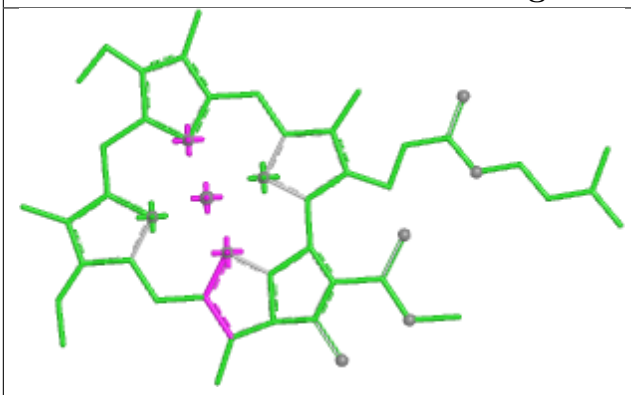


Torsions

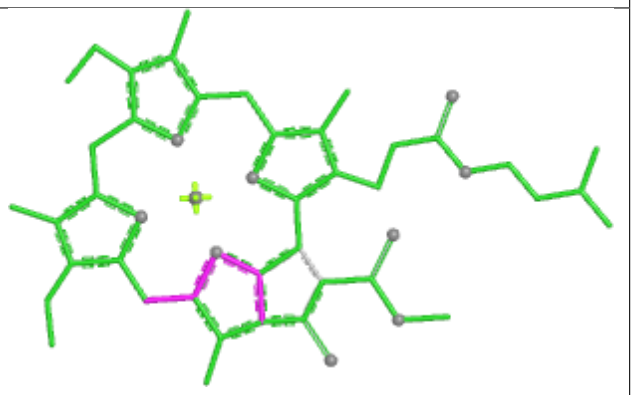


Rings

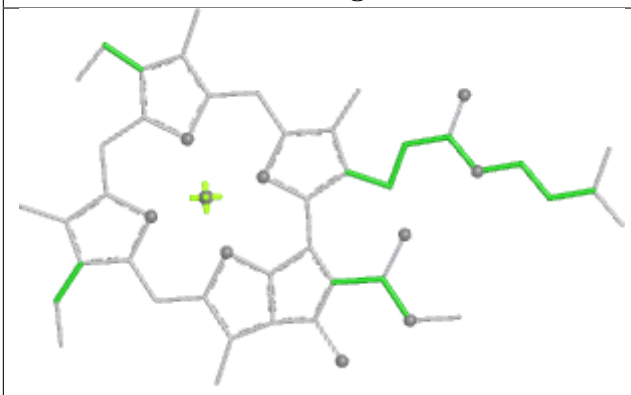
**Ligand CLA 7 608**



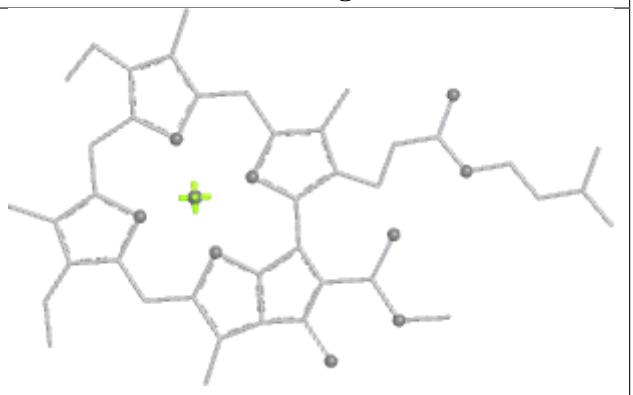
**Bond lengths**



**Bond angles**

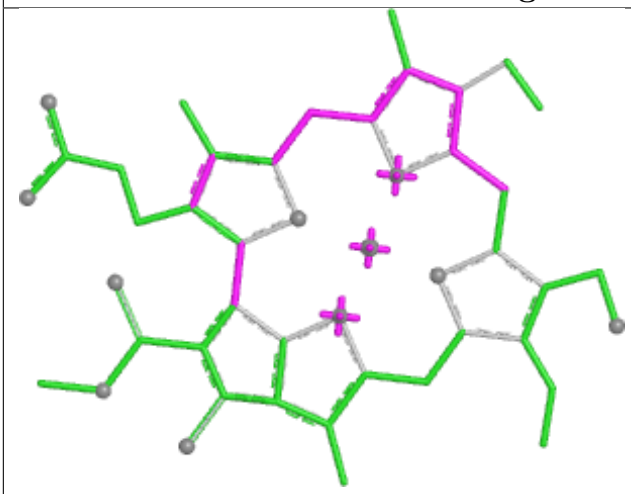


**Torsions**

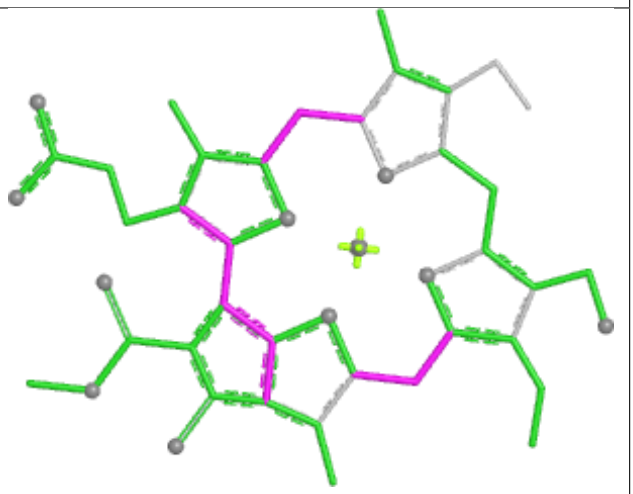


**Rings**

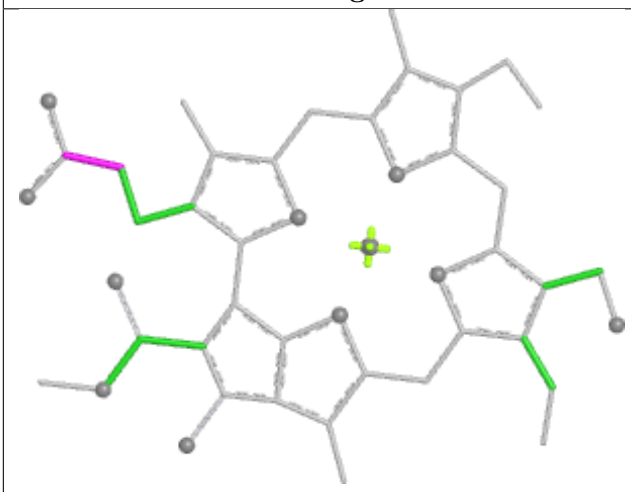
## Ligand CHL 72 607



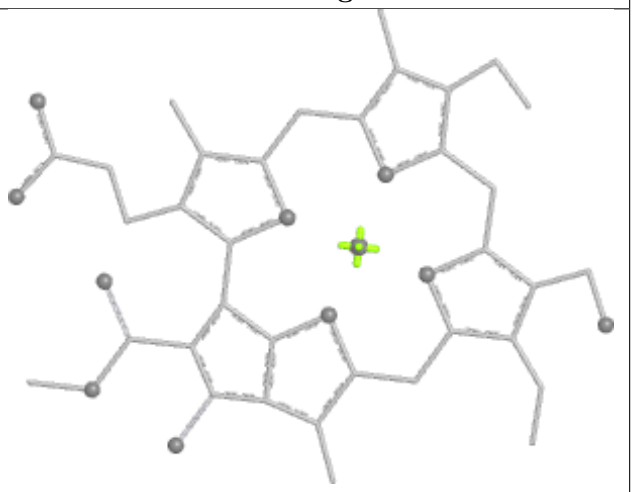
Bond lengths



Bond angles

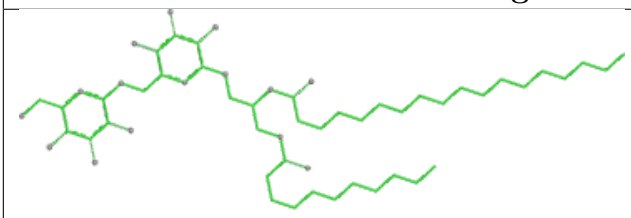


Torsions

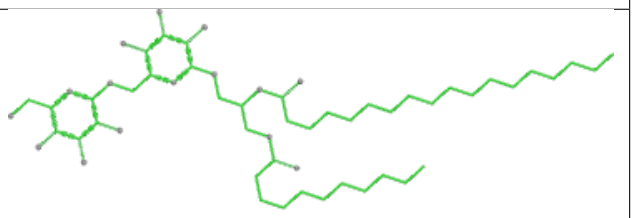


Rings

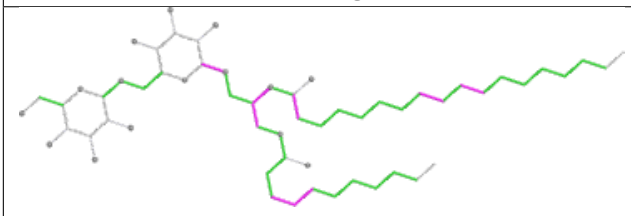
## Ligand DGD B2 850



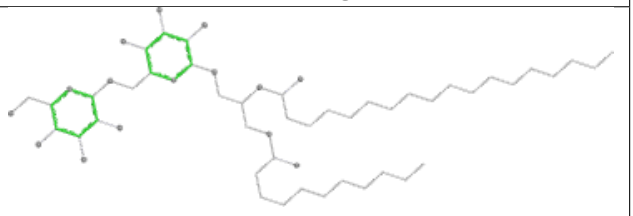
Bond lengths



Bond angles

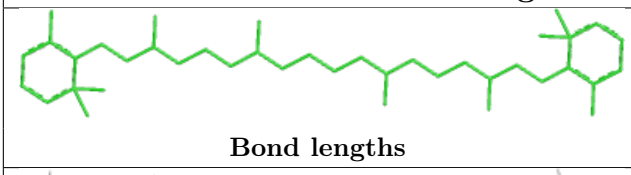


Torsions

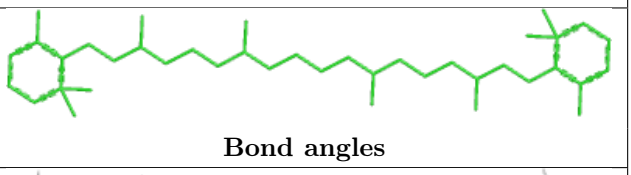


Rings

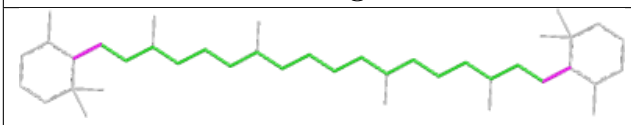
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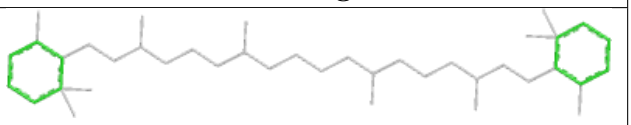
Bond lengths



Bond angles



Torsions



Rings

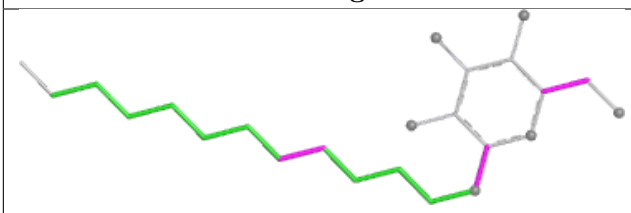
## Ligand LMU 6 631



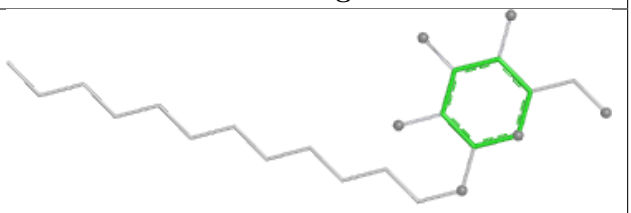
Bond lengths



Bond angles

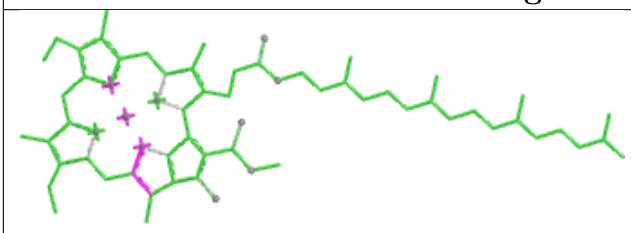


Torsions

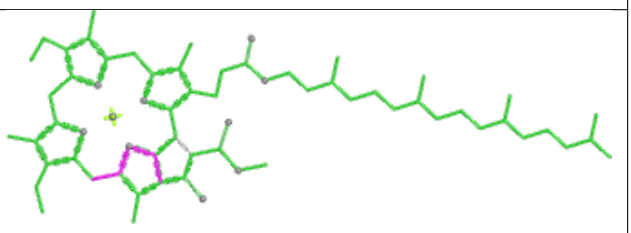


Rings

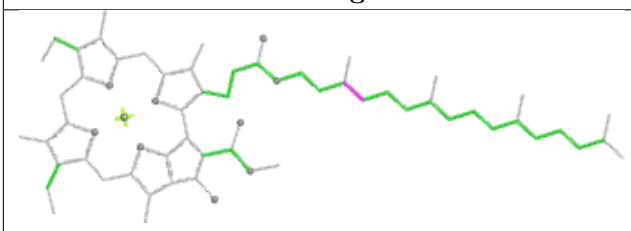
## Ligand CLA B 810



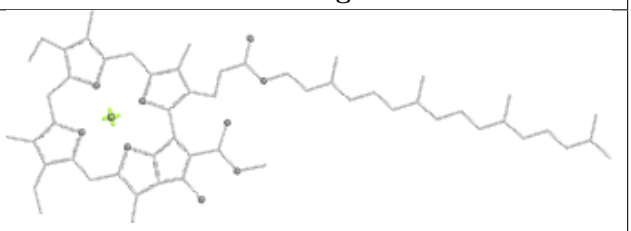
Bond lengths



Bond angles

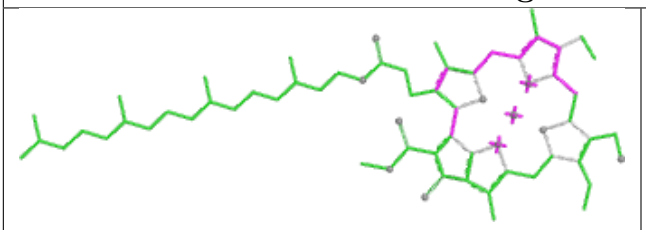


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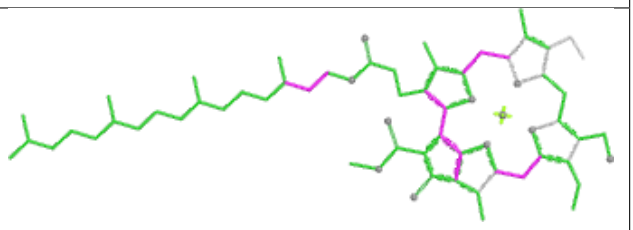


Rings

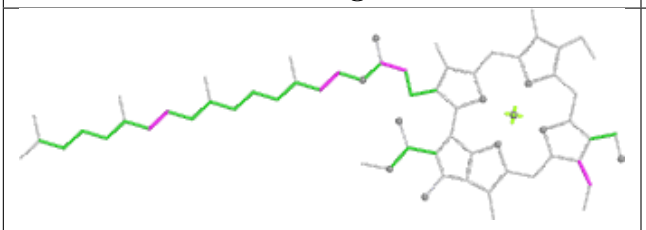
**Ligand CHL Z2 607**



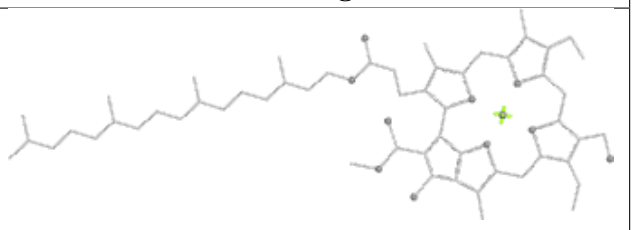
Bond lengths



Bond angles

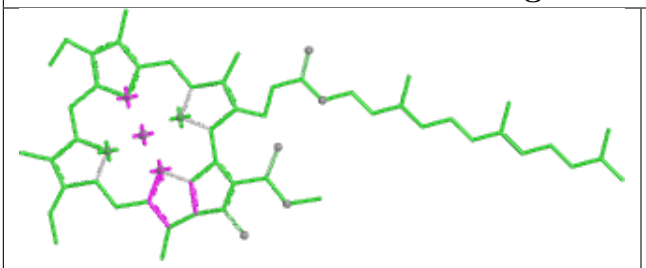


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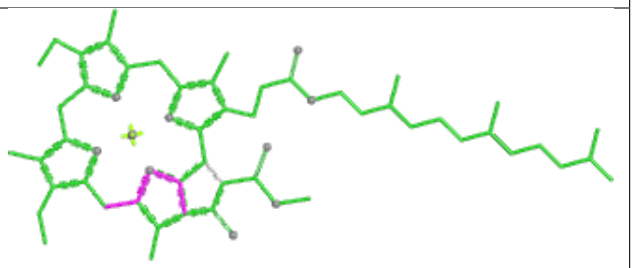


Rings

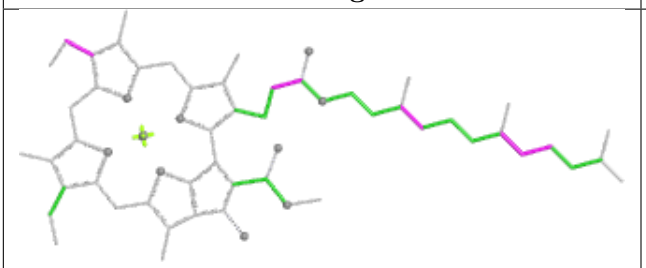
**Ligand CLA B 834**



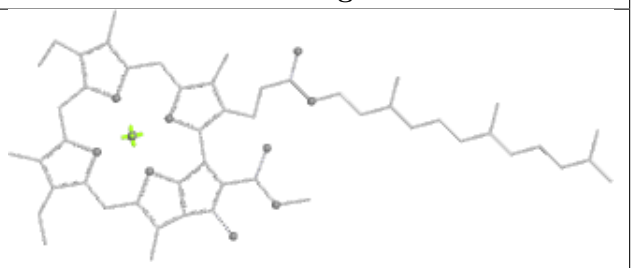
Bond lengths



Bond angles

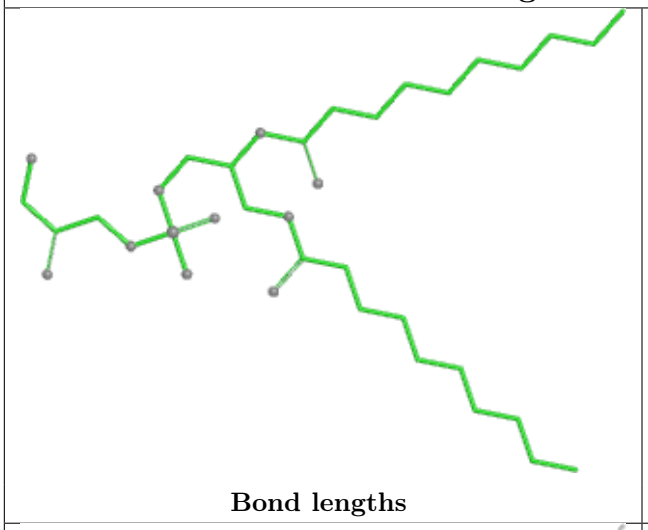


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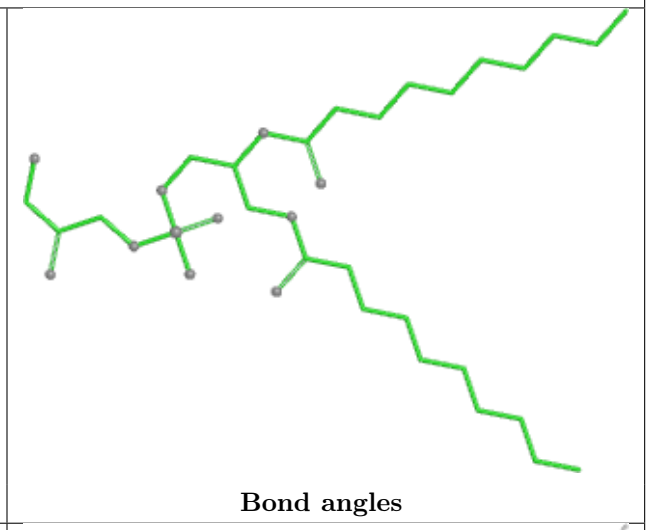


Rings

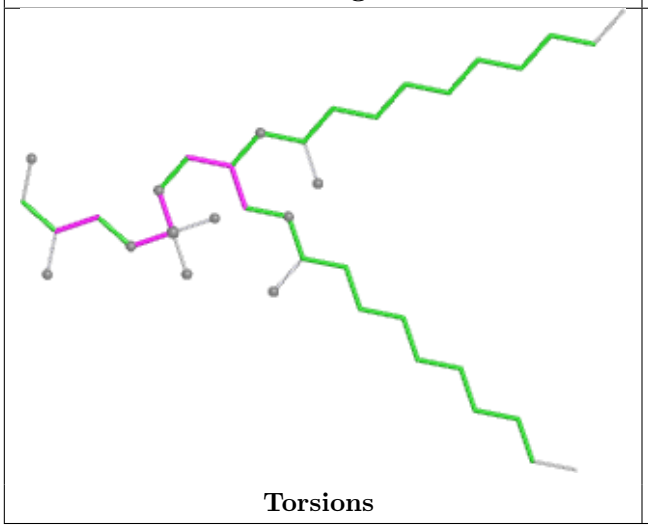
## Ligand LHG 52 623



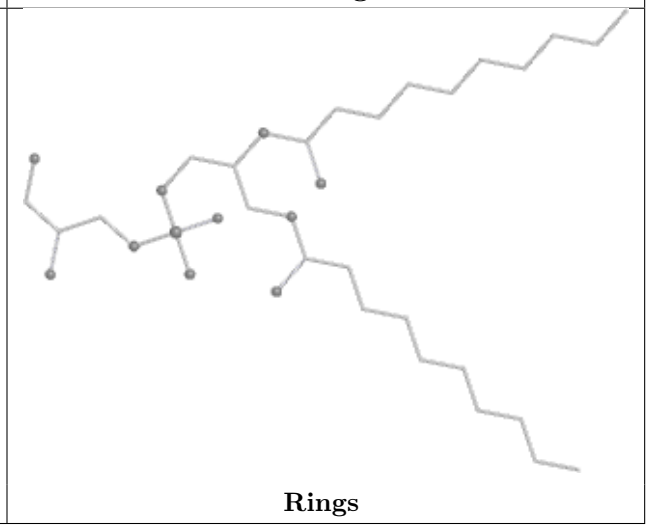
Bond lengths



Bond angles

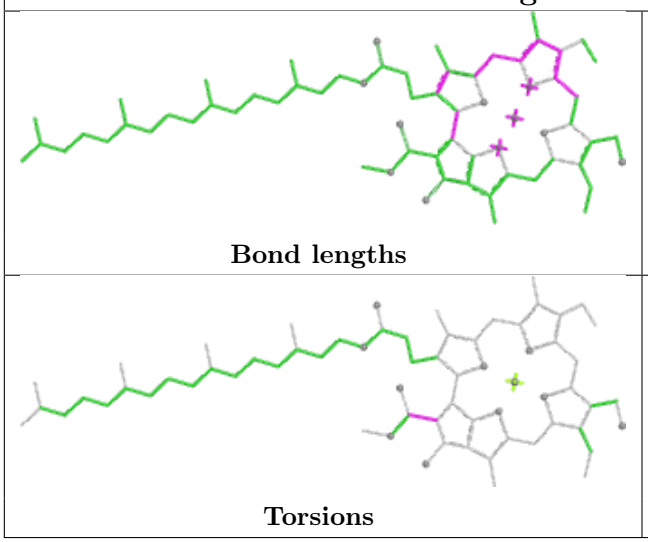


Torsions

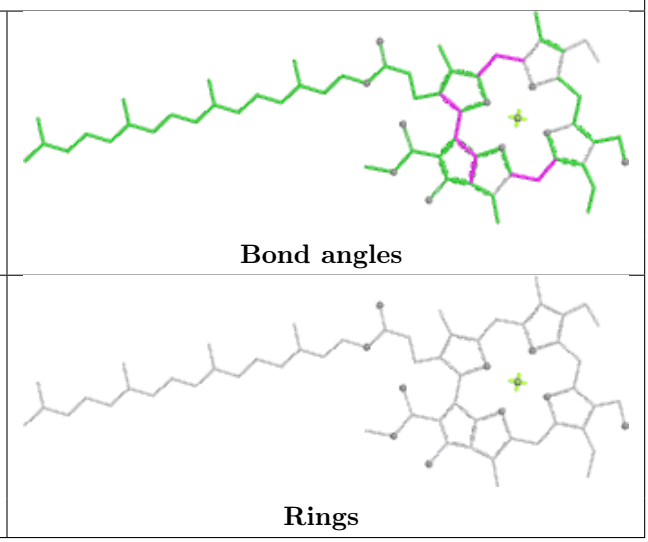


Rings

## Ligand CHL 42 607



Bond lengths



Bond angles

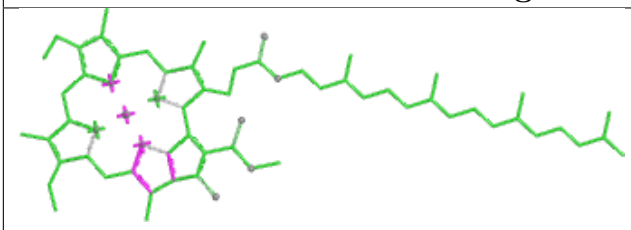


Torsions

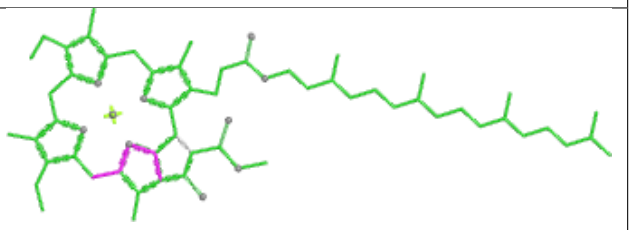


Rings

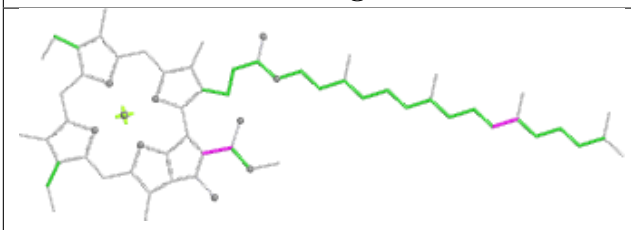
## Ligand CLA A2 804



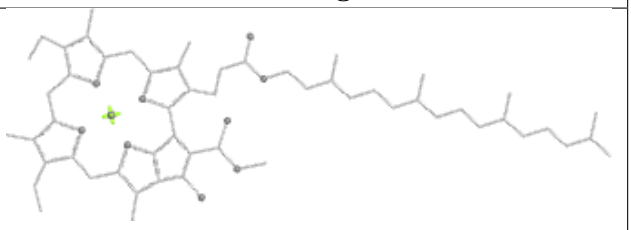
Bond lengths



Bond angles

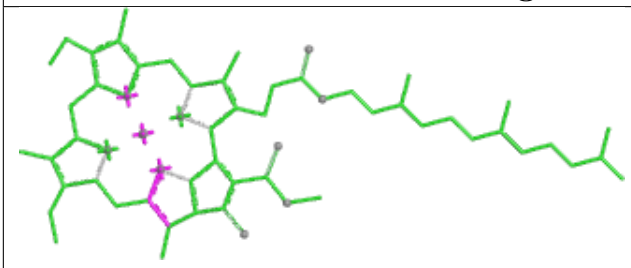


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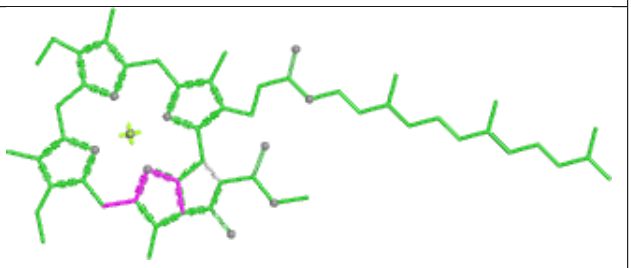


Rings

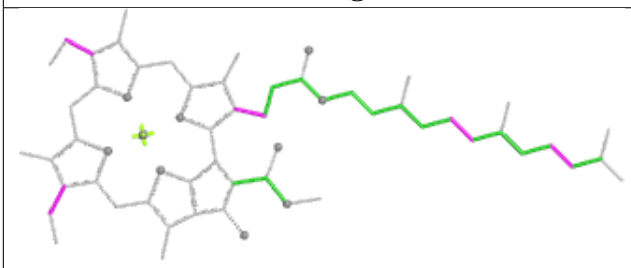
## Ligand CLA Z2 611



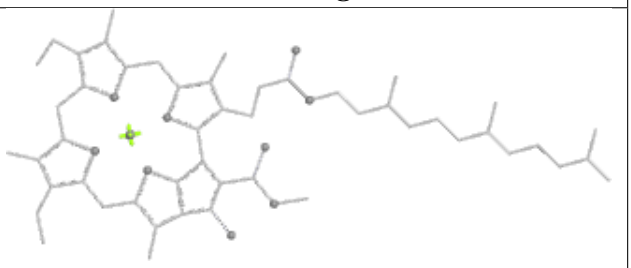
Bond lengths



Bond angles



Torsions



Rings

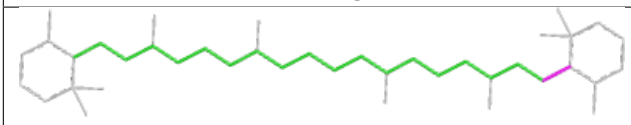
## Ligand BCR 32 719



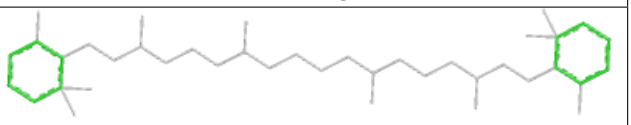
Bond lengths



Bond angles

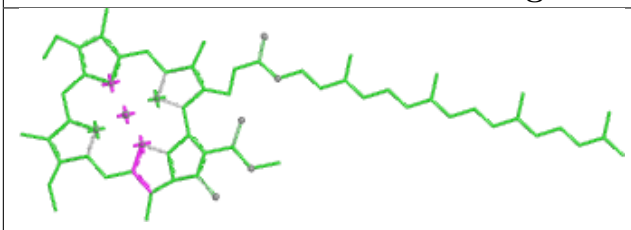


Torsions

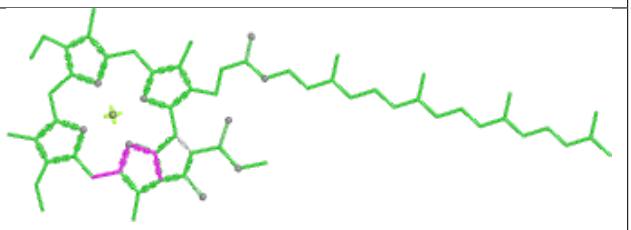


Rings

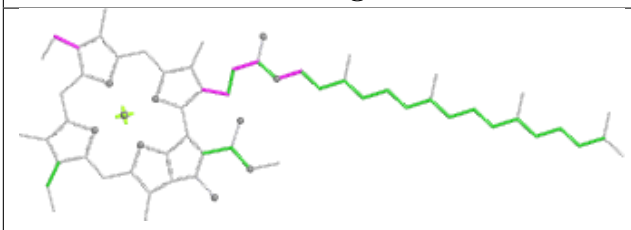
## Ligand CLA F 304



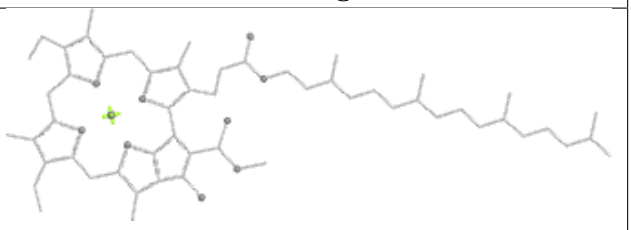
Bond lengths



Bond angles

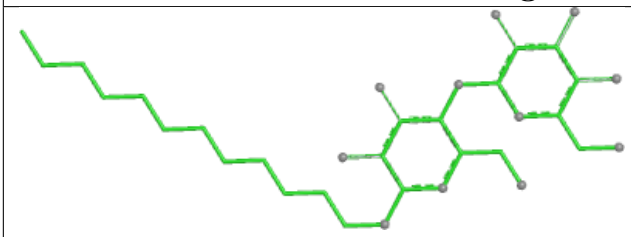


Torsions

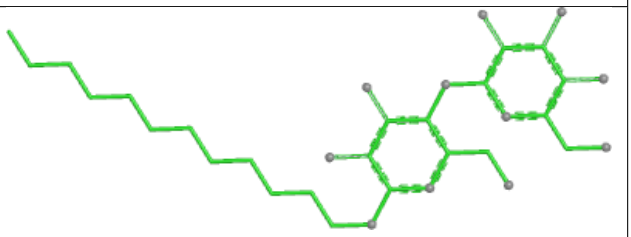


Rings

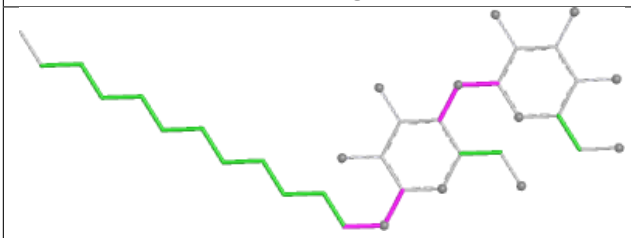
## Ligand LMU A 863



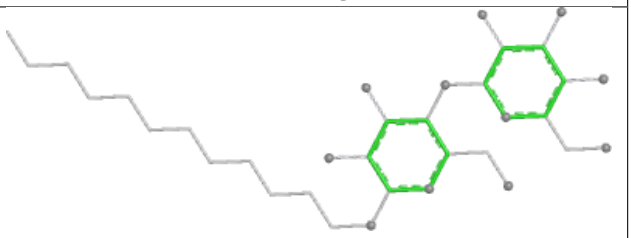
Bond lengths



Bond angles

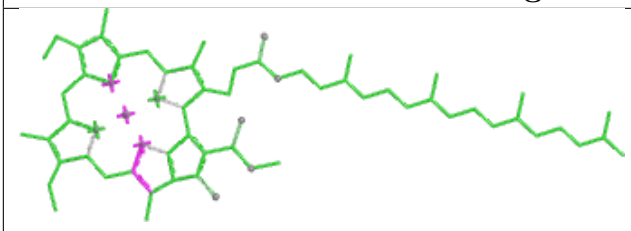


Torsions

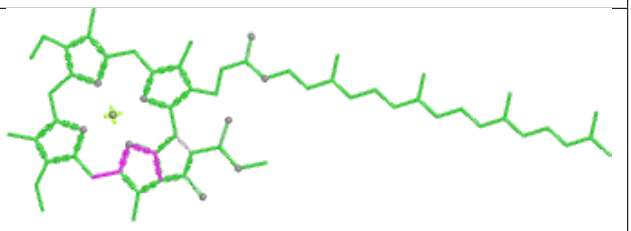


Rings

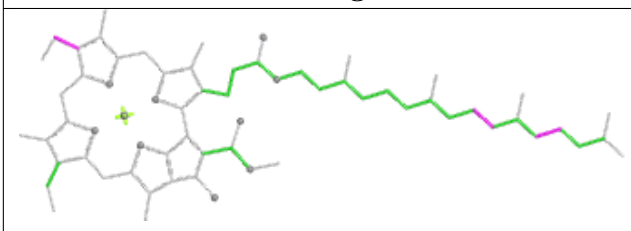
## Ligand CLA B 818



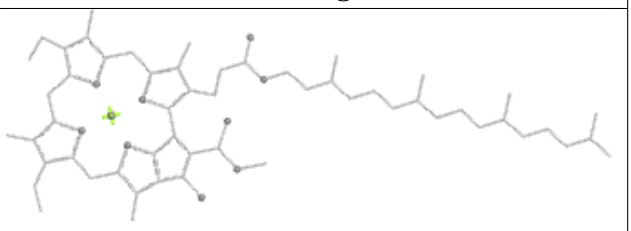
Bond lengths



Bond angles

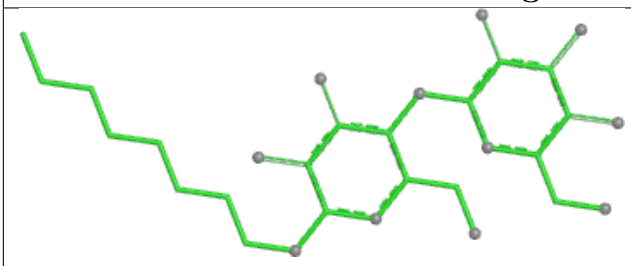


Torsions

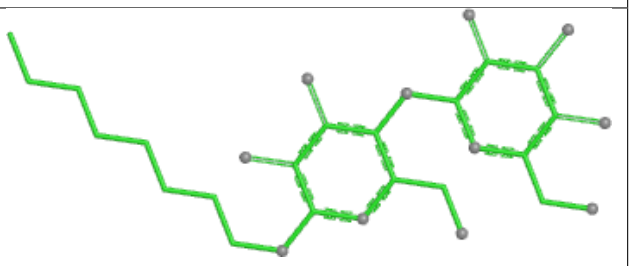


Rings

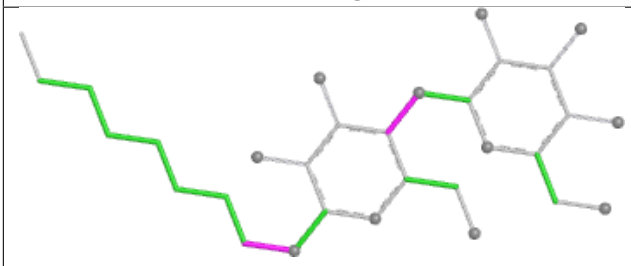
## Ligand LMU Z 622



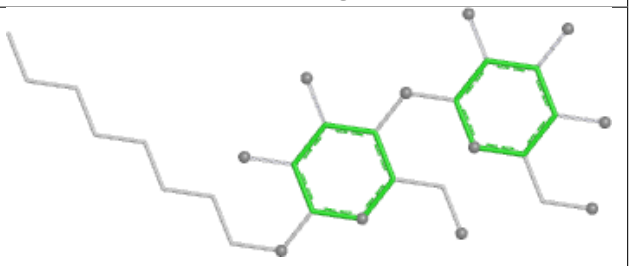
Bond lengths



Bond angles

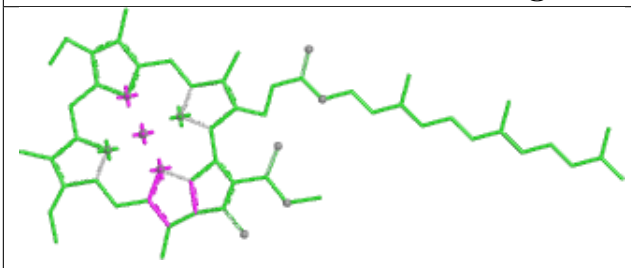


Torsions

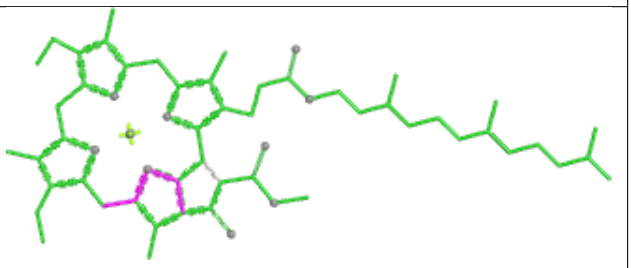


Rings

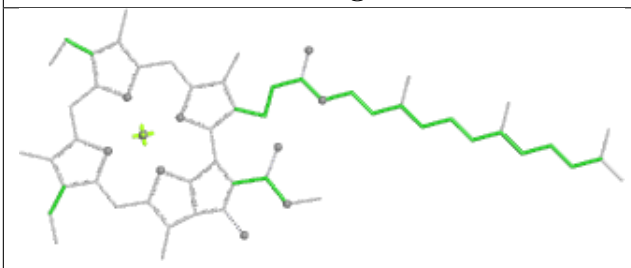
## Ligand CLA 9 610



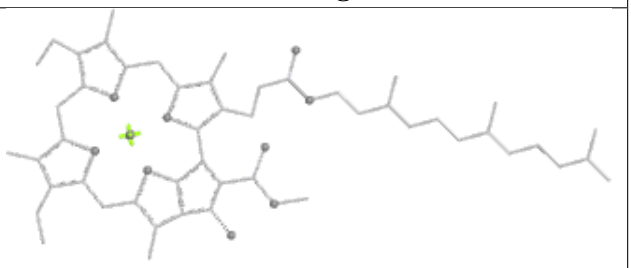
Bond lengths



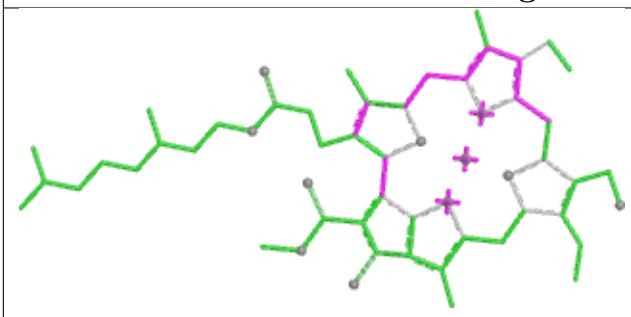
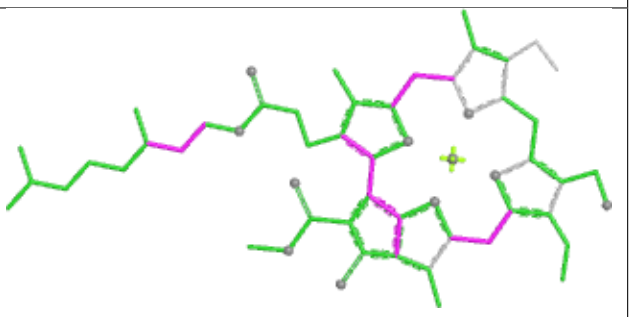
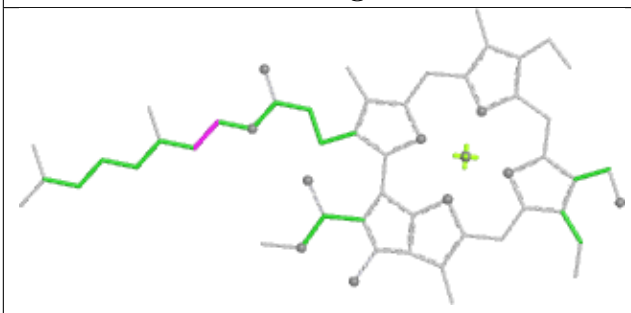
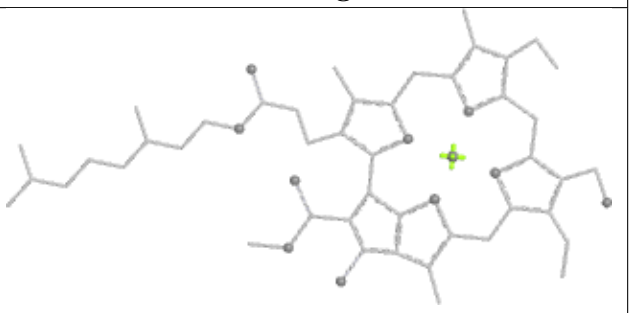
Bond angles

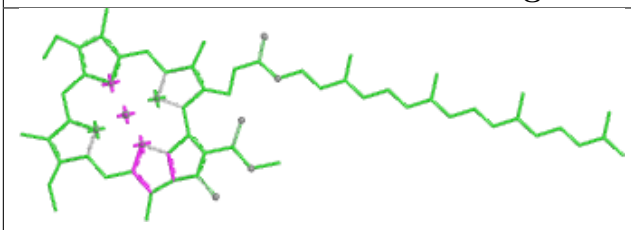
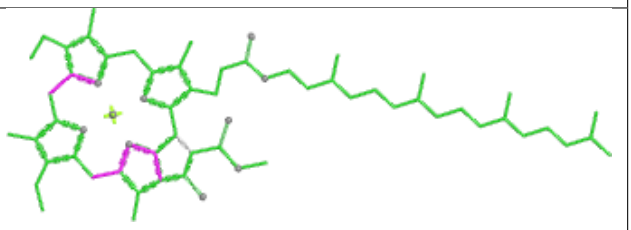
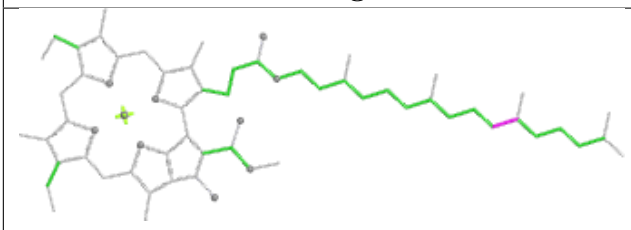
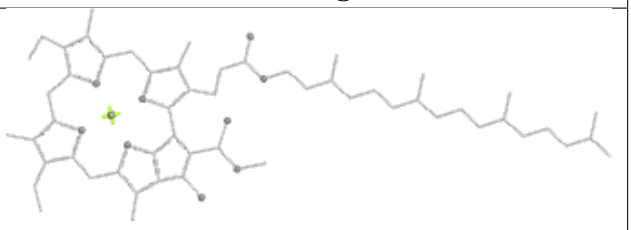


Torsions

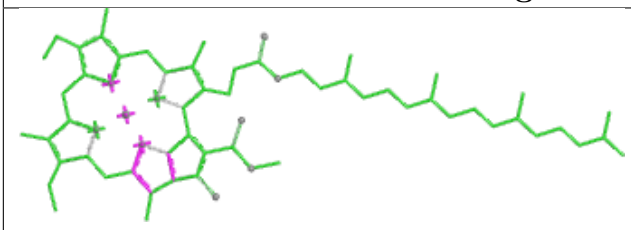


Rings

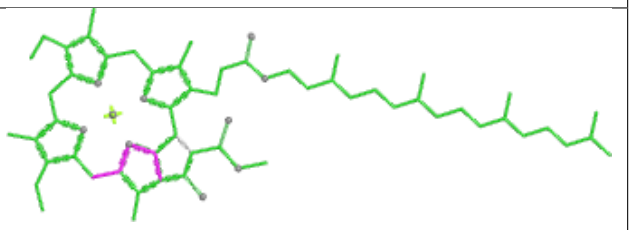
| Ligand CHL 42 606 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA A 839 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

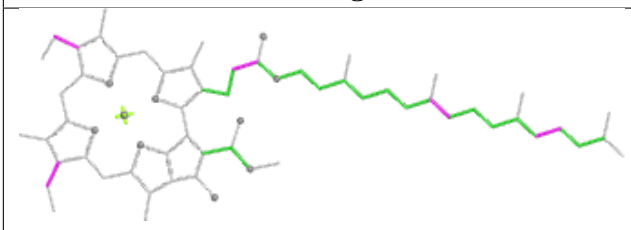
## Ligand CLA B2 817



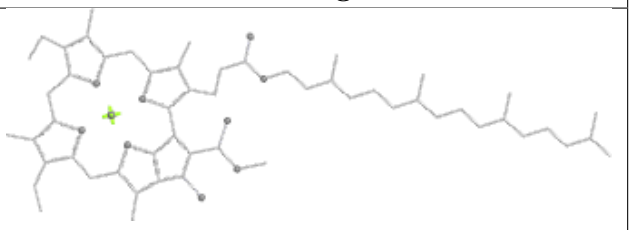
Bond lengths



Bond angles

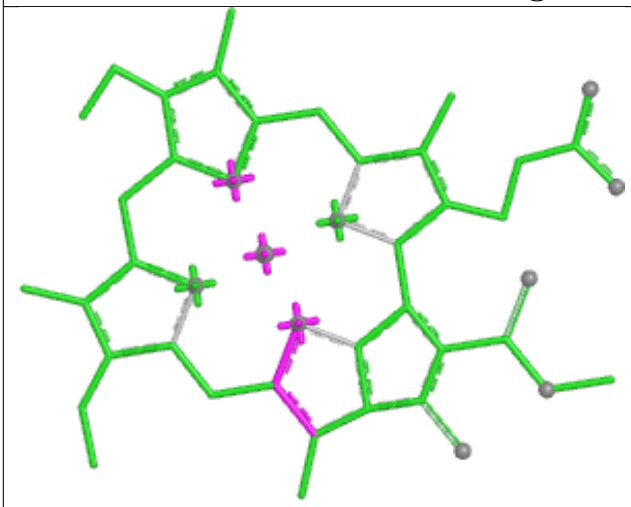


Torsions

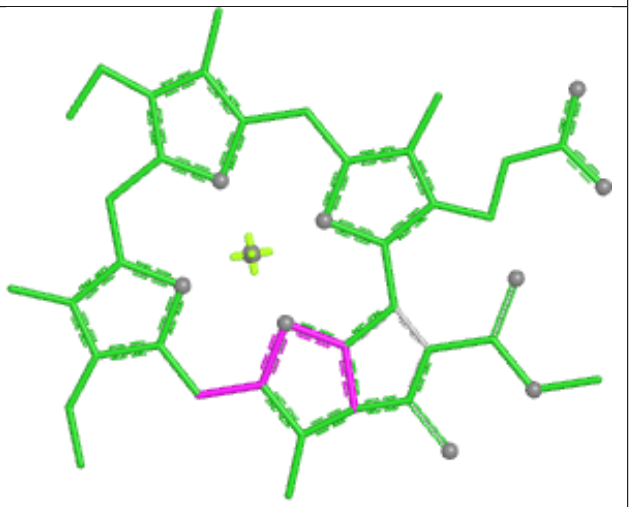


Rings

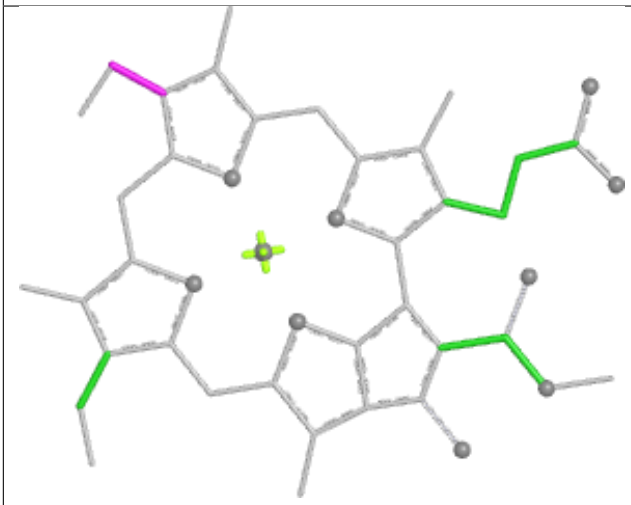
## Ligand CLA 7 609



Bond lengths



Bond angles

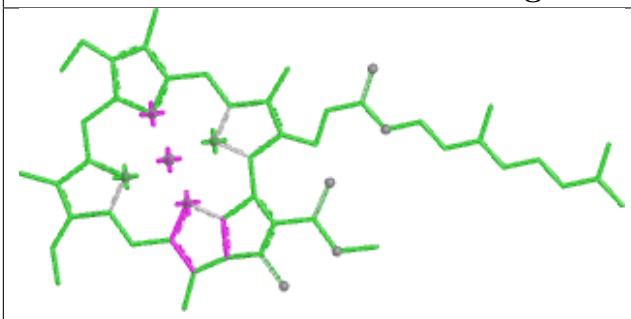


Torsions

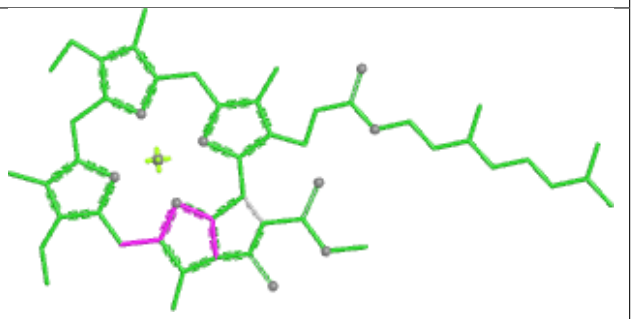


Rings

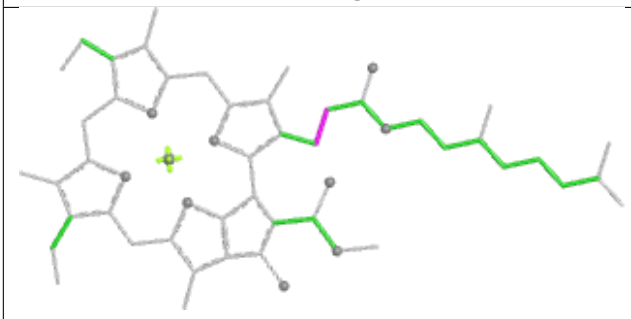
## Ligand CLA B 831



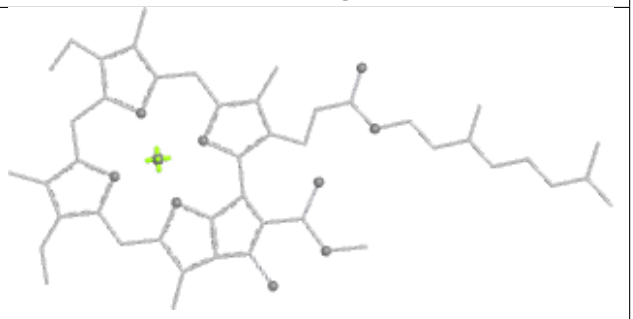
Bond lengths



Bond angles

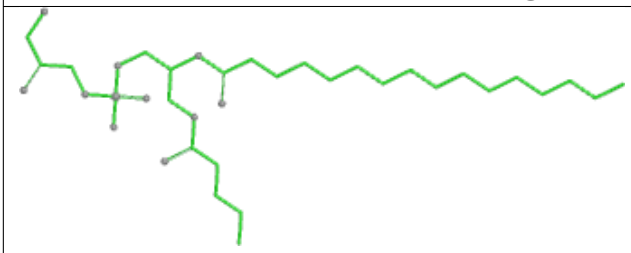


Torsions

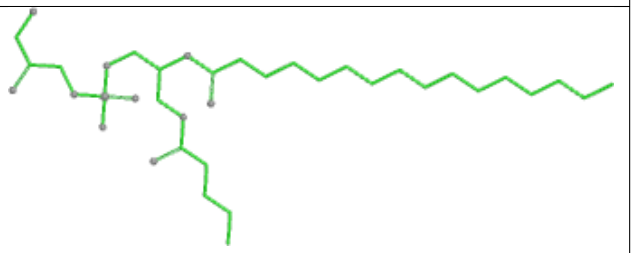


Rings

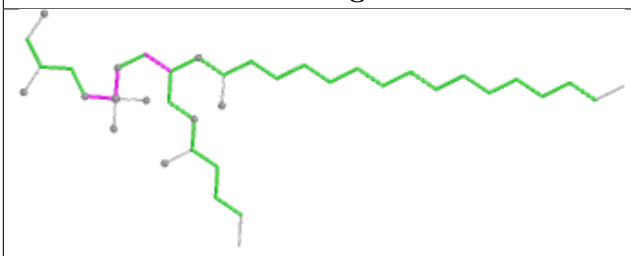
## Ligand LHG A 847



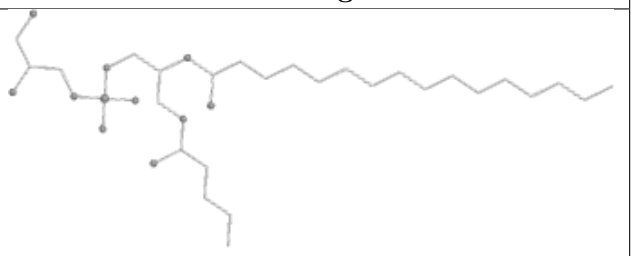
Bond lengths



Bond angles

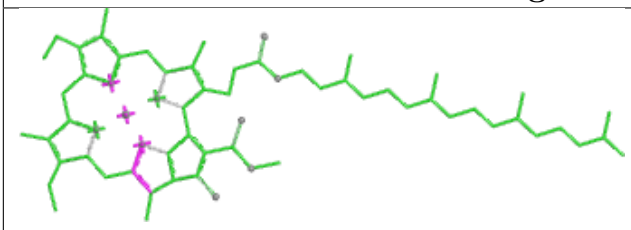


Torsions

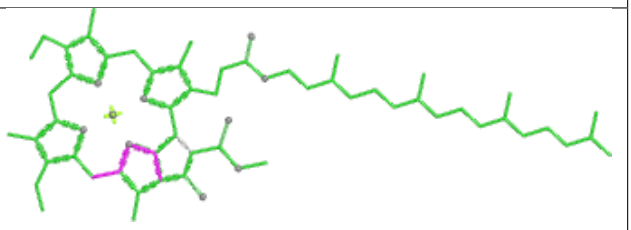


Rings

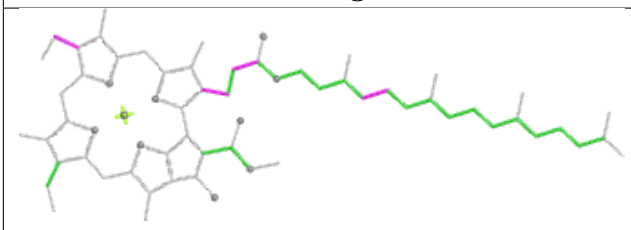
## Ligand CLA 3 611



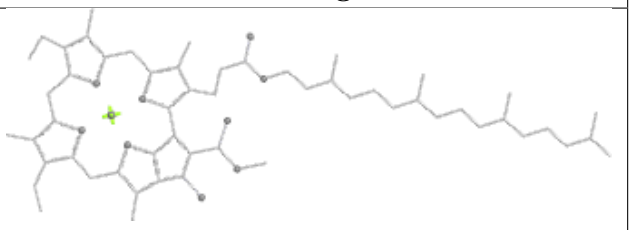
Bond lengths



Bond angles

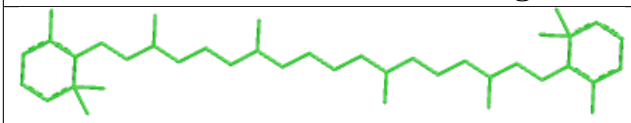


Torsions

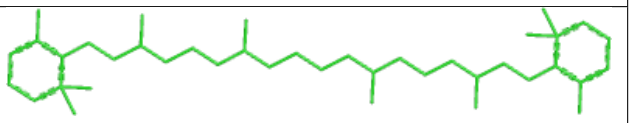


Rings

## Ligand BCR B2 844



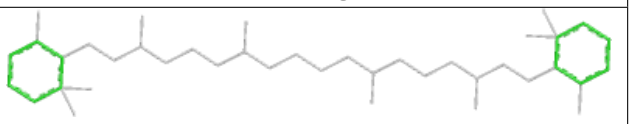
Bond lengths



Bond angles



Torsions

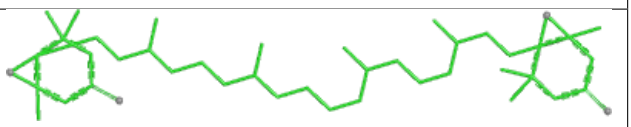


Rings

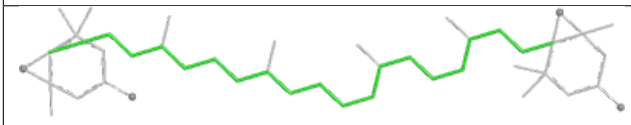
## Ligand XAT 5 624



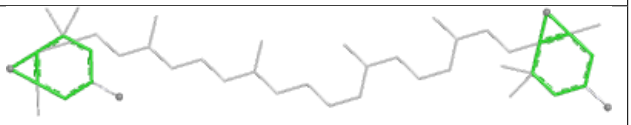
Bond lengths



Bond angles

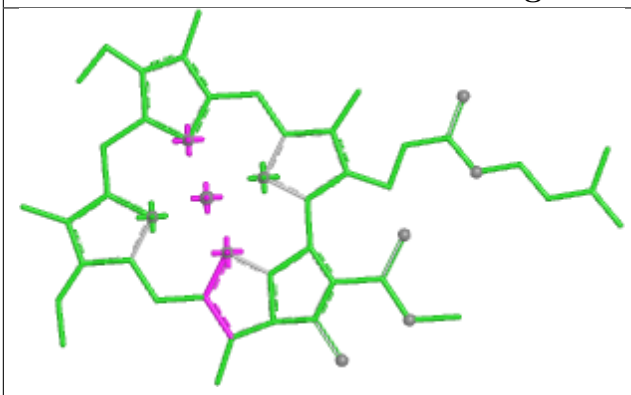


Torsions

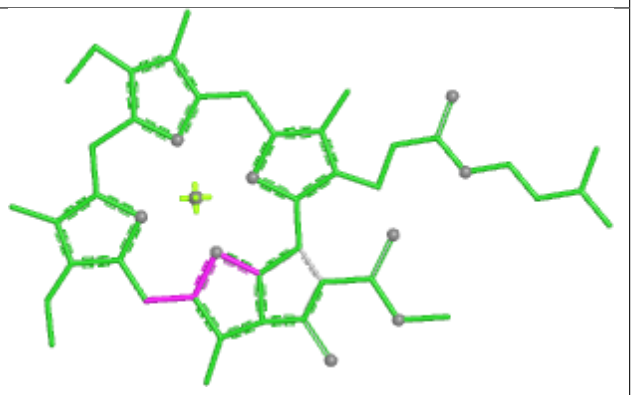


Rings

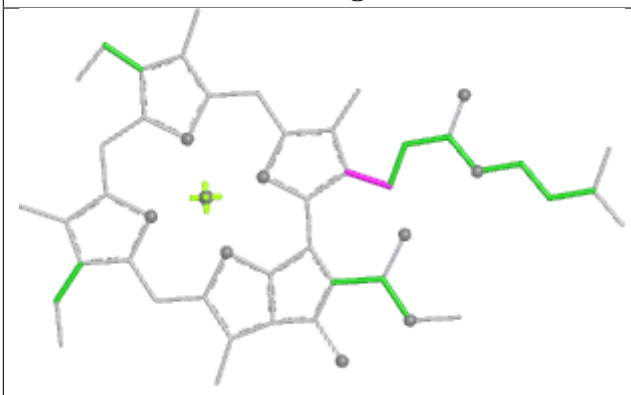
## Ligand CLA B 838



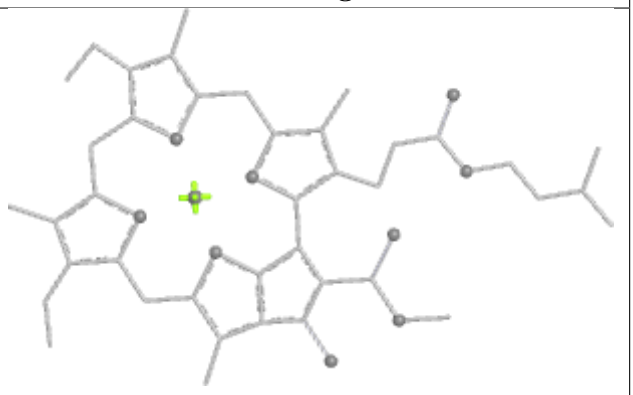
Bond lengths



Bond angles

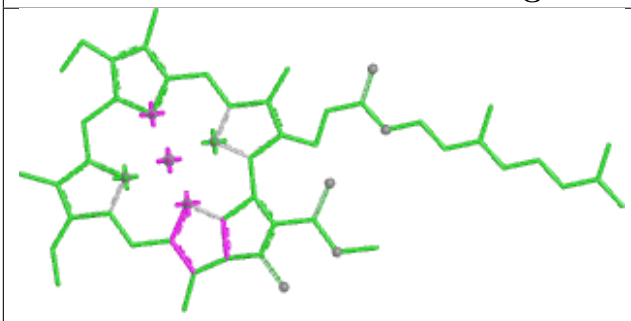


Torsions

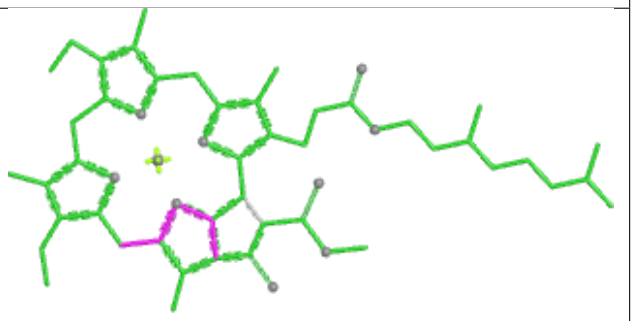


Rings

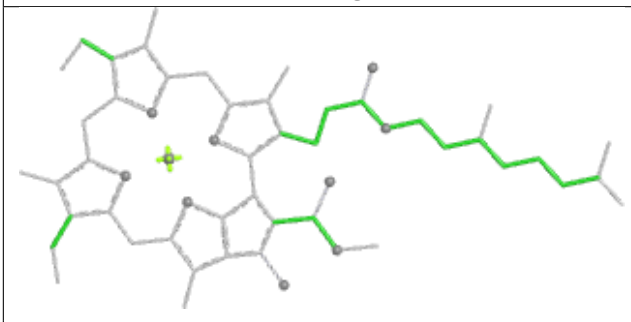
## Ligand CLA A 832



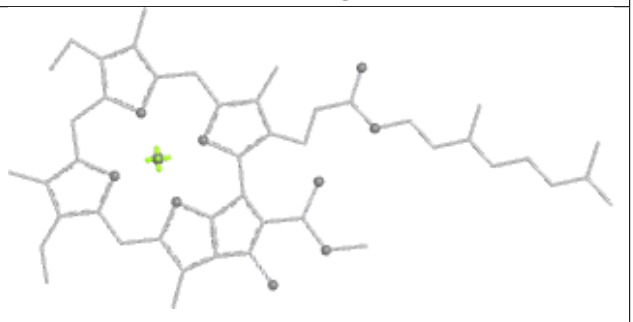
Bond lengths



Bond angles

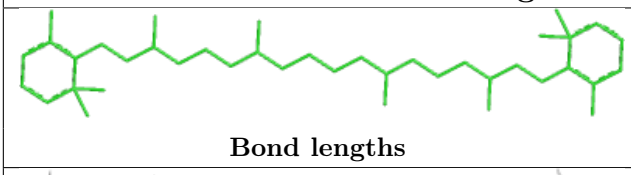


Torsions

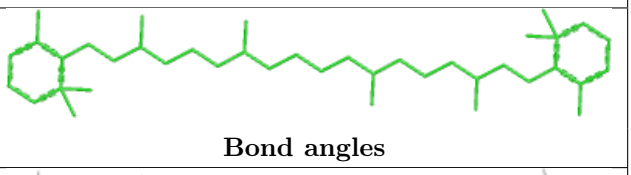


Rings

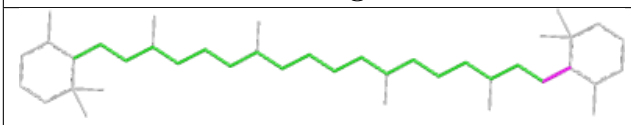
## Ligand BCR 62 623



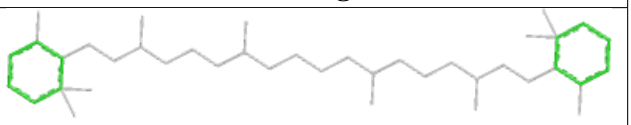
Bond lengths



Bond angles



Torsions

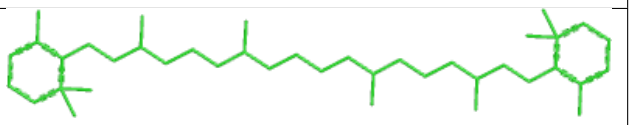


Rings

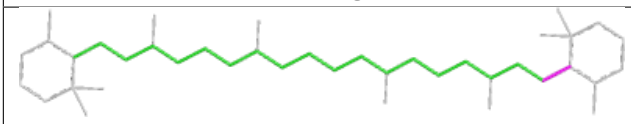
## Ligand BCR 72 623



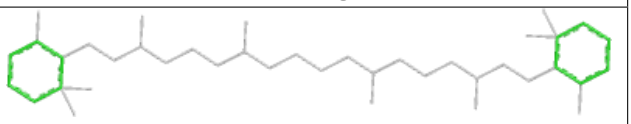
Bond lengths



Bond angles

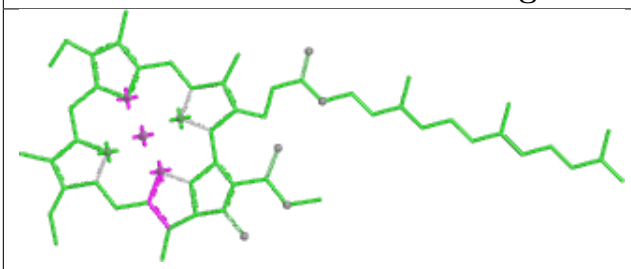


Torsions

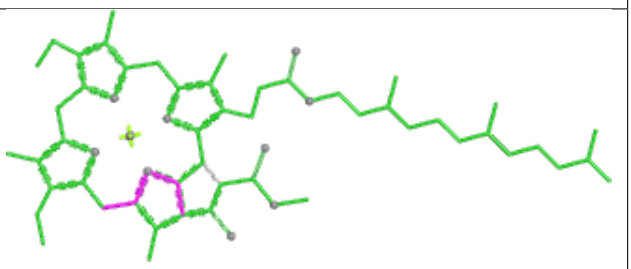


Rings

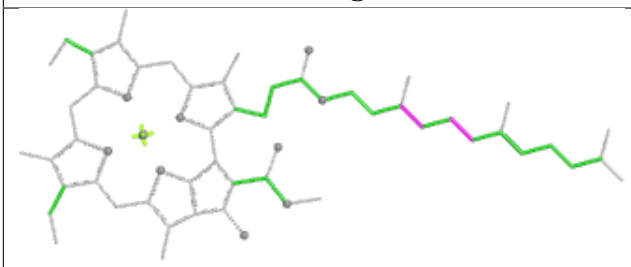
## Ligand CLA 42 610



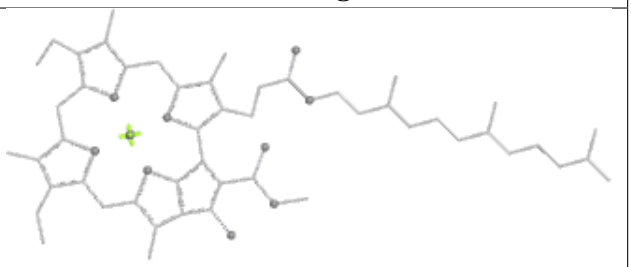
Bond lengths



Bond angles

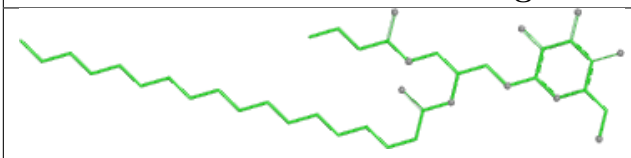


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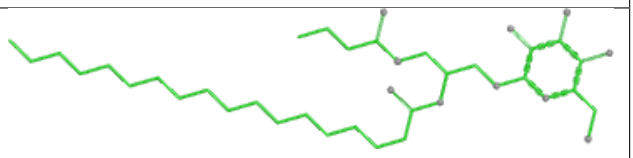


Rings

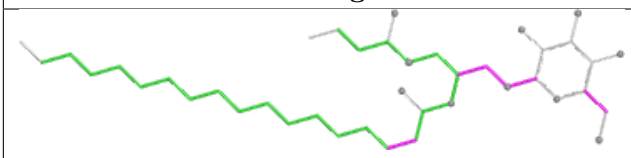
**Ligand LMG 42 624**



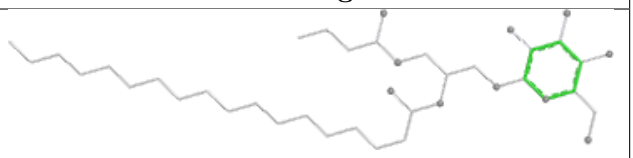
Bond lengths



Bond angles

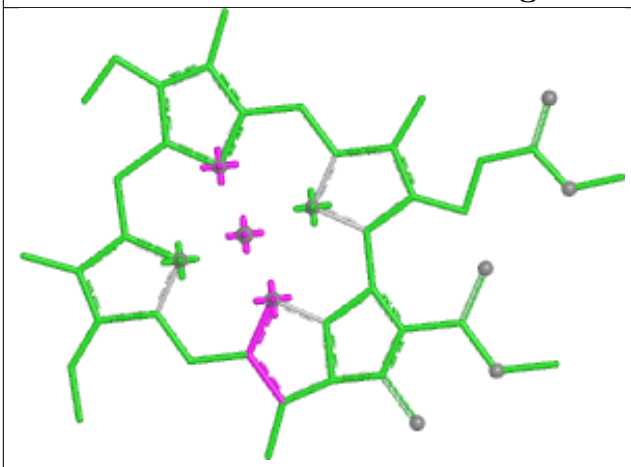


Torsions

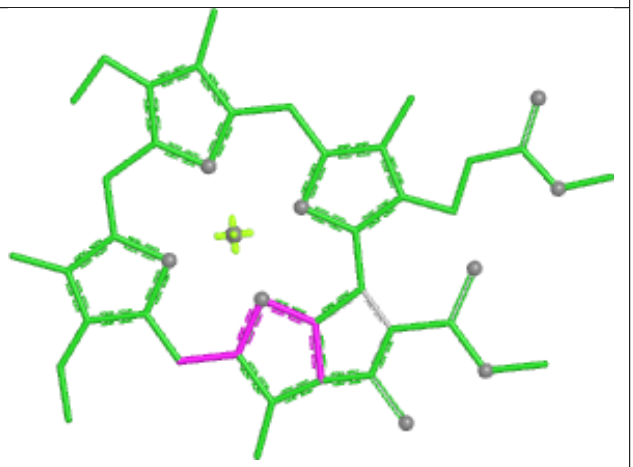


Rings

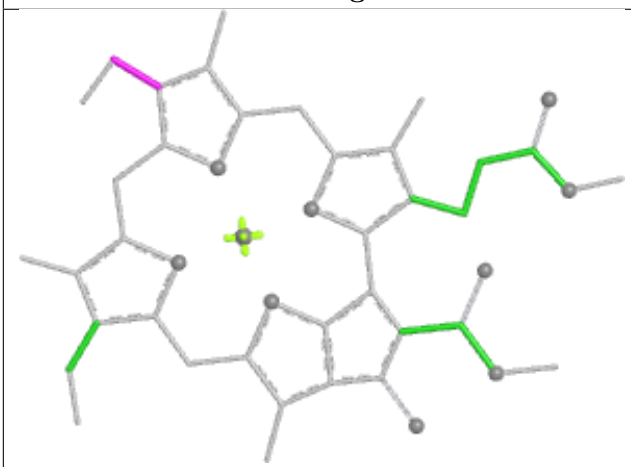
**Ligand CLA 92 601**



Bond lengths



Bond angles

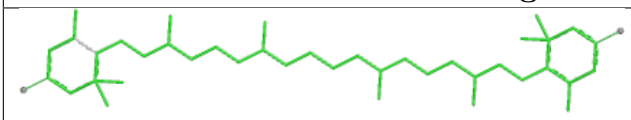


Torsions

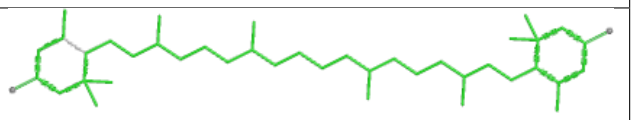


Rings

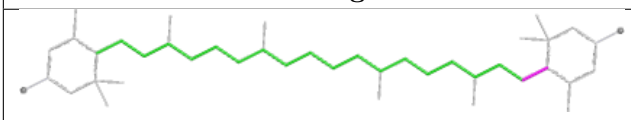
## Ligand LUT 12 619



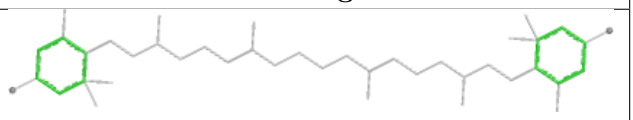
Bond lengths



Bond angles

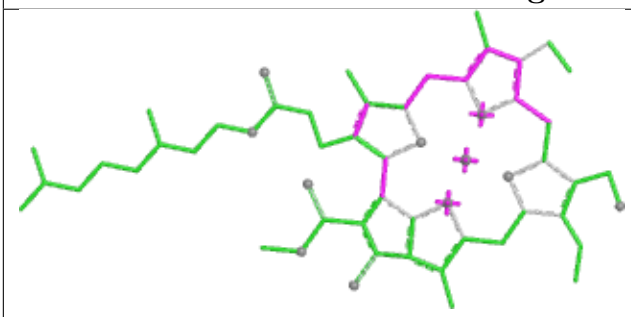


Torsions

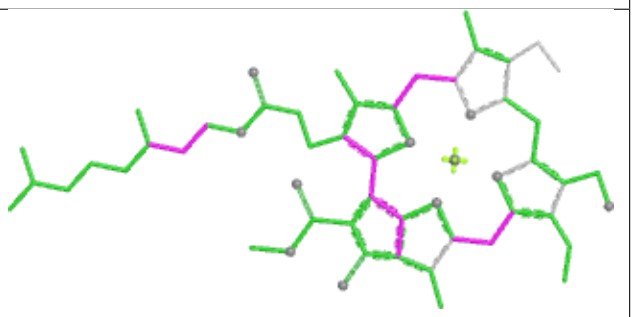


Rings

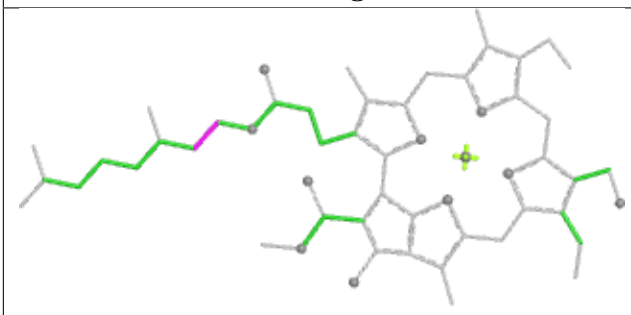
## Ligand CHL 4 606



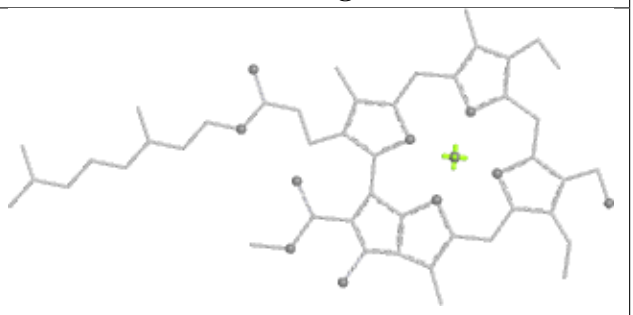
Bond lengths



Bond angles

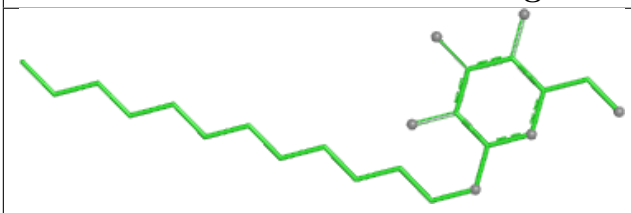


Torsions

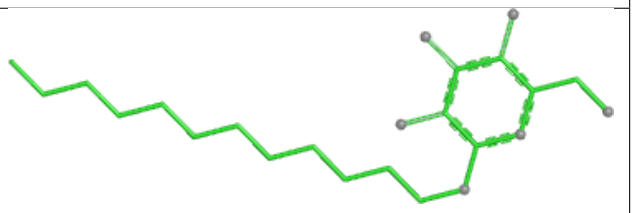


Rings

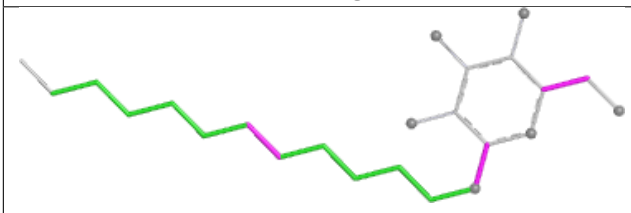
## Ligand LMU 9 624



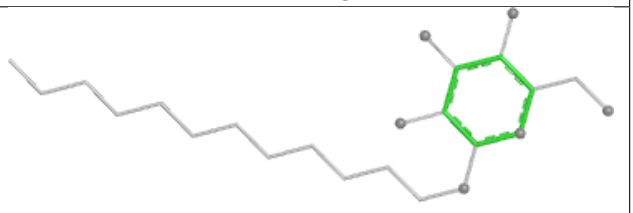
Bond lengths



Bond angles

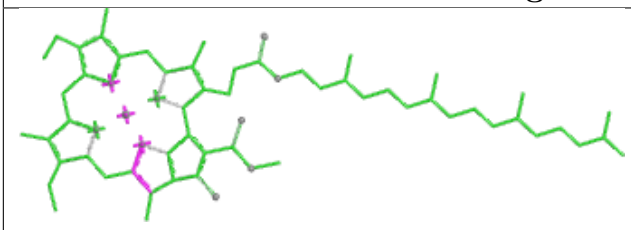


Torsions

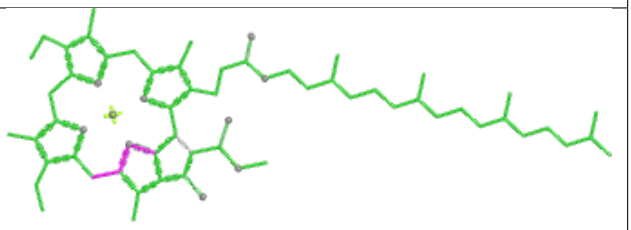


Rings

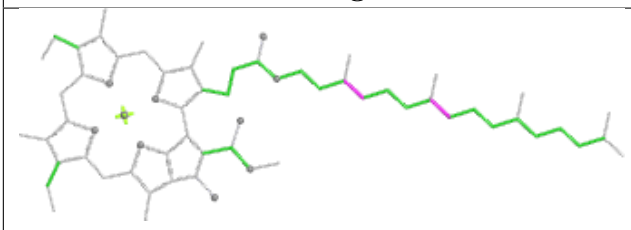
## Ligand CLA F 301



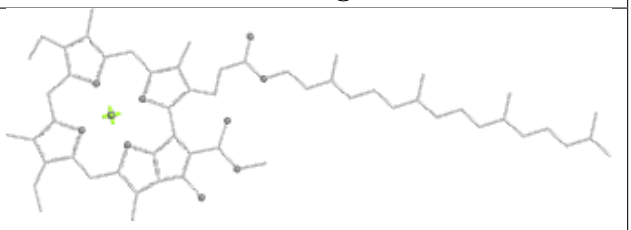
Bond lengths



Bond angles

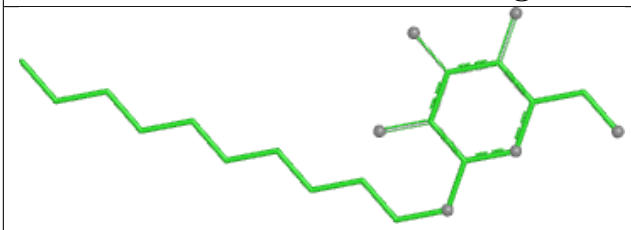


Torsions

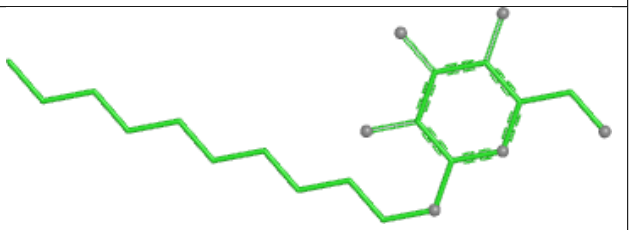


Rings

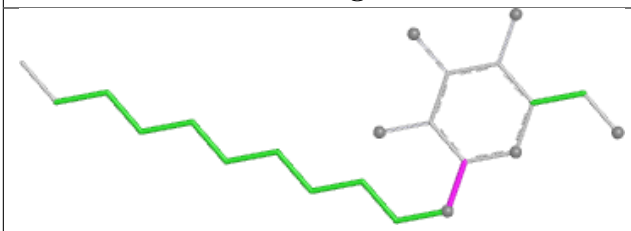
## Ligand LMU Z2 621



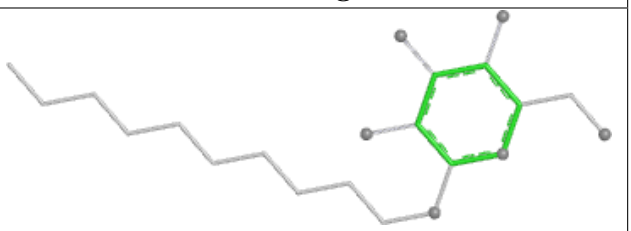
Bond lengths



Bond angles

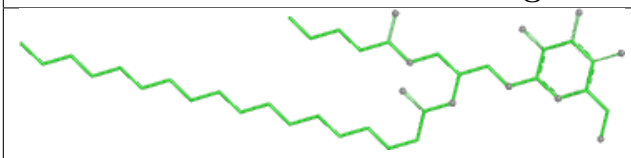


Torsions

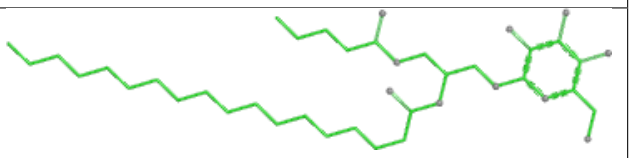


Rings

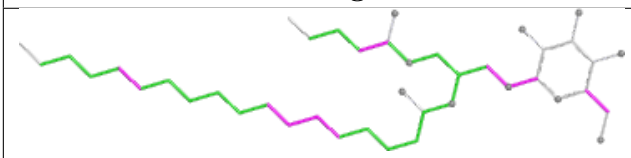
## Ligand LMG 8 629



Bond lengths



Bond angles

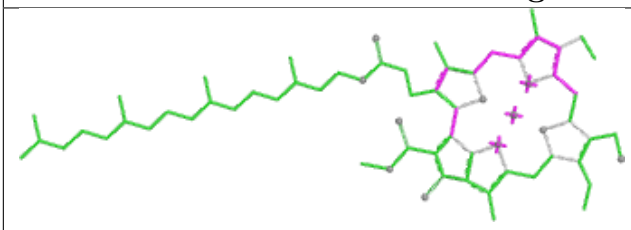


Torsions

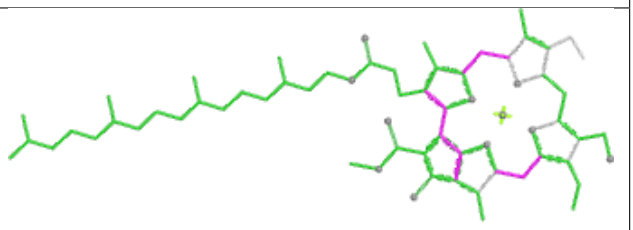


Rings

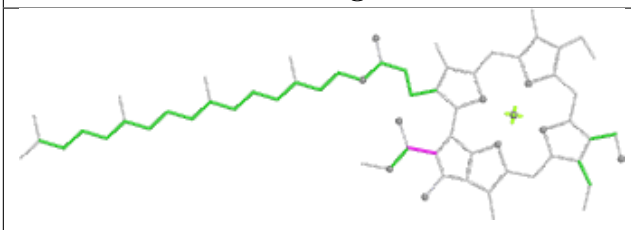
## Ligand CHL 4 607



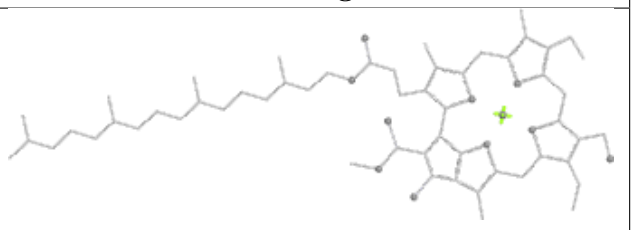
Bond lengths



Bond angles



Torsions

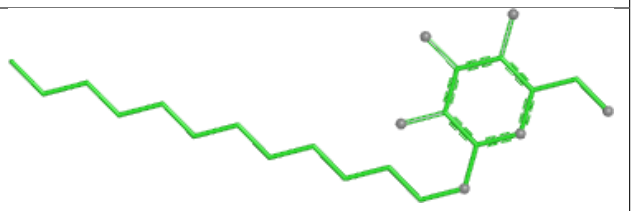


Rings

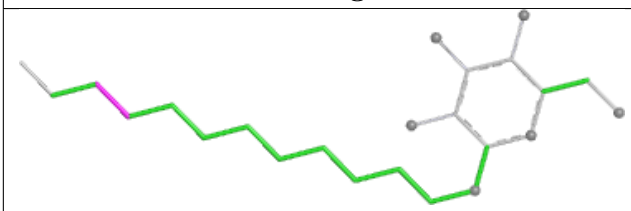
## Ligand LMU 1 623



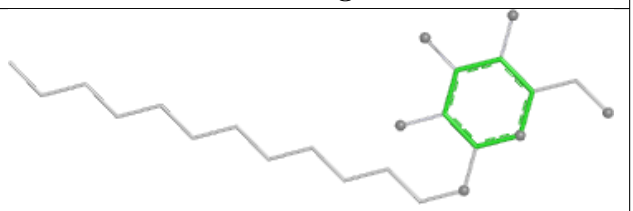
Bond lengths



Bond angles

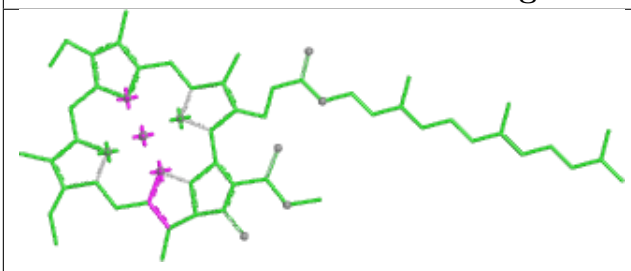


Torsions

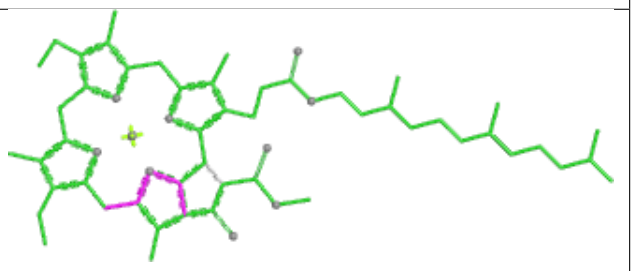


Rings

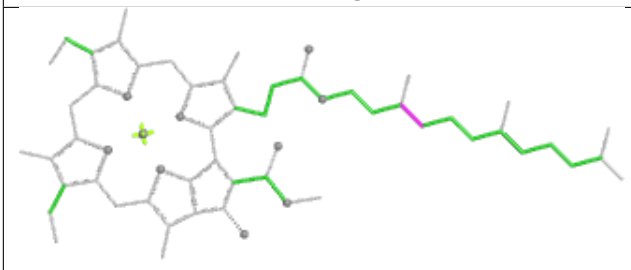
## Ligand CLA 52 610



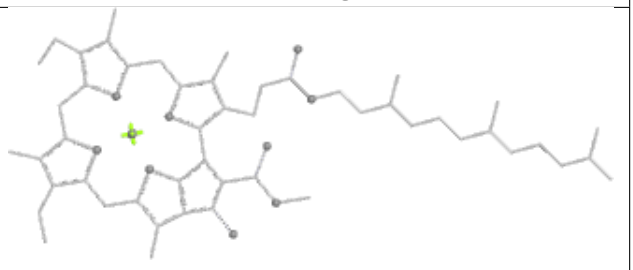
Bond lengths



Bond angles

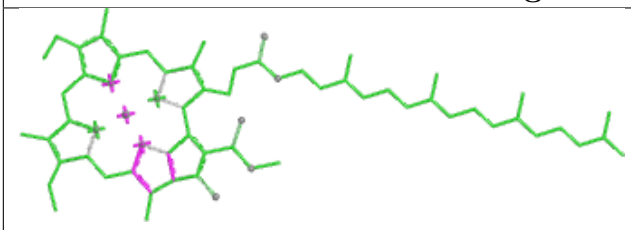


Torsions

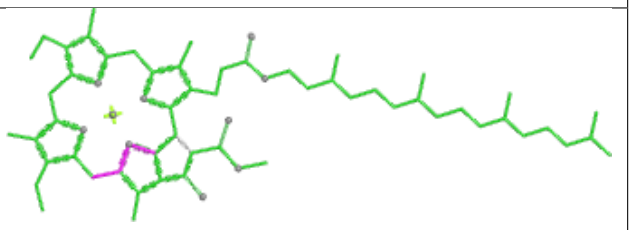


Rings

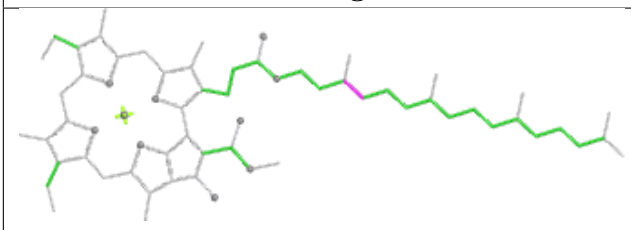
## Ligand CLA B 812



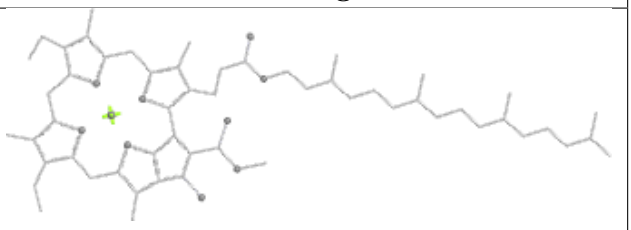
Bond lengths



Bond angles

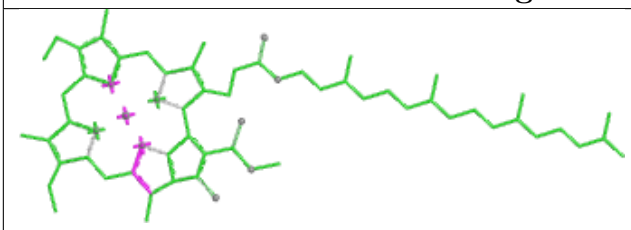


Torsions

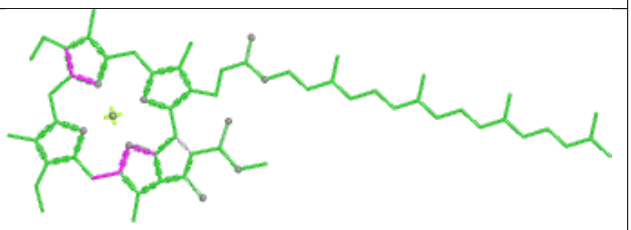


Rings

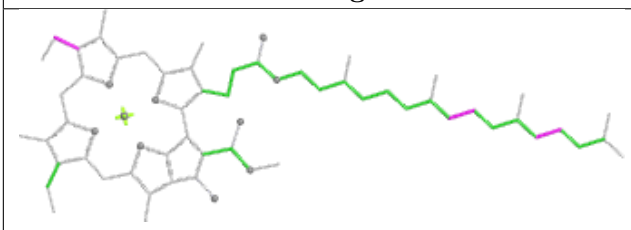
## Ligand CLA B2 826



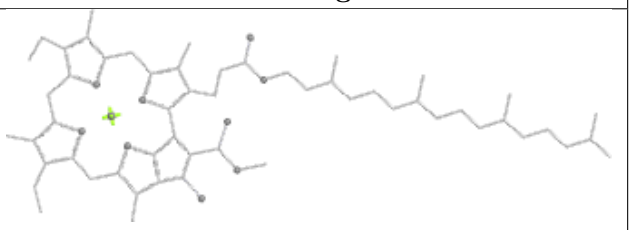
Bond lengths



Bond angles



Torsions



Rings

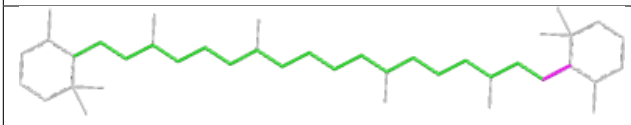
## Ligand BCR 3 718



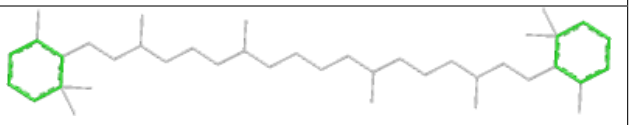
Bond lengths



Bond angles

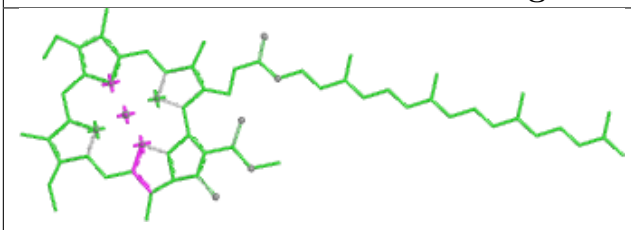


Torsions

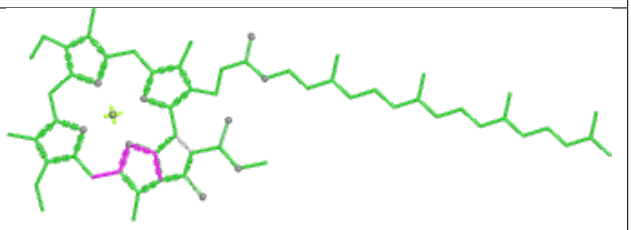


Rings

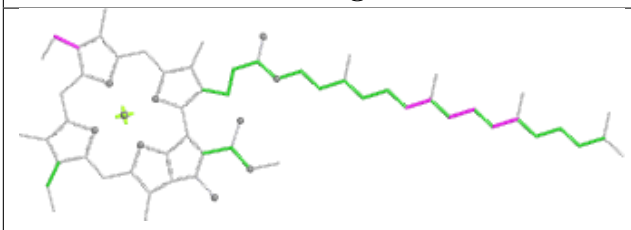
## Ligand CLA 7 611



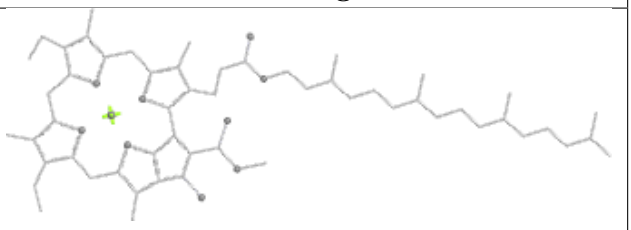
Bond lengths



Bond angles

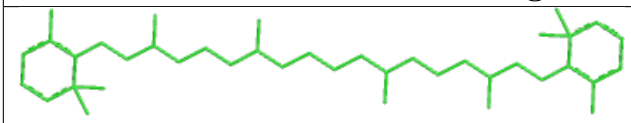


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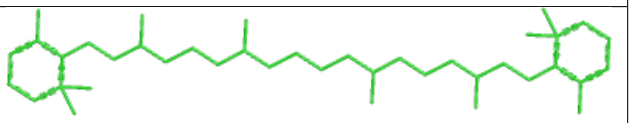


Rings

## Ligand BCR 6 623



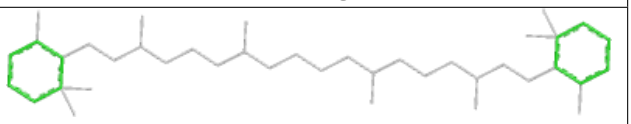
Bond lengths



Bond angles

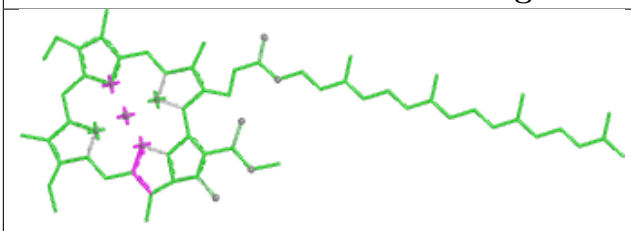


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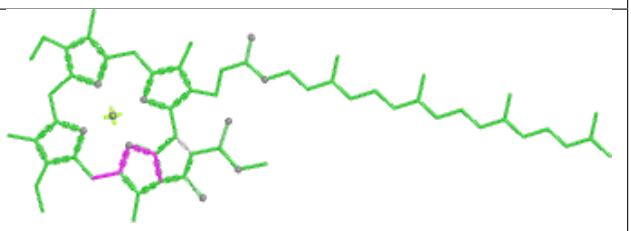


Rings

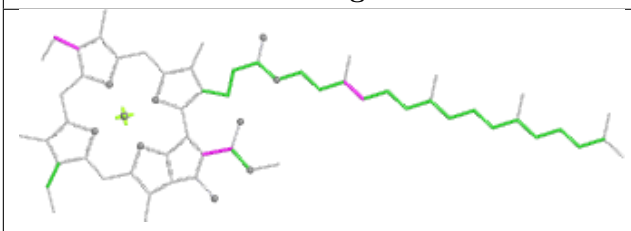
## Ligand CLA A2 835



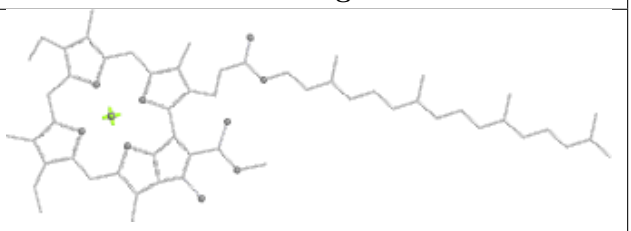
Bond lengths



Bond angles

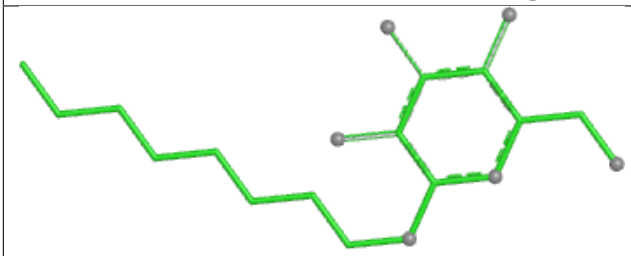


Torsions

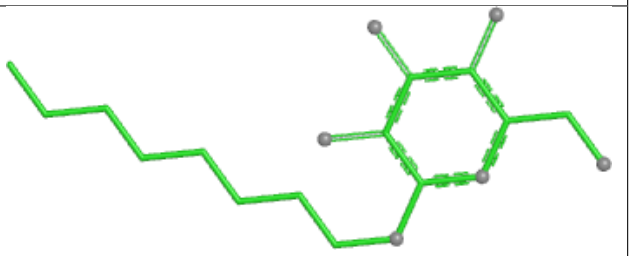


Rings

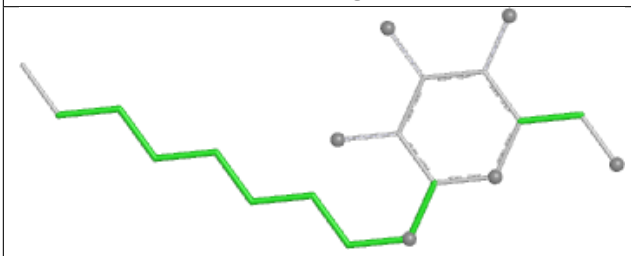
## Ligand LMU 4 626



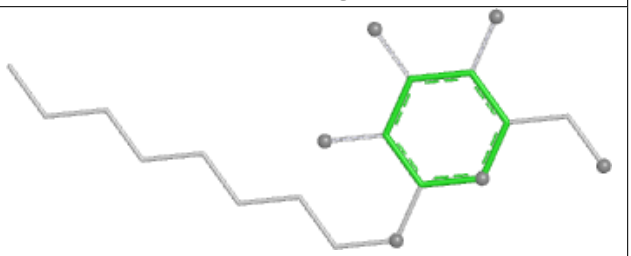
Bond lengths



Bond angles

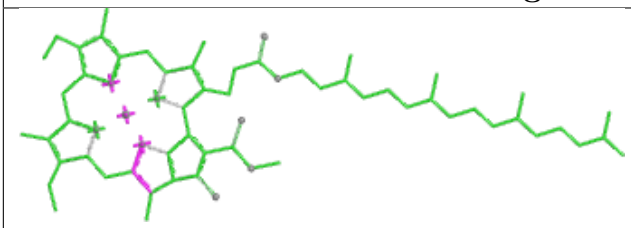


Torsions

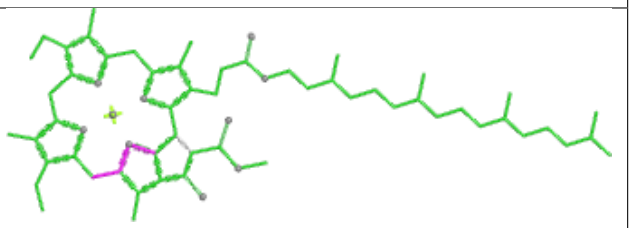


Rings

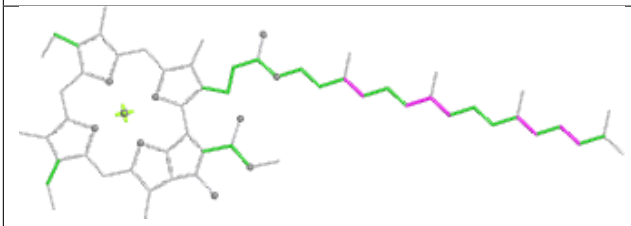
## Ligand CLA A 840



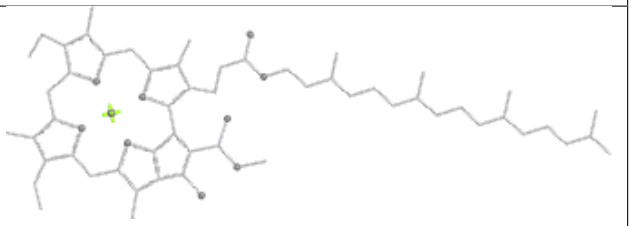
Bond lengths



Bond angles

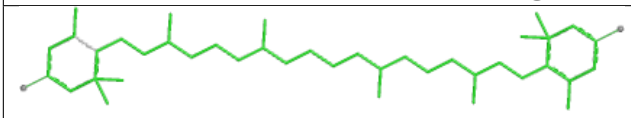


Torsions

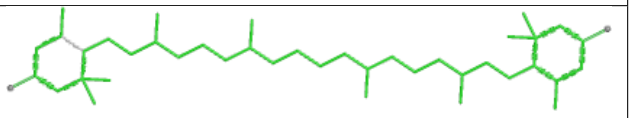


Rings

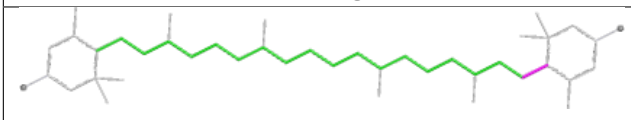
## Ligand LUT 1 617



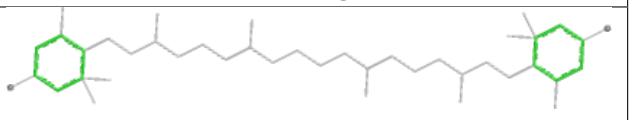
Bond lengths



Bond angles

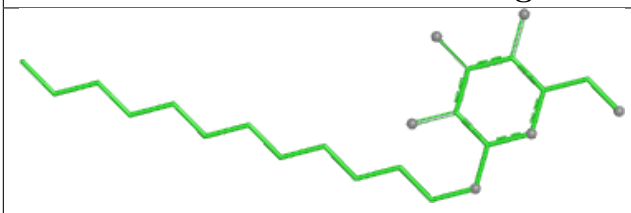


Torsions

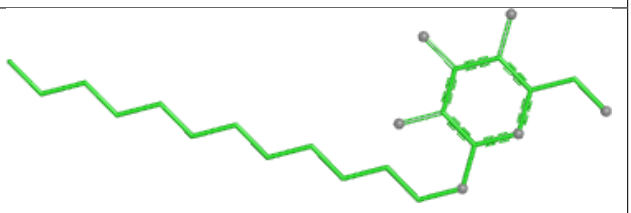


Rings

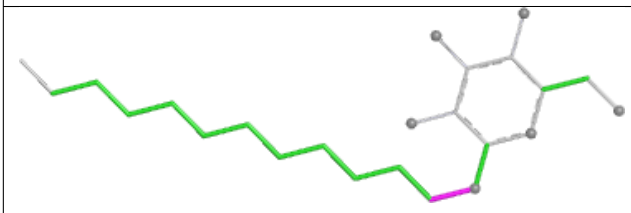
## Ligand LMU 52 627



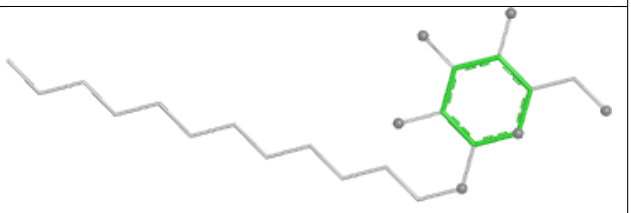
Bond lengths



Bond angles

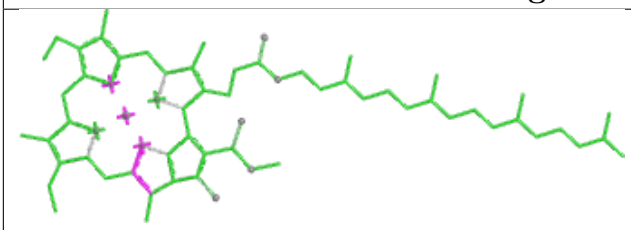


Torsions

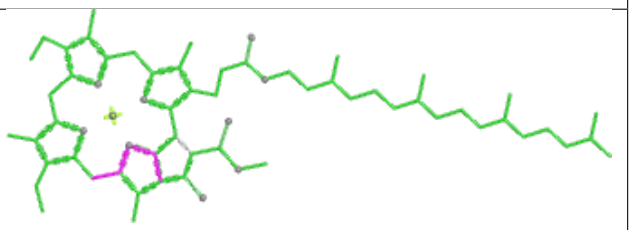


Rings

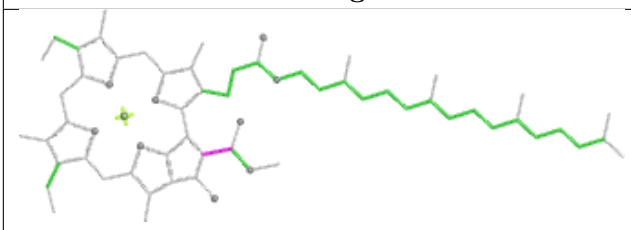
## Ligand CLA 6 602



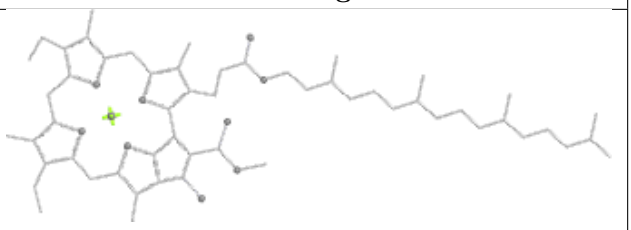
Bond lengths



Bond angles

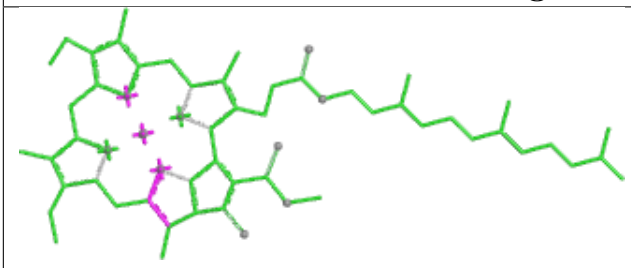


Torsions

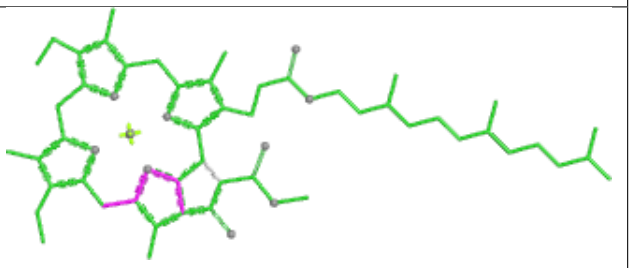


Rings

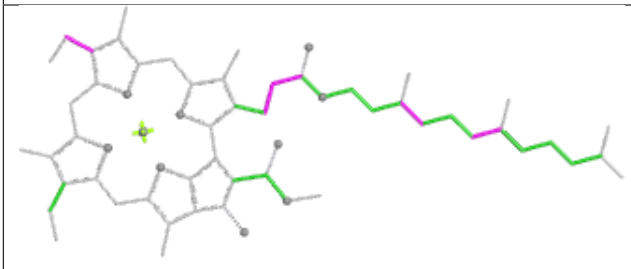
## Ligand CLA 1 614



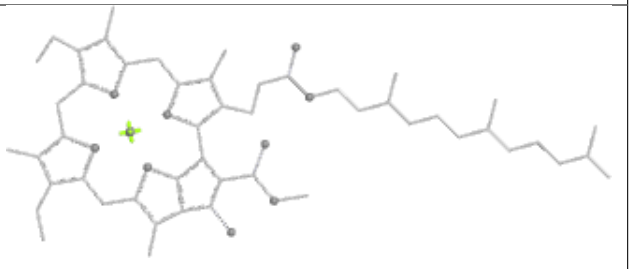
Bond lengths



Bond angles

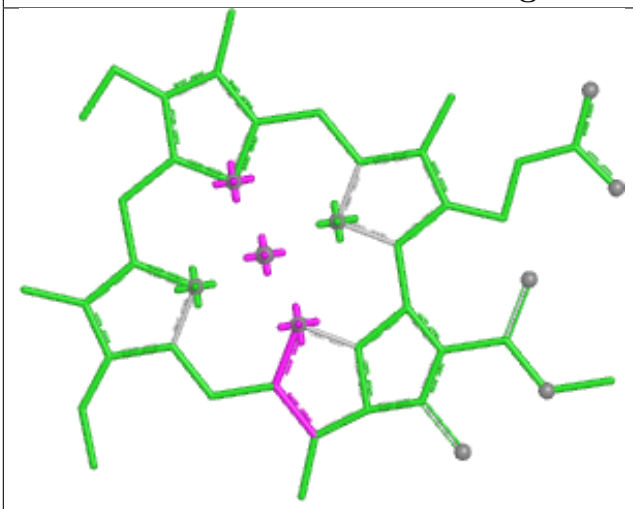


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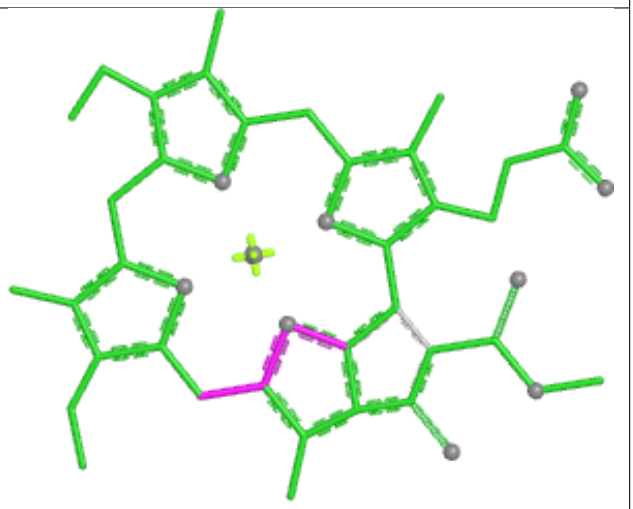


Rings

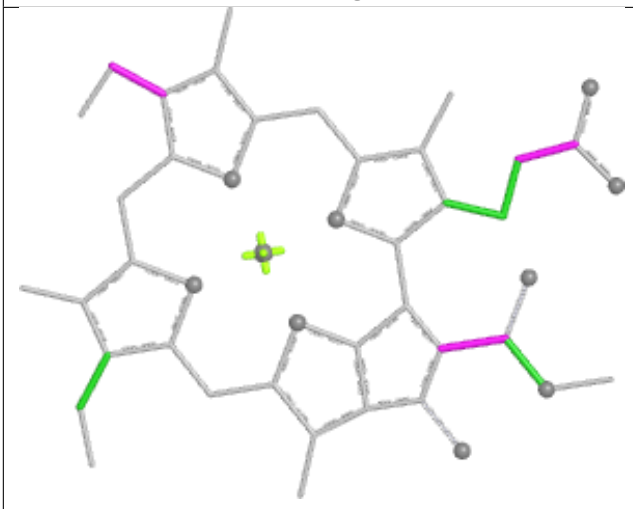
## Ligand CLA 12 612



Bond lengths



Bond angles

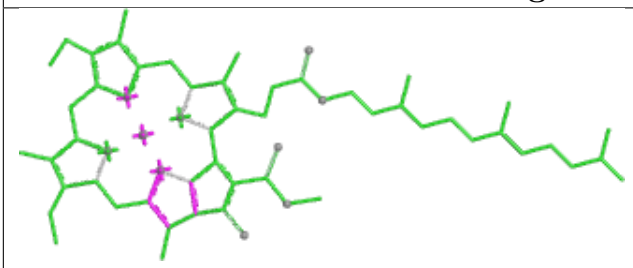


Torsions

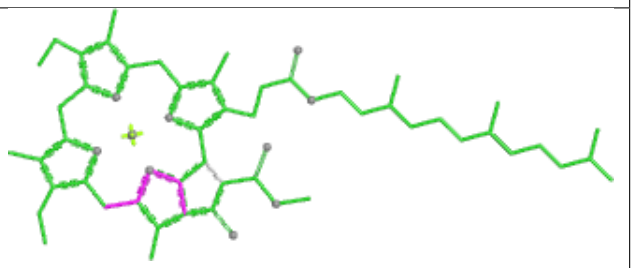


Rings

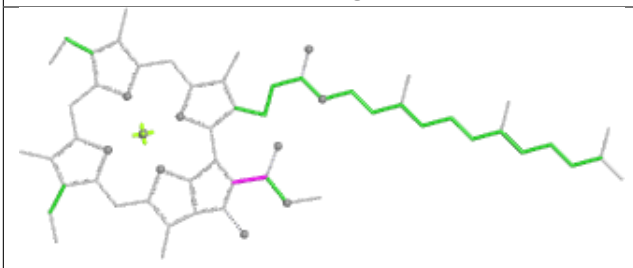
## Ligand CLA 3 602



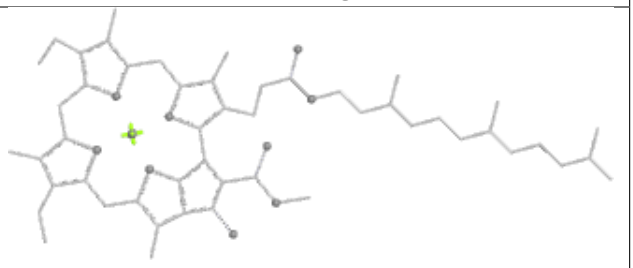
Bond lengths



Bond angles

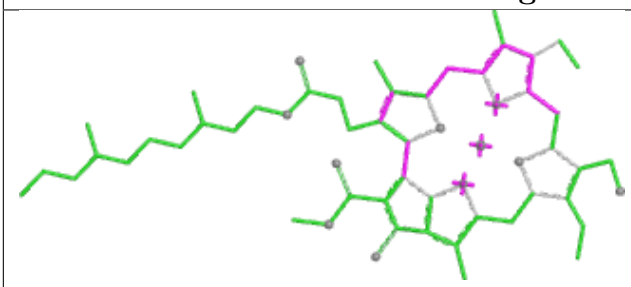


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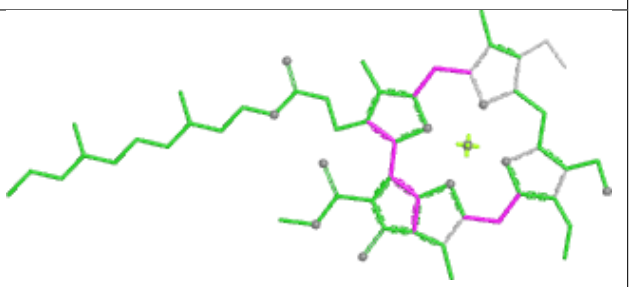


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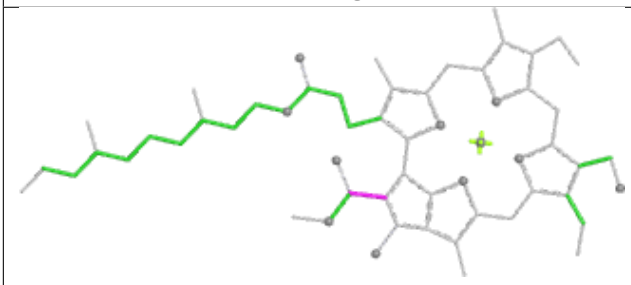
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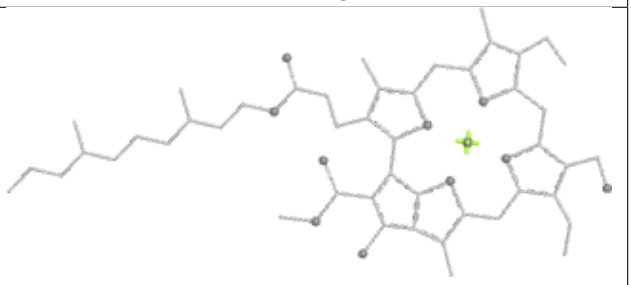
Bond lengths



Bond angles



Torsions

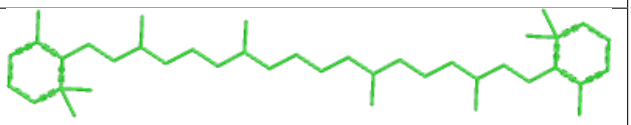


Rings

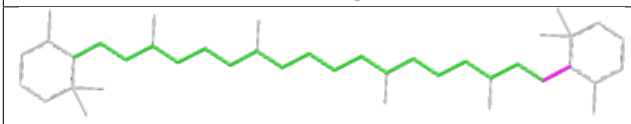
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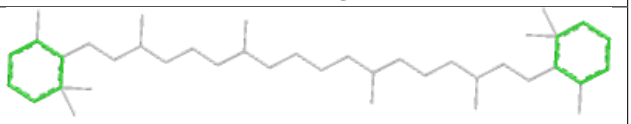
Bond lengths



Bond angles

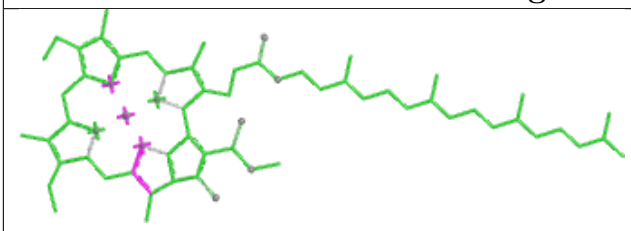


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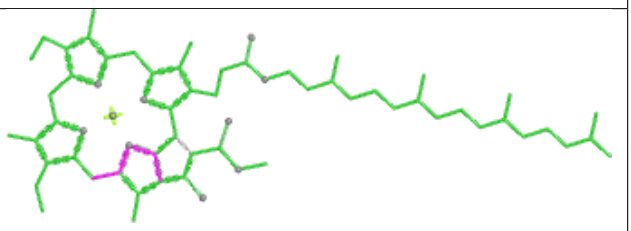


Rings

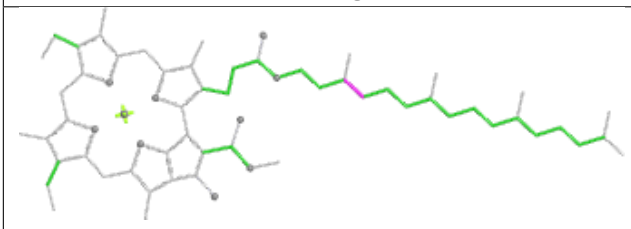
## Ligand CLA 6 604



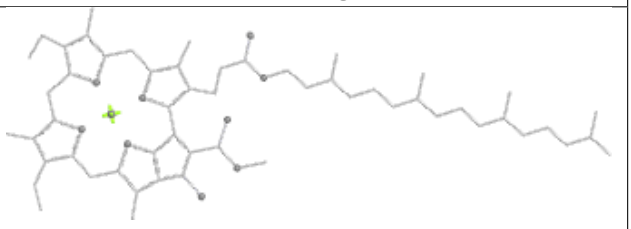
Bond lengths



Bond angles

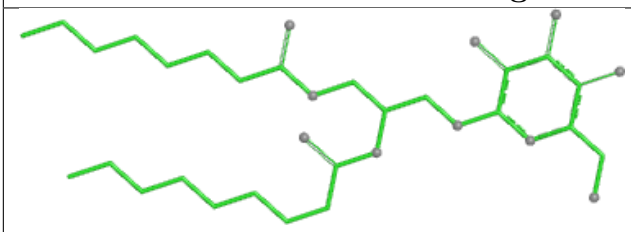


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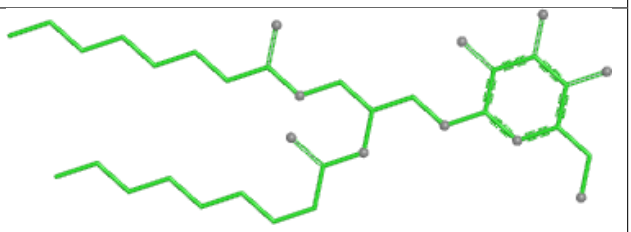


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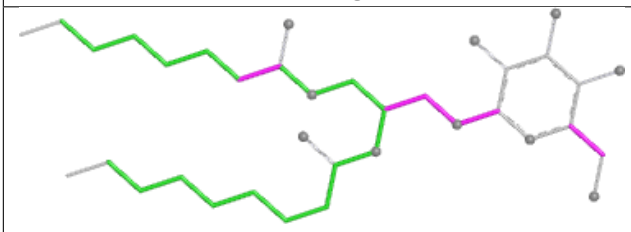
## Ligand LMG A2 860



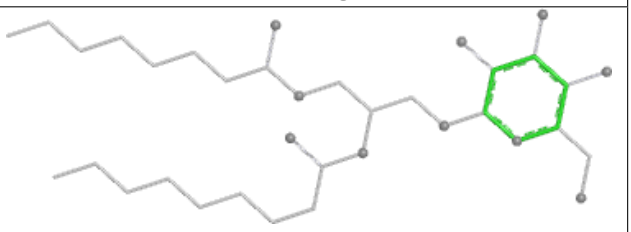
Bond lengths



Bond angles

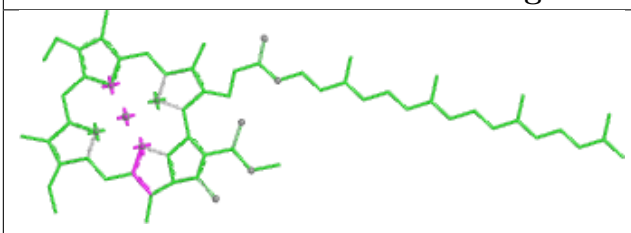


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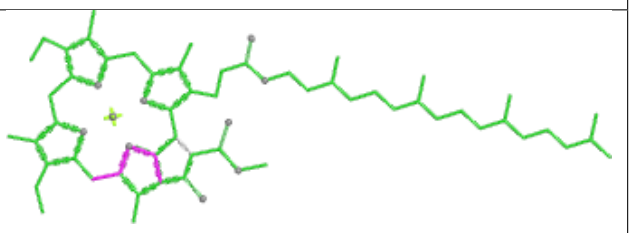


Rings

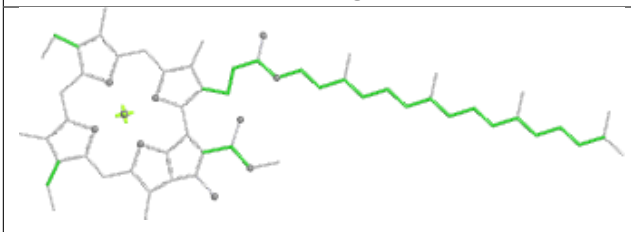
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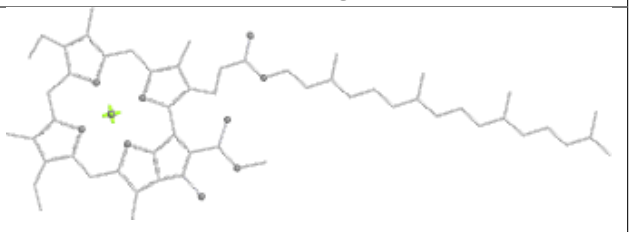
Bond lengths



Bond angles

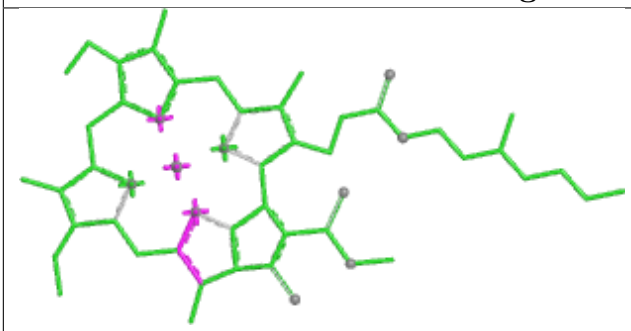


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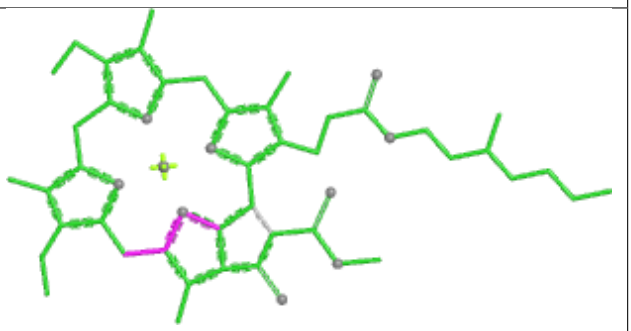


Rings

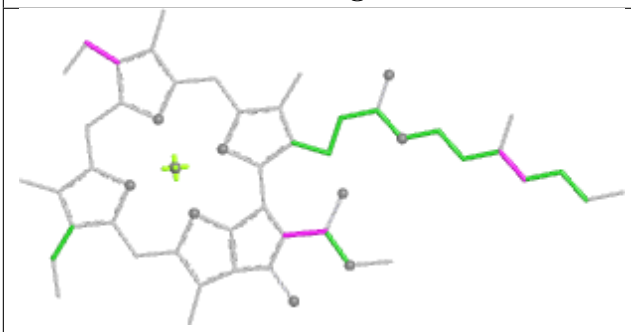
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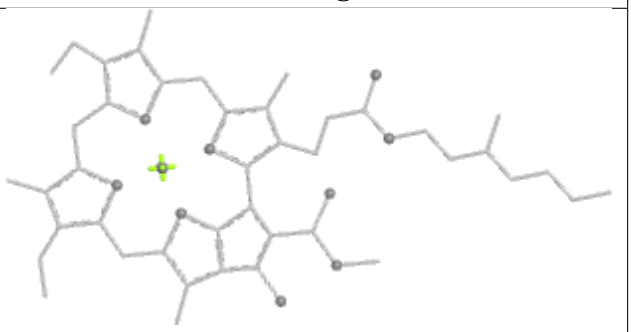
**Bond lengths**



**Bond angles**

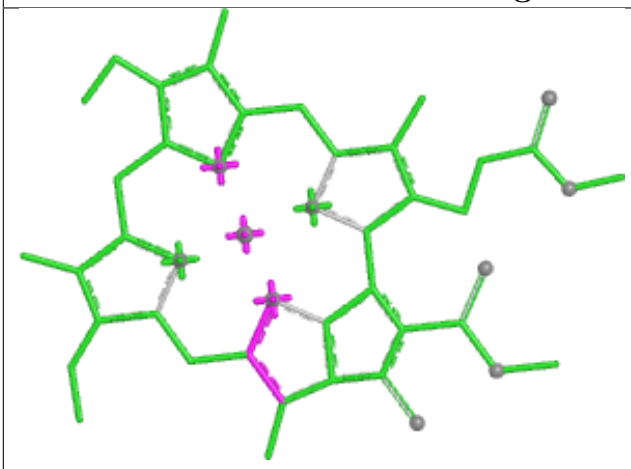


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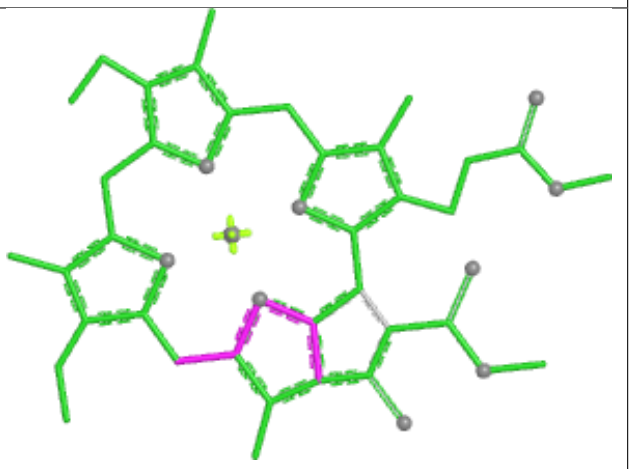


**Rings**

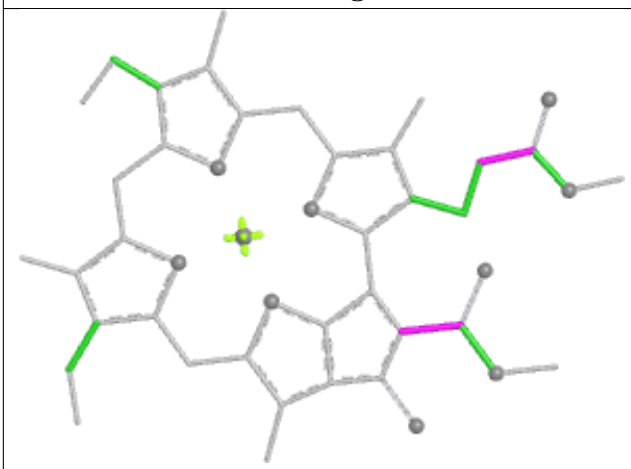
## Ligand CLA G2 204



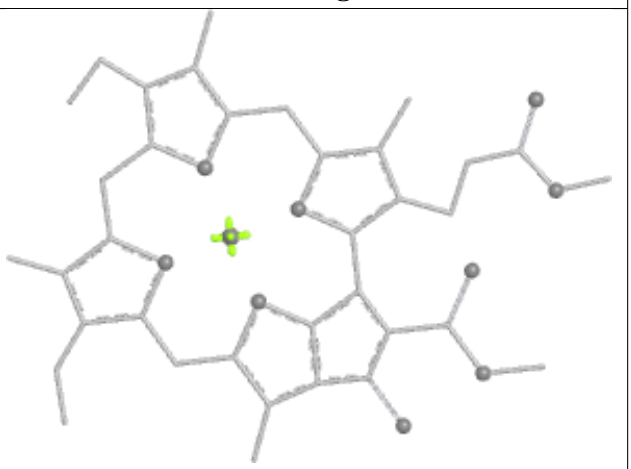
Bond lengths



Bond angles

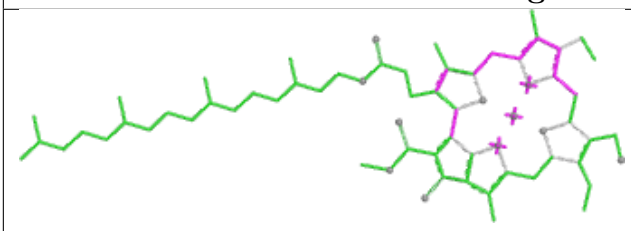


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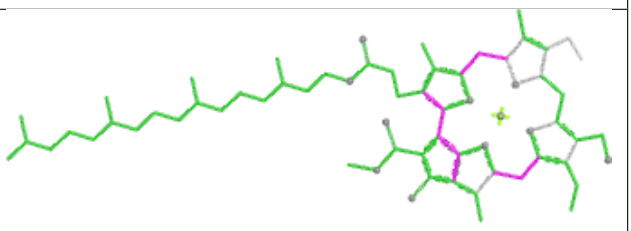


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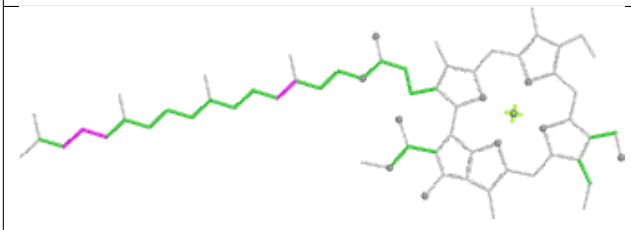
## Ligand CHL 3 608



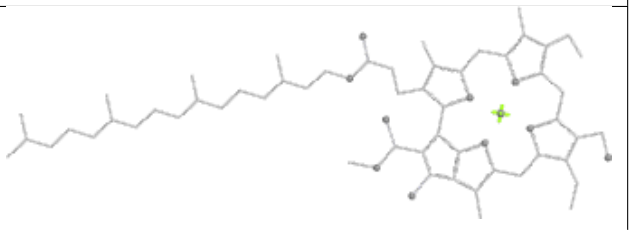
Bond lengths



Bond angles

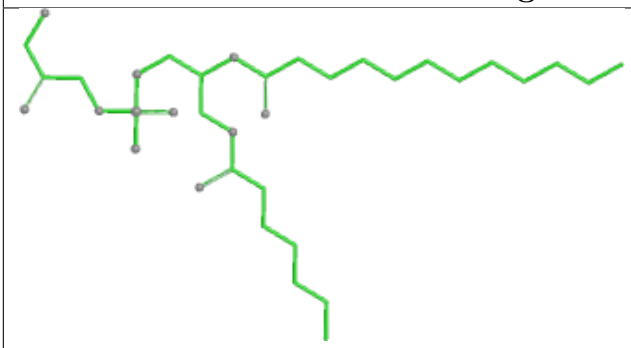


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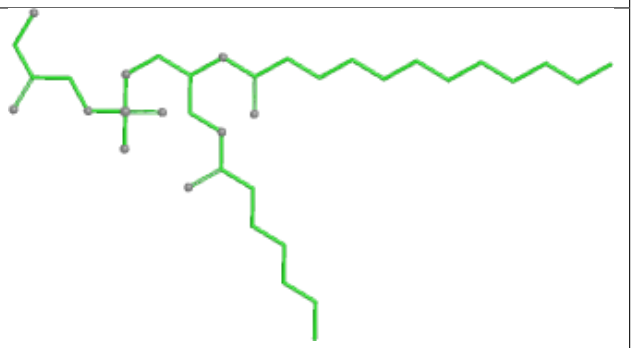


Rings

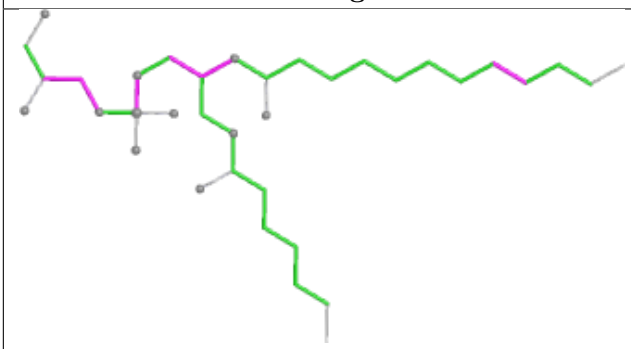
## Ligand LHG 62 629



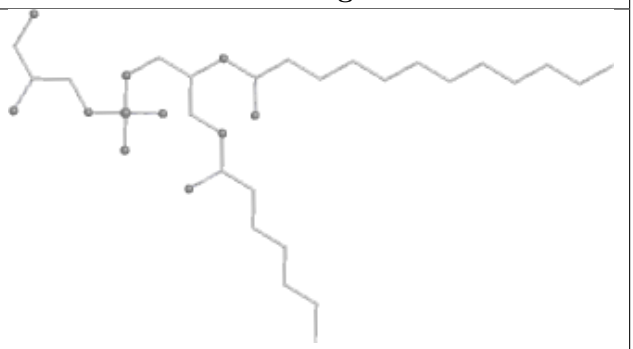
Bond lengths



Bond angles

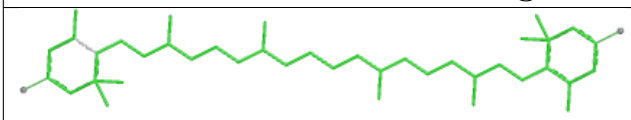


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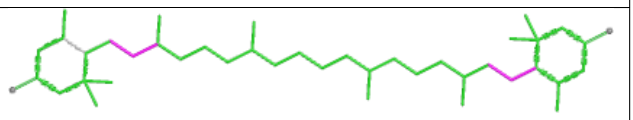


Rings

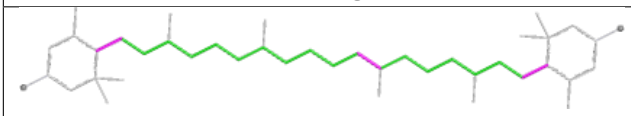
## Ligand LUT F2 305



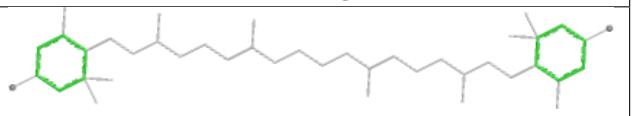
Bond lengths



Bond angles

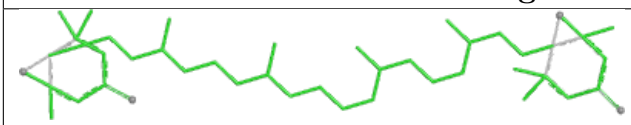


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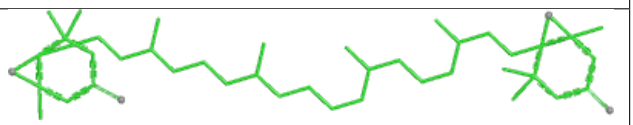


Rings

## Ligand XAT 82 618



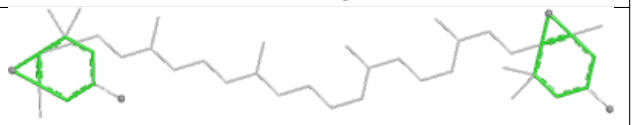
Bond lengths



Bond angles

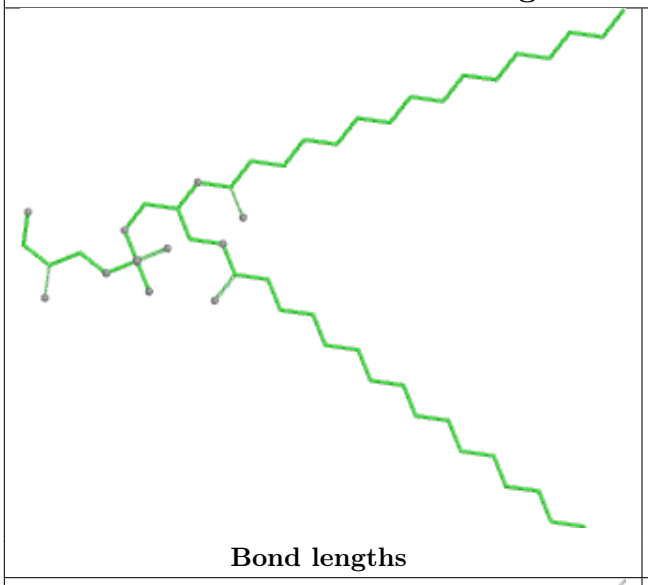


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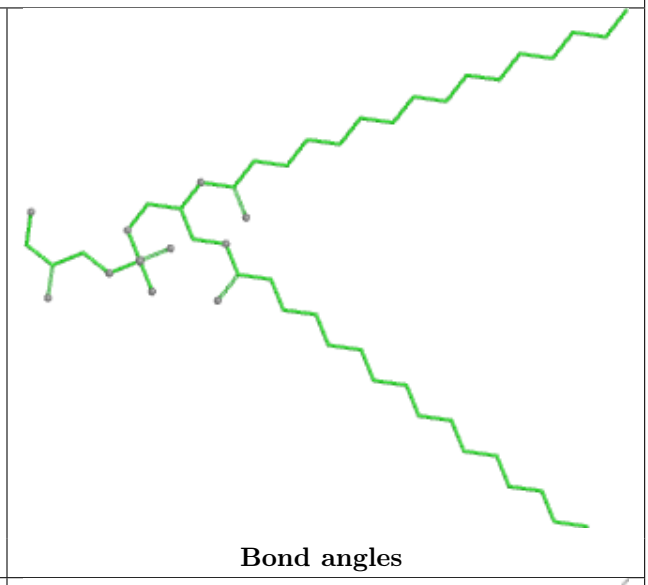


Rings

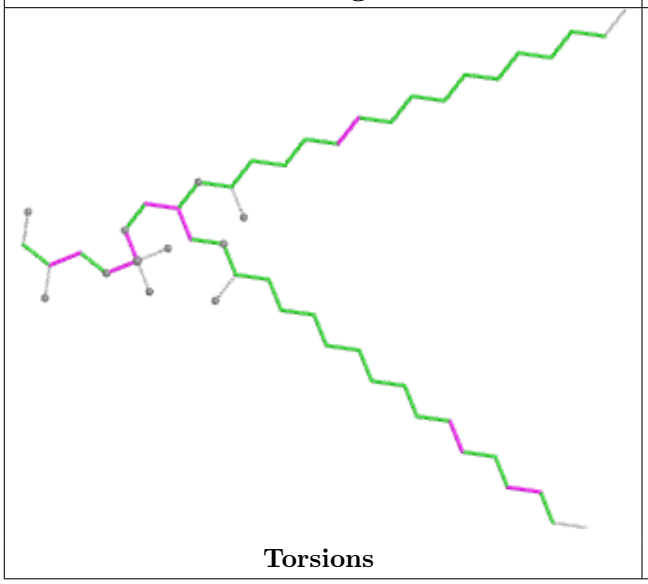
**Ligand LHG 72 625**



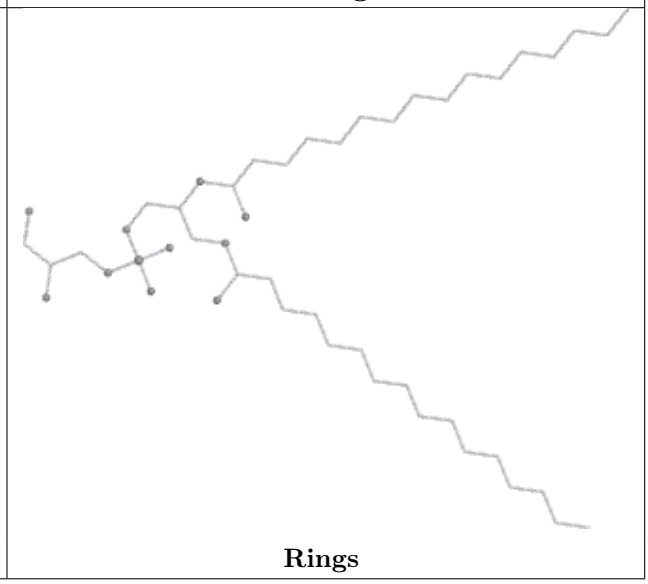
**Bond lengths**



**Bond angles**

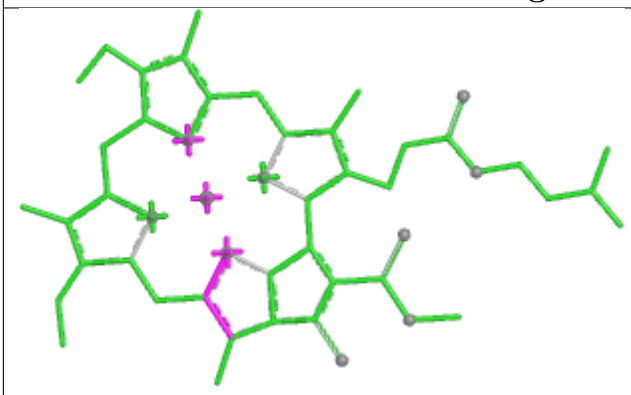


**Torsions**

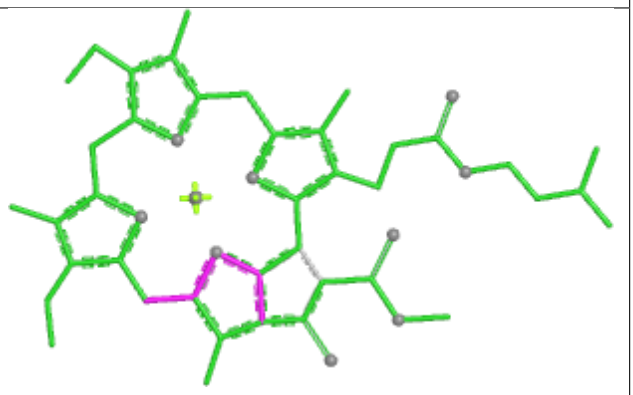


**Rings**

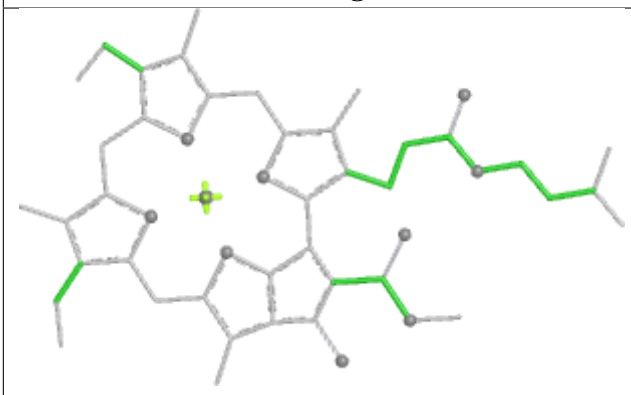
## Ligand CLA 1 604



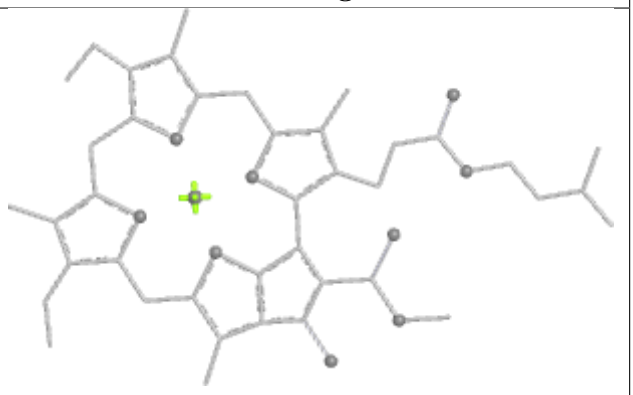
Bond lengths



Bond angles



Torsions

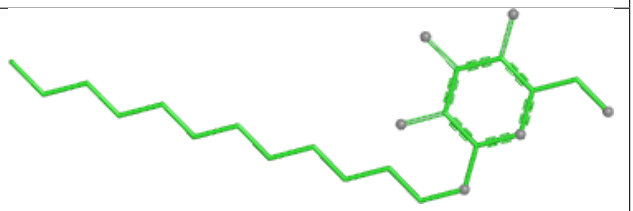


Rings

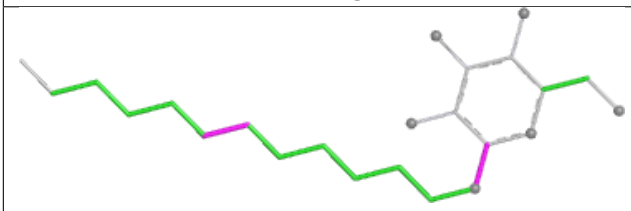
## Ligand LMU K2 208



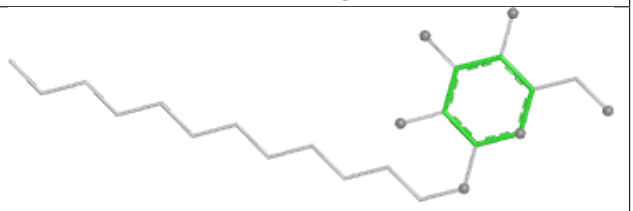
Bond lengths



Bond angles

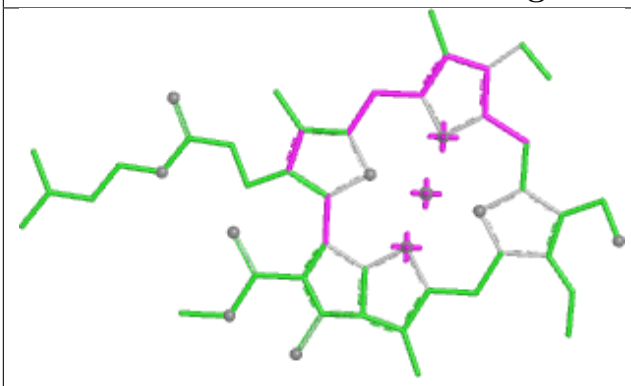


Torsions

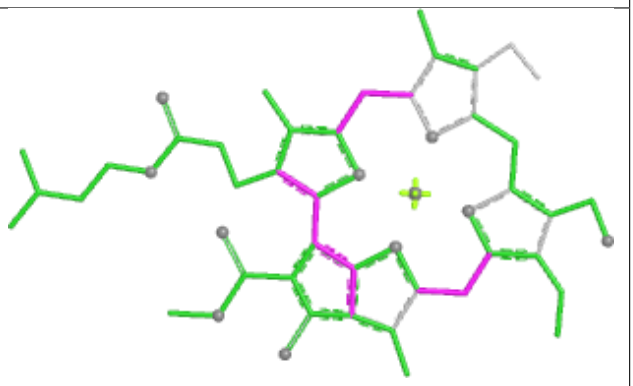


Rings

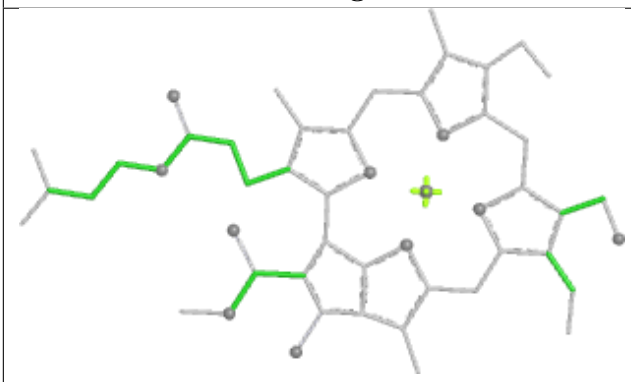
**Ligand CHL 6 608**



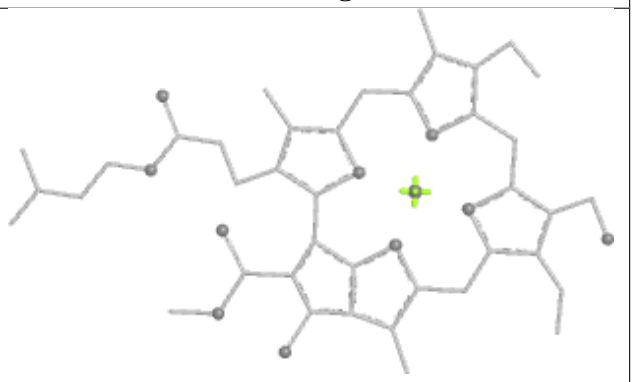
**Bond lengths**



**Bond angles**

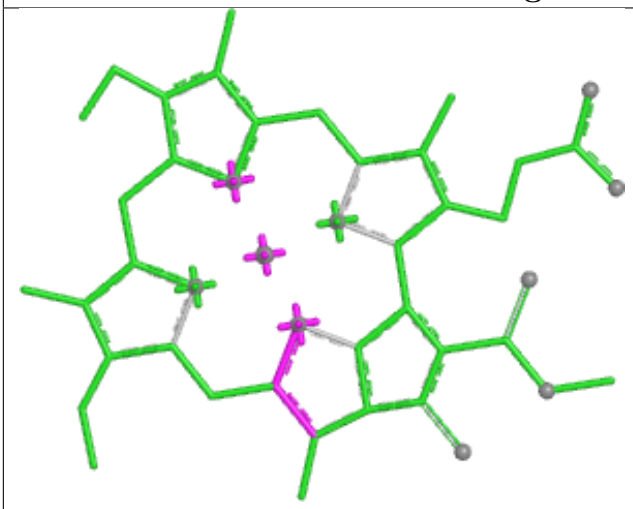


**Torsions**

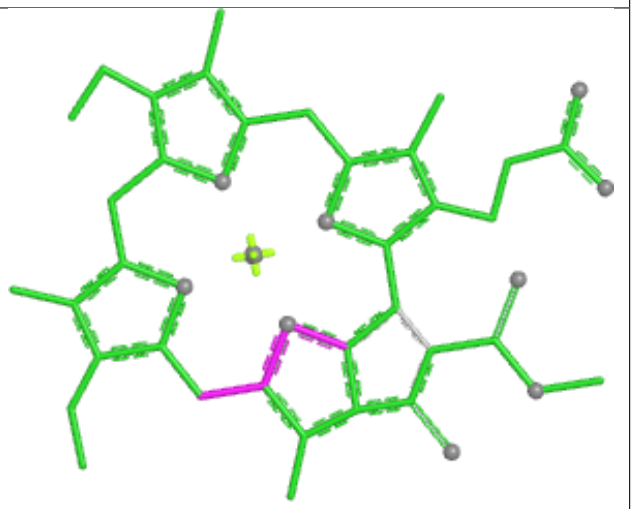


**Rings**

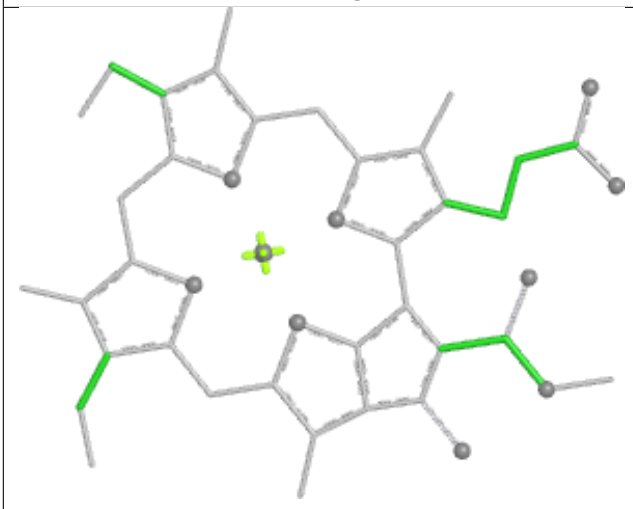
**Ligand CLA B 835**



**Bond lengths**



**Bond angles**

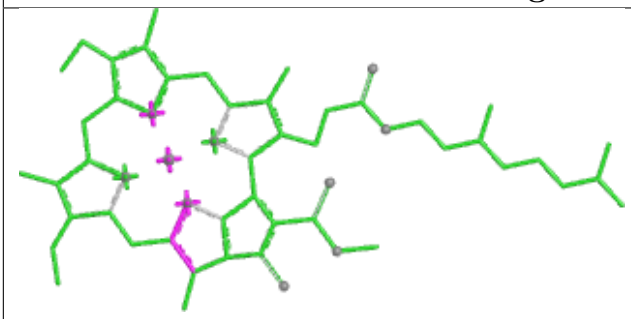


**Torsions**

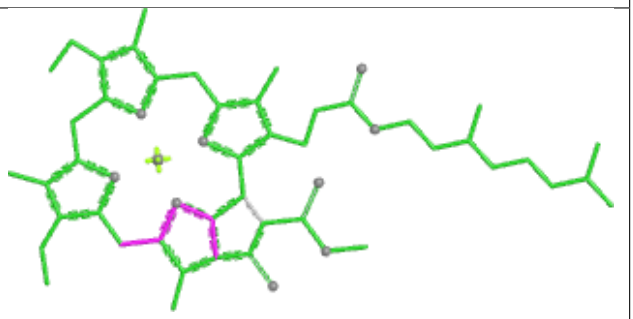


**Rings**

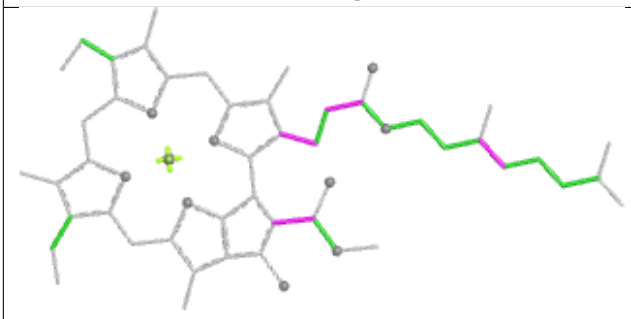
## Ligand CLA 4 614



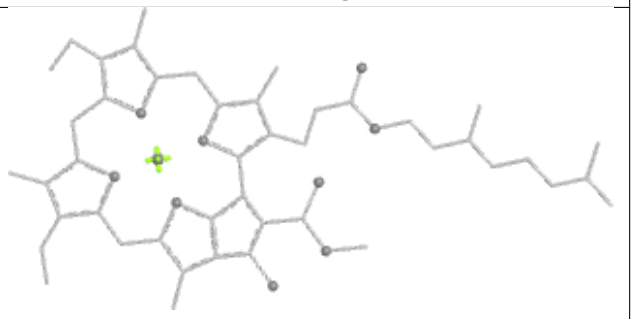
Bond lengths



Bond angles

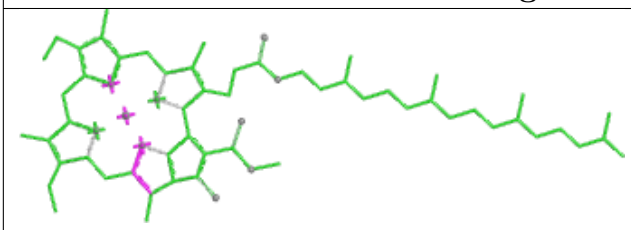


Torsions

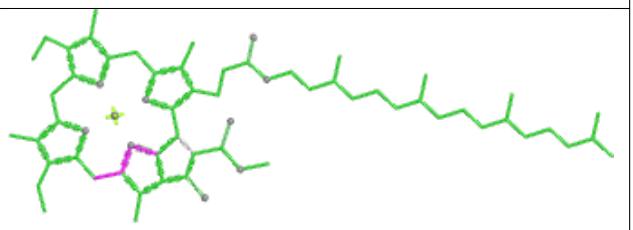


Rings

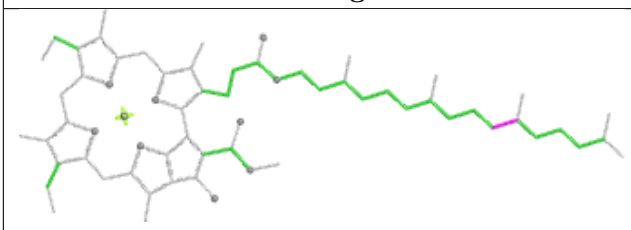
## Ligand CLA 82 610



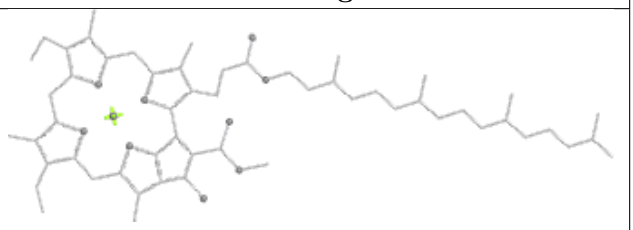
Bond lengths



Bond angles



Torsions



Rings

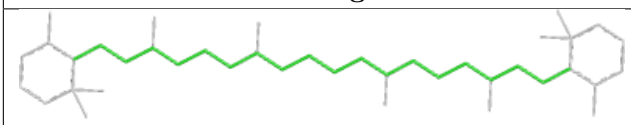
## Ligand BCR I 172



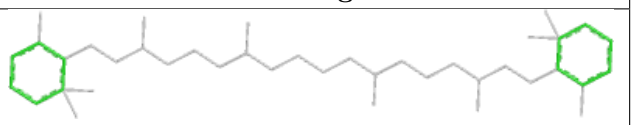
Bond lengths



Bond angles

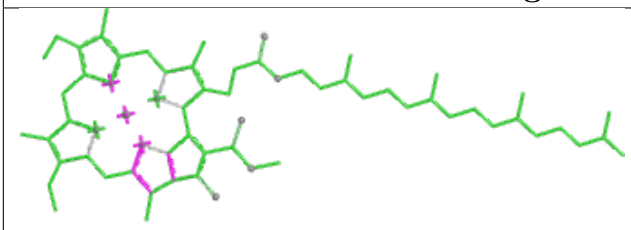


Torsions

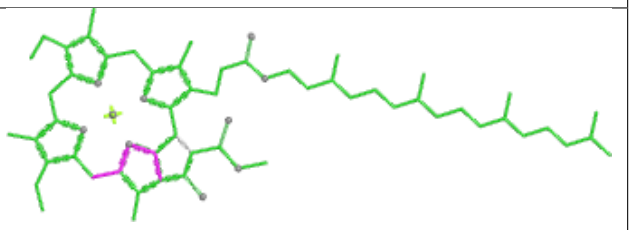


Rings

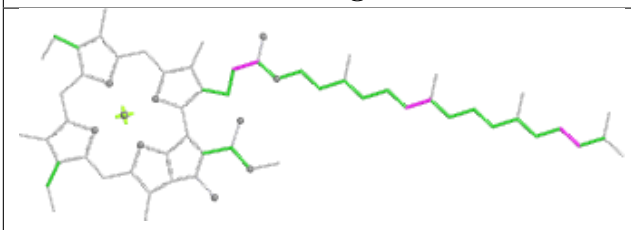
## Ligand CLA A 813



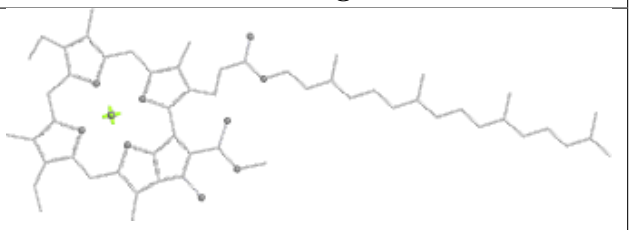
Bond lengths



Bond angles

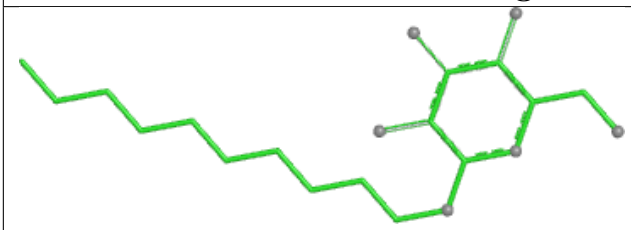


Torsions

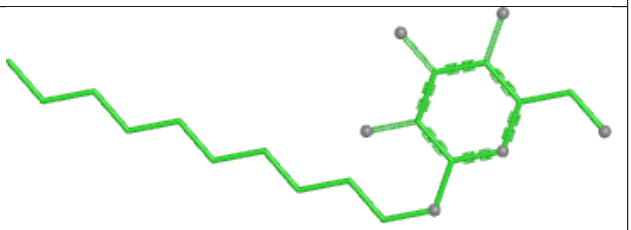


Rings

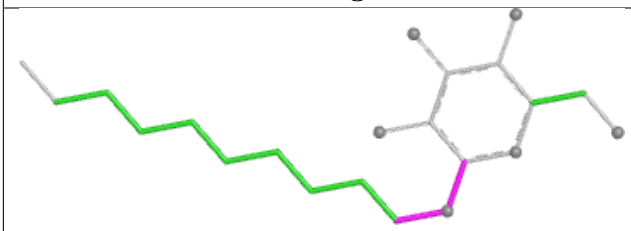
## Ligand LMU 12 627



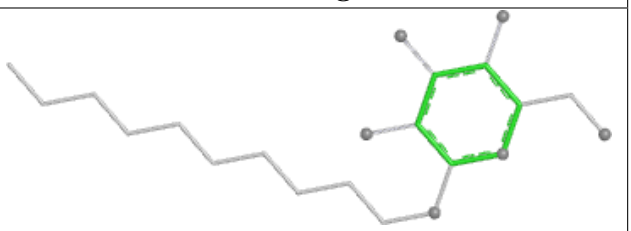
Bond lengths



Bond angles

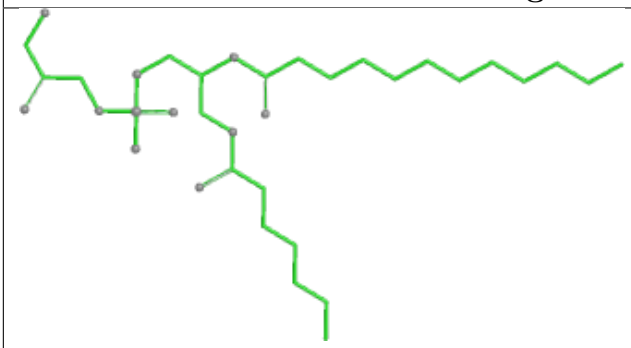


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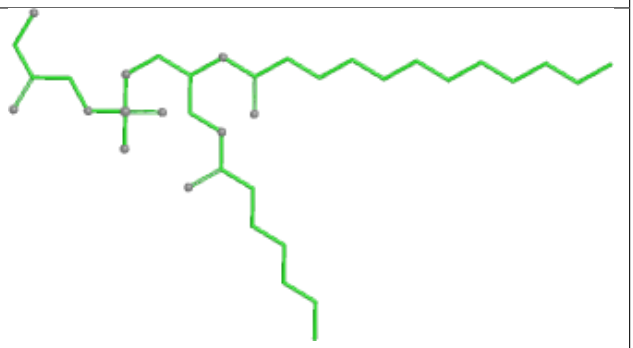


Rings

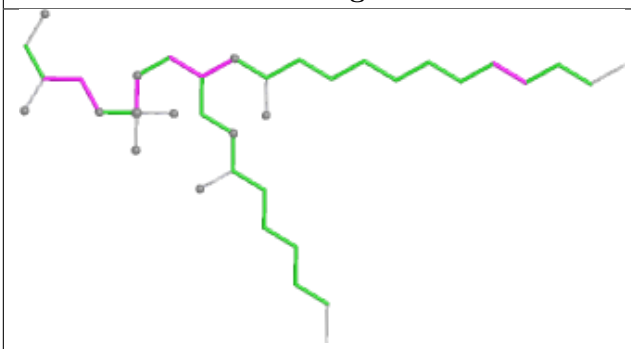
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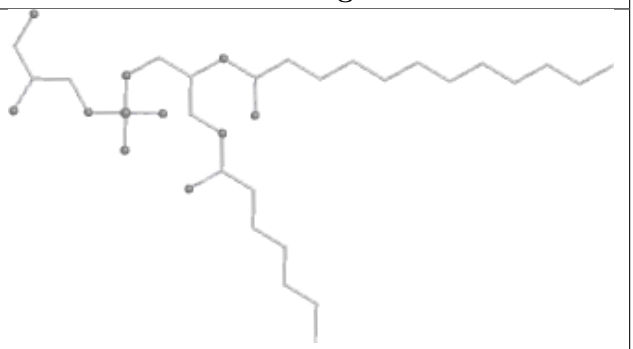
Bond lengths



Bond angles

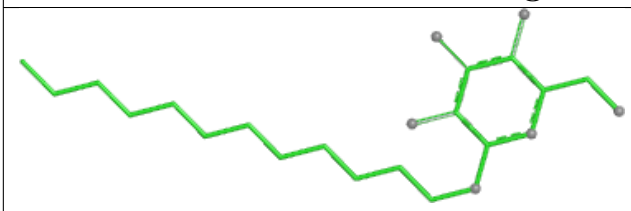


Torsions

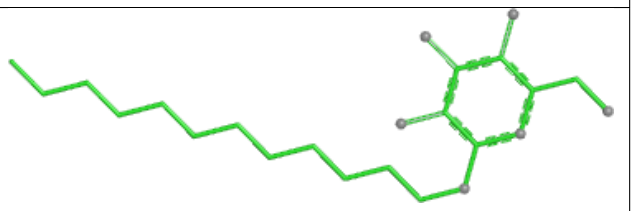


Rings

## Ligand LMU 5 627



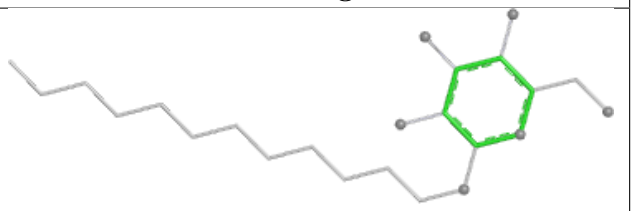
Bond lengths



Bond angles

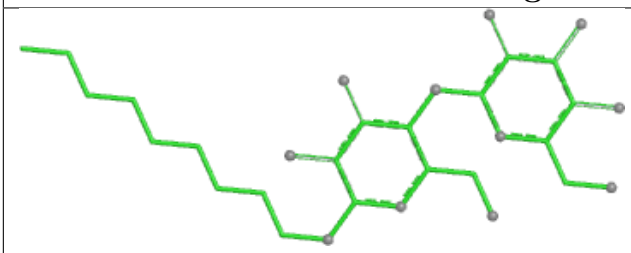


Torsions

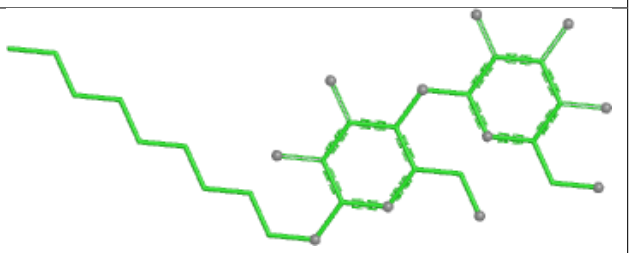


Rings

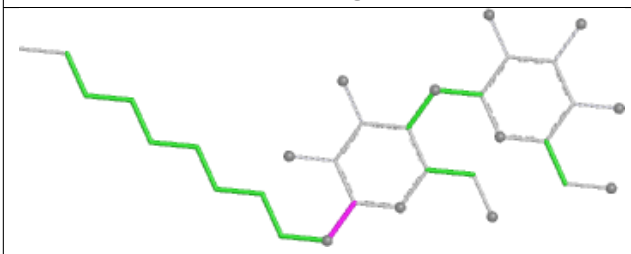
## Ligand LMU 7 627



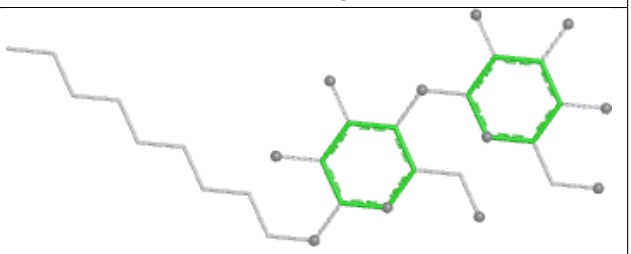
Bond lengths



Bond angles

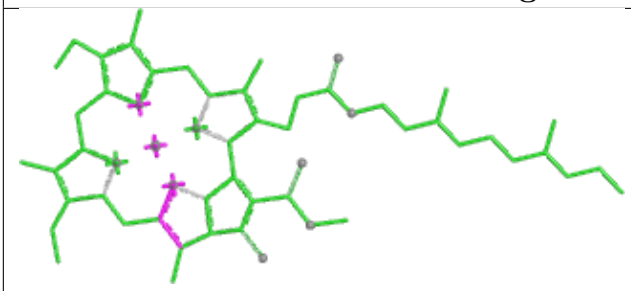


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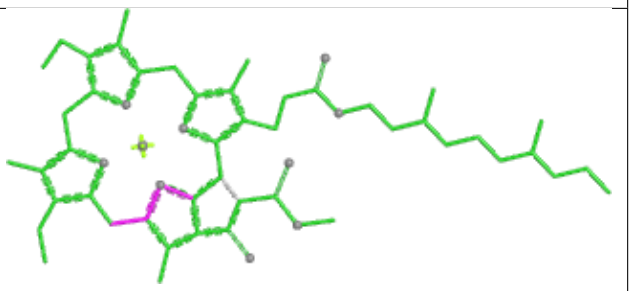


Rings

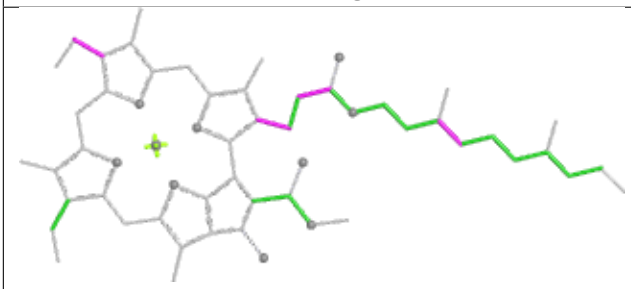
## Ligand CLA 82 614



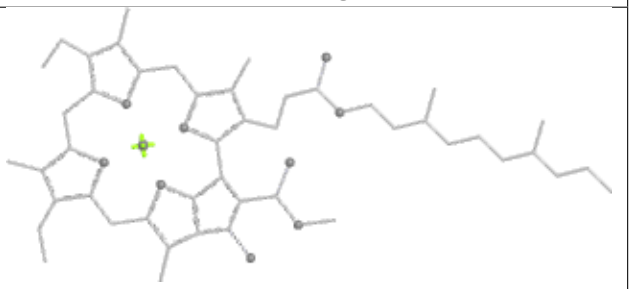
Bond lengths



Bond angles

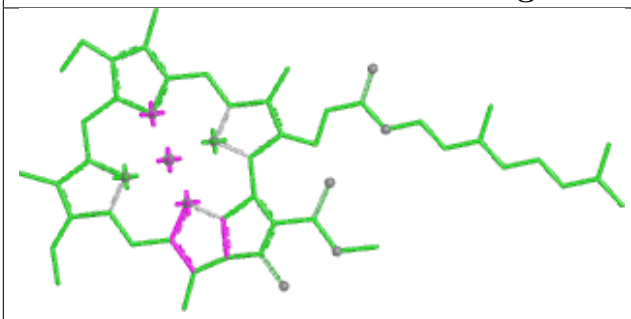


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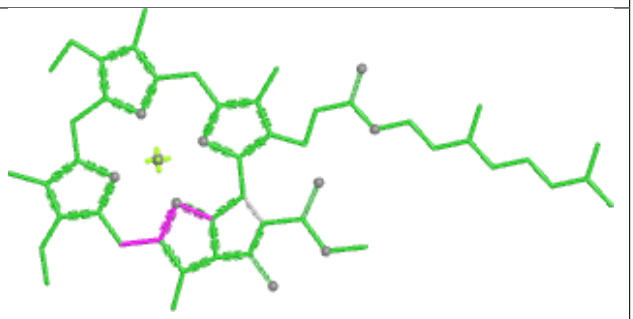


Rings

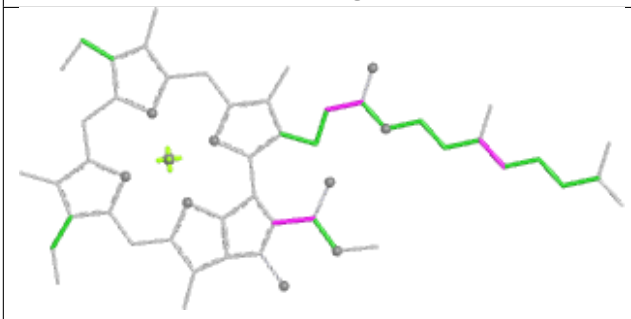
**Ligand CLA Z2 603**



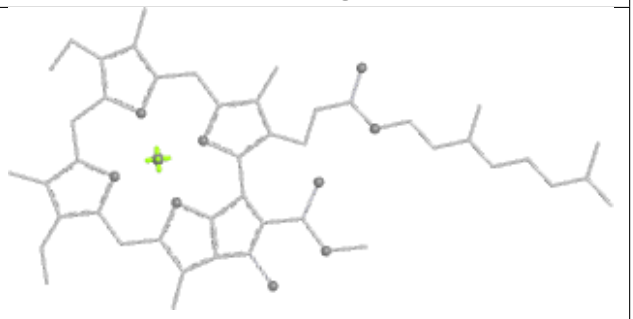
**Bond lengths**



**Bond angles**

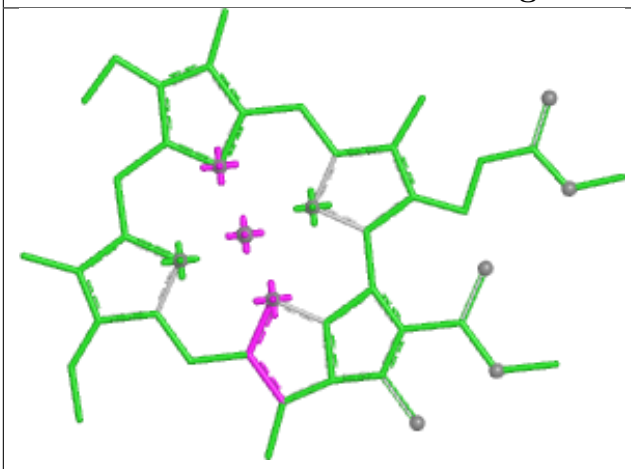


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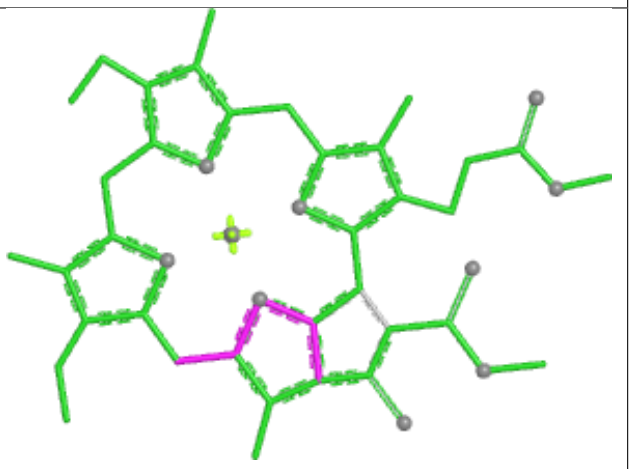


**Rings**

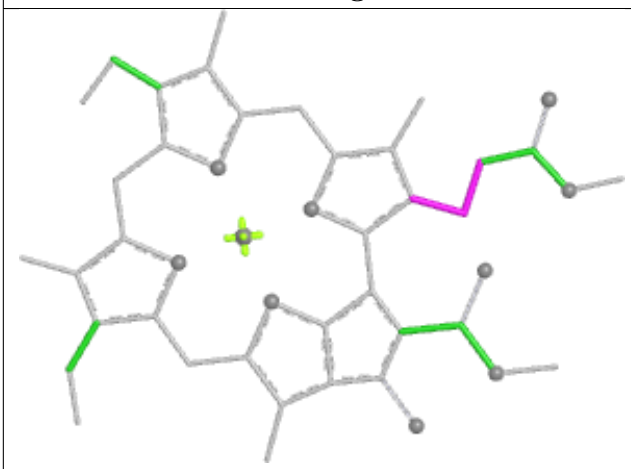
**Ligand CLA 72 616**



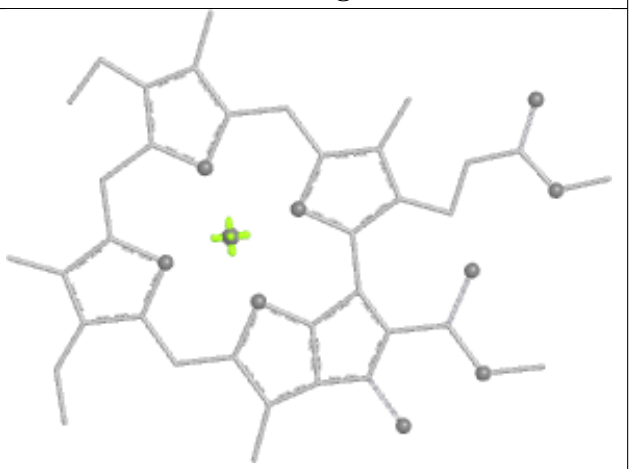
**Bond lengths**



**Bond angles**

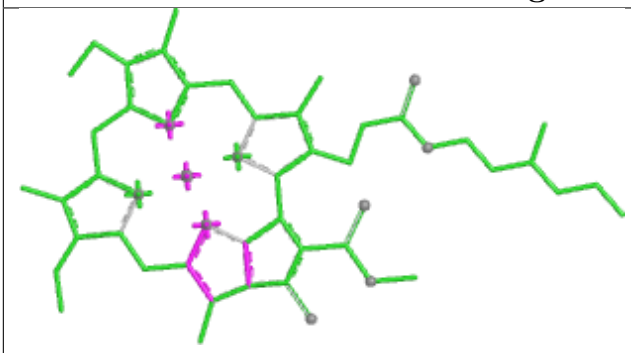


**Torsions**

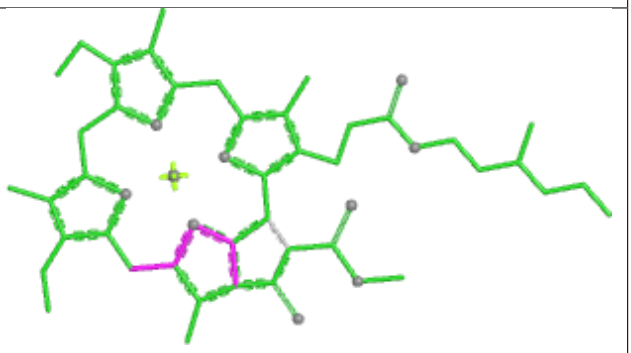


**Rings**

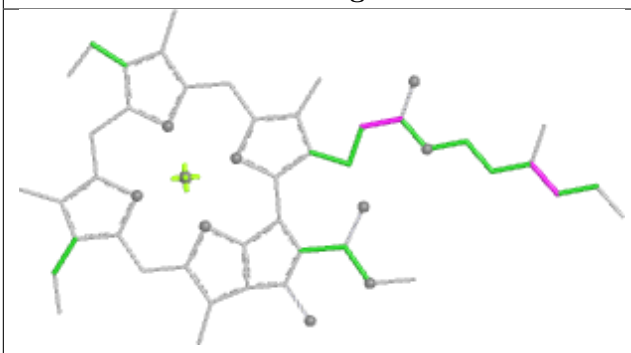
## Ligand CLA 7 603



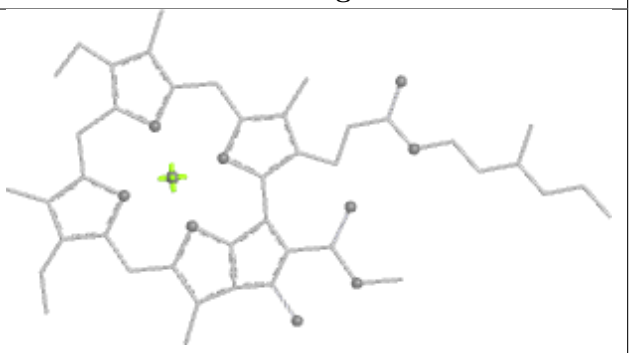
Bond lengths



Bond angles

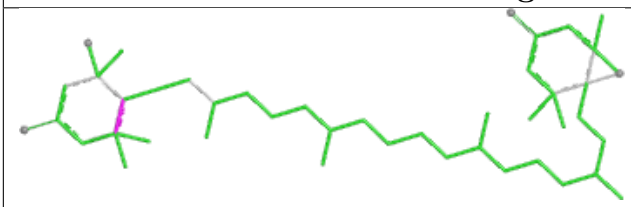


Torsions

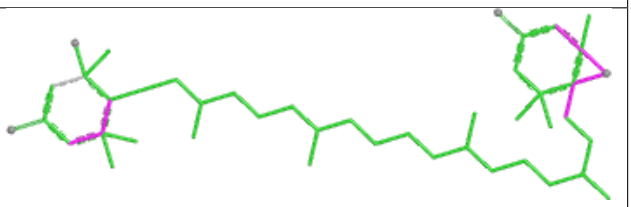


Rings

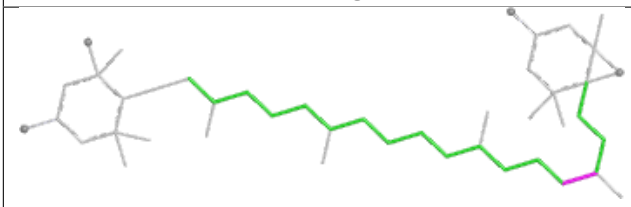
## Ligand NEX 52 625



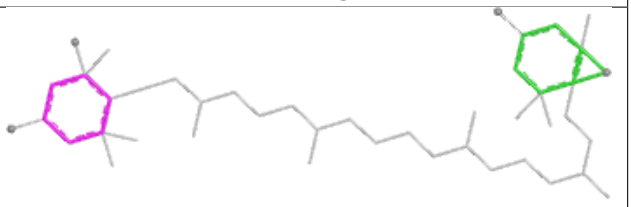
Bond lengths



Bond angles

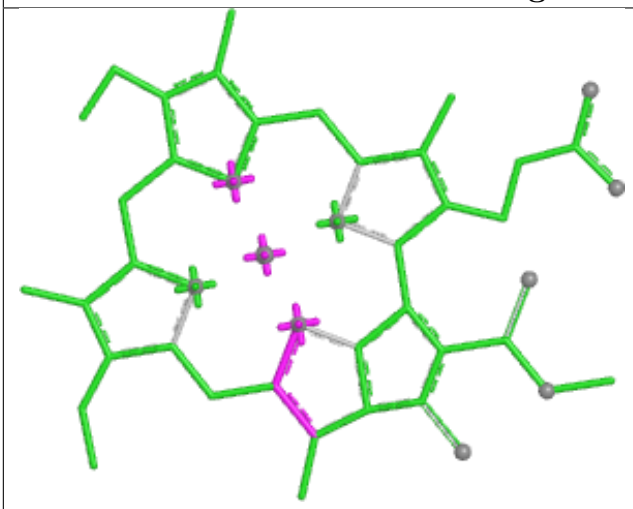


Torsions

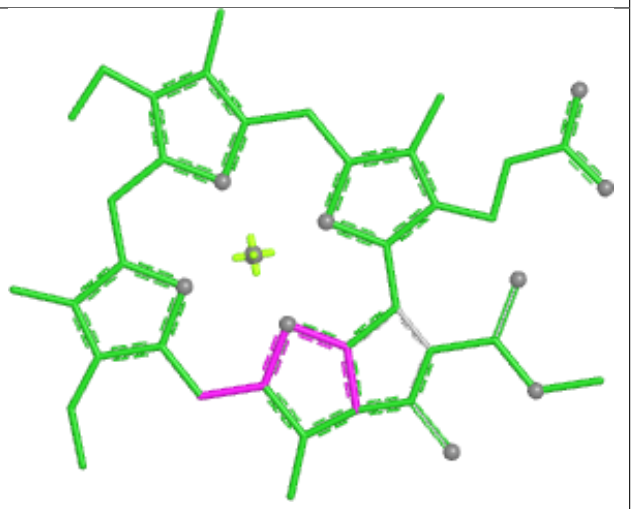


Rings

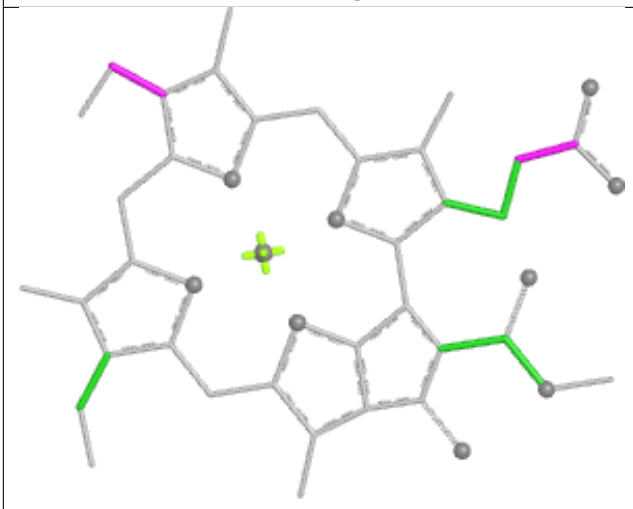
## Ligand CLA 9 614



Bond lengths



Bond angles

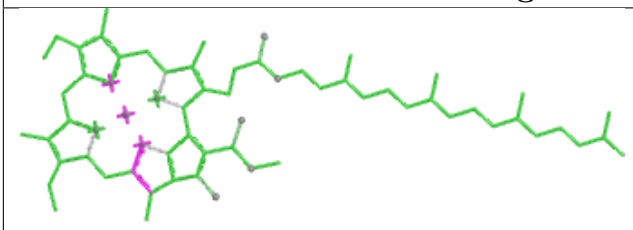


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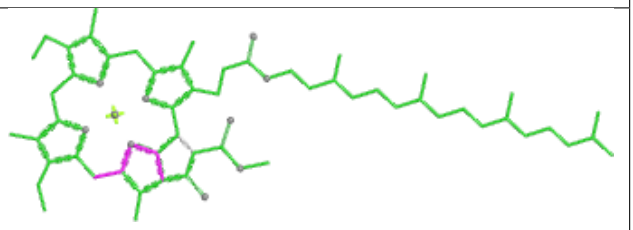


Rings

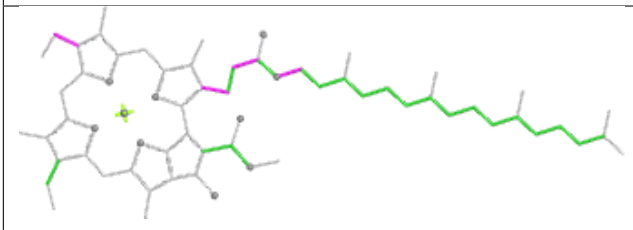
## Ligand CLA F2 304



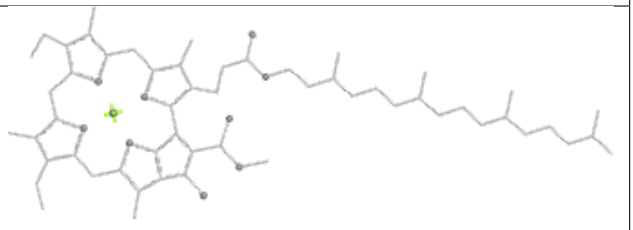
Bond lengths



Bond angles

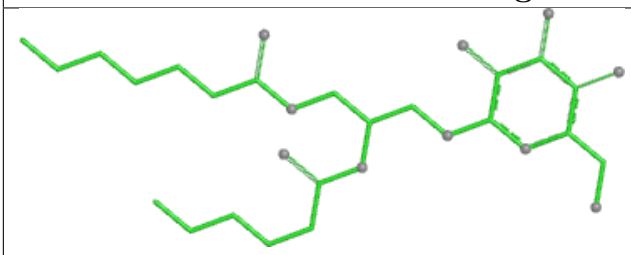


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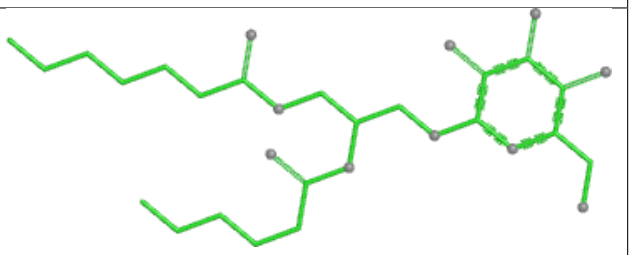


Rings

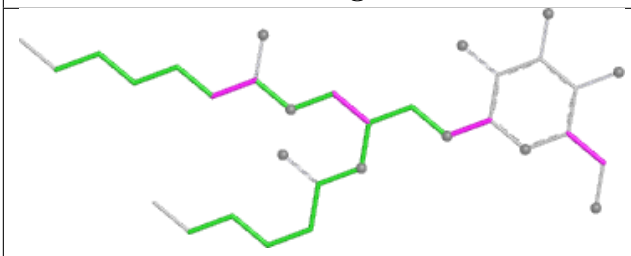
## Ligand LMG 82 626



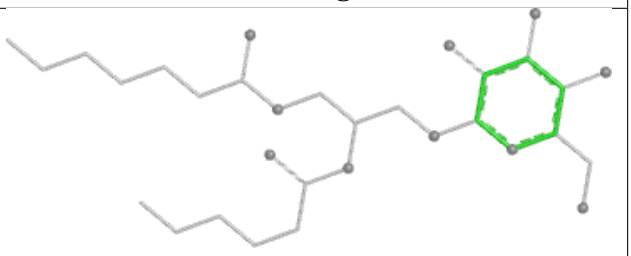
Bond lengths



Bond angles

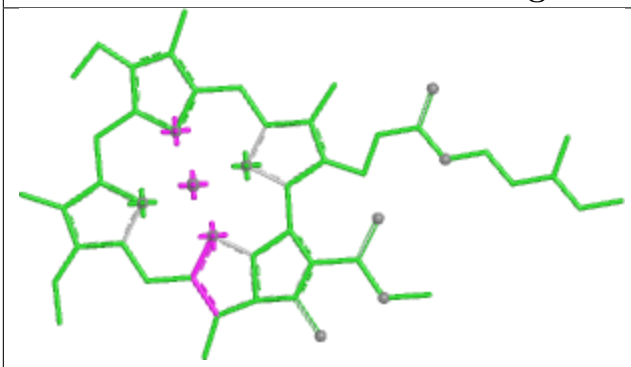


Torsions

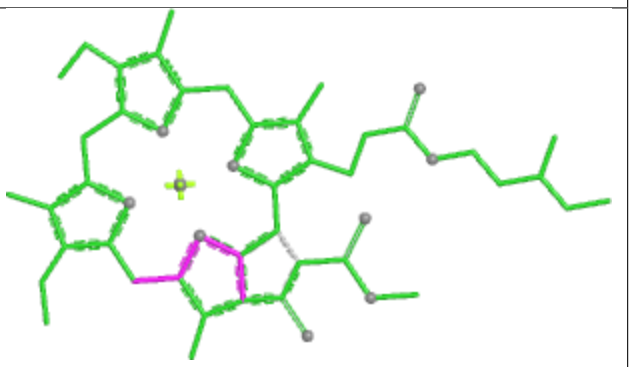


Rings

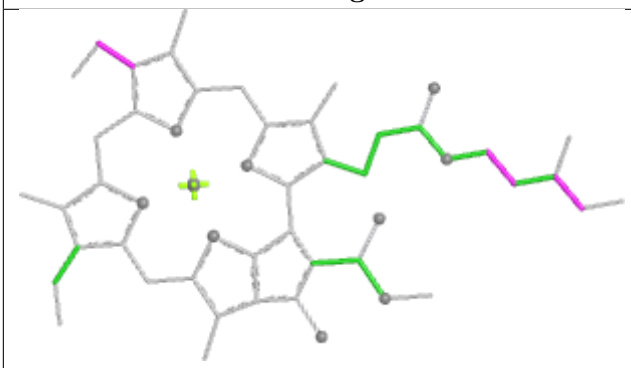
## Ligand CLA 9 609



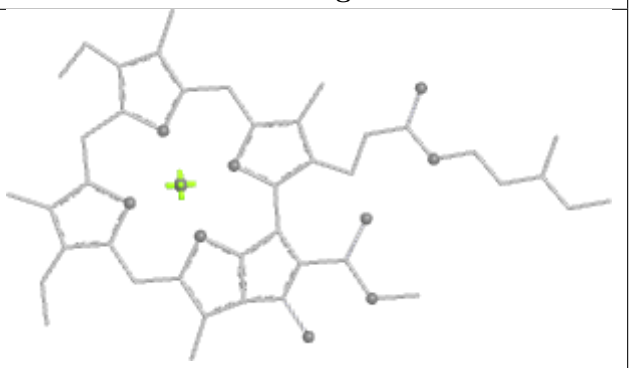
Bond lengths



Bond angles

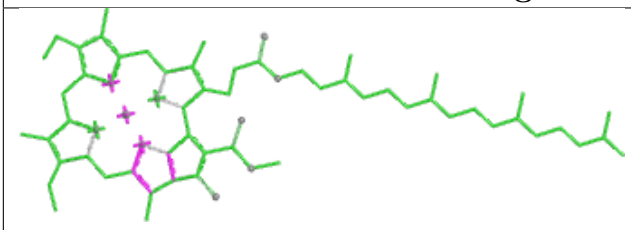


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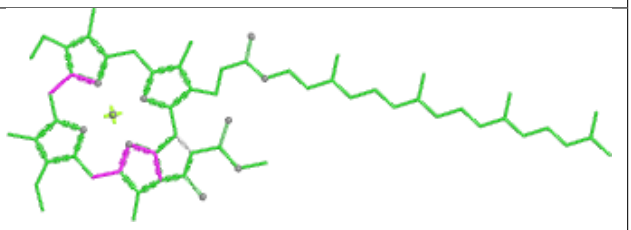


Rings

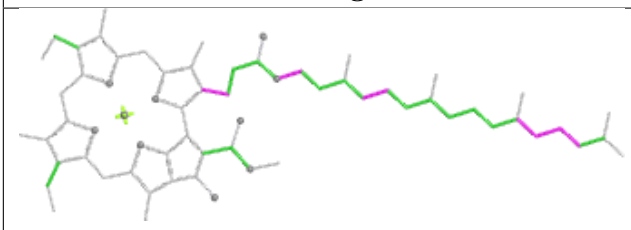
**Ligand CLA A2 812**



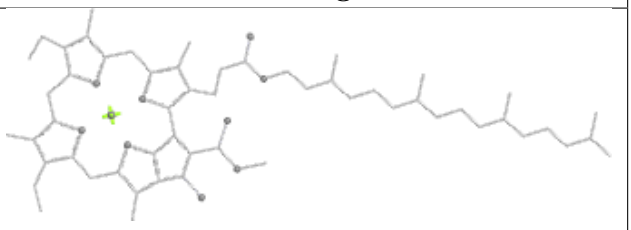
Bond lengths



Bond angles

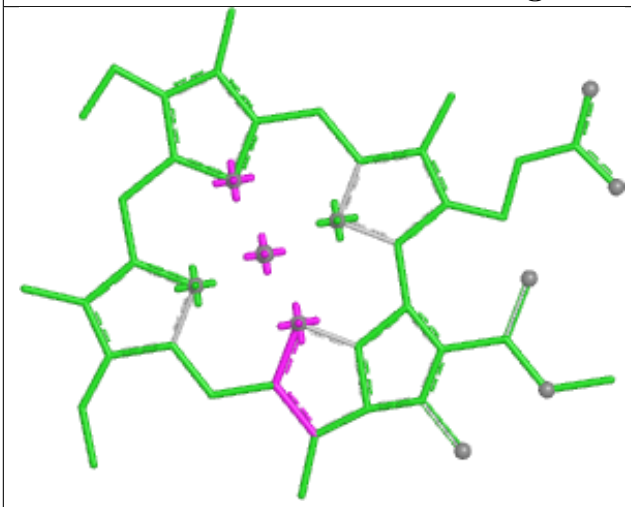


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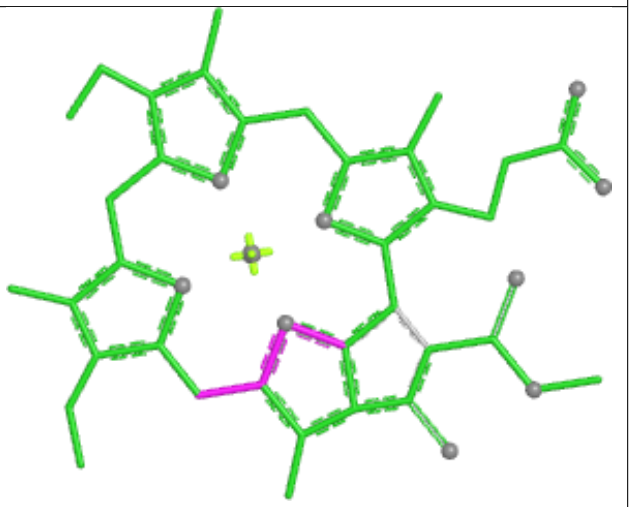


Rings

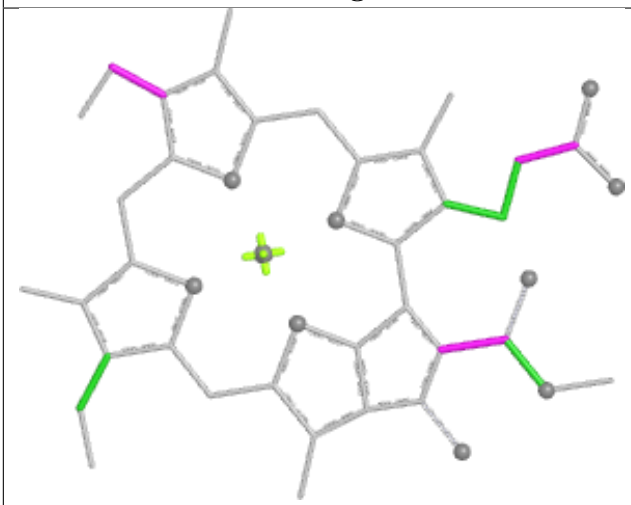
**Ligand CLA Z 612**



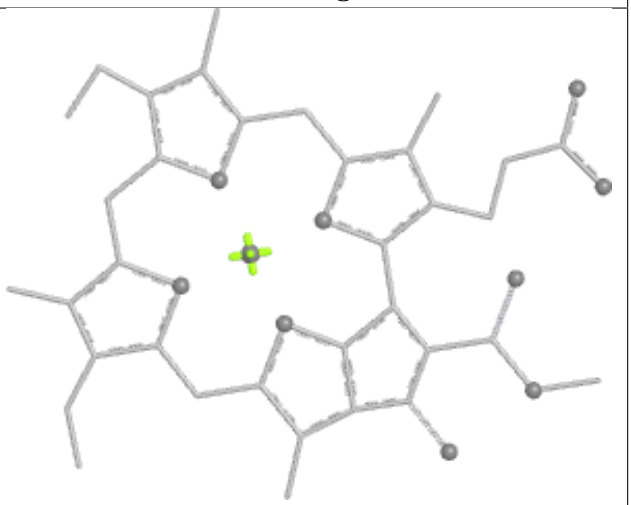
Bond lengths



Bond angles

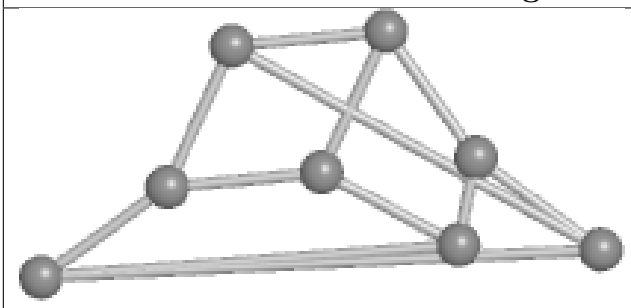


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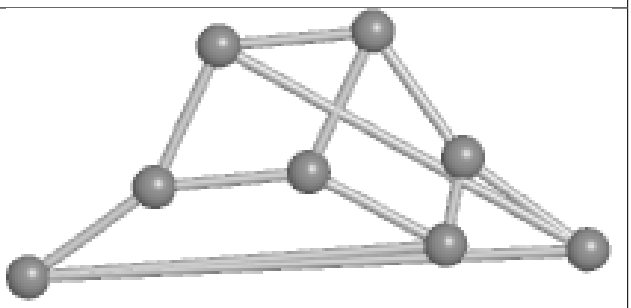


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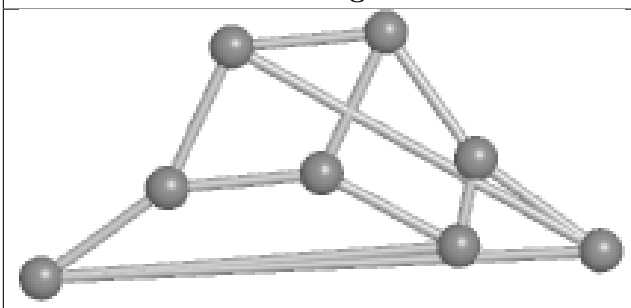
**Ligand SF4 C2 101**



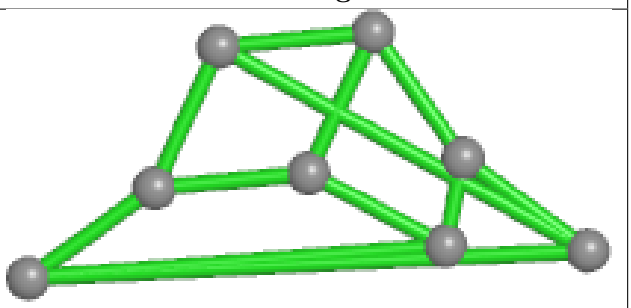
Bond lengths



Bond angles

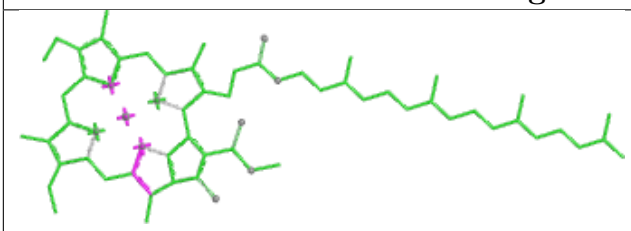


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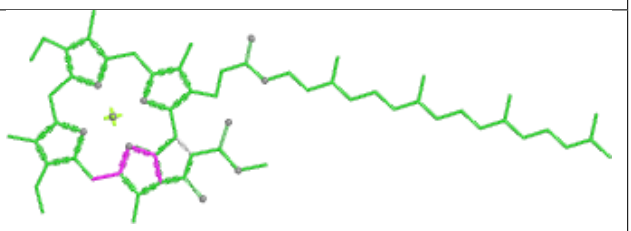


Rings

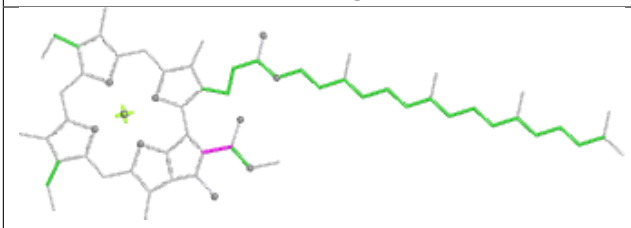
**Ligand CLA 7 602**



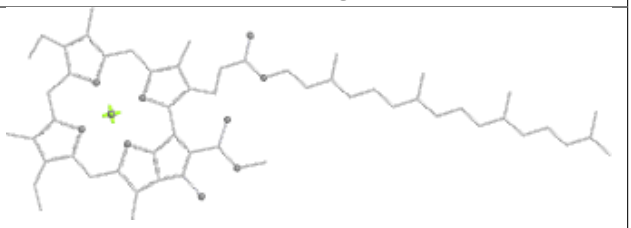
Bond lengths



Bond angles

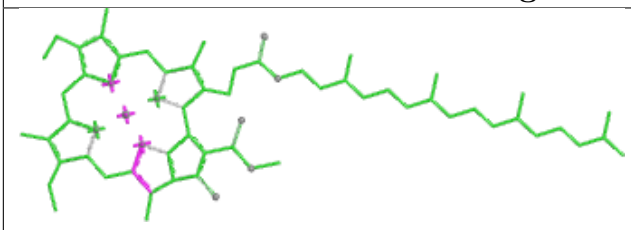


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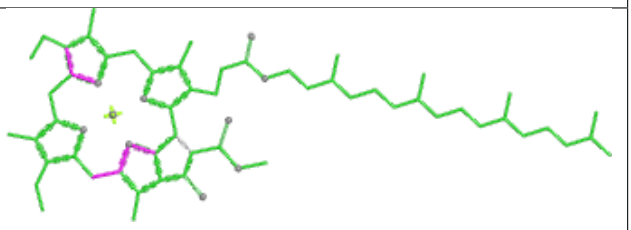


Rings

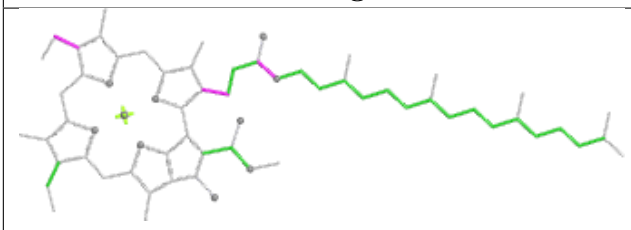
## Ligand CLA 72 610



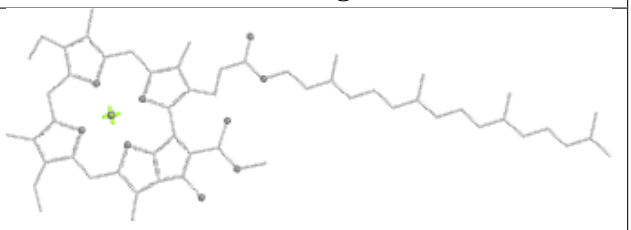
Bond lengths



Bond angles

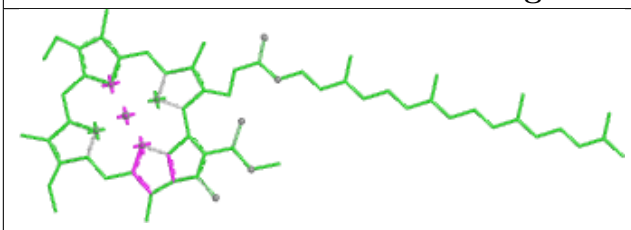


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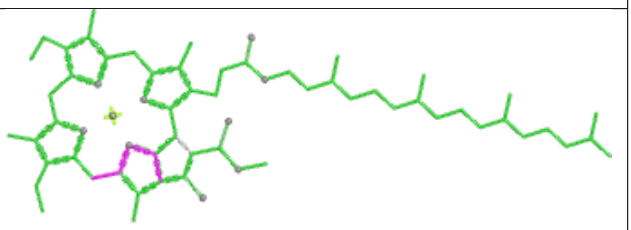


Rings

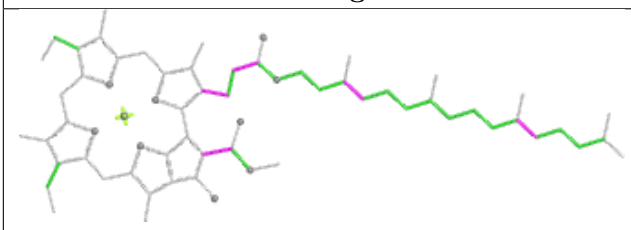
## Ligand CLA B 805



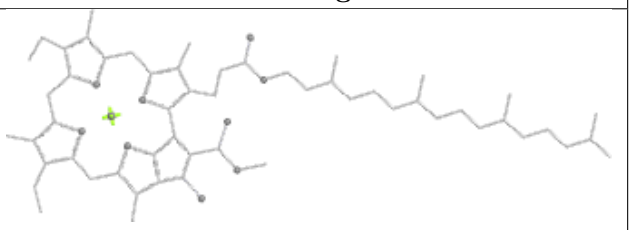
Bond lengths



Bond angles

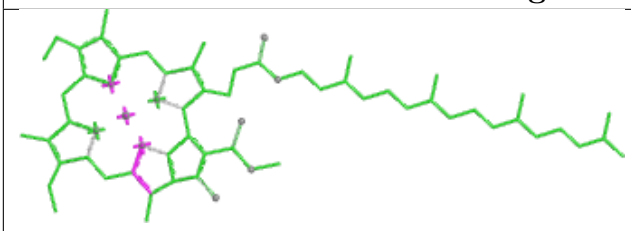


Torsions

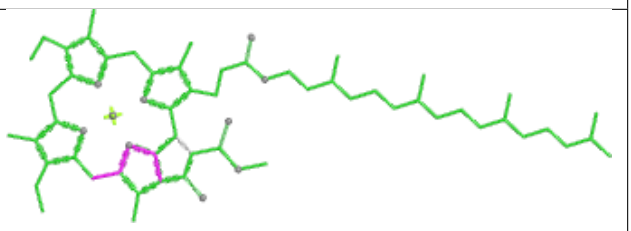


Rings

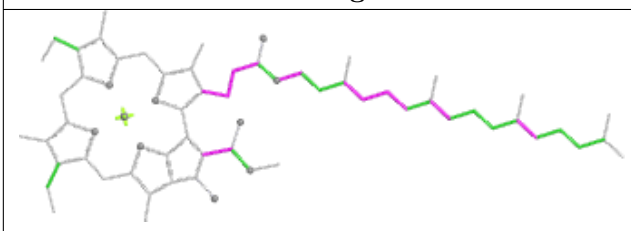
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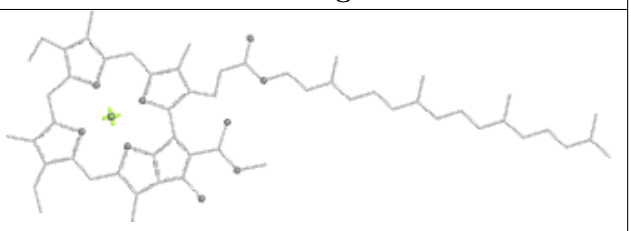
Bond lengths



Bond angles

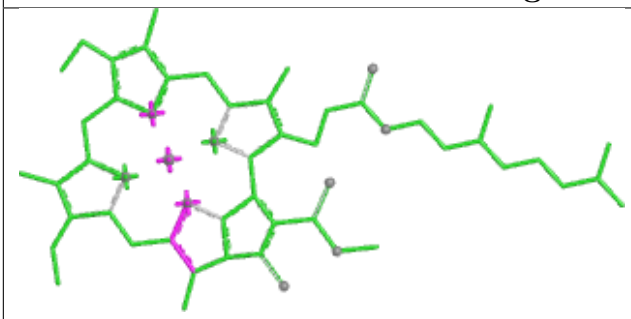


Torsions

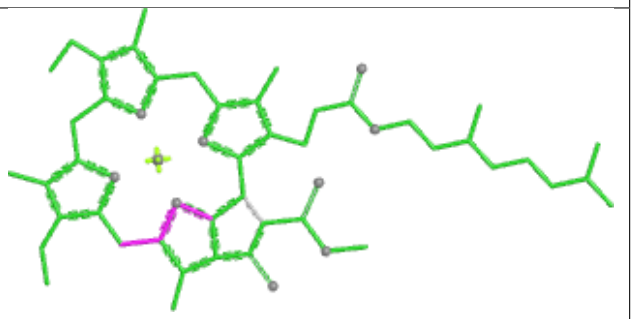


Rings

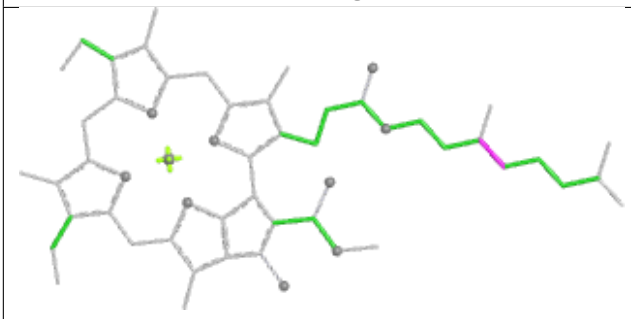
## Ligand CLA A 815



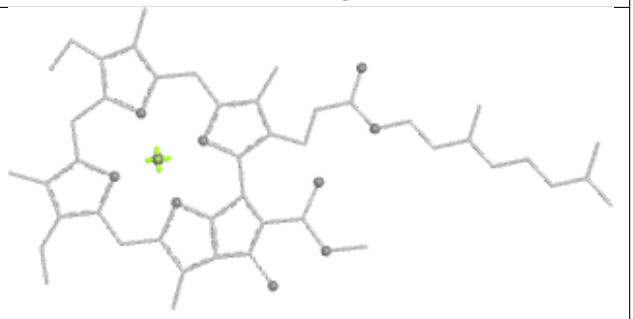
Bond lengths



Bond angles

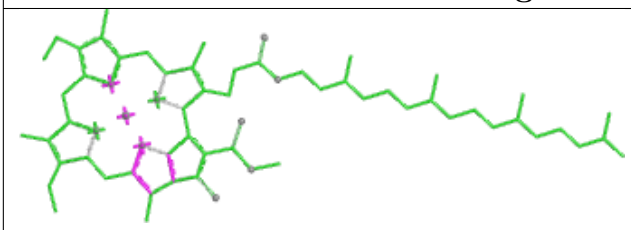


Torsions

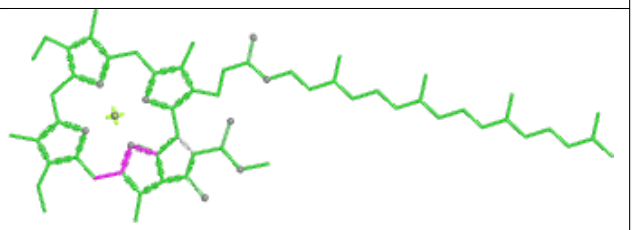


Rings

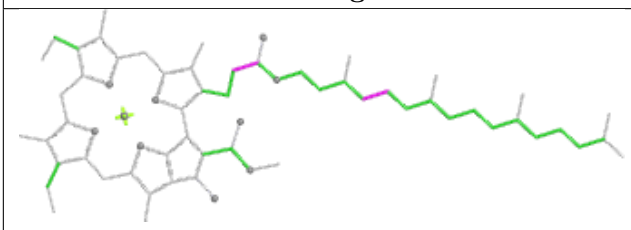
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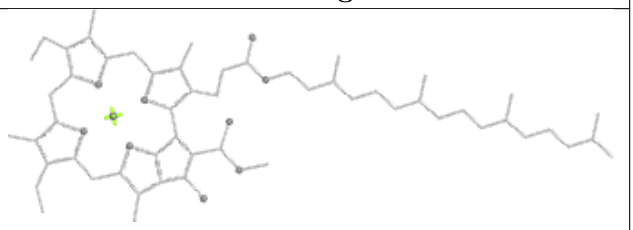
Bond lengths



Bond angles

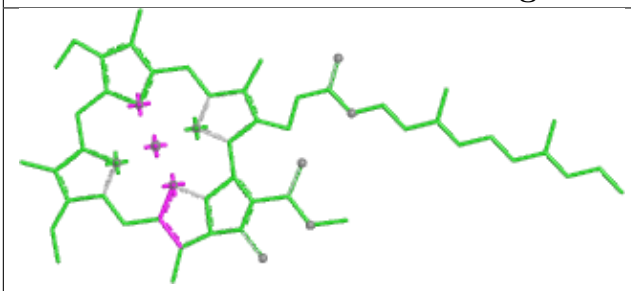


Torsions

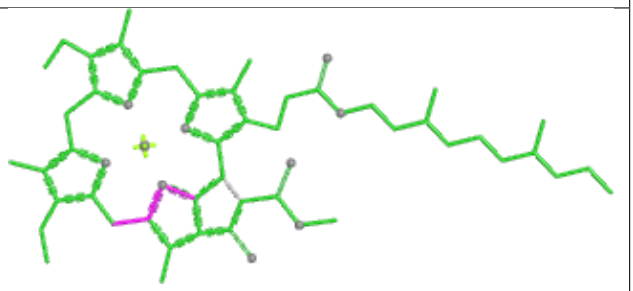


Rings

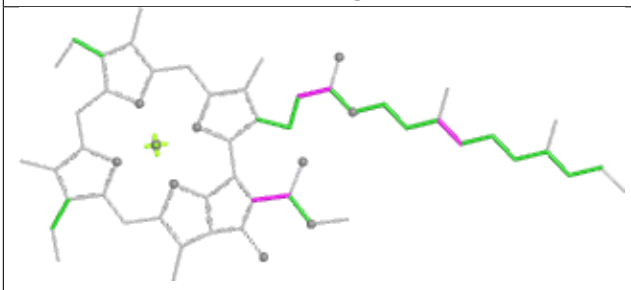
**Ligand CLA 12 603**



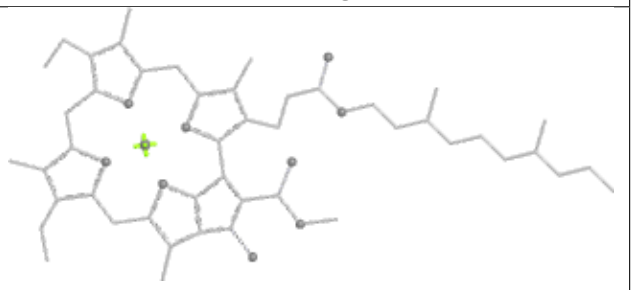
Bond lengths



Bond angles

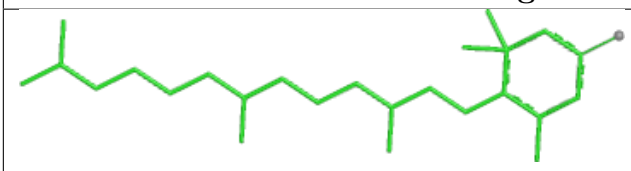


Torsions

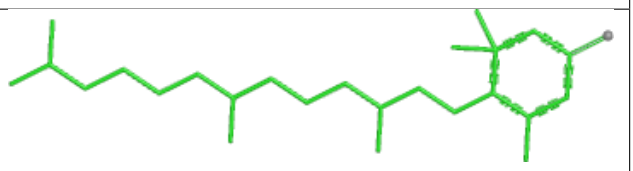


Rings

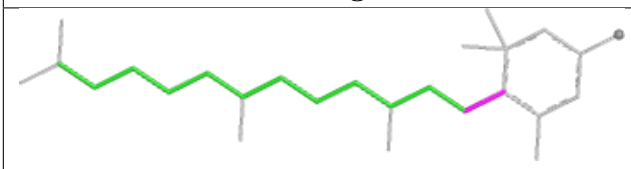
**Ligand LUT Z2 619**



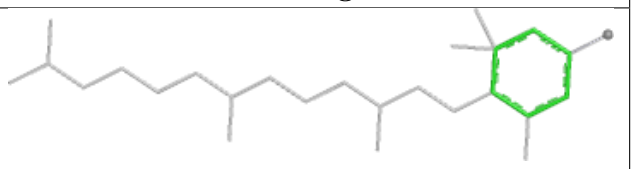
Bond lengths



Bond angles

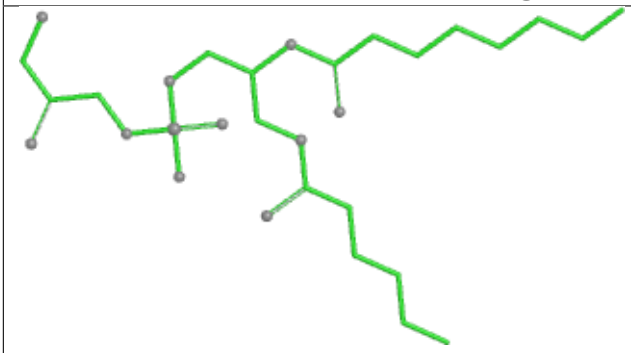


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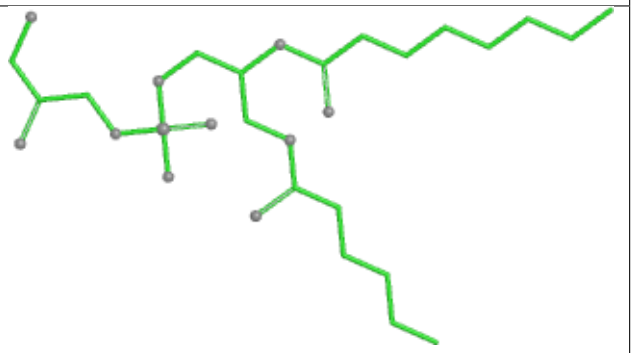


Rings

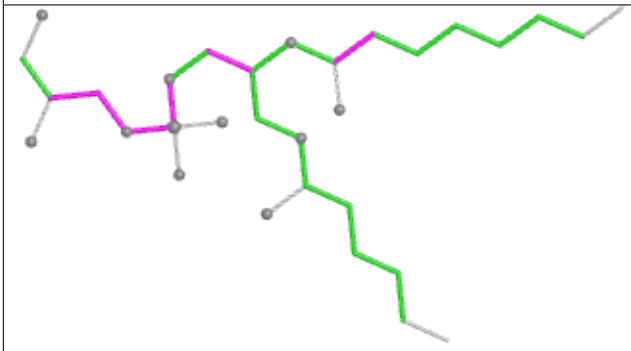
**Ligand LHG 32 721**



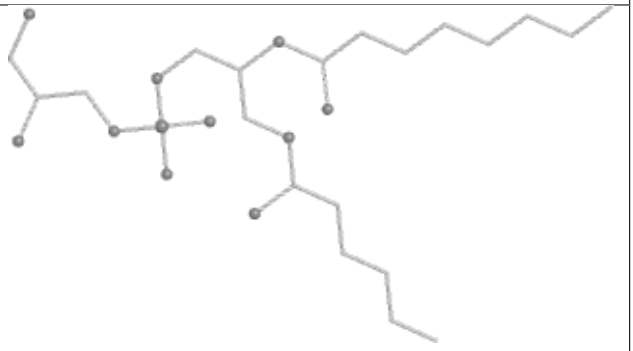
Bond lengths



Bond angles

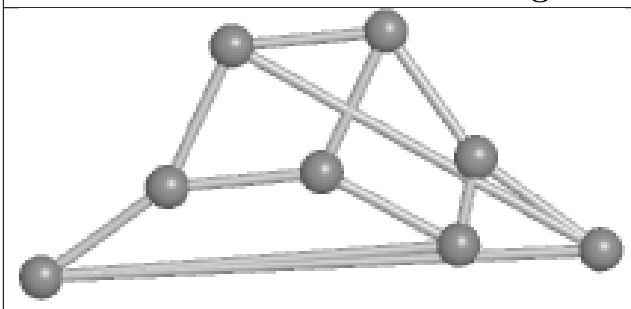


Torsions

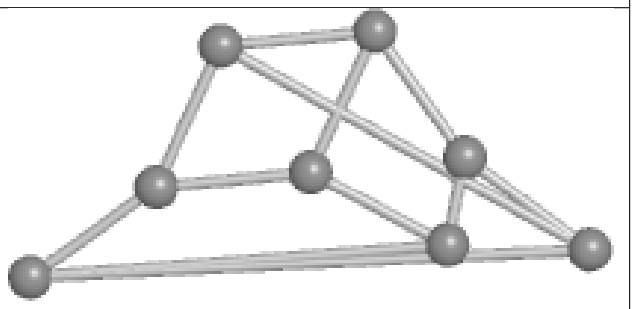


Rings

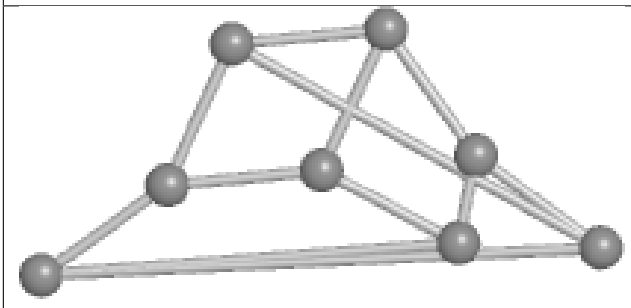
**Ligand SF4 C 102**



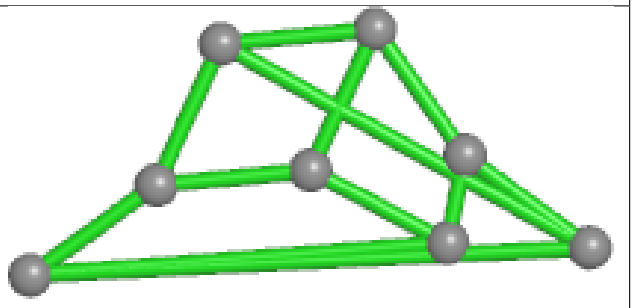
Bond lengths



Bond angles

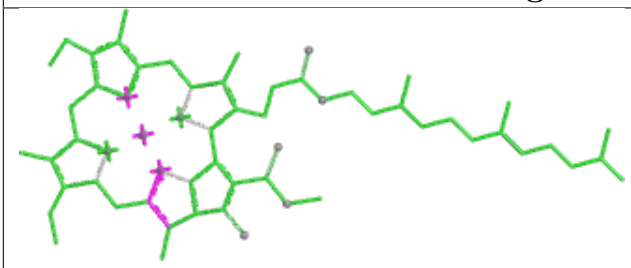


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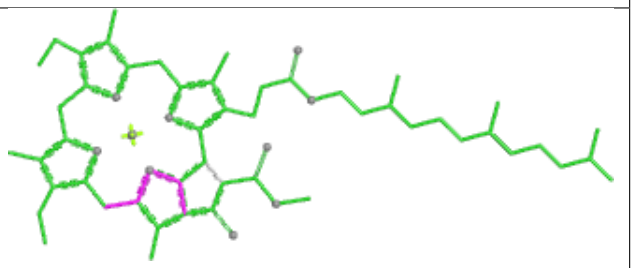


Rings

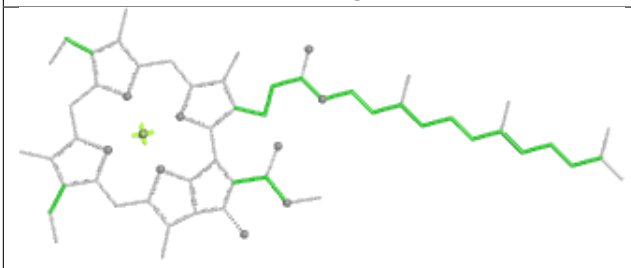
## Ligand CLA Z 610



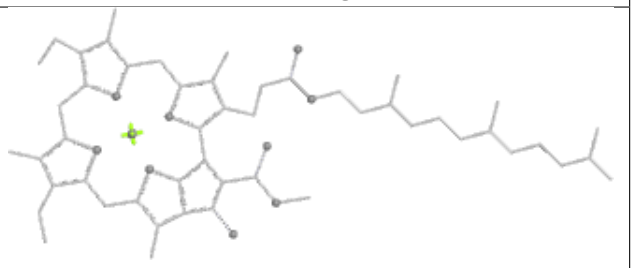
Bond lengths



Bond angles

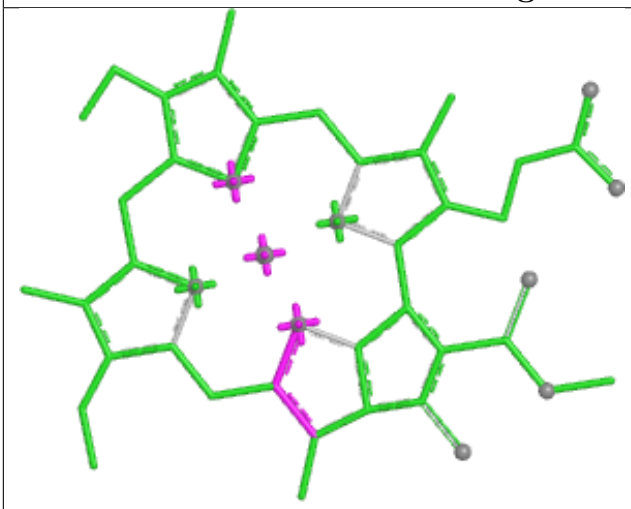


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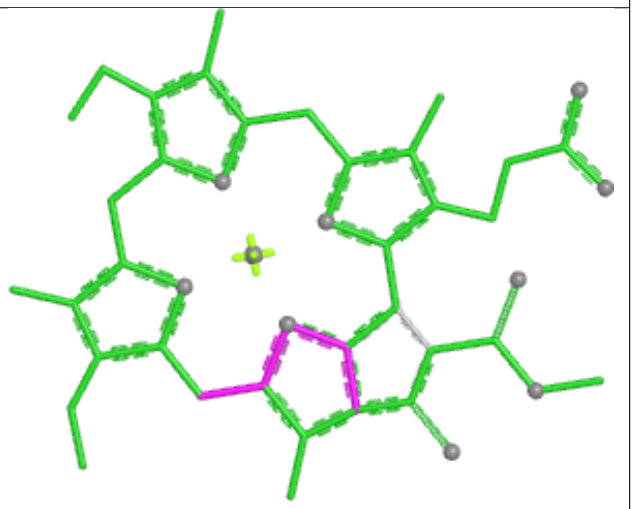


Rings

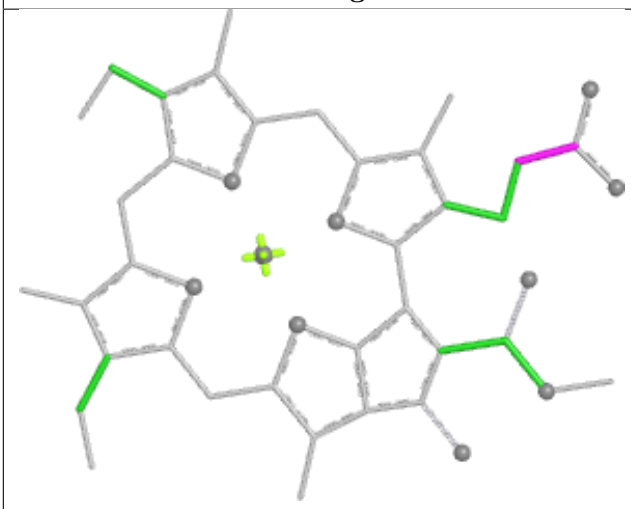
## Ligand CLA L2 204



Bond lengths



Bond angles

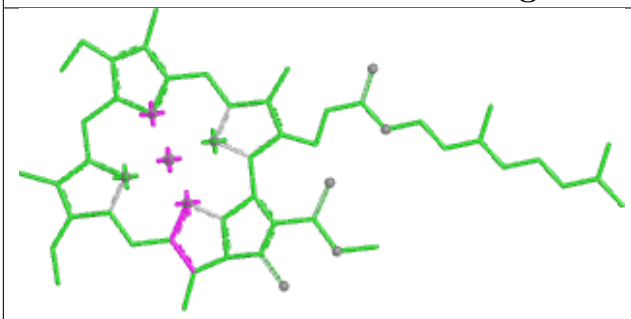


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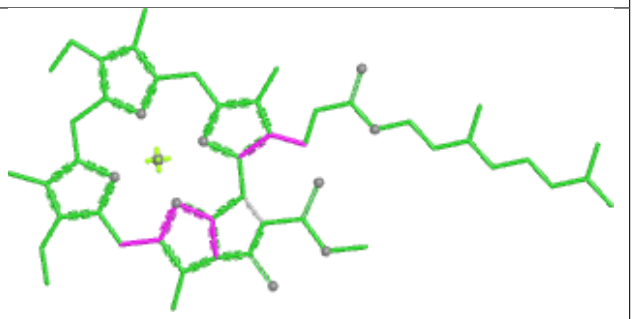


Rings

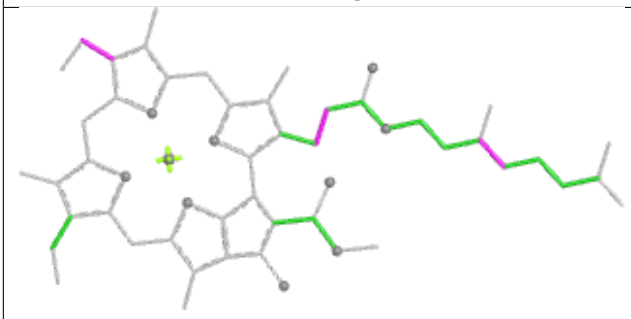
## Ligand CLA 62 609



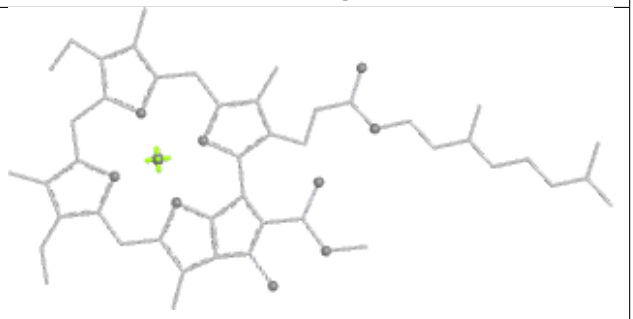
Bond lengths



Bond angles

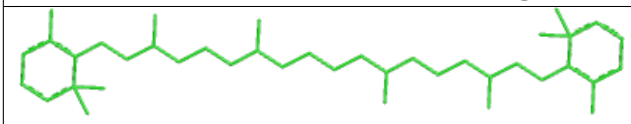


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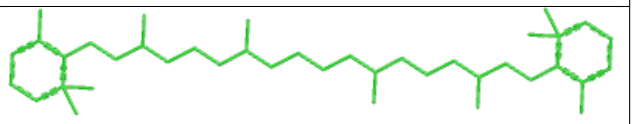


Rings

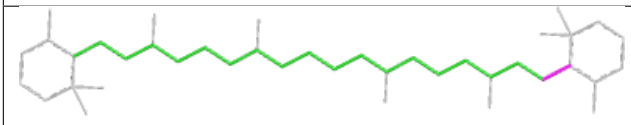
## Ligand BCR L2 205



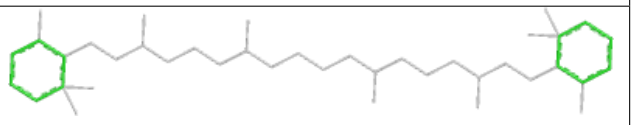
Bond lengths



Bond angles

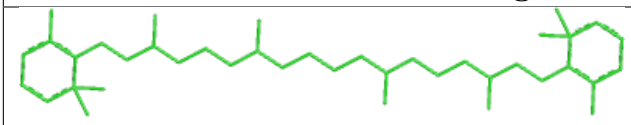


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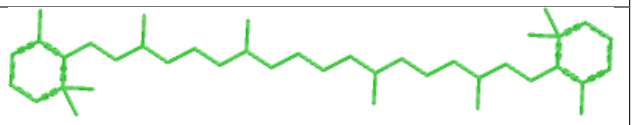


Rings

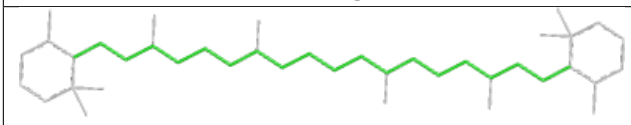
## Ligand BCR A2 850



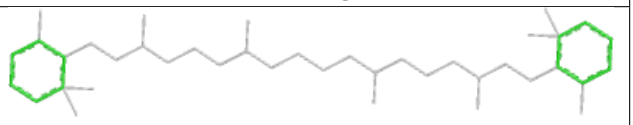
Bond lengths



Bond angles

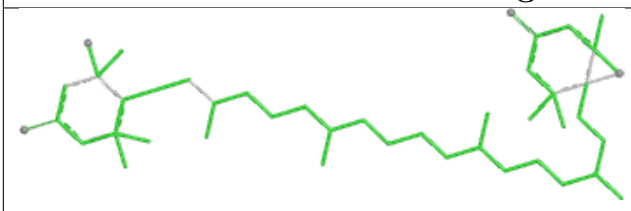


Torsions

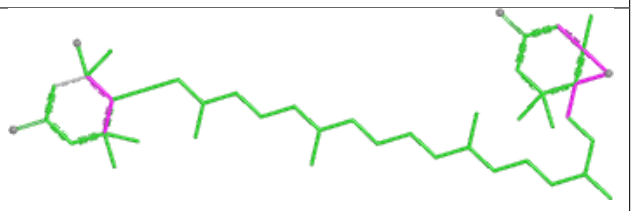


Rings

## Ligand NEX 62 625



Bond lengths



Bond angles

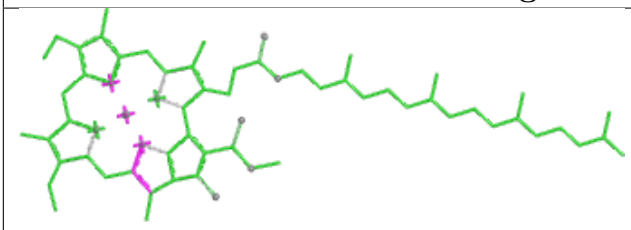


Torsions

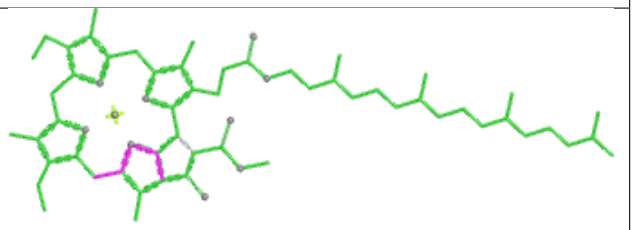


Rings

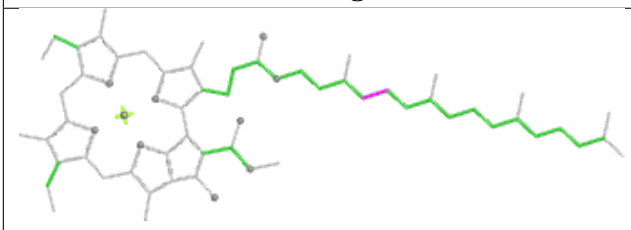
## Ligand CLA 32 604



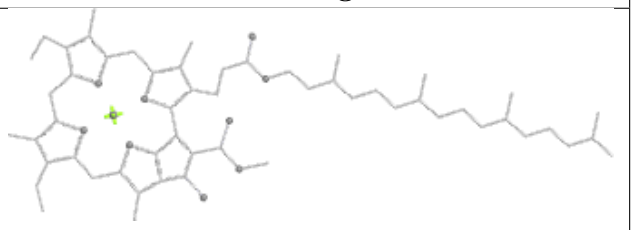
Bond lengths



Bond angles

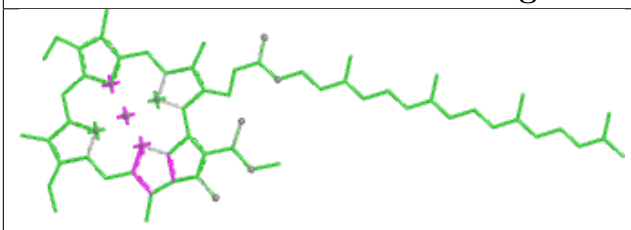


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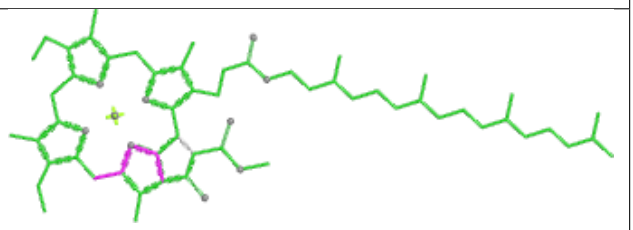


Rings

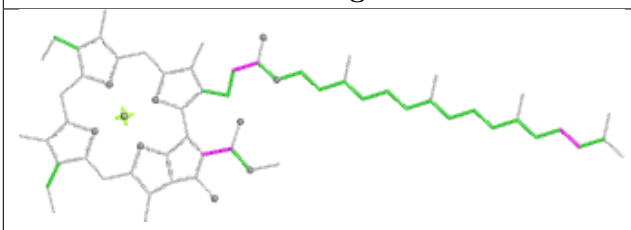
## Ligand CLA 82 603



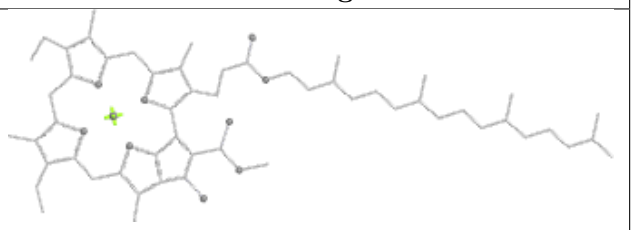
Bond lengths



Bond angles

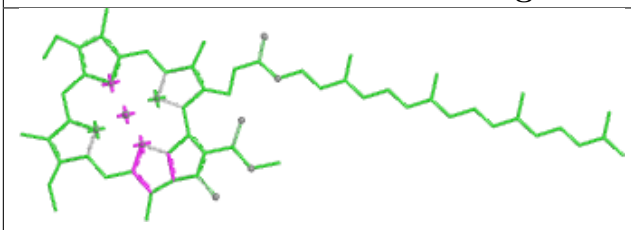


Torsions

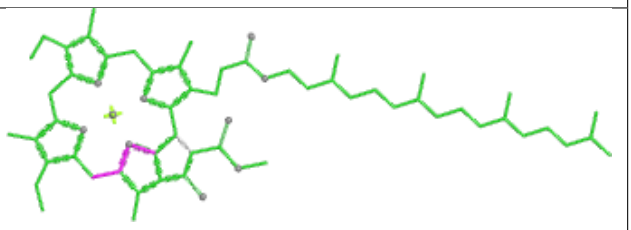


Rings

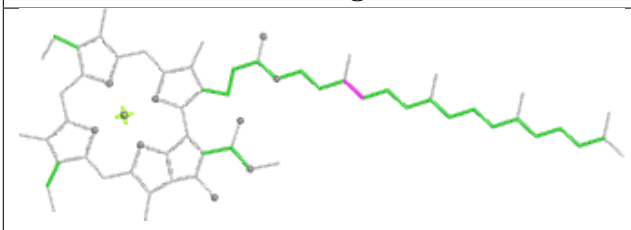
## Ligand CLA B2 812



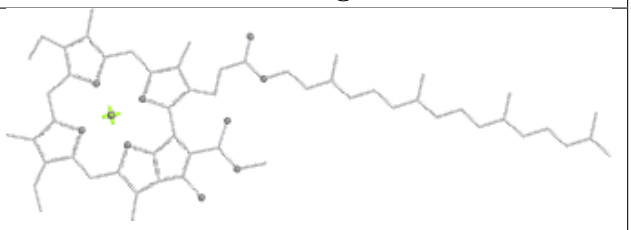
Bond lengths



Bond angles

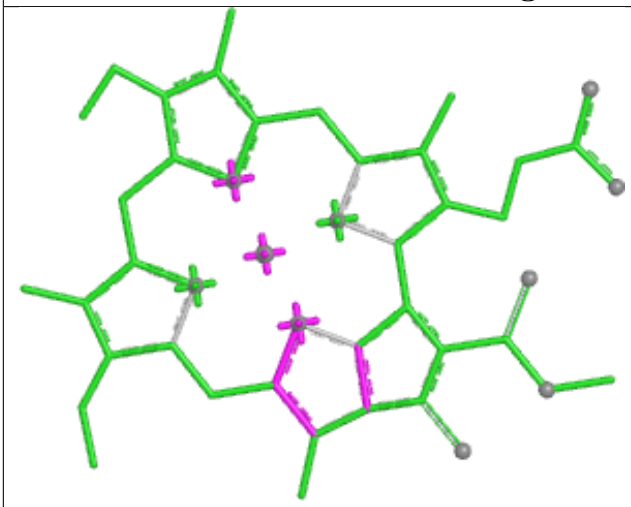


Torsions

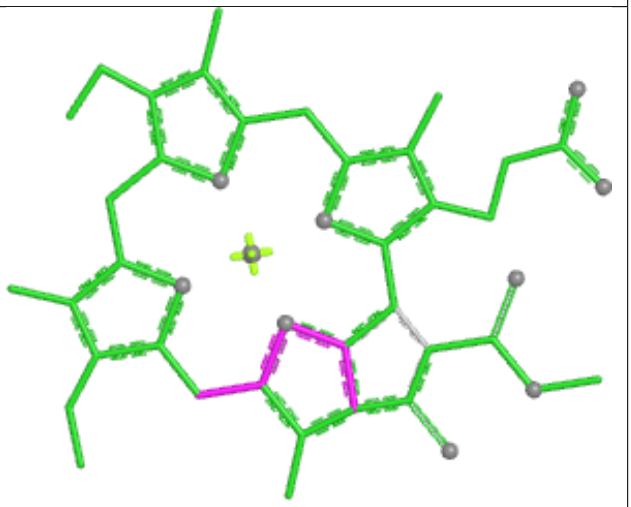


Rings

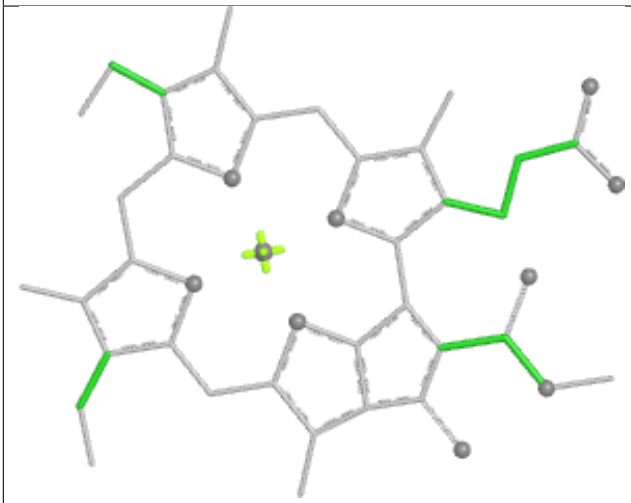
## Ligand CLA 82 616



Bond lengths



Bond angles

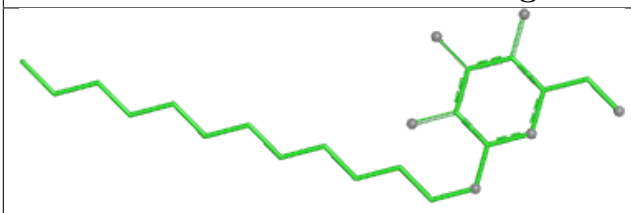


Torsions

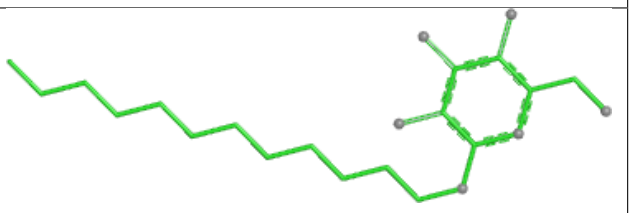


Rings

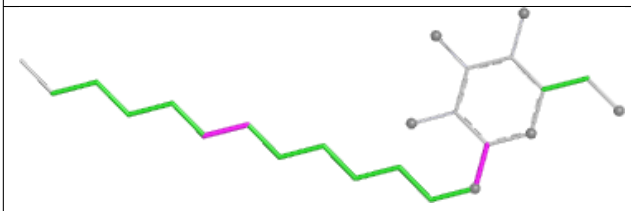
## Ligand LMU A 865



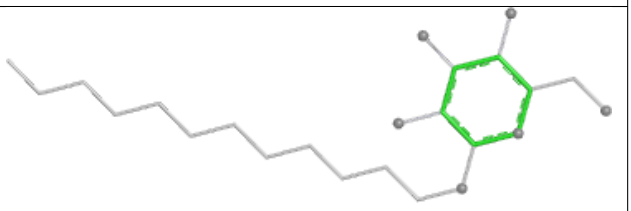
Bond lengths



Bond angles

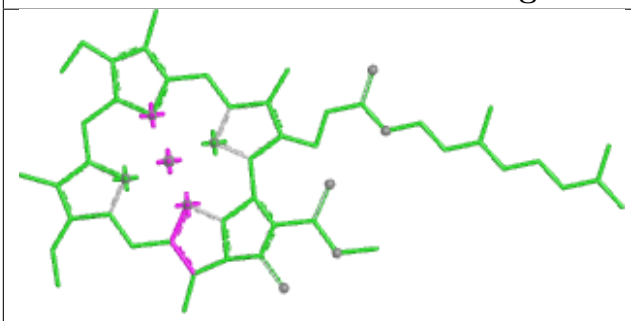


Torsions

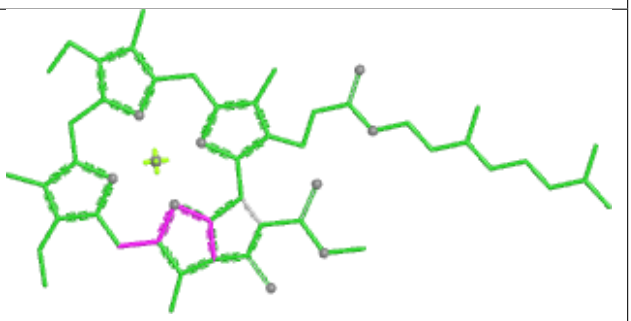


Rings

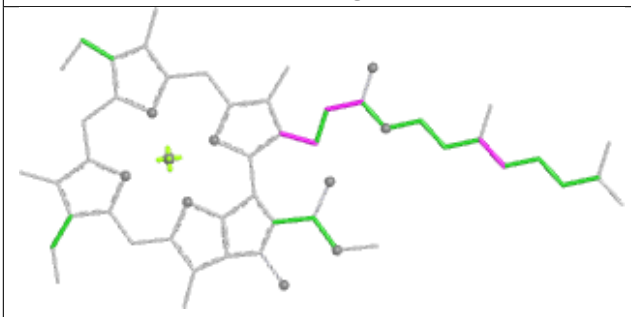
## Ligand CLA 52 604



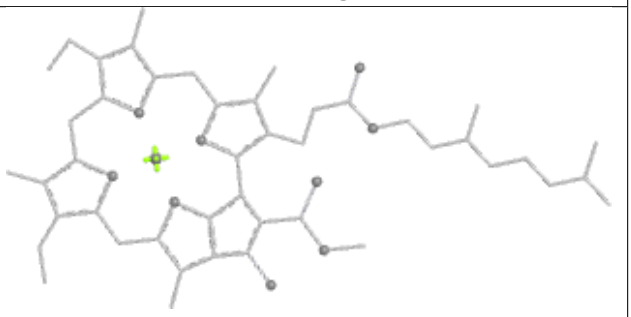
Bond lengths



Bond angles

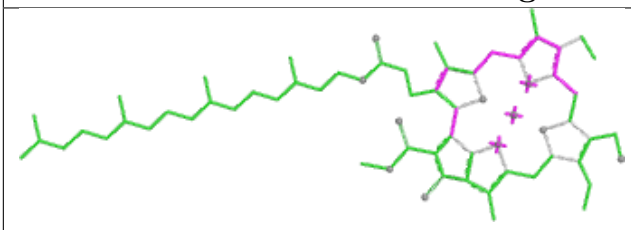


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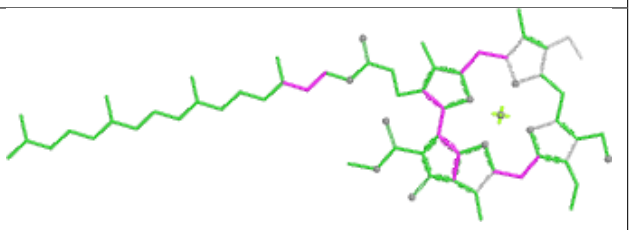


Rings

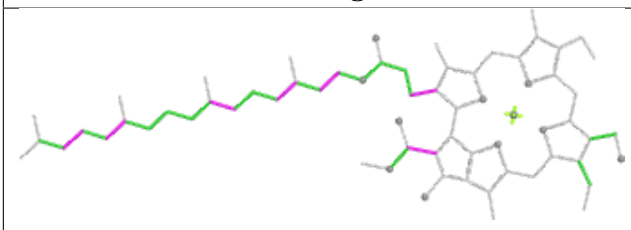
**Ligand CHL 62 607**



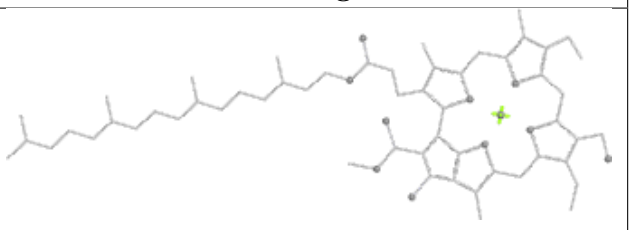
Bond lengths



Bond angles

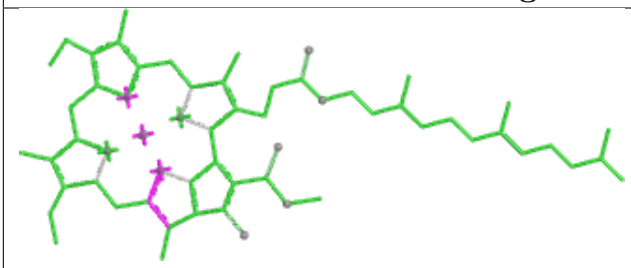


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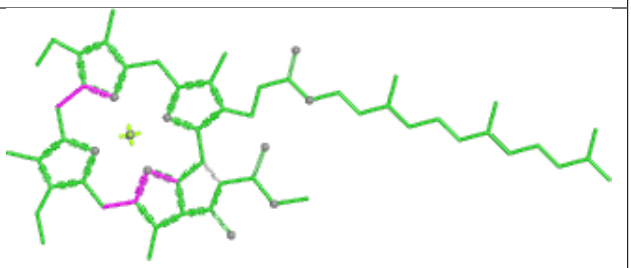


Rings

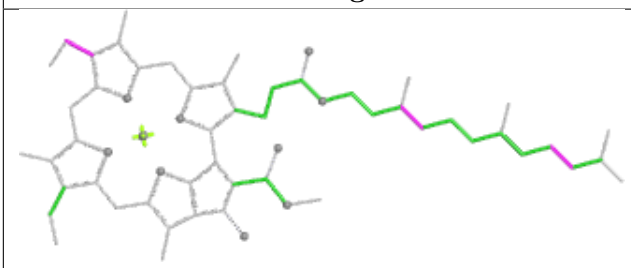
**Ligand CLA 32 613**



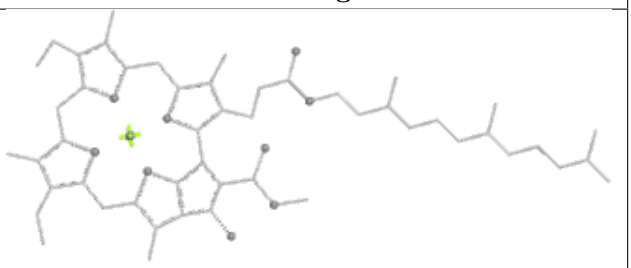
Bond lengths



Bond angles

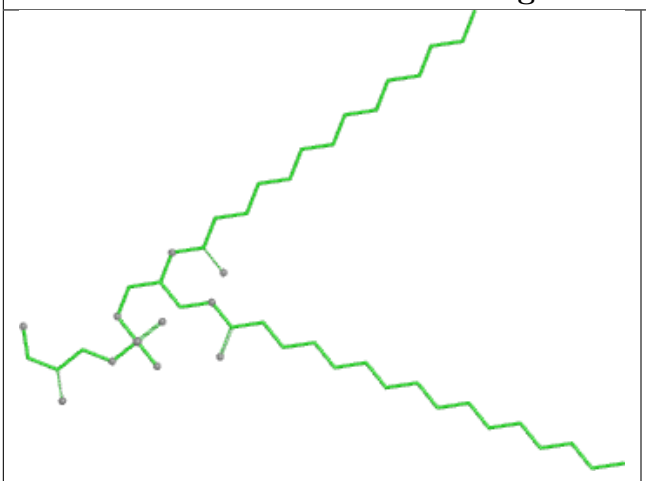


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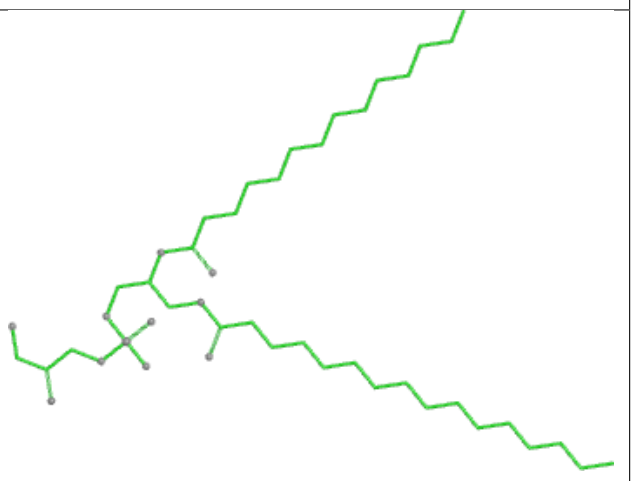


Rings

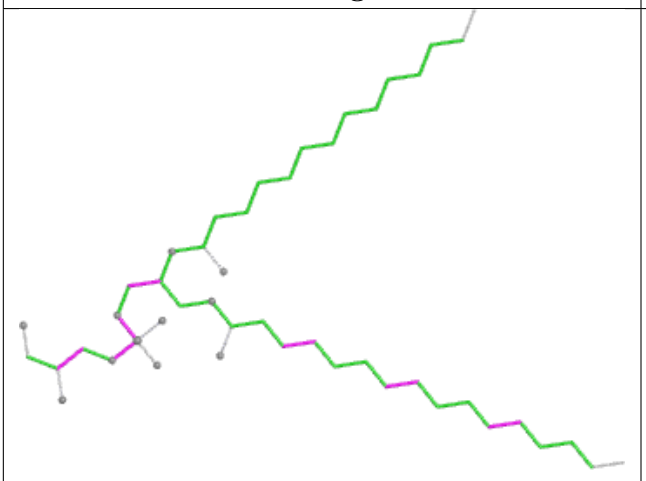
**Ligand LHG 32 623**



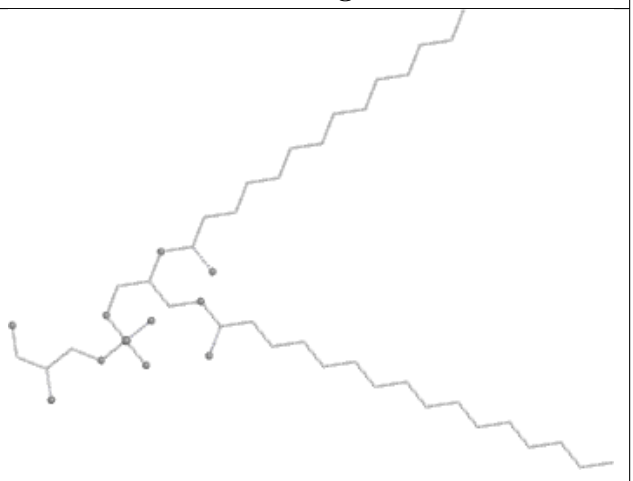
Bond lengths



Bond angles

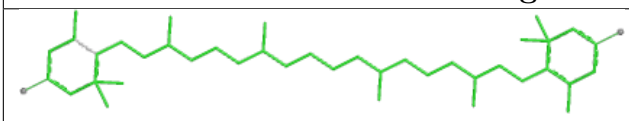


Torsions

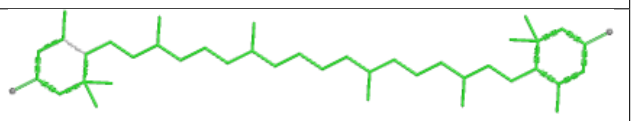


Rings

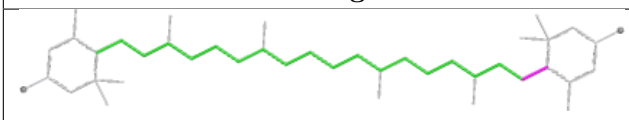
**Ligand LUT 42 619**



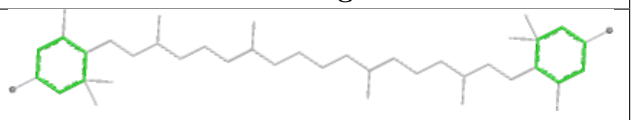
Bond lengths



Bond angles

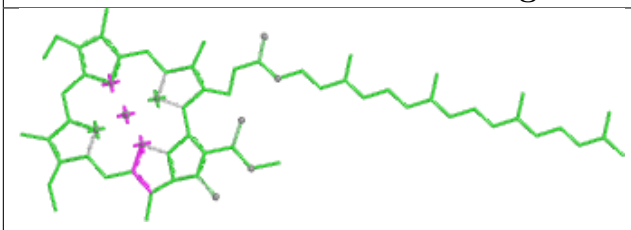


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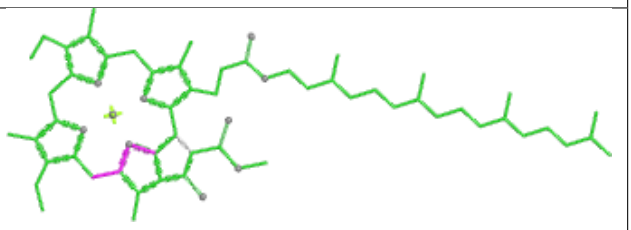


Rings

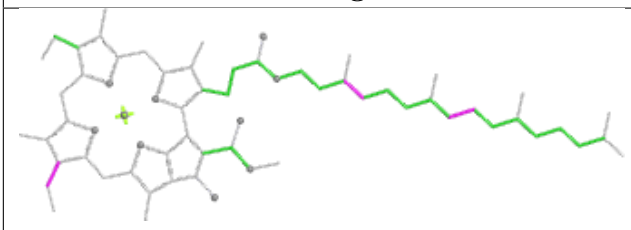
## Ligand CLA 32 603



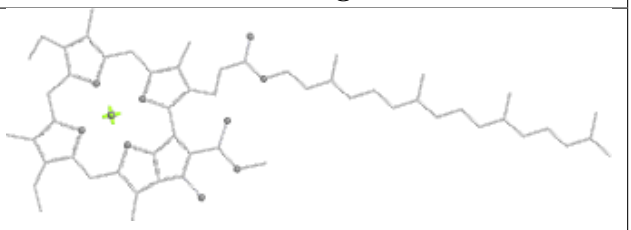
Bond lengths



Bond angles

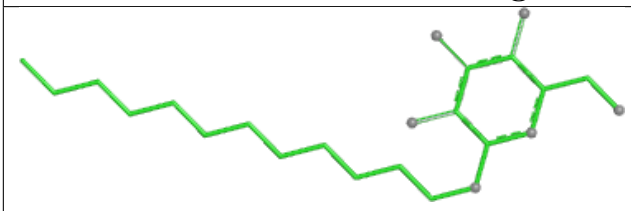


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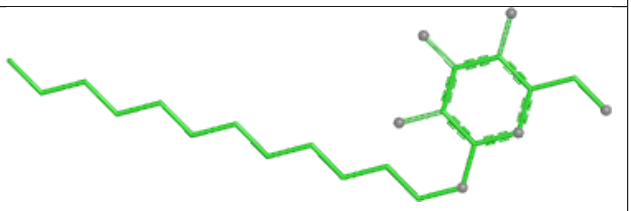


Rings

## Ligand LMU G2 206



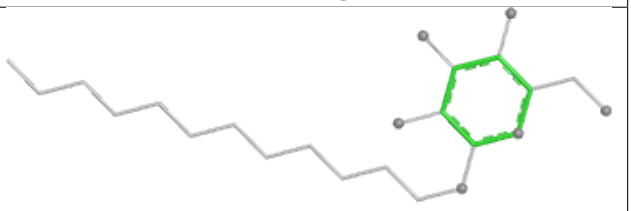
Bond lengths



Bond angles

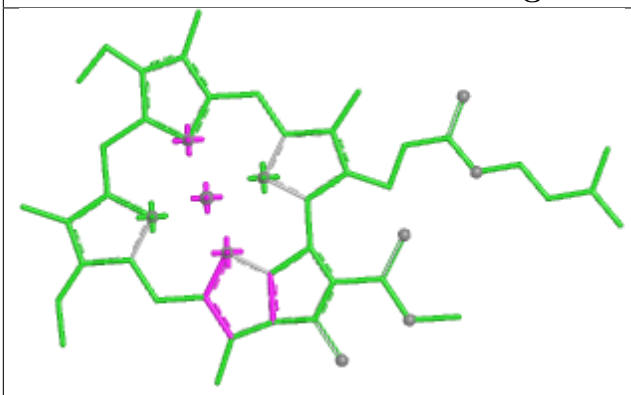


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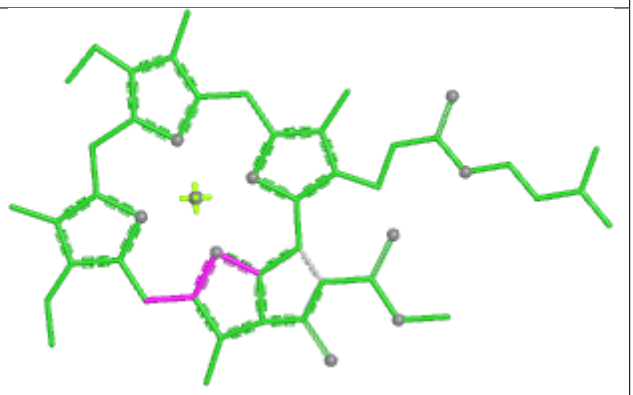


Rings

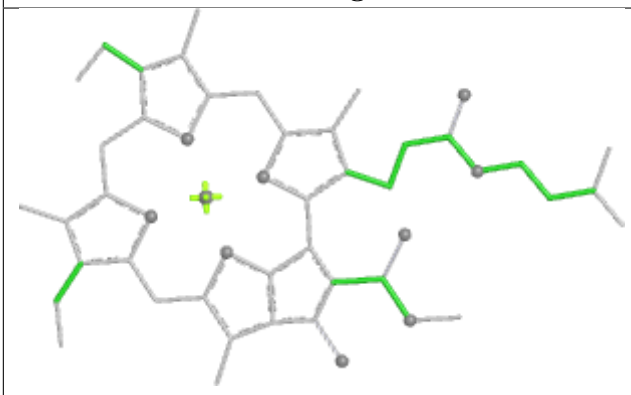
## Ligand CLA A 808



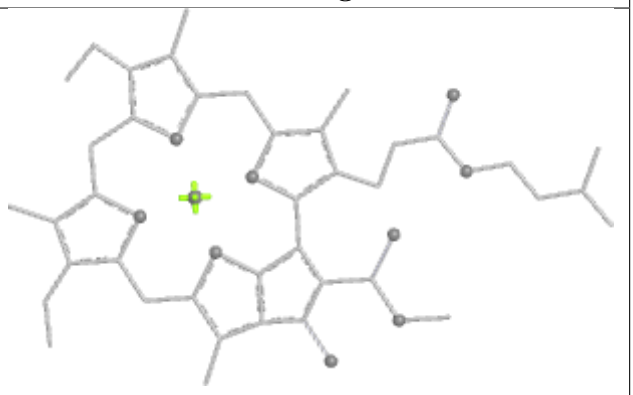
Bond lengths



Bond angles

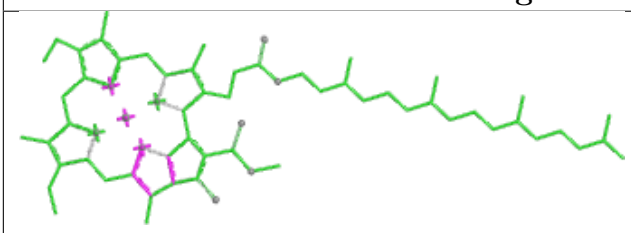


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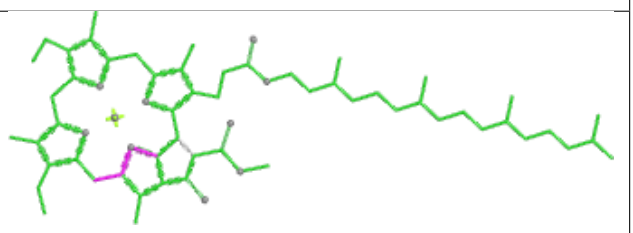


Rings

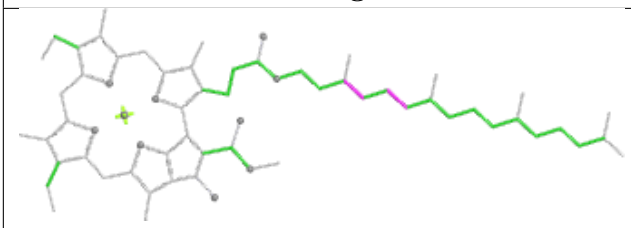
## Ligand CLA B2 829



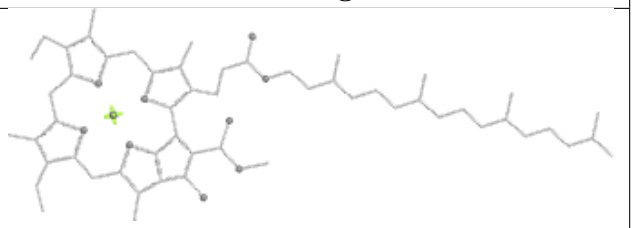
Bond lengths



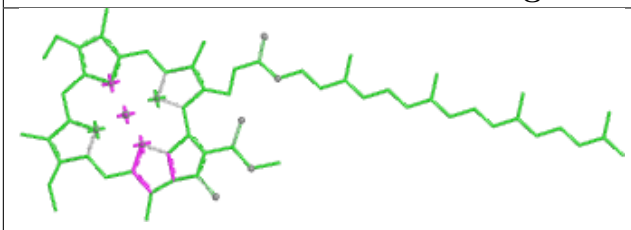
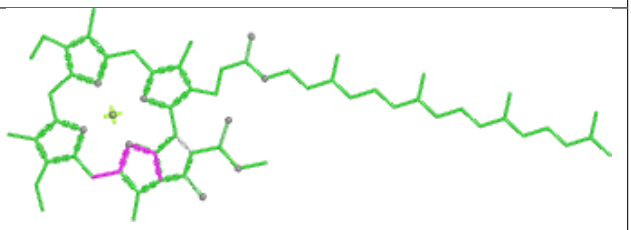
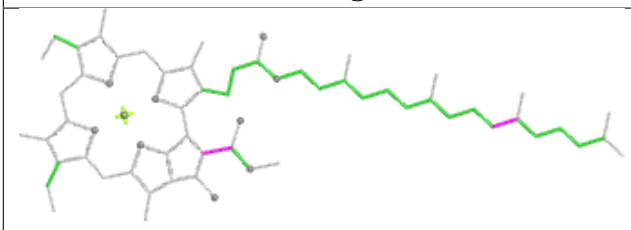
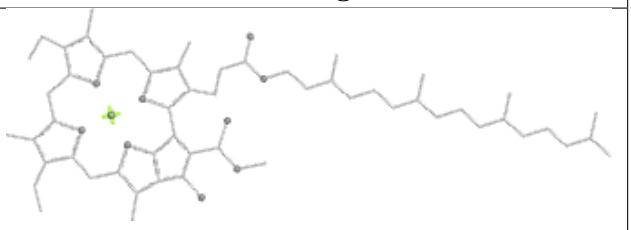
Bond angles

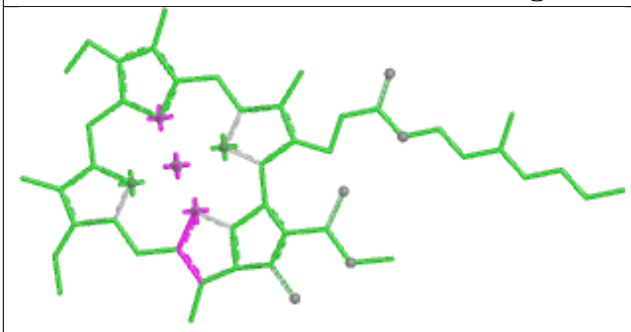
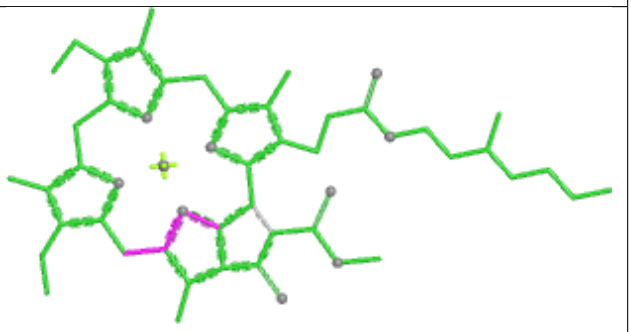
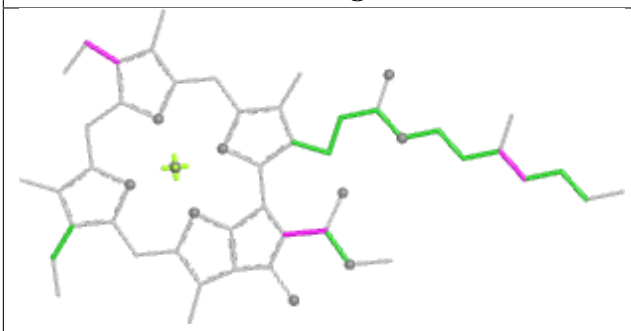
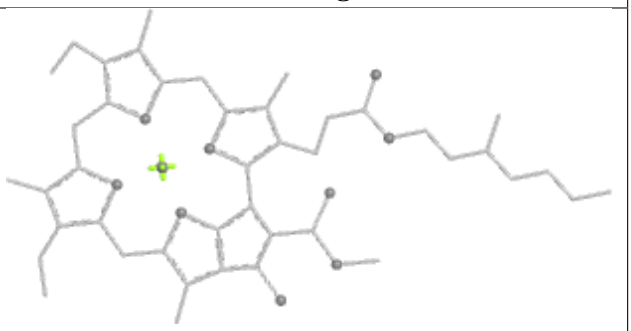


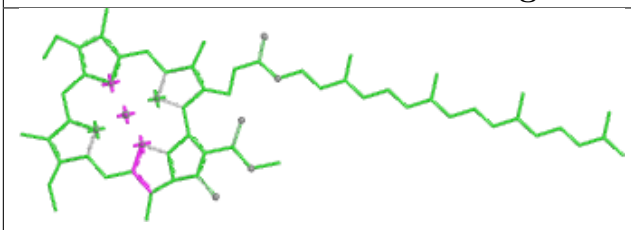
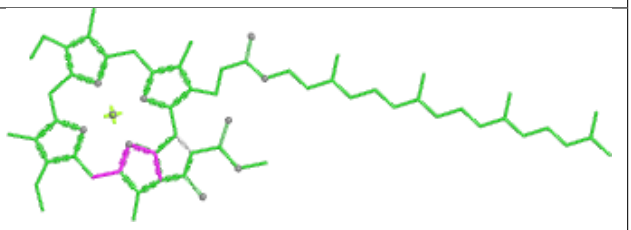
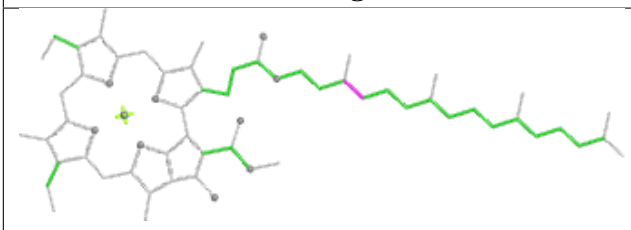
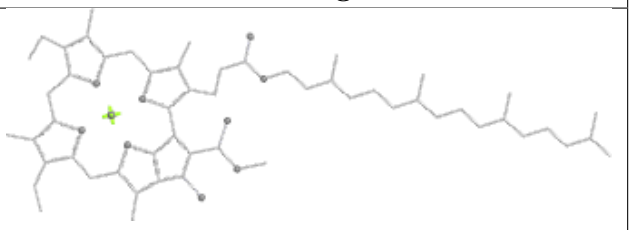
Torsions

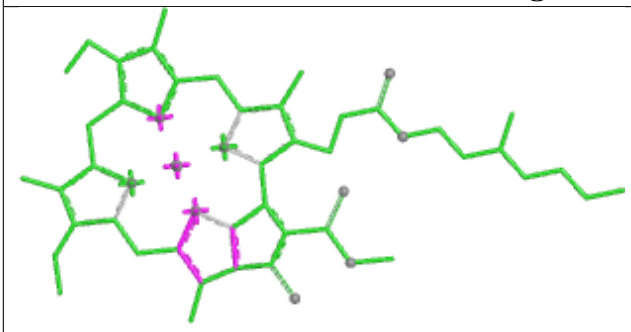
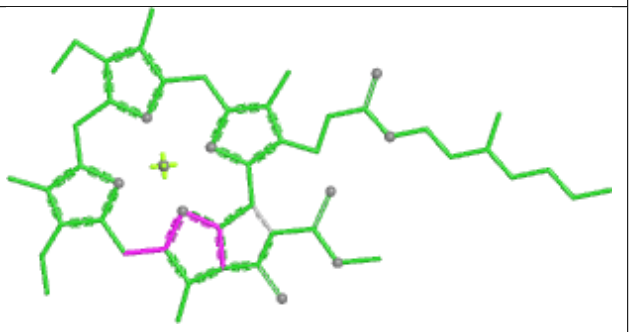
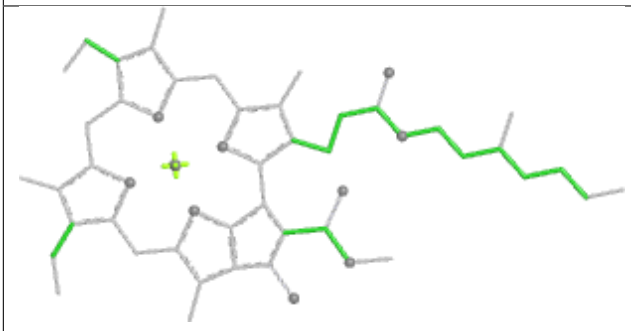
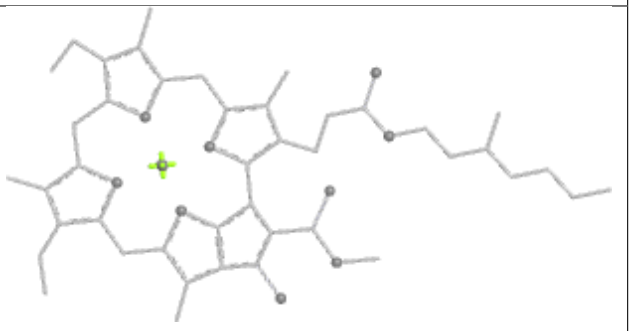


Rings

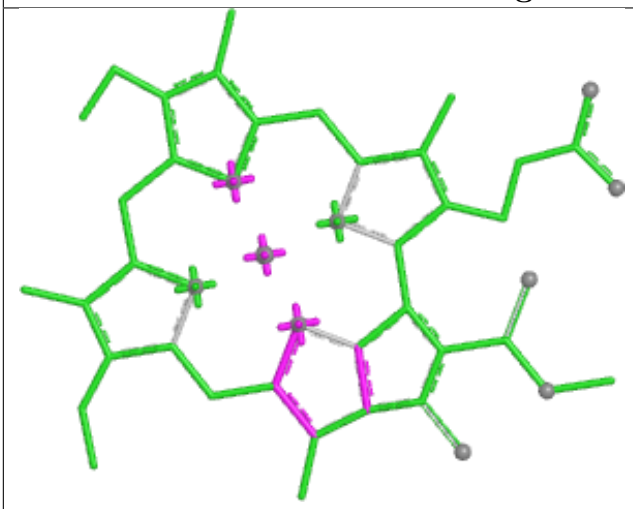
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|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 7 620 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

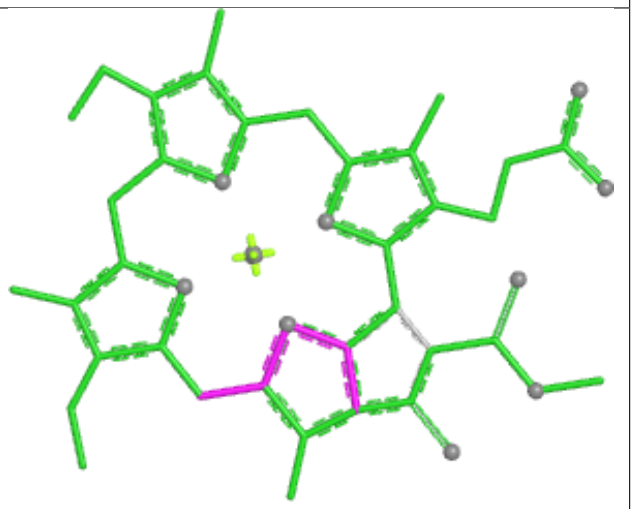
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|  Torsions |  Rings |

| Ligand CLA 9 604 | |
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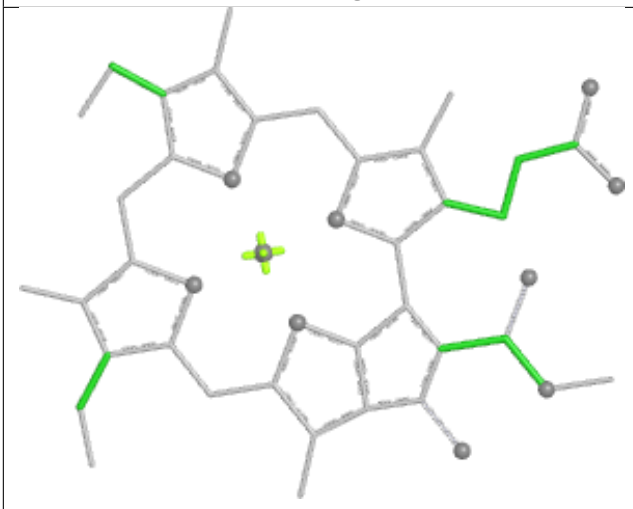
## Ligand CLA B2 830



Bond lengths



Bond angles

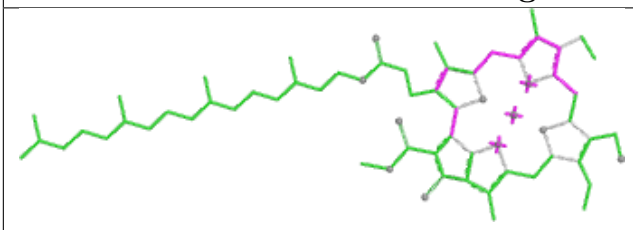


Torsions

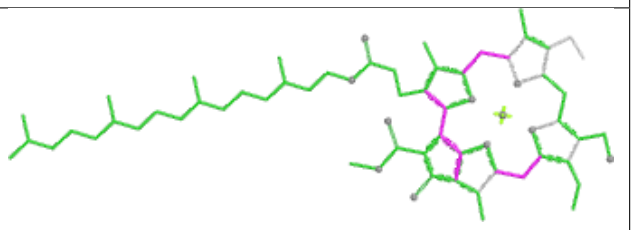


Rings

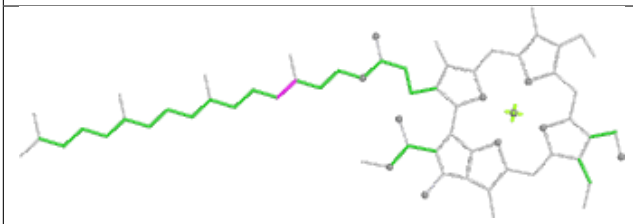
## Ligand CHL 82 606



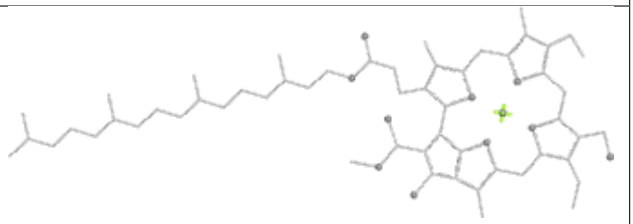
Bond lengths



Bond angles

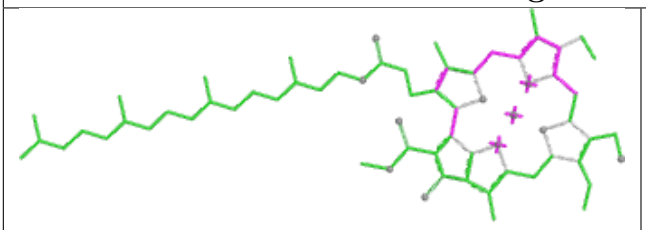


Torsions

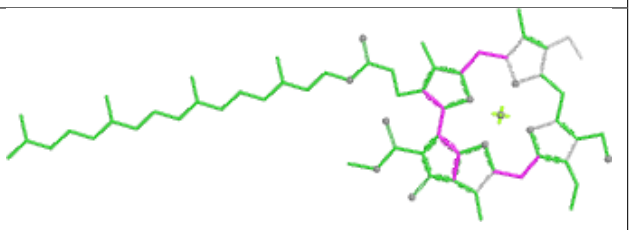


Rings

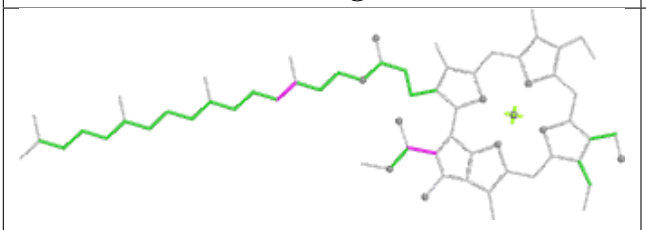
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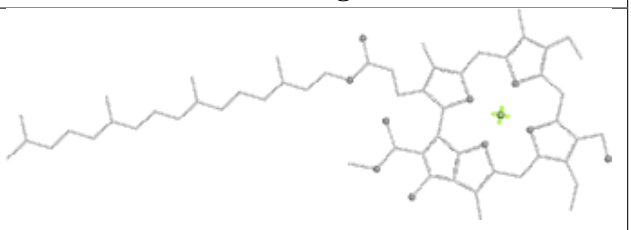
Bond lengths



Bond angles

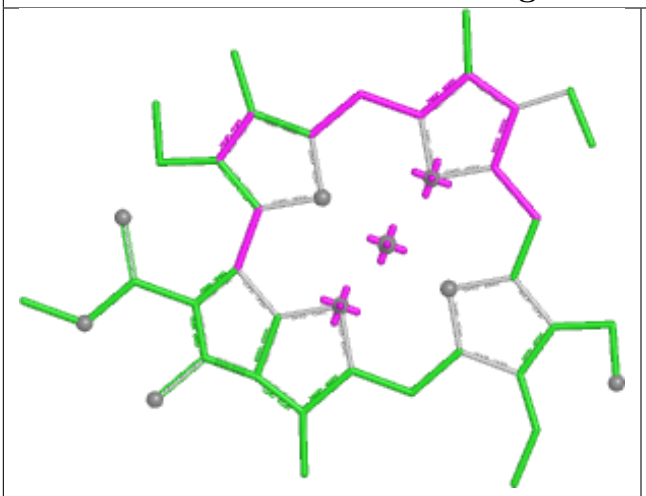


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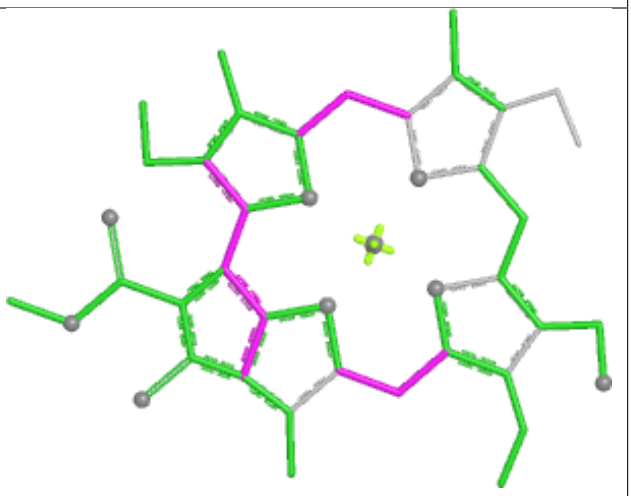


Rings

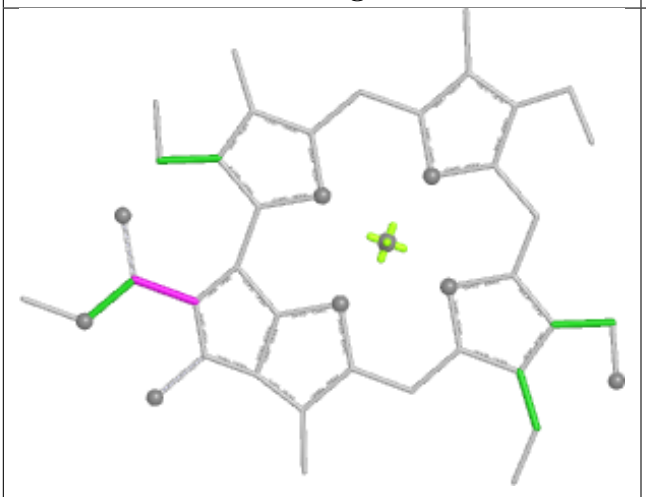
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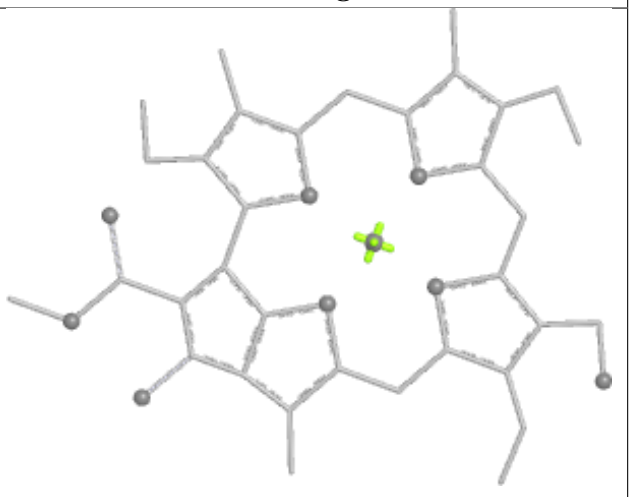
Bond lengths



Bond angles

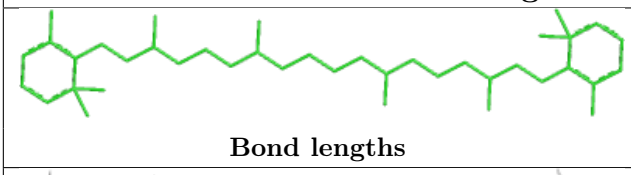


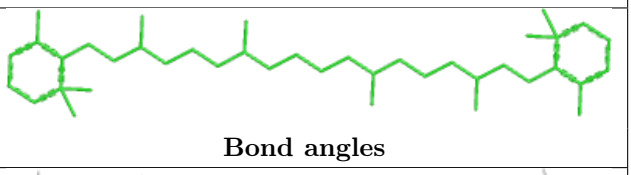
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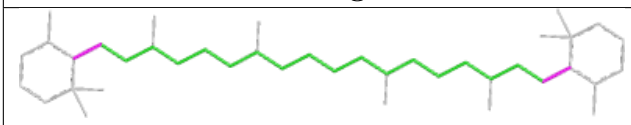


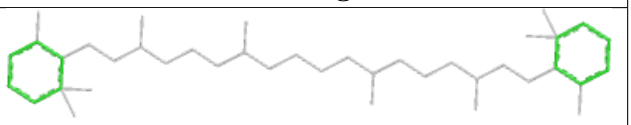
Rings

## Ligand BCR K 207


Bond lengths

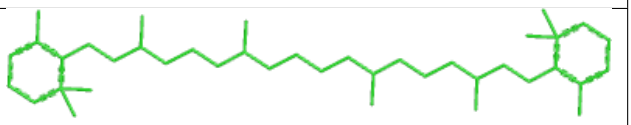

Bond angles

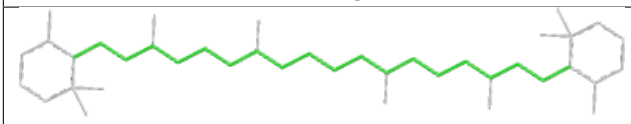

Torsions

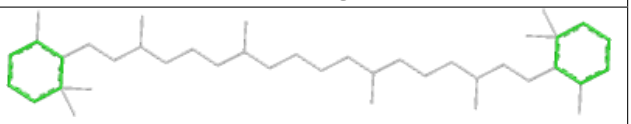

Rings

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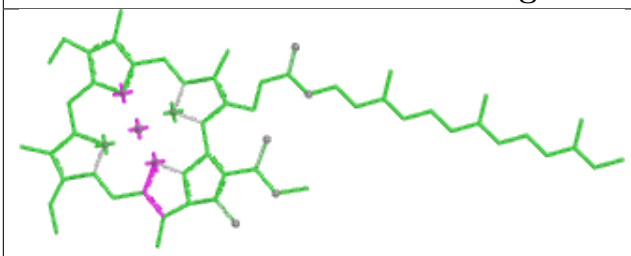

Bond lengths

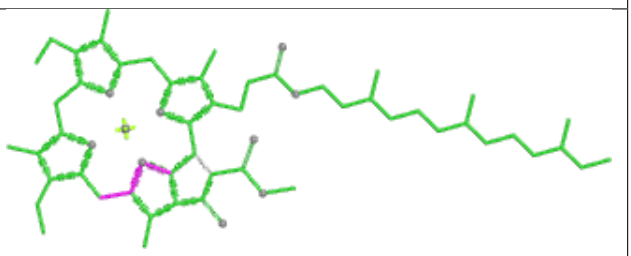

Bond angles

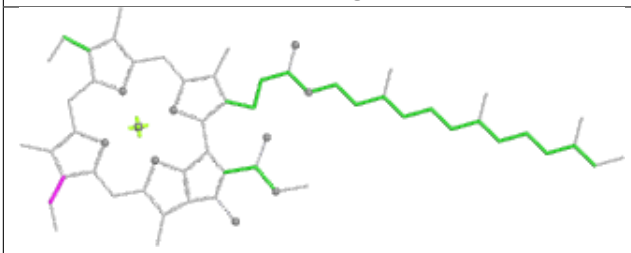

Torsions

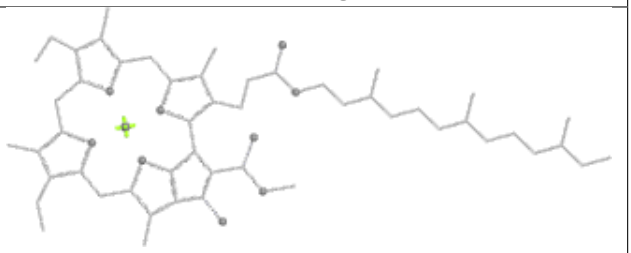

Rings

## Ligand CLA 32 609

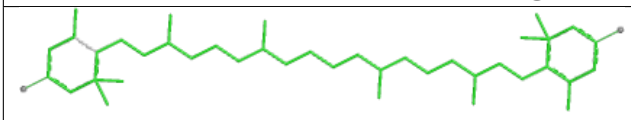

Bond lengths

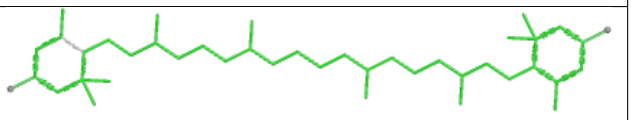

Bond angles

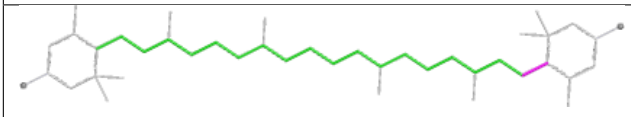

Torsions

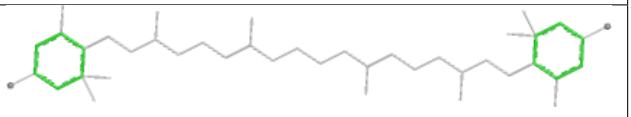

Rings

## Ligand LUT 9 616

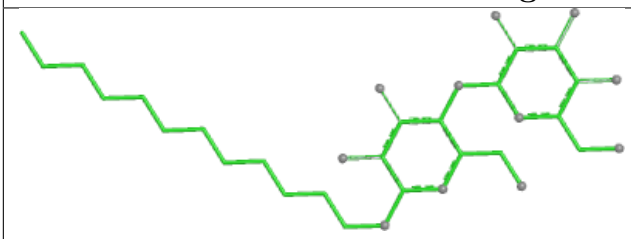

Bond lengths


Bond angles

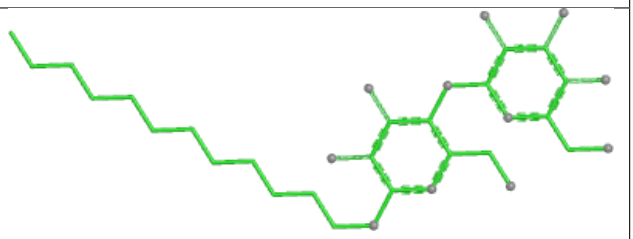

Torsions


Rings

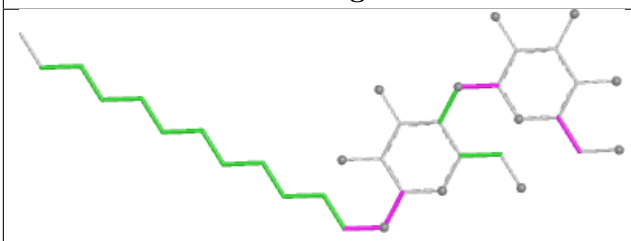
## Ligand LMU A 858



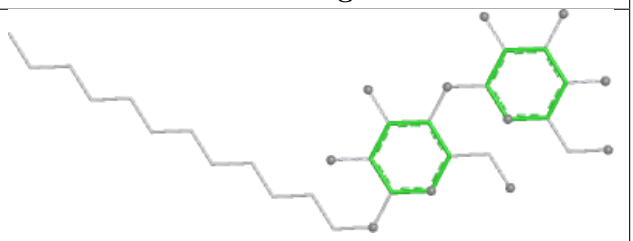
Bond lengths



Bond angles

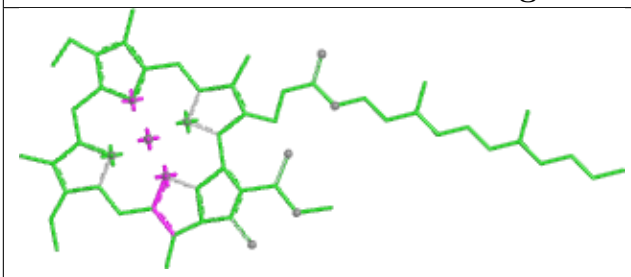


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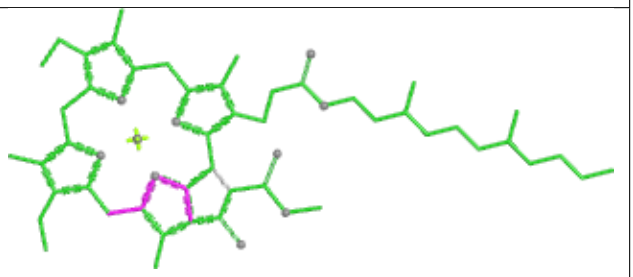


Rings

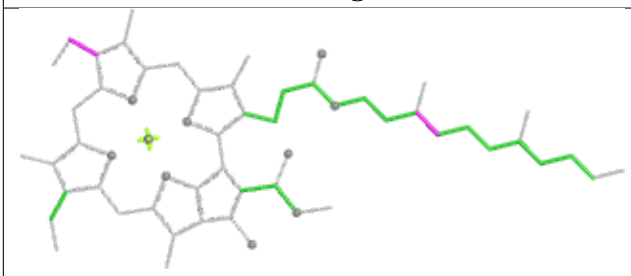
## Ligand CLA 62 611



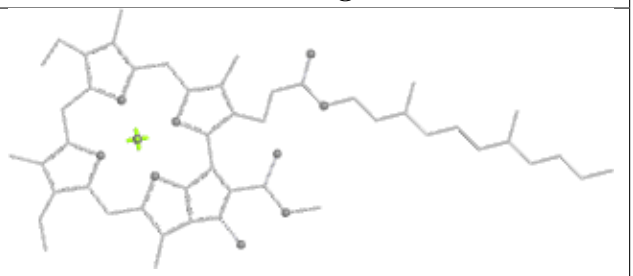
Bond lengths



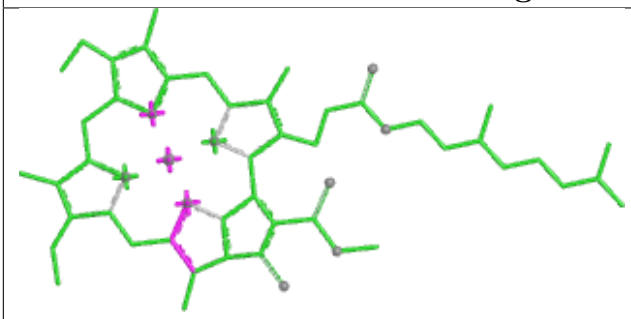
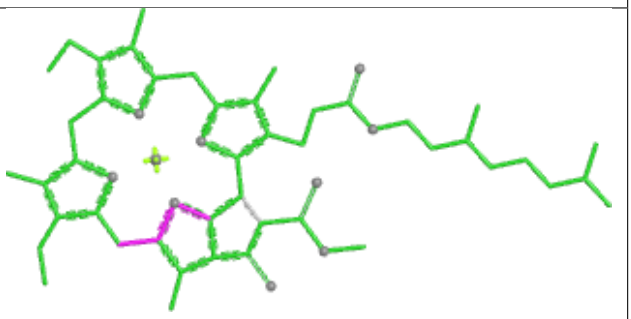
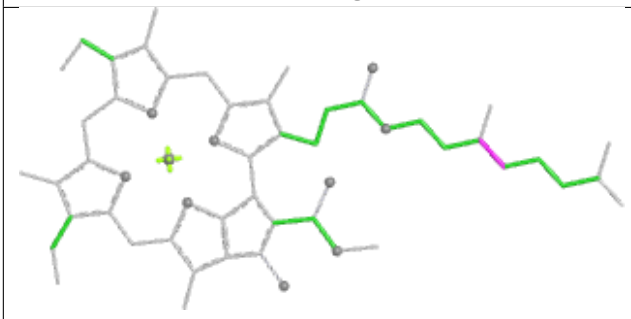
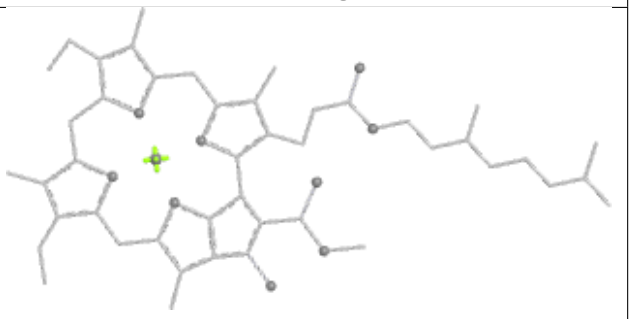
Bond angles

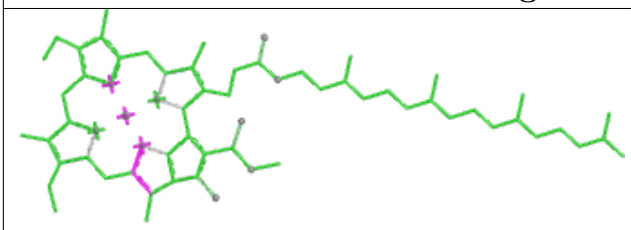
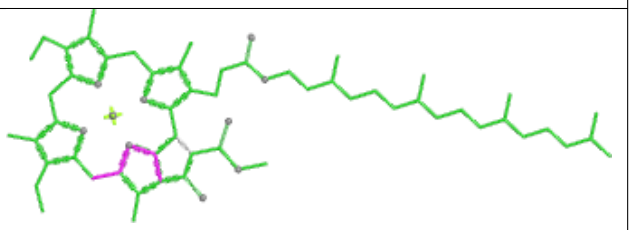
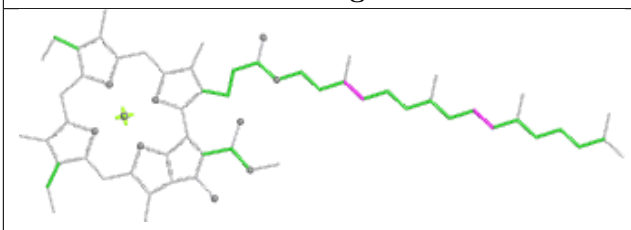
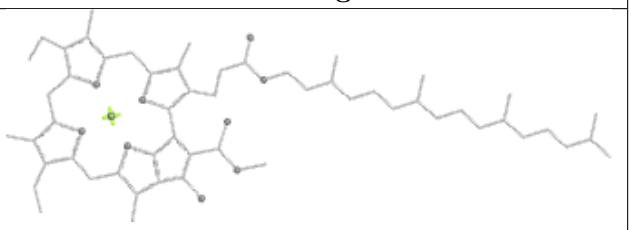


Torsions

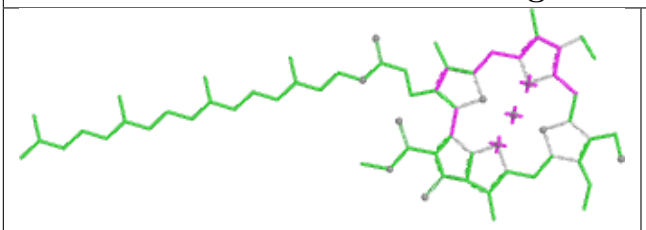


Rings

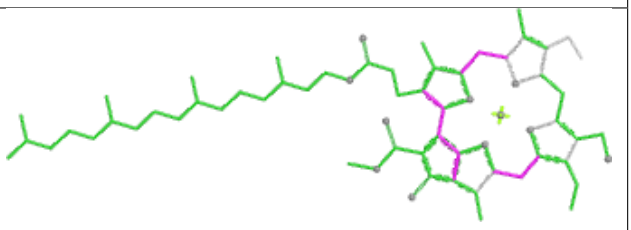
| Ligand CLA A2 815 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 52 609 | |
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|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

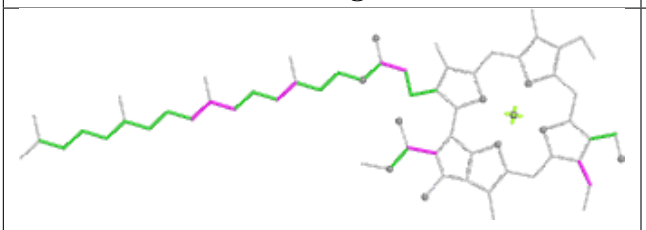
**Ligand CHL 5 607**



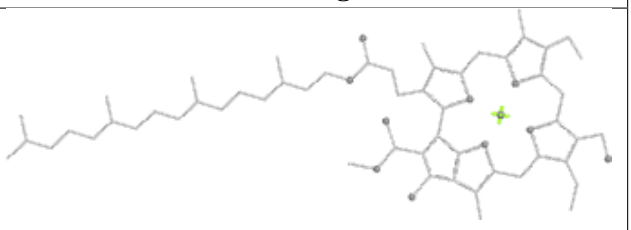
Bond lengths



Bond angles



Torsions

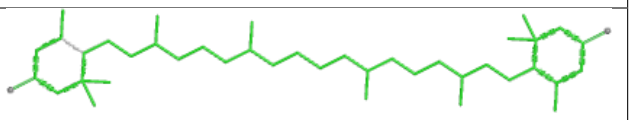


Rings

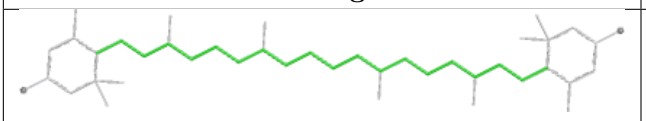
**Ligand LUT 3 720**



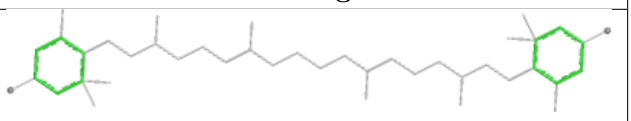
Bond lengths



Bond angles

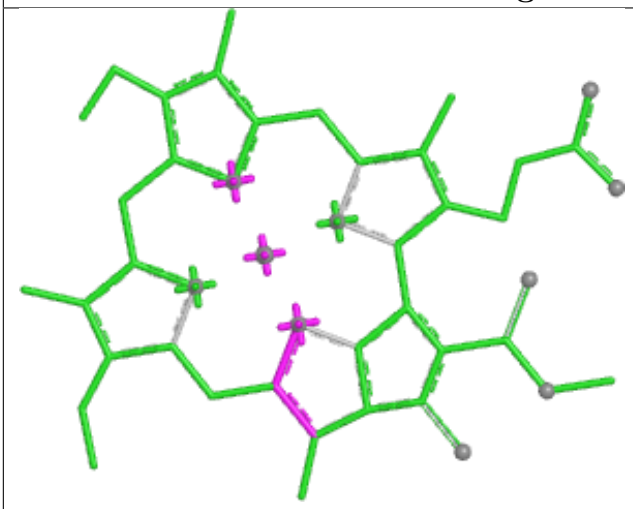


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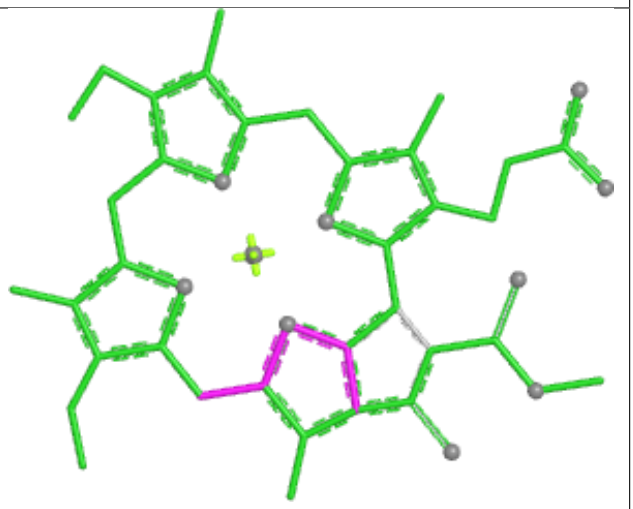


Rings

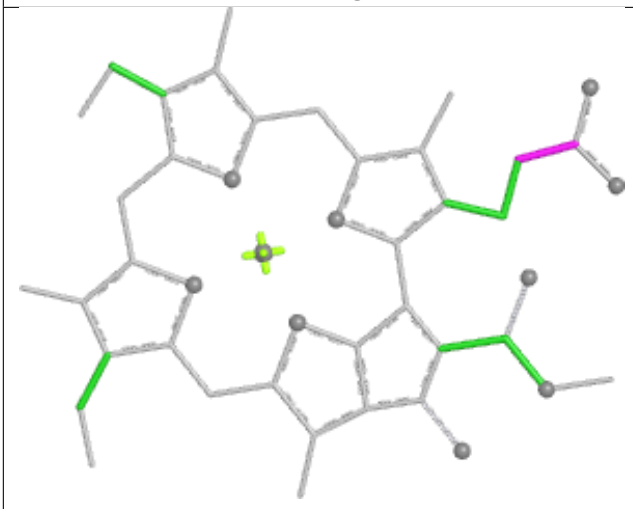
## Ligand CLA F2 303



Bond lengths



Bond angles

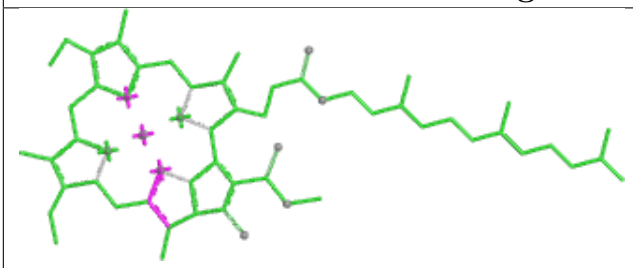


Torsions

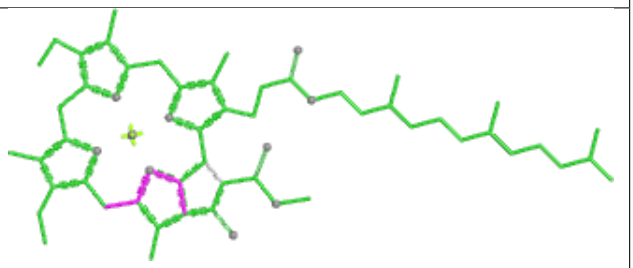


Rings

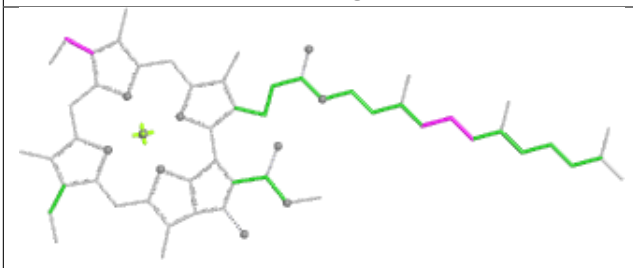
## Ligand CLA Z2 616



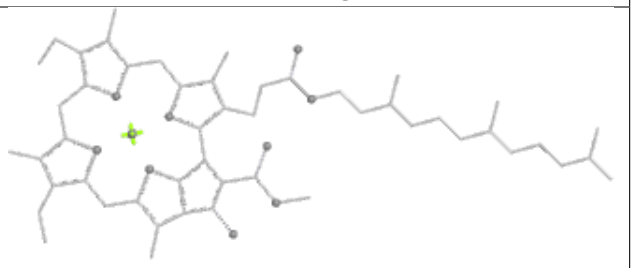
Bond lengths



Bond angles

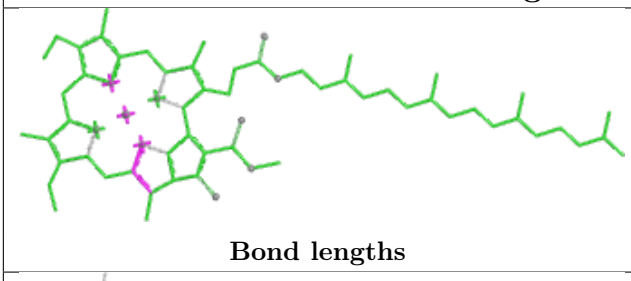


Torsions

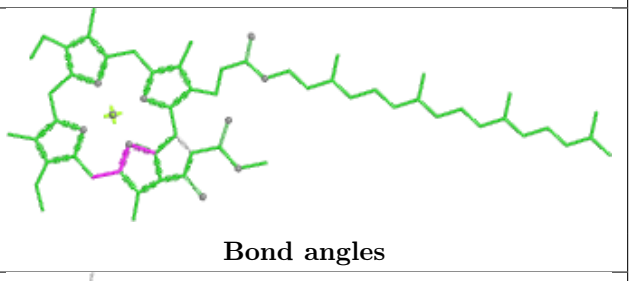


Rings

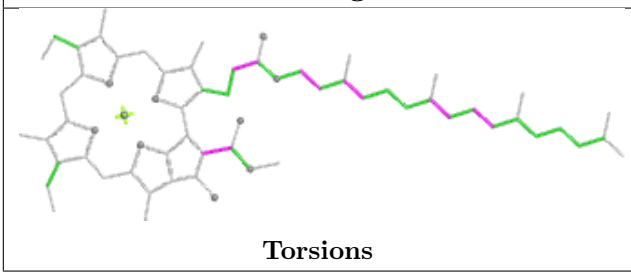
## Ligand CLA A 826



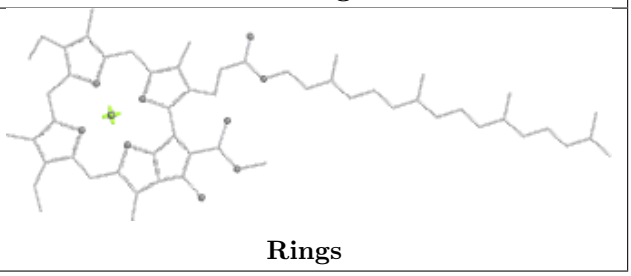
Bond lengths



Bond angles

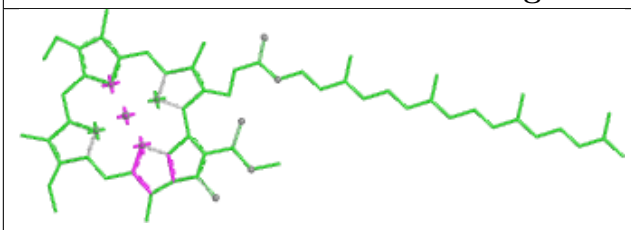


Torsions

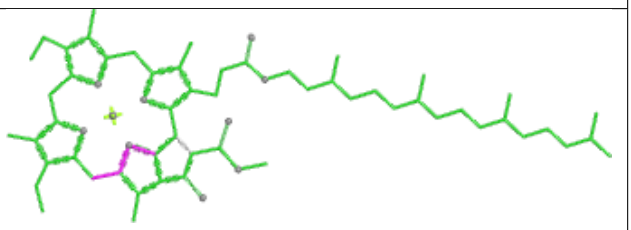


Rings

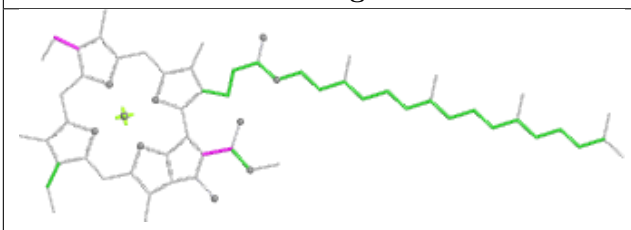
## Ligand CLA A 842



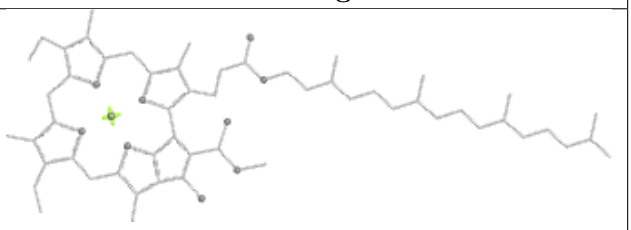
Bond lengths



Bond angles

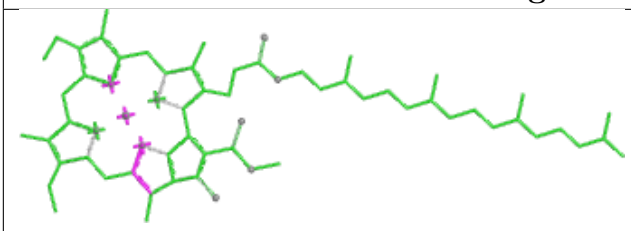


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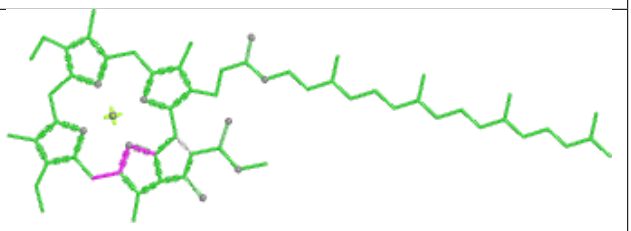


Rings

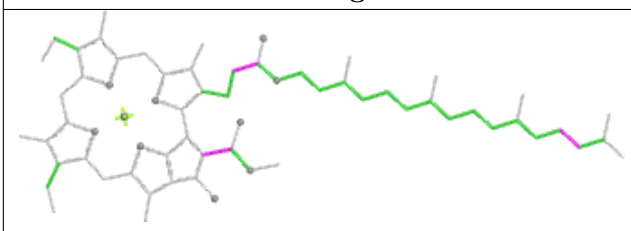
## Ligand CLA 8 603



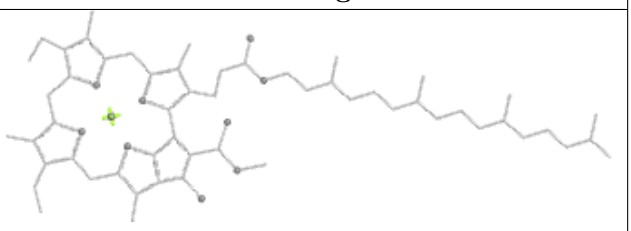
Bond lengths



Bond angles

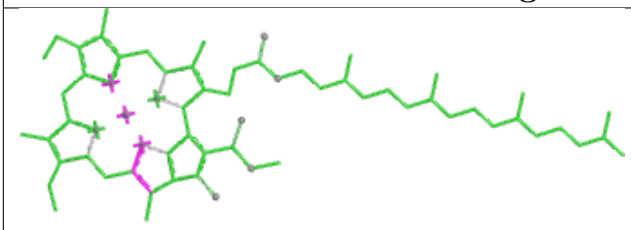


Torsions

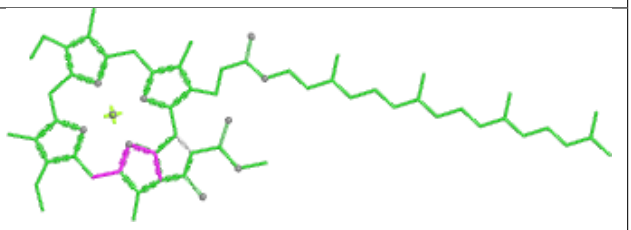


Rings

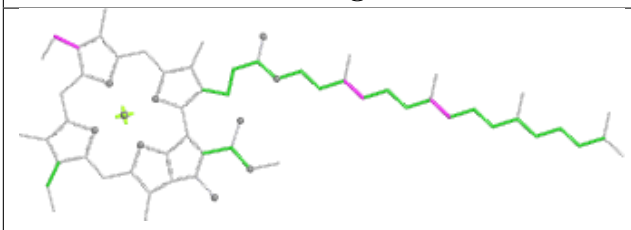
## Ligand CLA 62 613



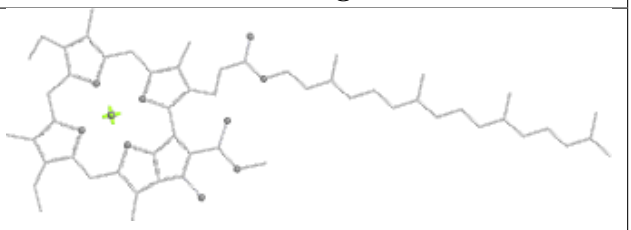
Bond lengths



Bond angles

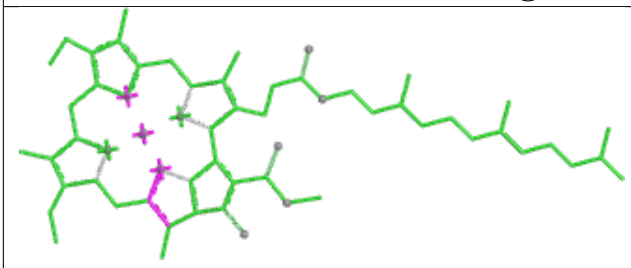


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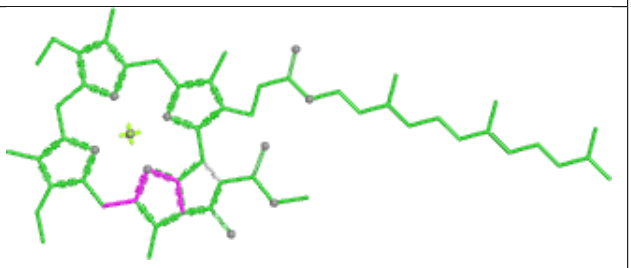


Rings

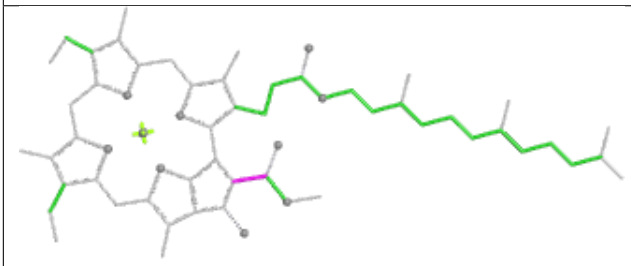
## Ligand CLA 42 602



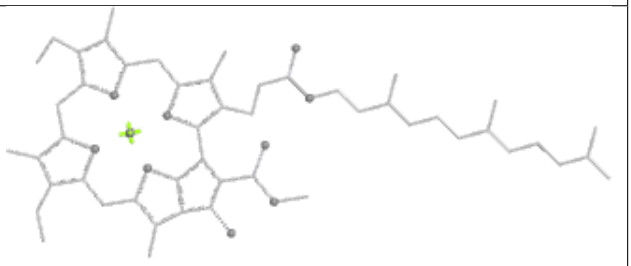
Bond lengths



Bond angles



Torsions

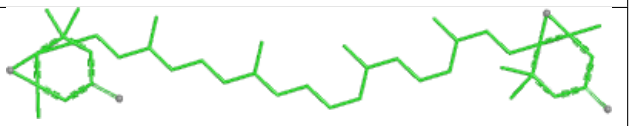


Rings

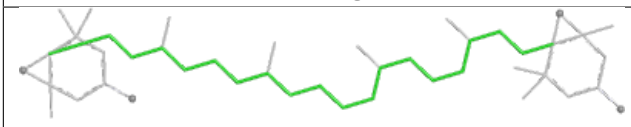
## Ligand XAT 8 618



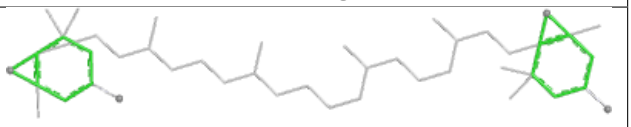
Bond lengths



Bond angles

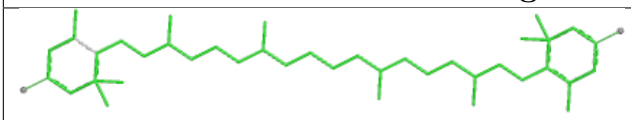


Torsions

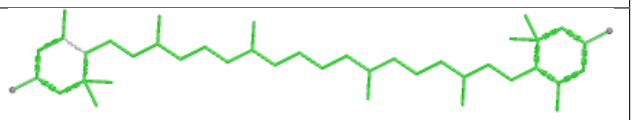


Rings

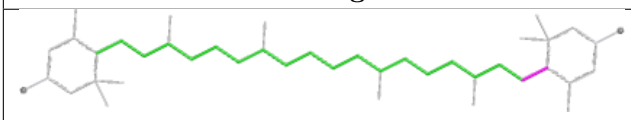
**Ligand LUT 62 621**



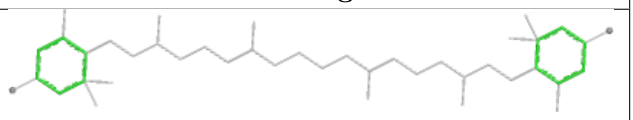
Bond lengths



Bond angles

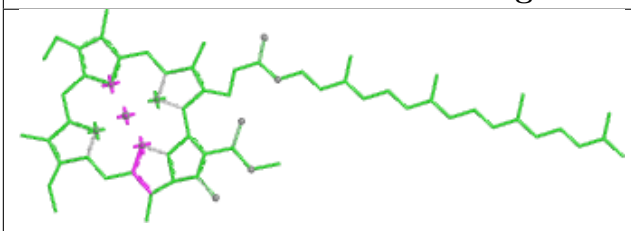


Torsions

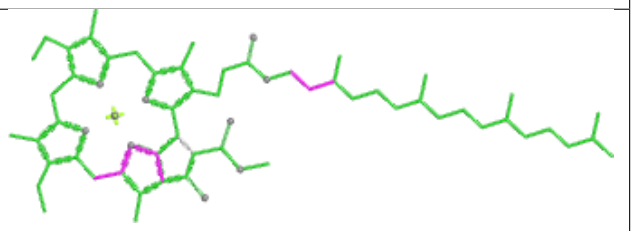


Rings

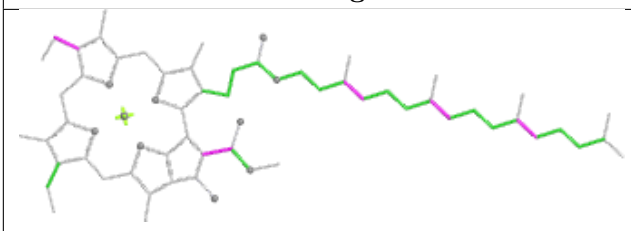
**Ligand CLA B2 841**



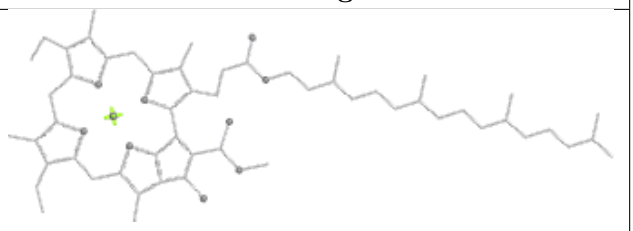
Bond lengths



Bond angles

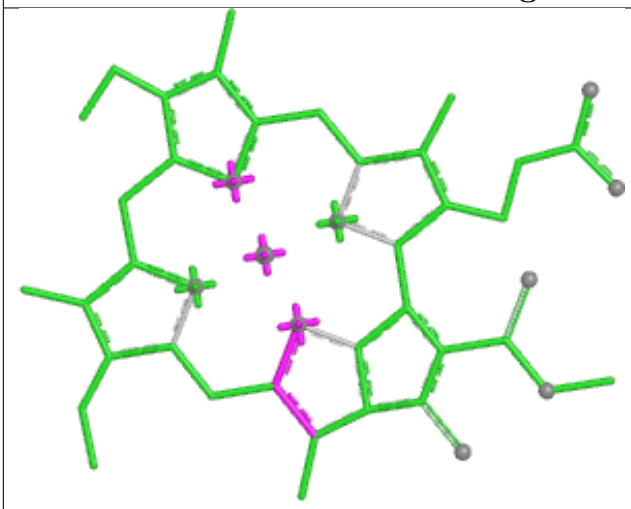


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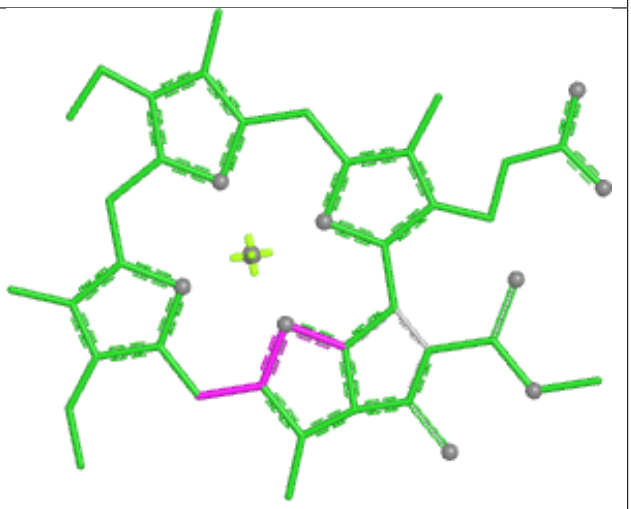


Rings

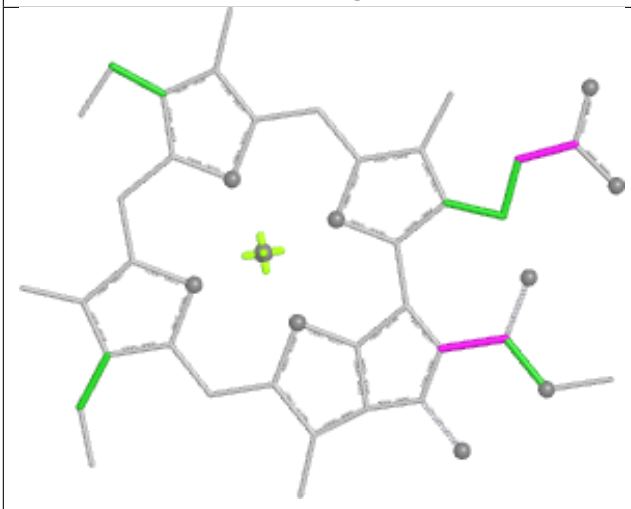
**Ligand CLA 42 612**



**Bond lengths**



**Bond angles**

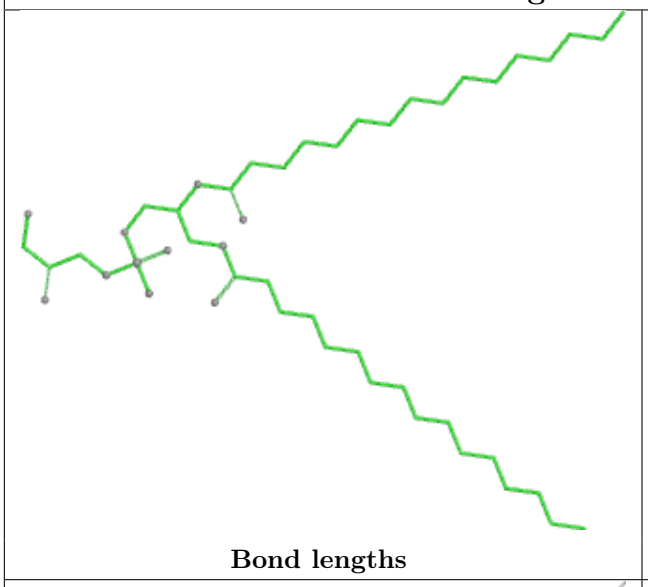


**Torsions**

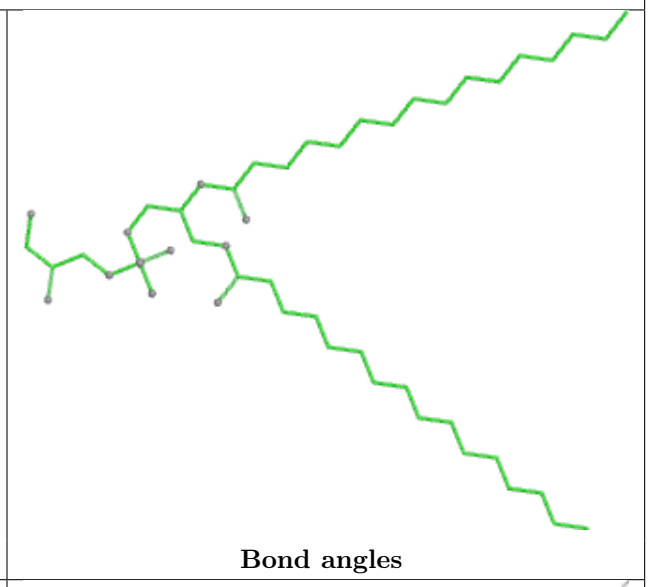


**Rings**

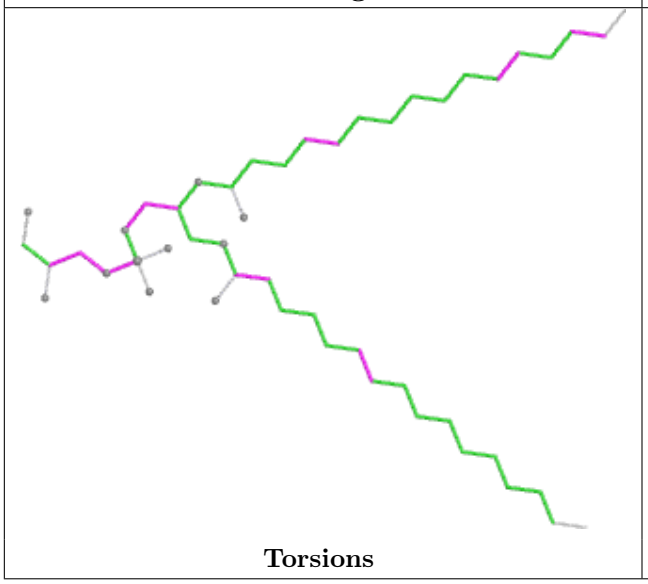
**Ligand LHG 4 622**



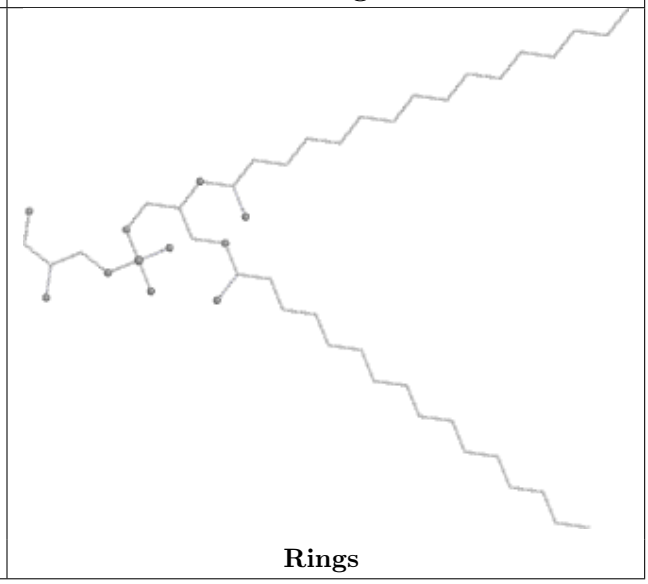
**Bond lengths**



**Bond angles**

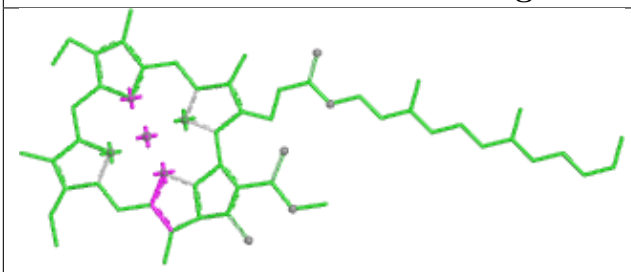


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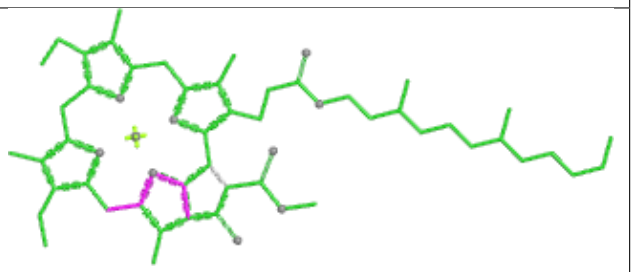


**Rings**

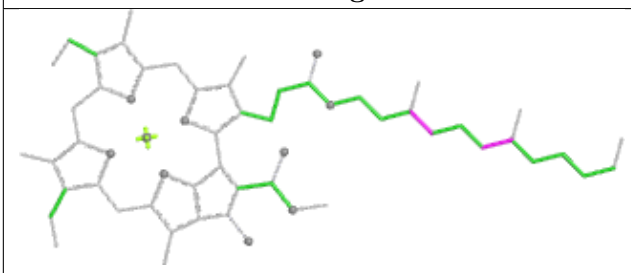
## Ligand CLA B2 822



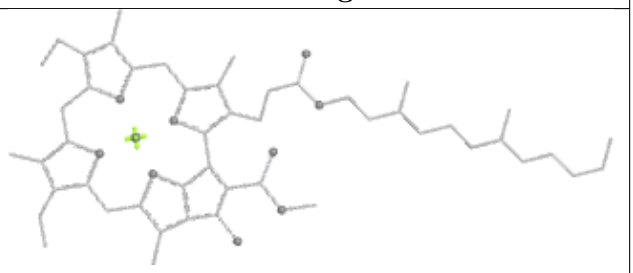
Bond lengths



Bond angles

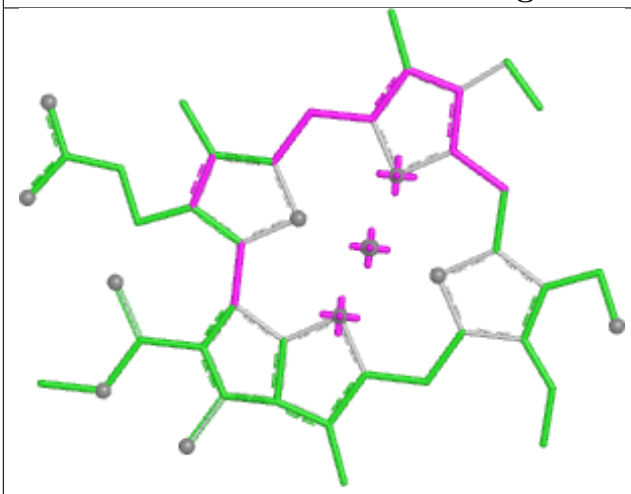


Torsions

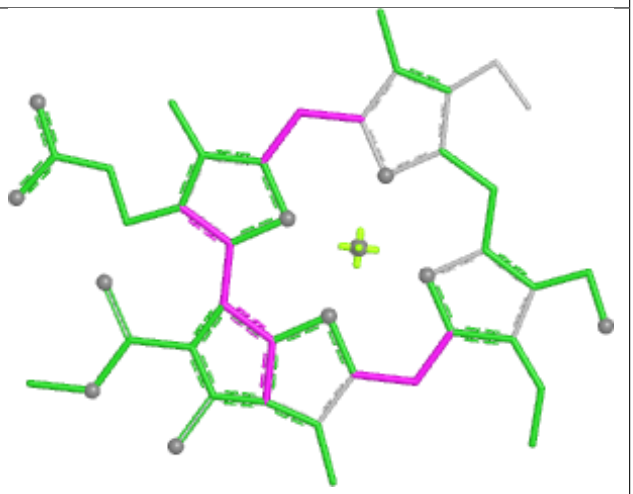


Rings

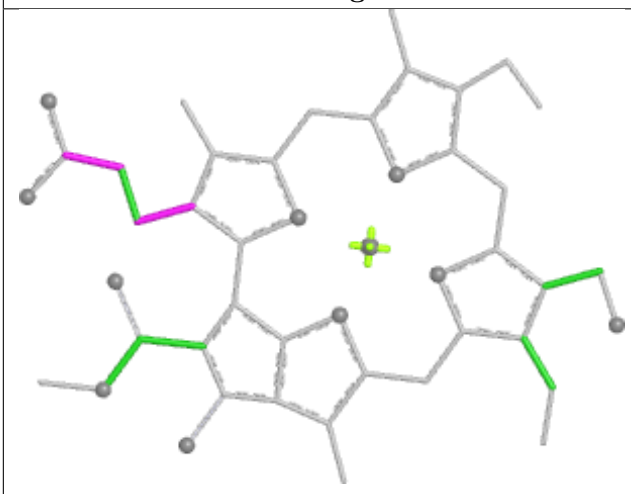
## Ligand CHL Z2 606



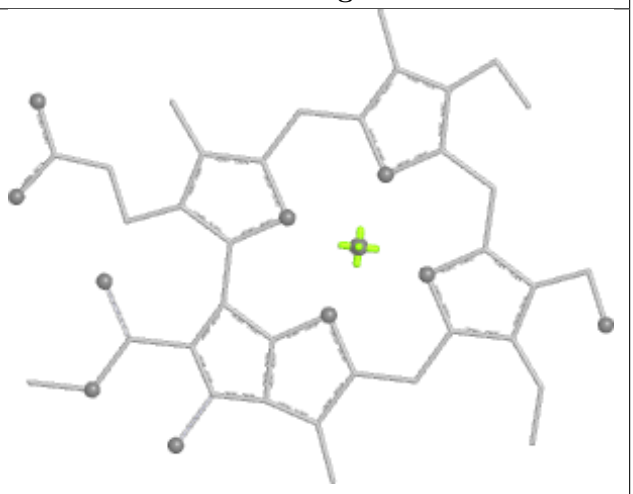
Bond lengths



Bond angles

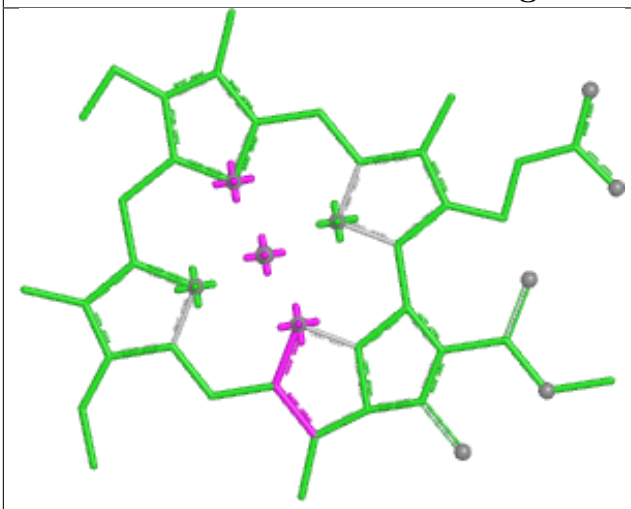


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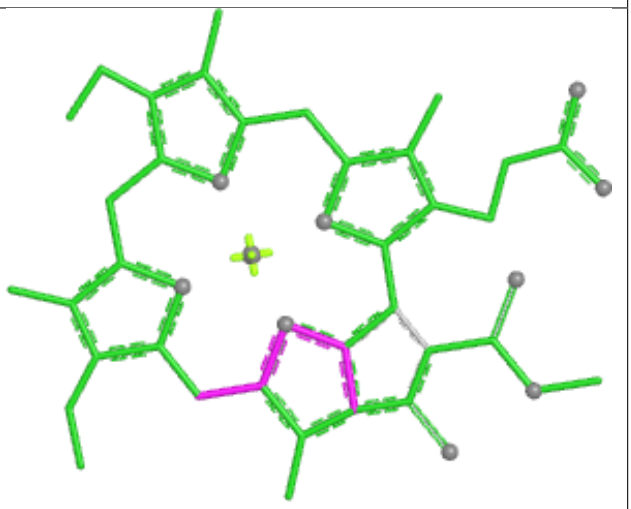


Rings

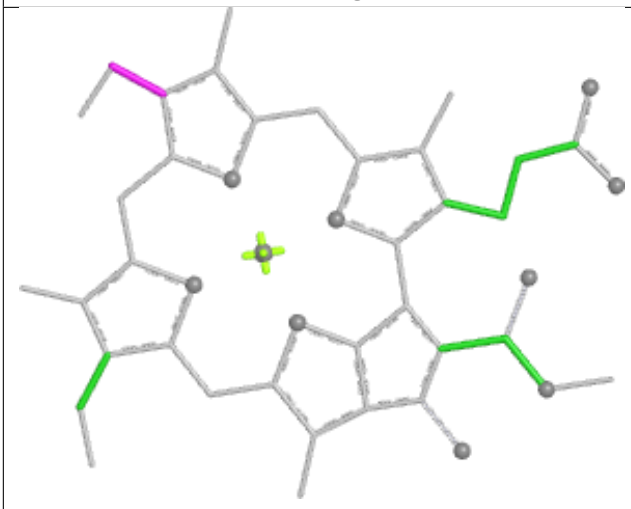
**Ligand CLA 32 614**



**Bond lengths**



**Bond angles**

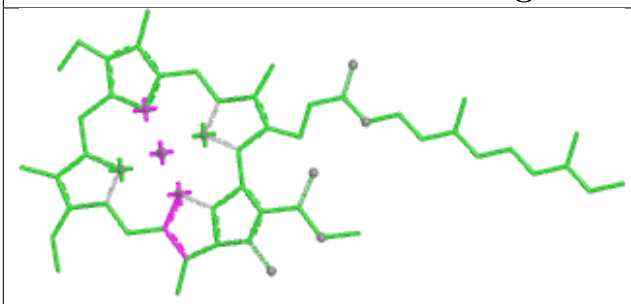


**Torsions**

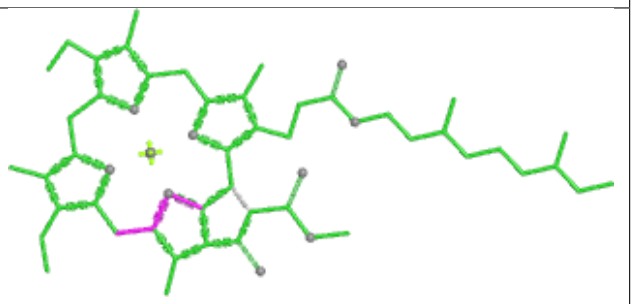


**Rings**

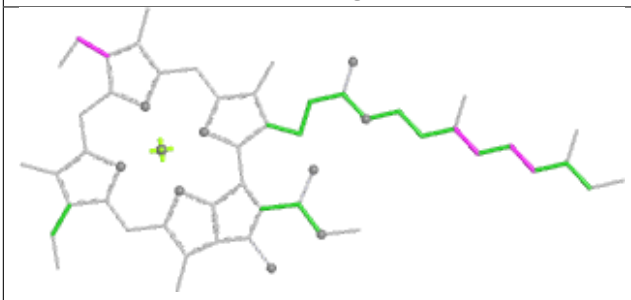
## Ligand CLA B2 820



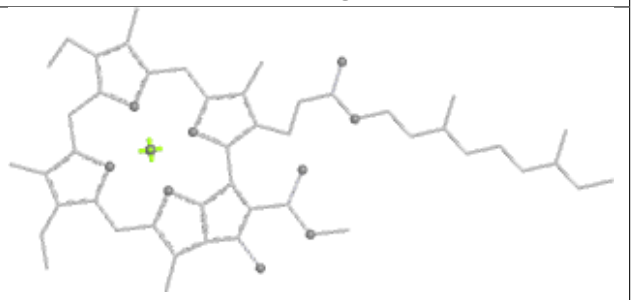
Bond lengths



Bond angles

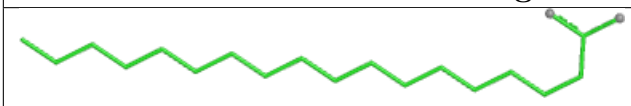


Torsions

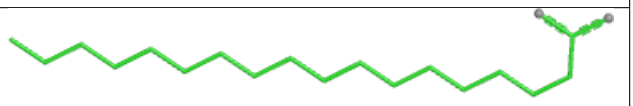


Rings

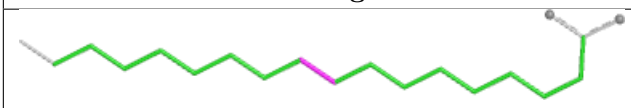
## Ligand LMG 62 633



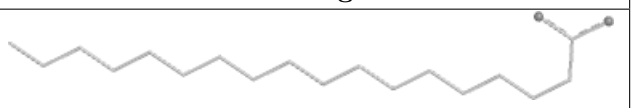
Bond lengths



Bond angles

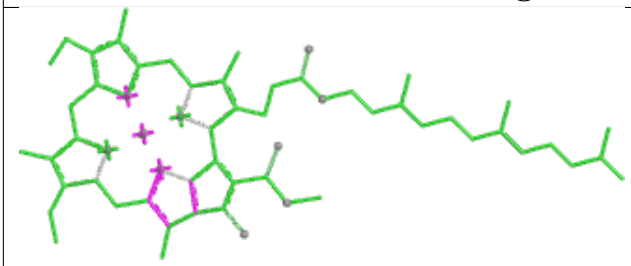


Torsions

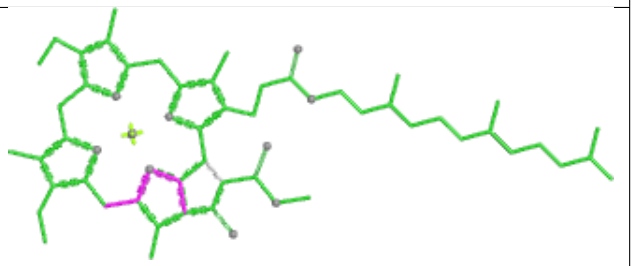


Rings

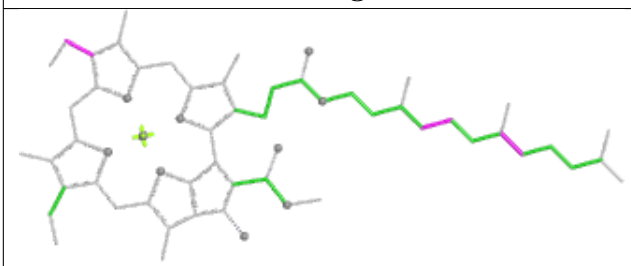
## Ligand CLA B2 819



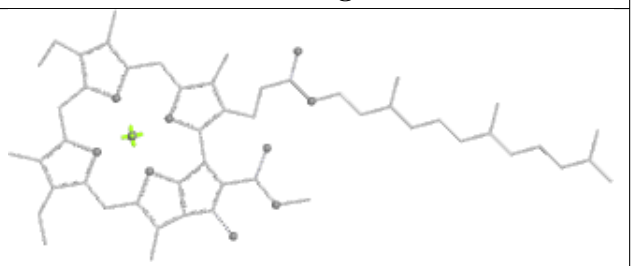
Bond lengths



Bond angles

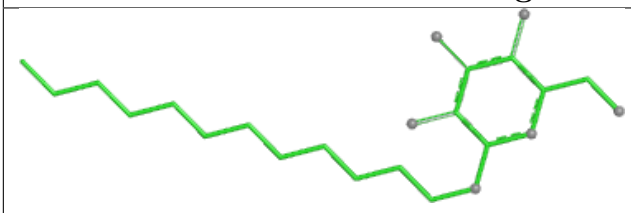


Torsions

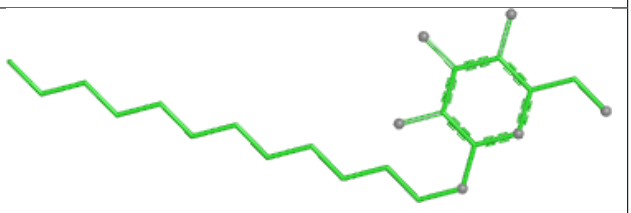


Rings

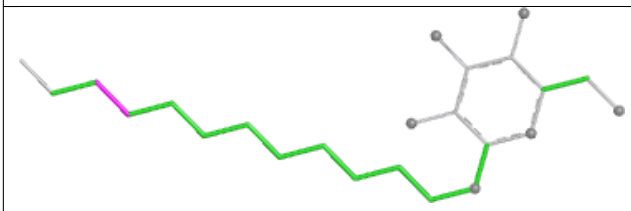
## Ligand LMU 12 623



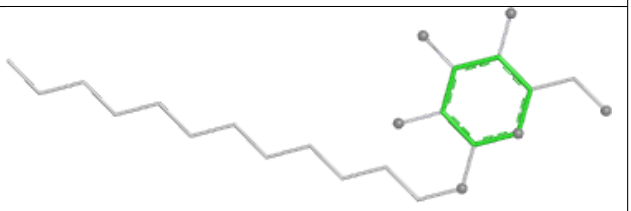
Bond lengths



Bond angles

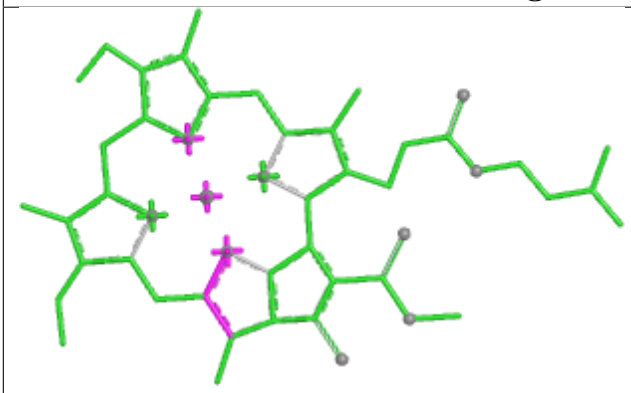


Torsions

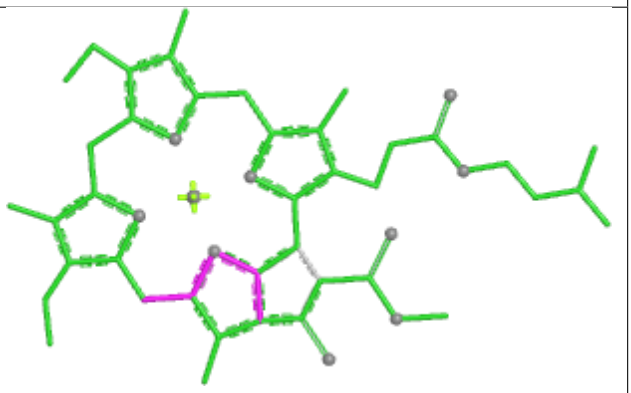


Rings

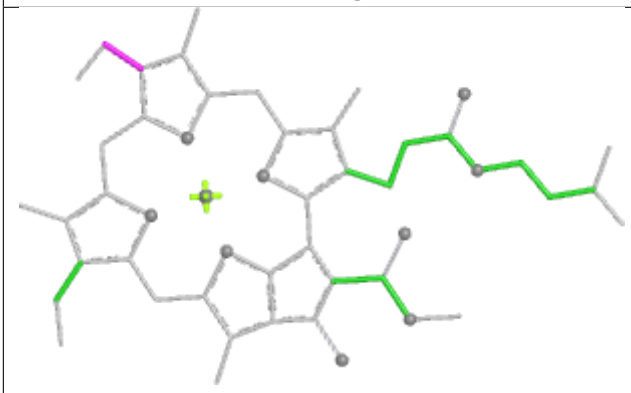
## Ligand CLA Z 608



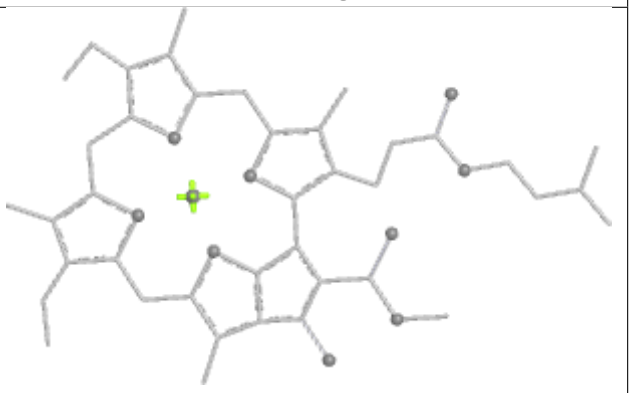
Bond lengths



Bond angles

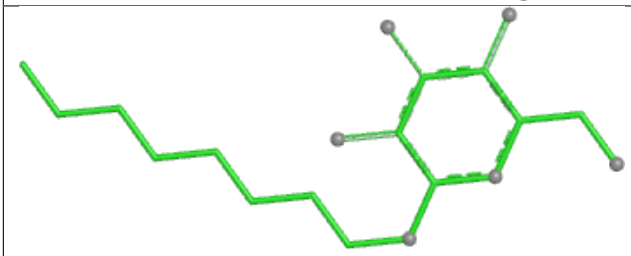


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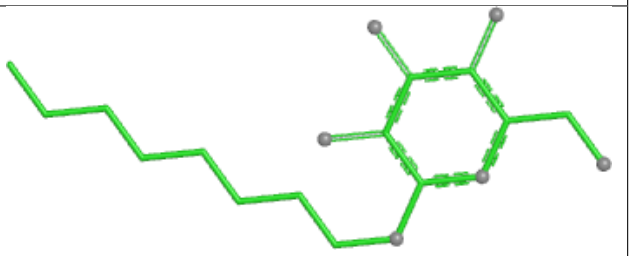


Rings

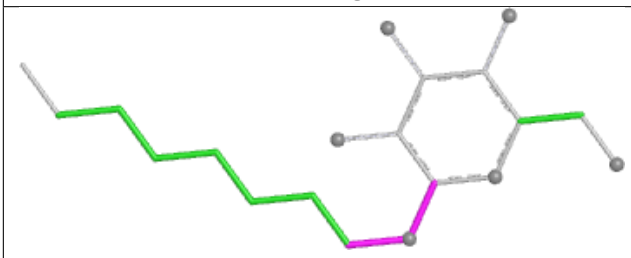
## Ligand LMU 62 632



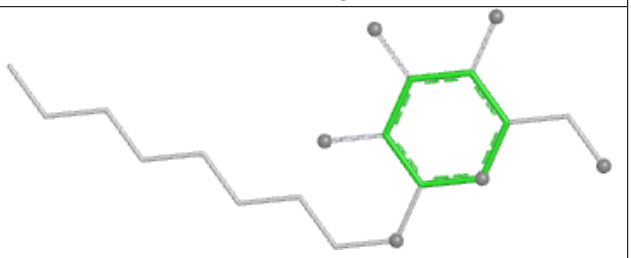
Bond lengths



Bond angles

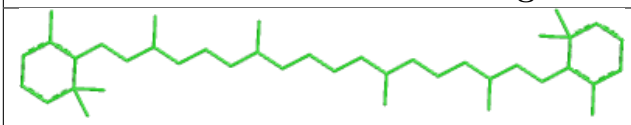


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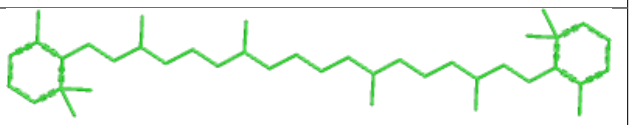


Rings

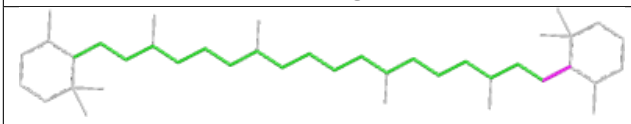
## Ligand BCR 52 622



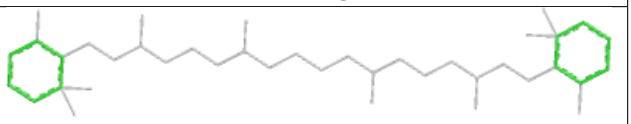
Bond lengths



Bond angles



Torsions



Rings

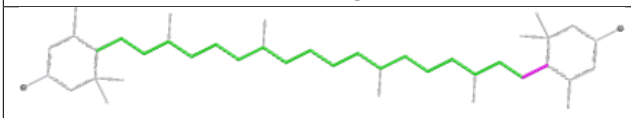
## Ligand LUT 3 621



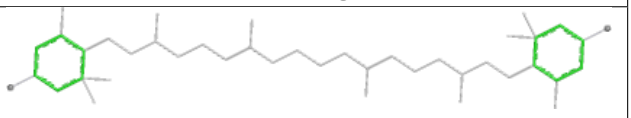
Bond lengths



Bond angles

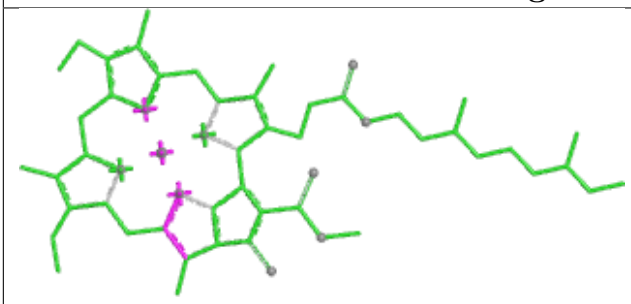


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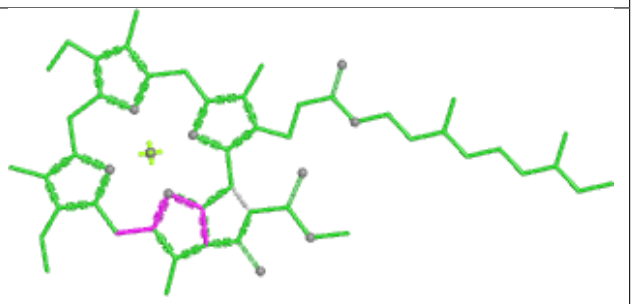


Rings

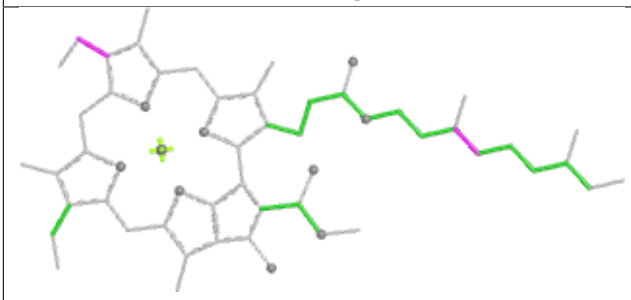
## Ligand CLA 5 613



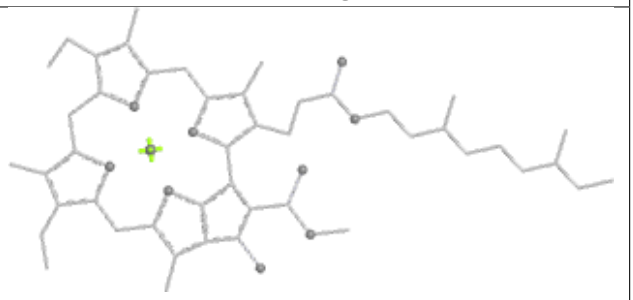
Bond lengths



Bond angles

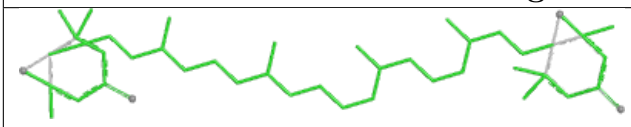


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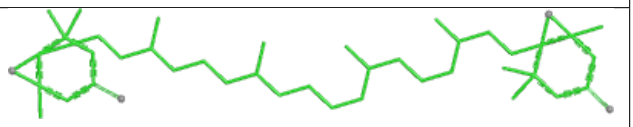


Rings

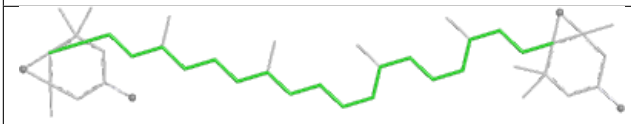
## Ligand XAT 7 622



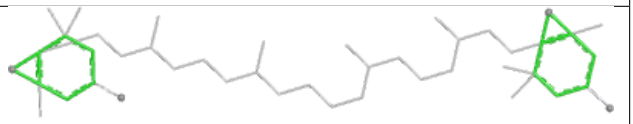
Bond lengths



Bond angles

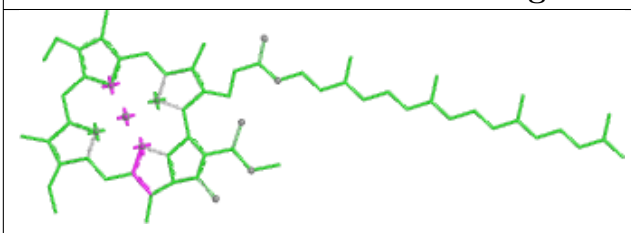


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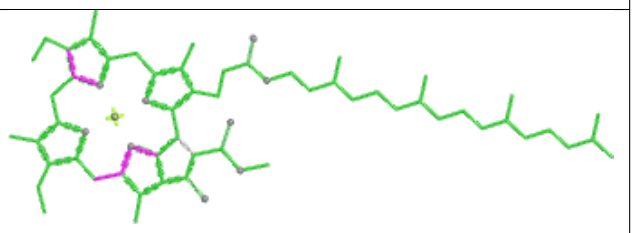


Rings

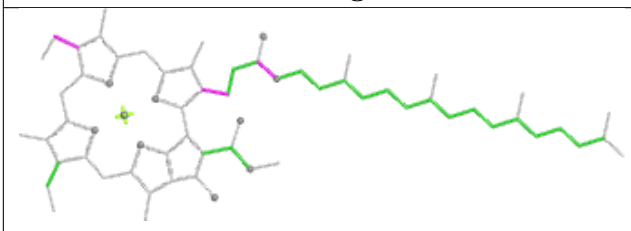
## Ligand CLA 7 610



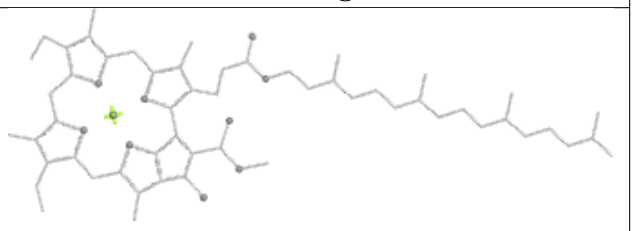
Bond lengths



Bond angles

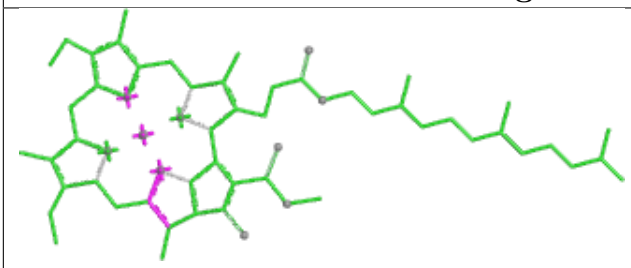


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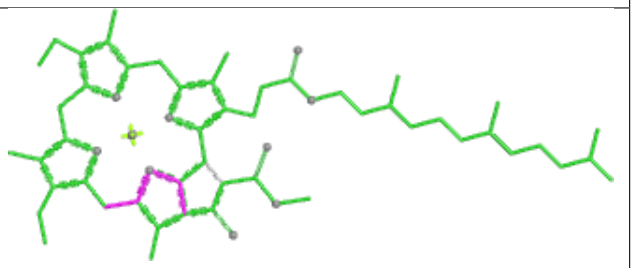


Rings

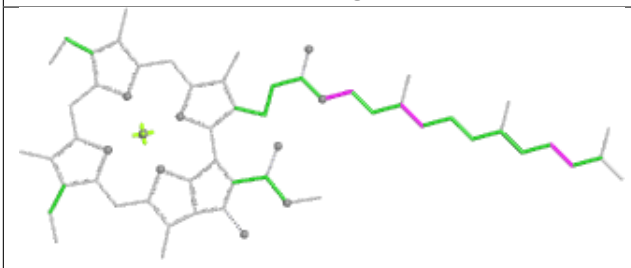
## Ligand CLA B2 836



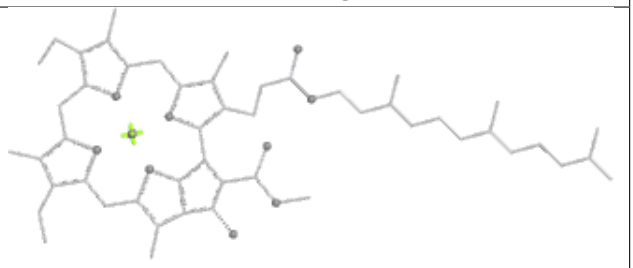
Bond lengths



Bond angles

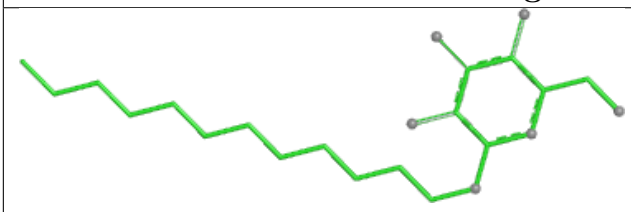


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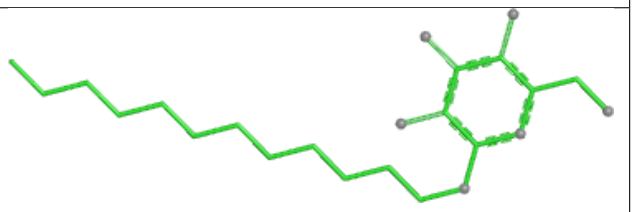


Rings

## Ligand LMU 1 626



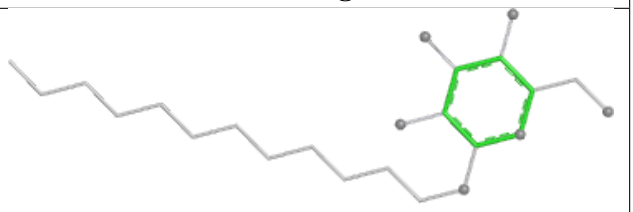
Bond lengths



Bond angles

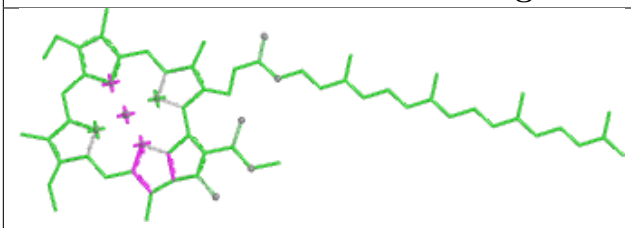


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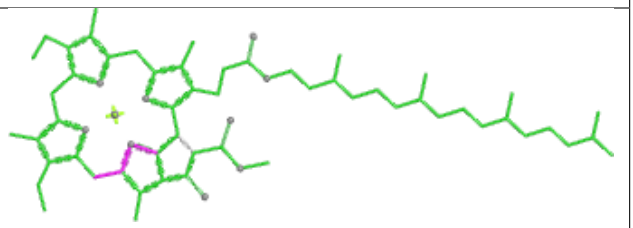


Rings

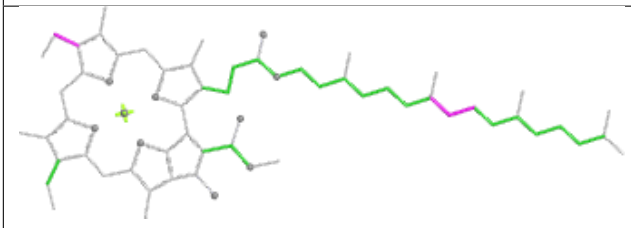
## Ligand CLA B2 802



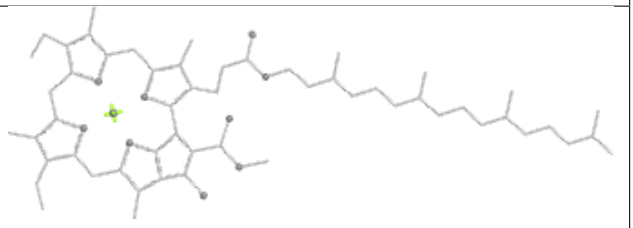
Bond lengths



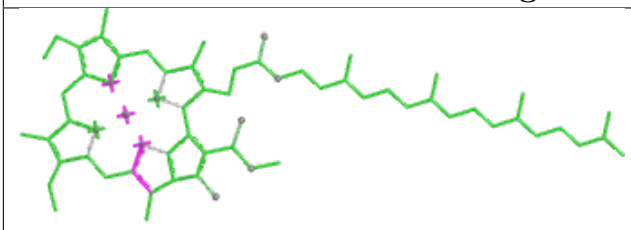
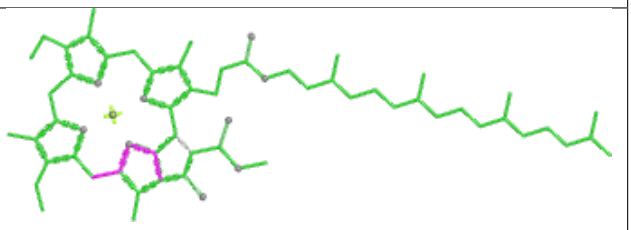
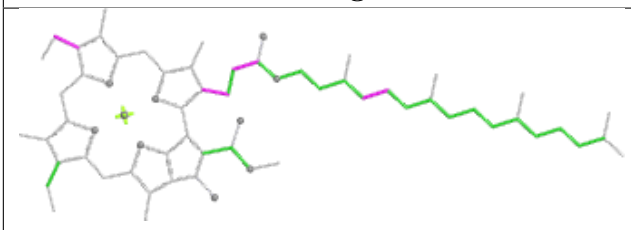
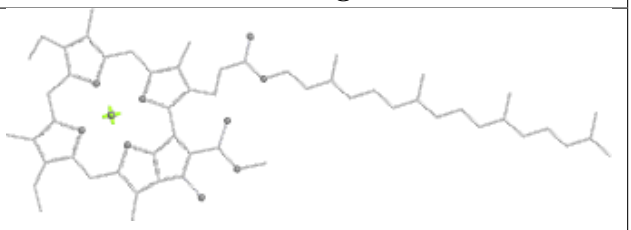
Bond angles

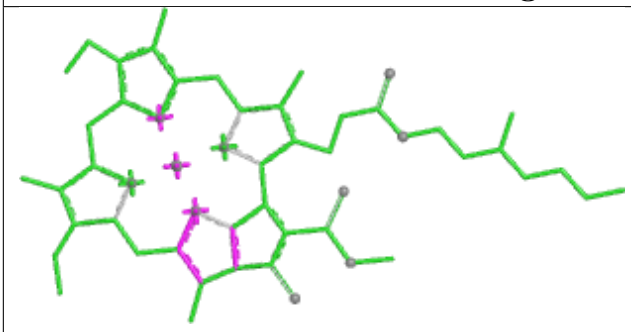
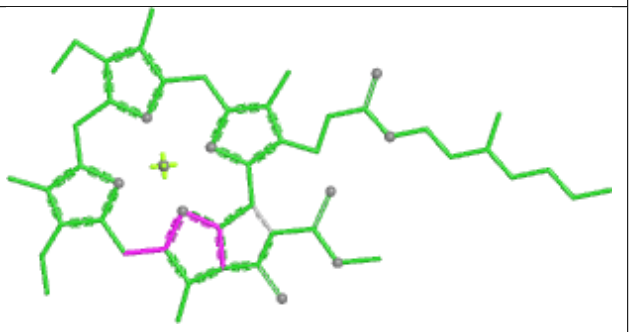
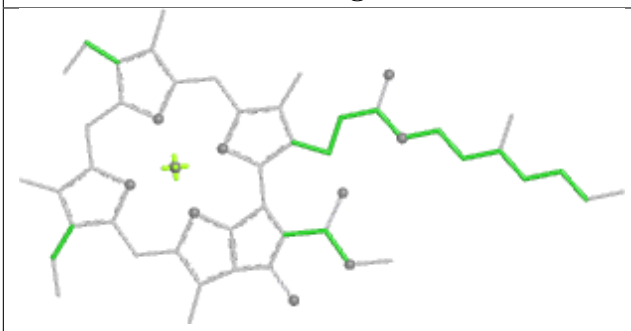
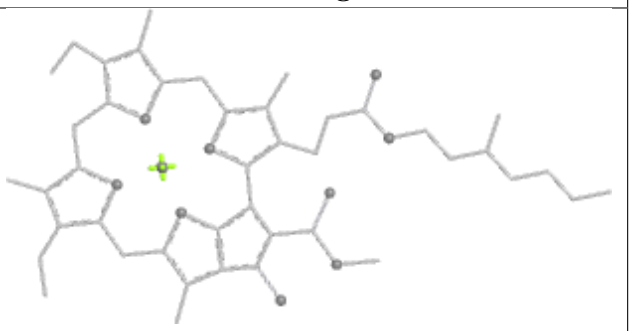


Torsions

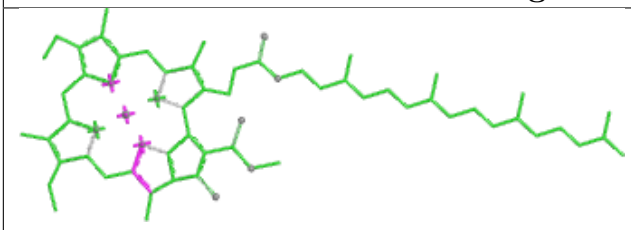


Rings

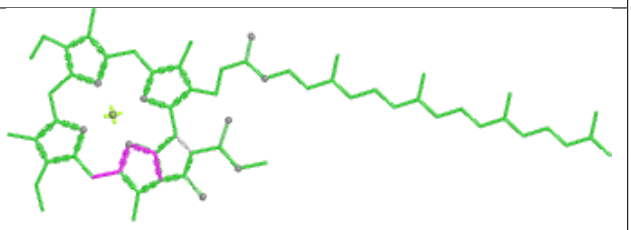
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|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 92 604 | |
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|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

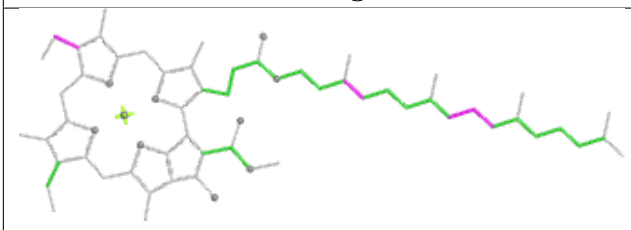
**Ligand CLA 5 617**



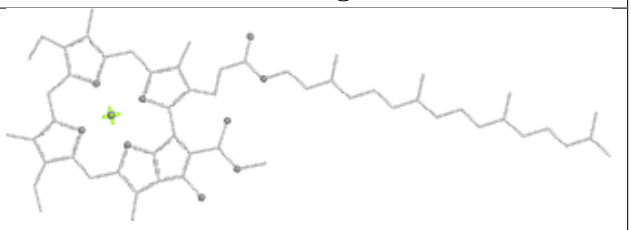
Bond lengths



Bond angles

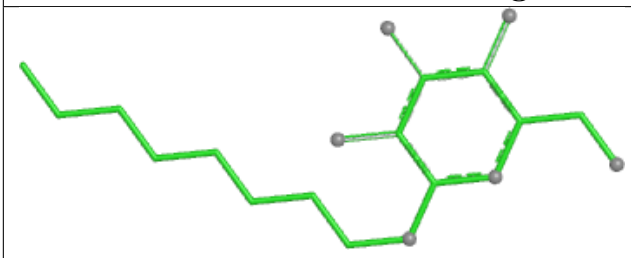


Torsions

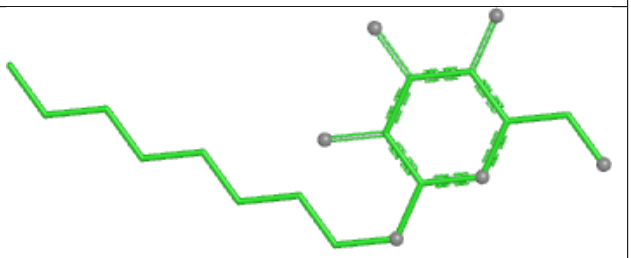


Rings

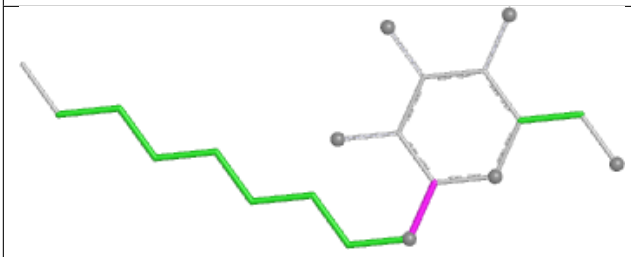
**Ligand LMU A2 862**



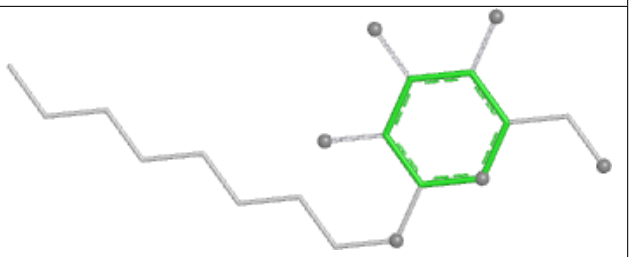
Bond lengths



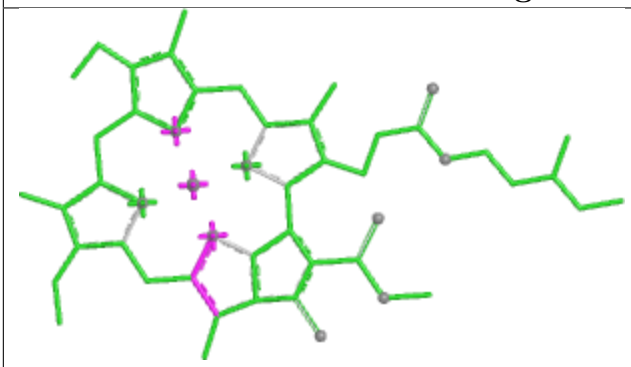
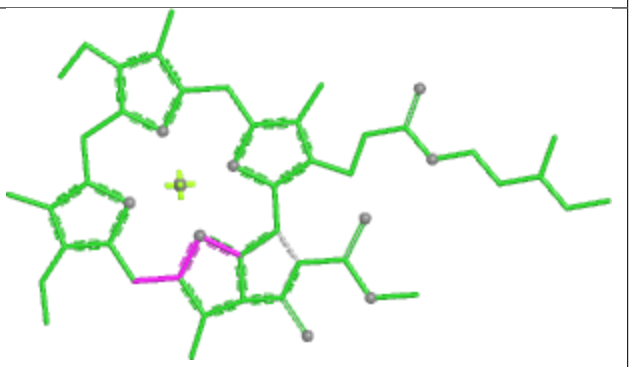
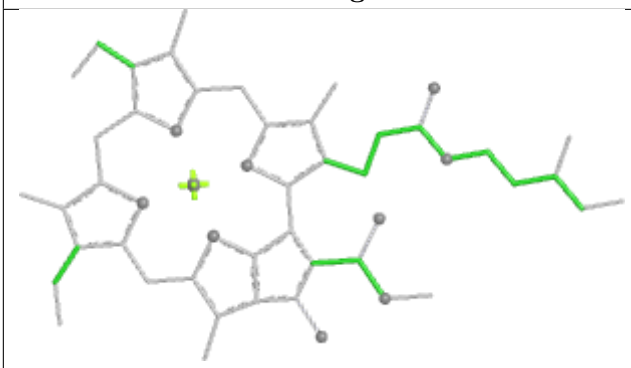
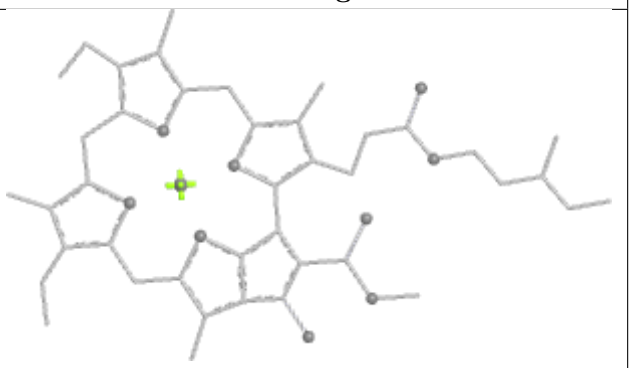
Bond angles

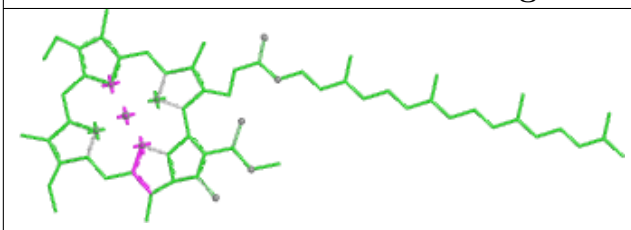
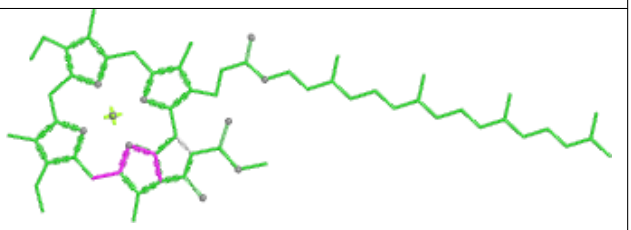
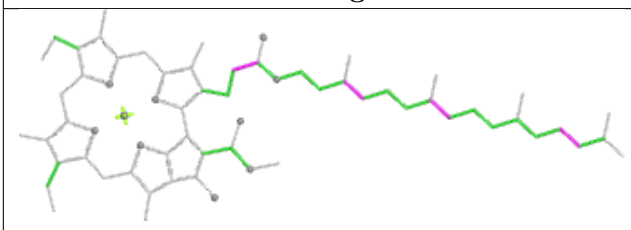
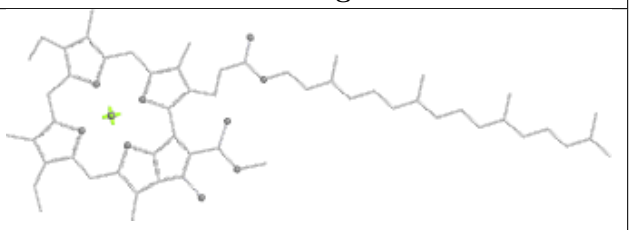


Torsions

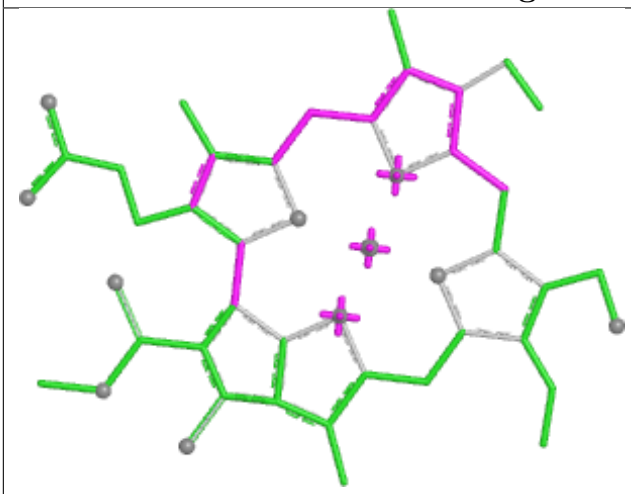


Rings

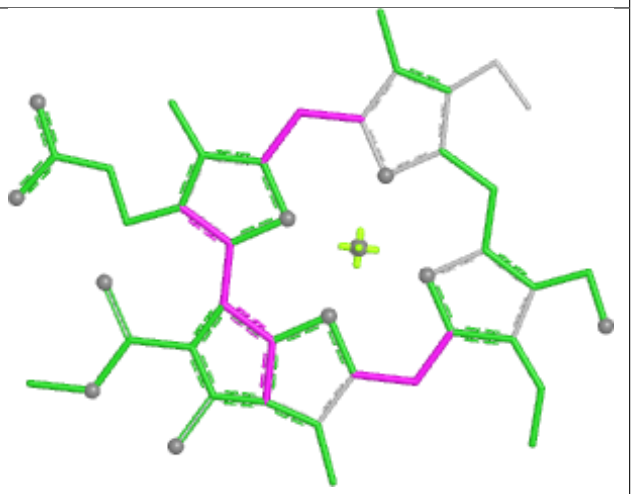
| Ligand CLA A2 838 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 12 609 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

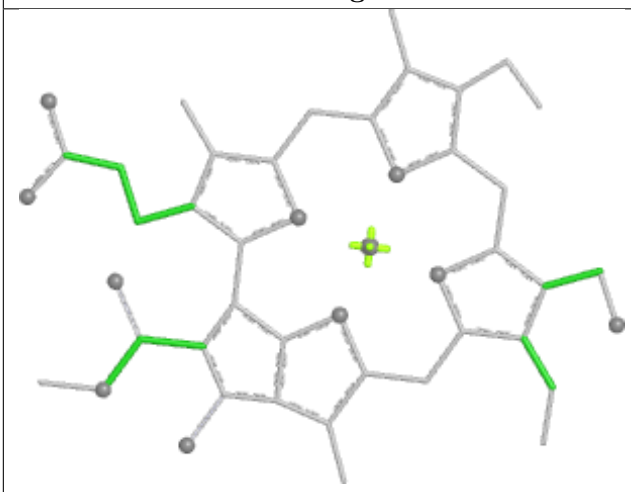
## Ligand CHL 12 606



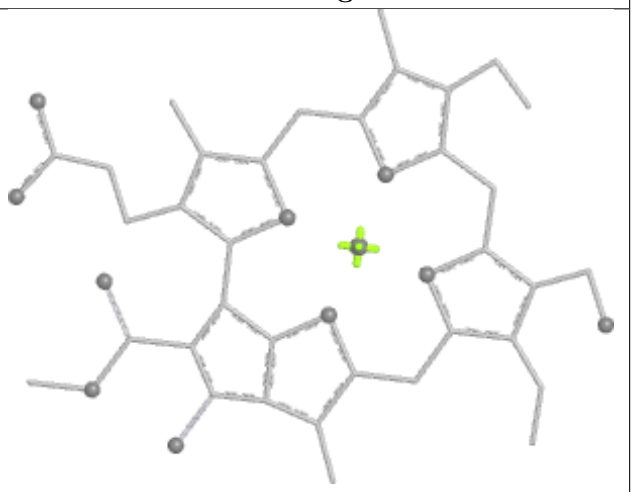
Bond lengths



Bond angles

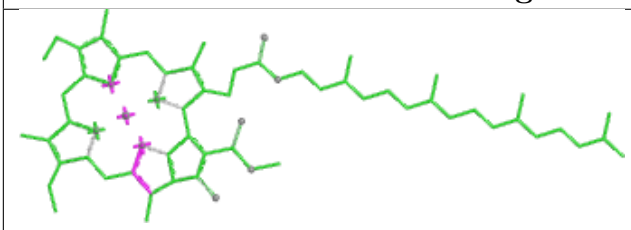


Torsions

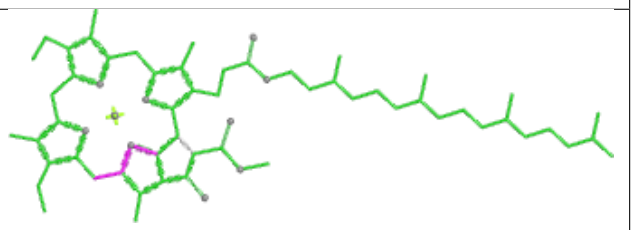


Rings

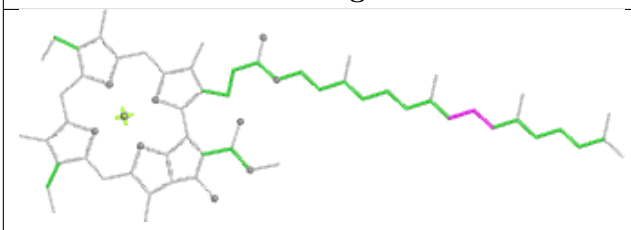
## Ligand CLA B2 803



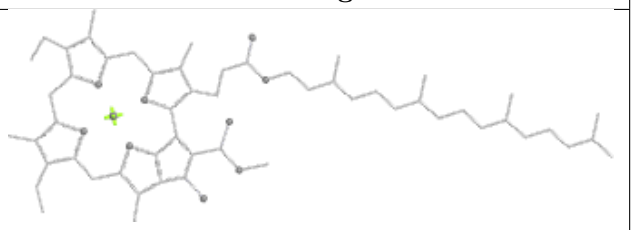
Bond lengths



Bond angles

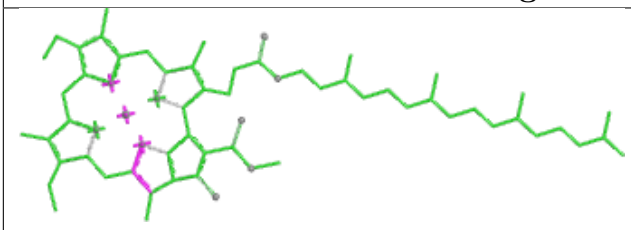


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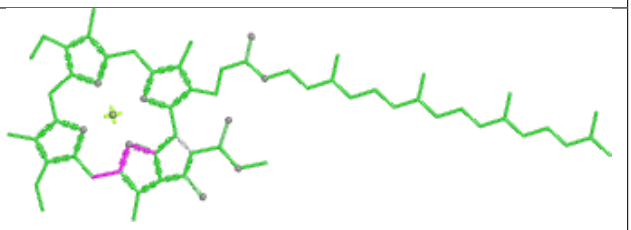


Rings

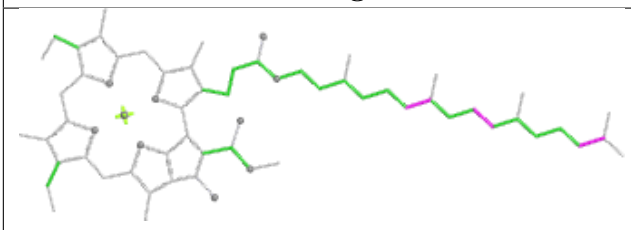
**Ligand CLA 52 601**



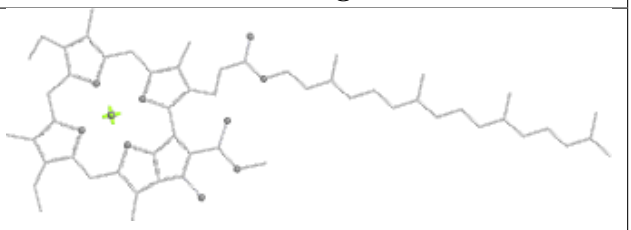
Bond lengths



Bond angles

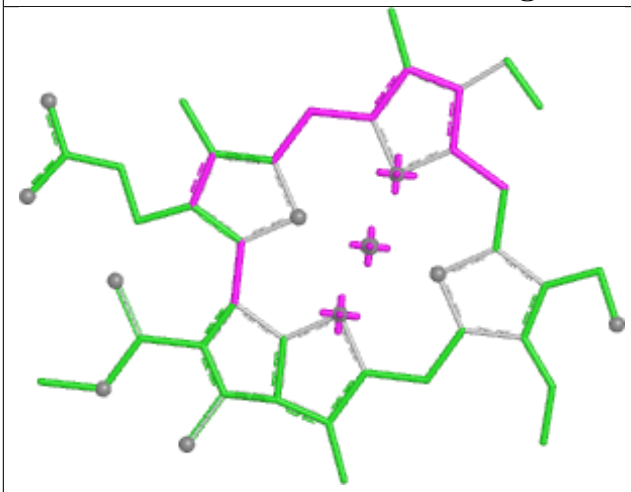


Torsions

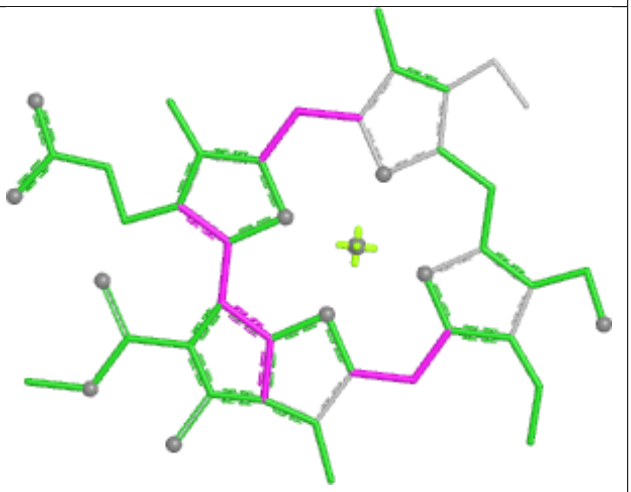


Rings

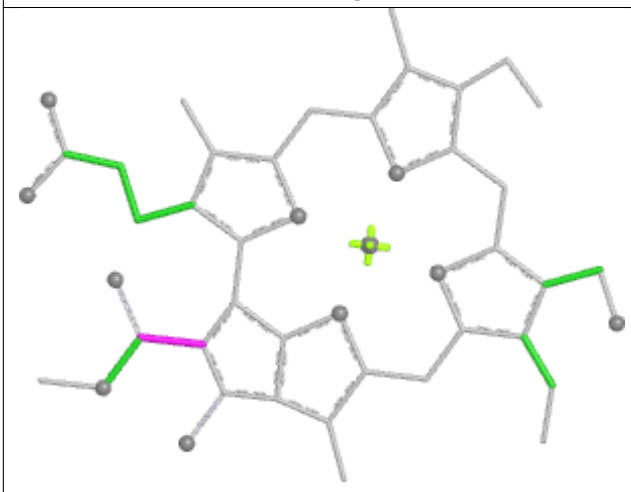
**Ligand CHL 52 606**



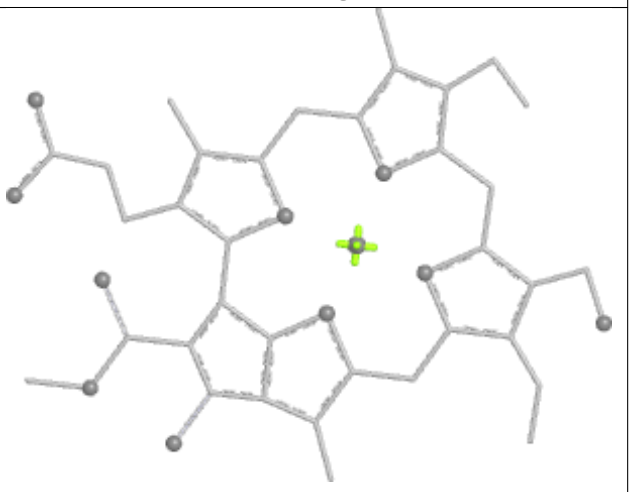
Bond lengths



Bond angles

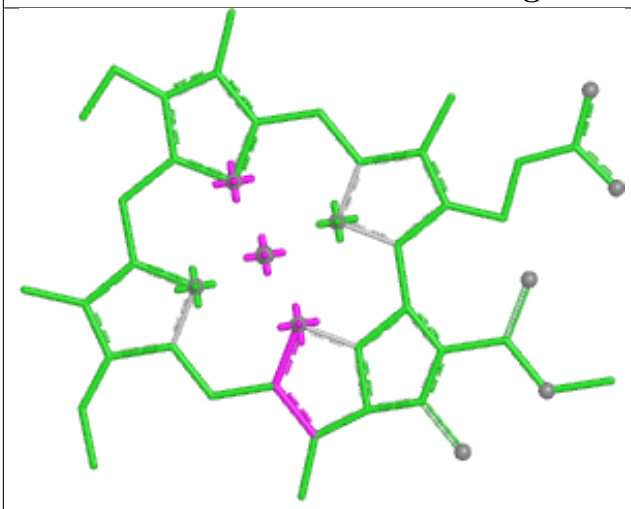


Torsions

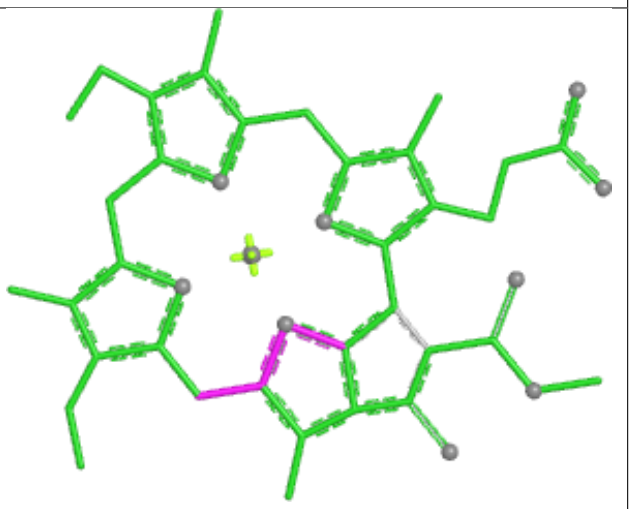


Rings

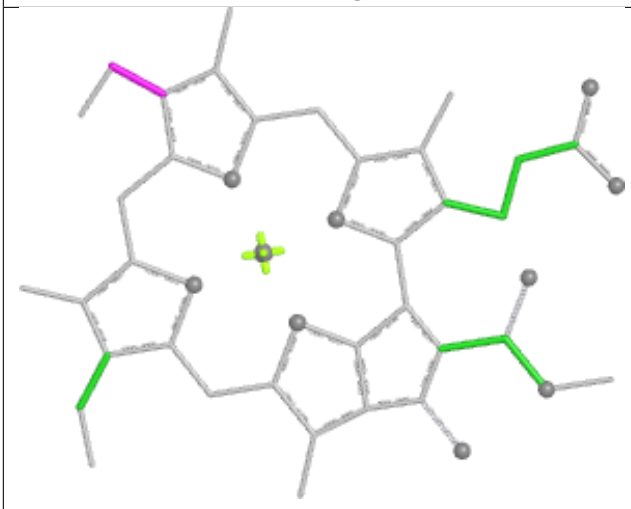
**Ligand CLA K 201**



**Bond lengths**



**Bond angles**

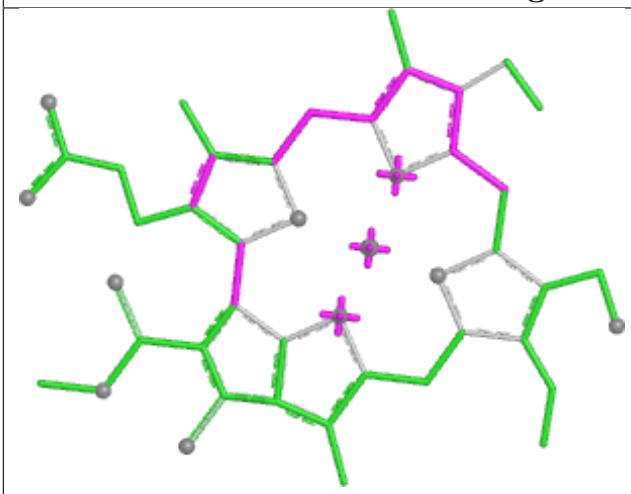


**Torsions**

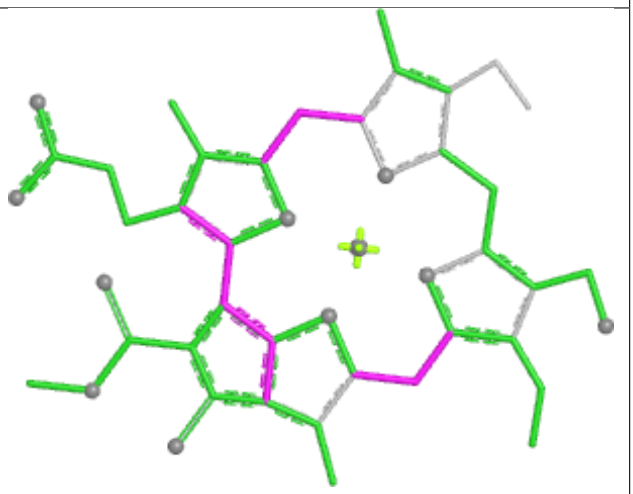


**Rings**

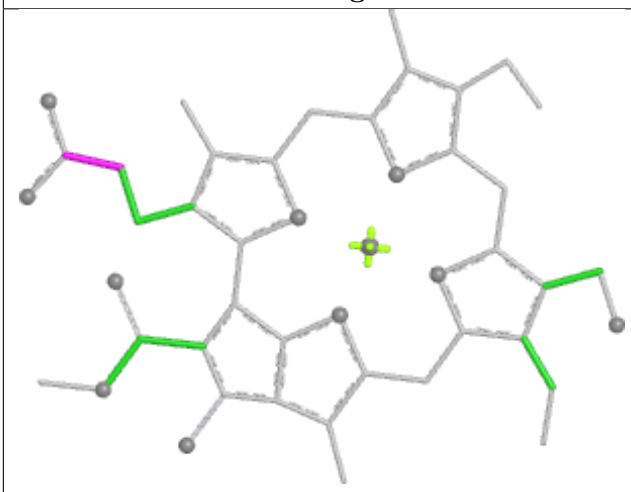
## Ligand CHL 7 606



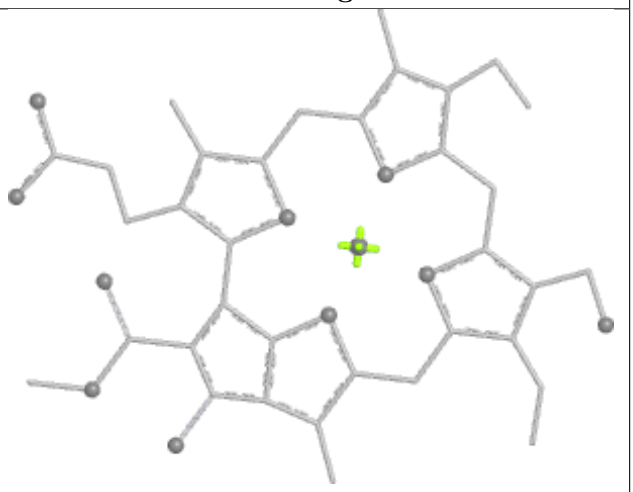
Bond lengths



Bond angles

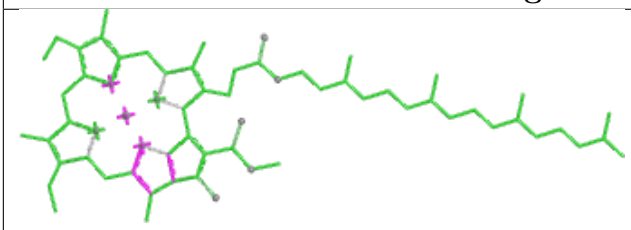


Torsions

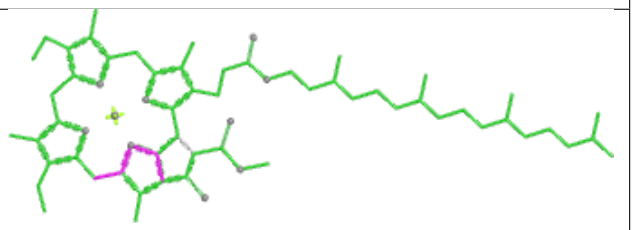


Rings

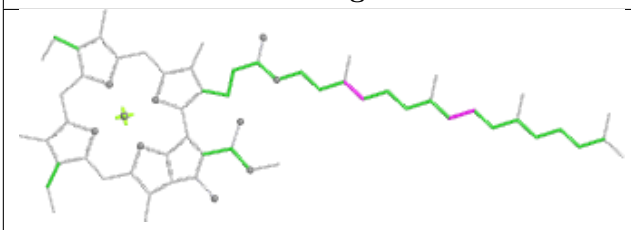
## Ligand CLA B 813



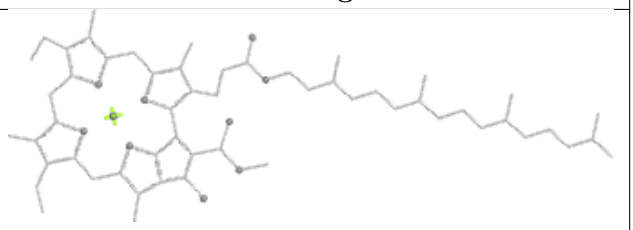
Bond lengths



Bond angles

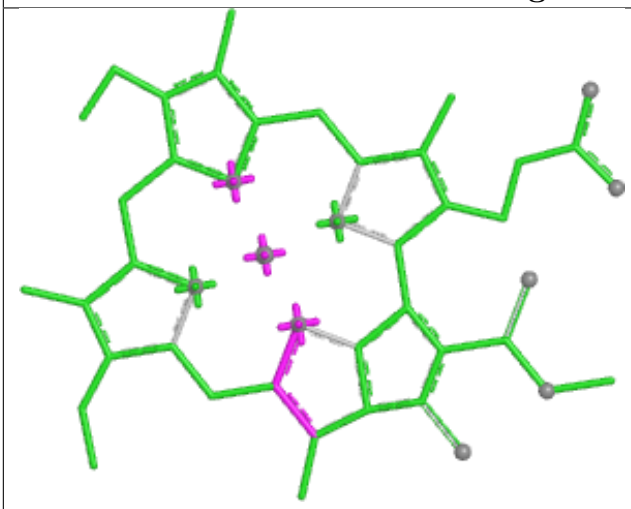


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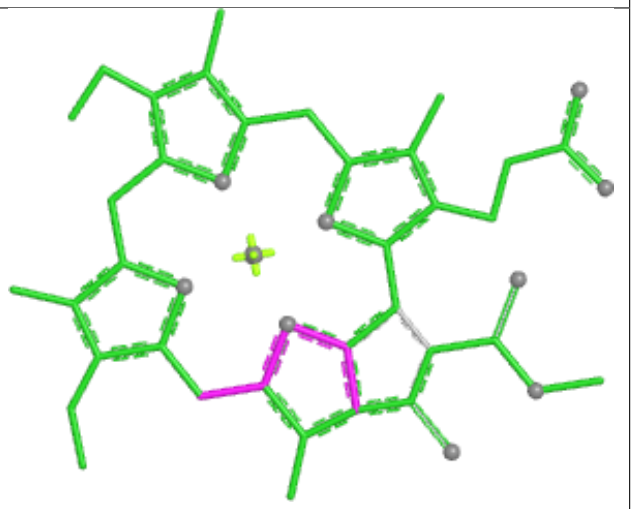


Rings

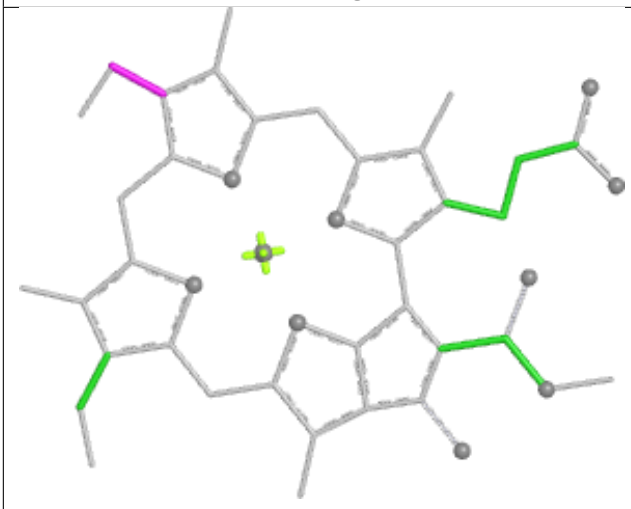
## Ligand CLA 6 617



Bond lengths



Bond angles

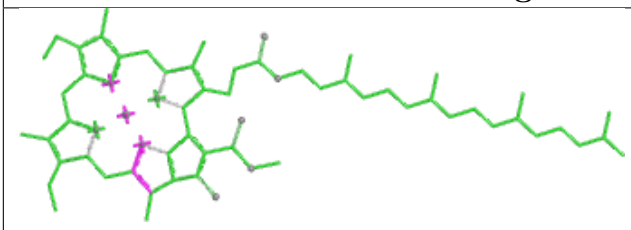


Torsions

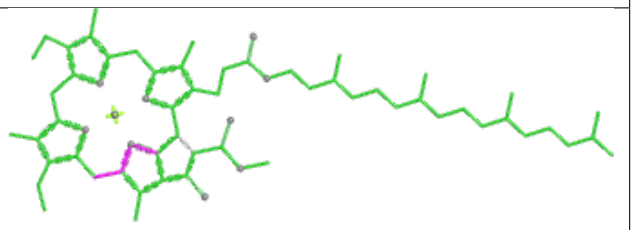


Rings

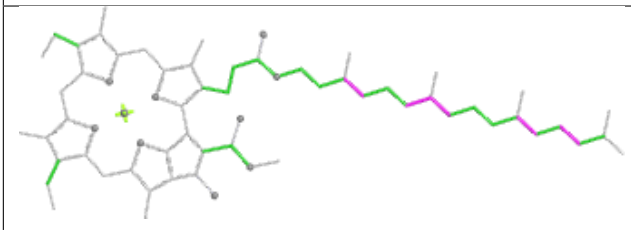
## Ligand CLA A2 840



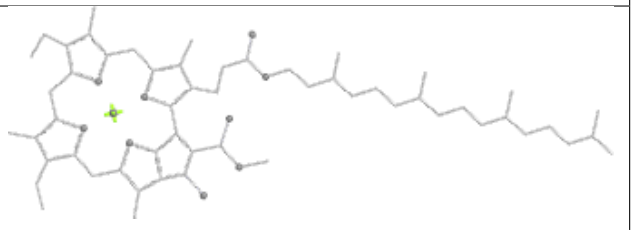
Bond lengths



Bond angles

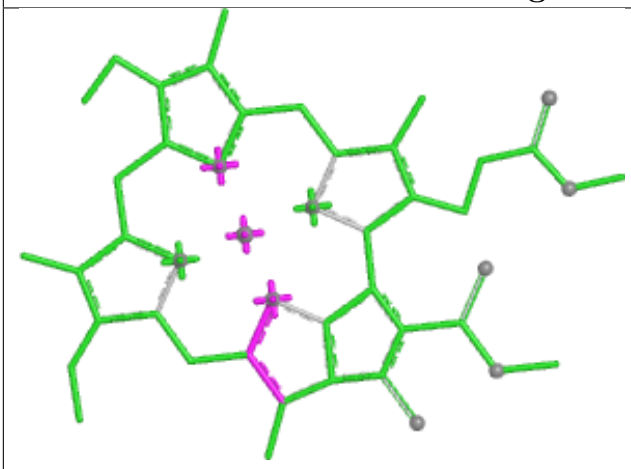


Torsions

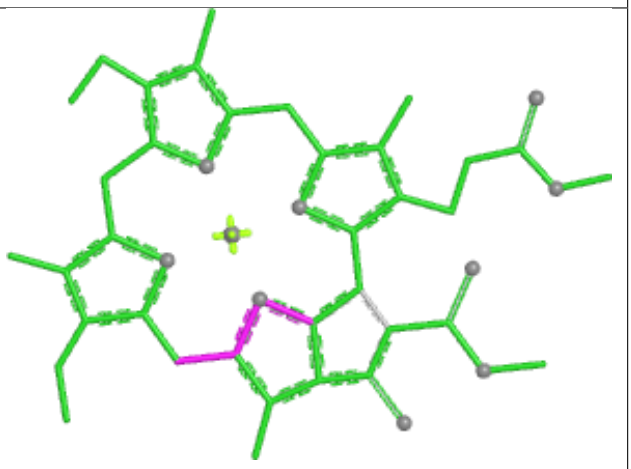


Rings

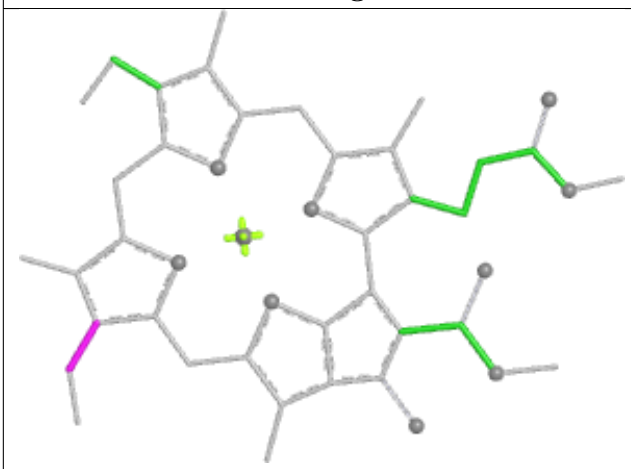
## Ligand CLA 3 617



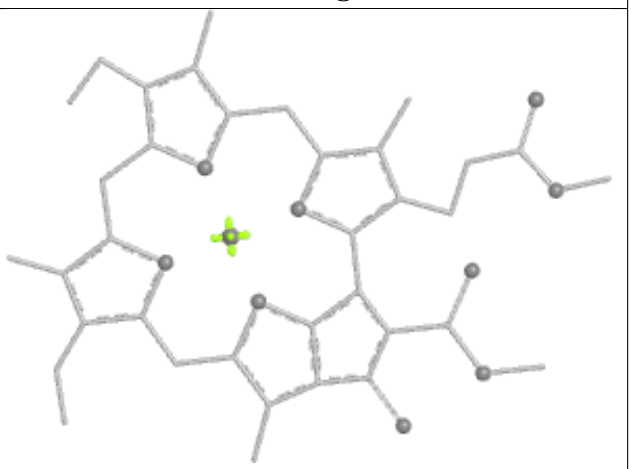
Bond lengths



Bond angles

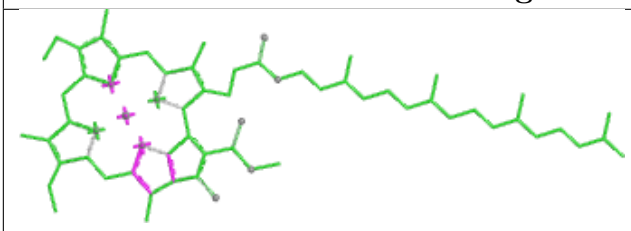


Torsions

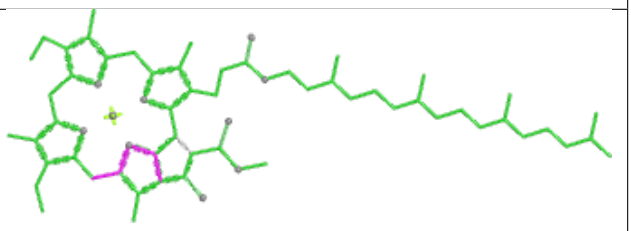


Rings

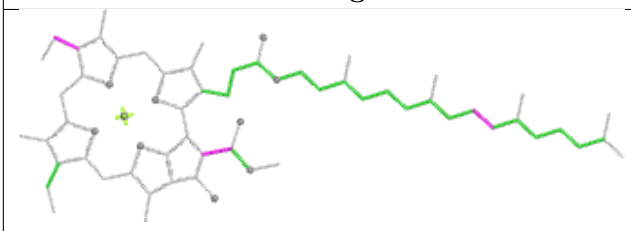
## Ligand CLA B2 821



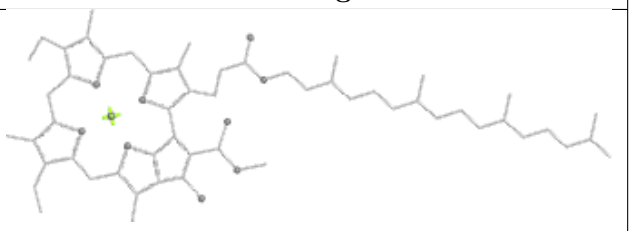
Bond lengths



Bond angles

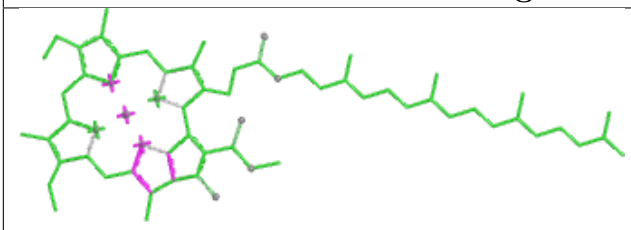


Torsions

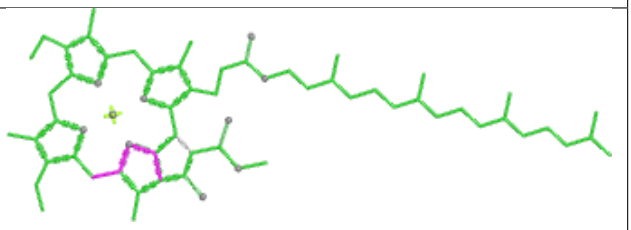


Rings

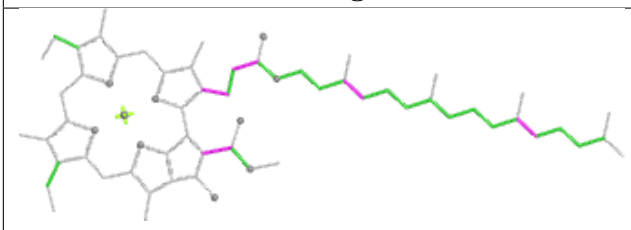
**Ligand CLA B2 805**



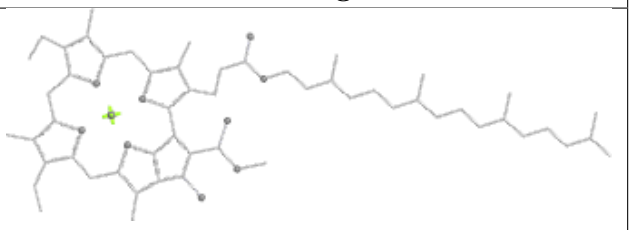
Bond lengths



Bond angles

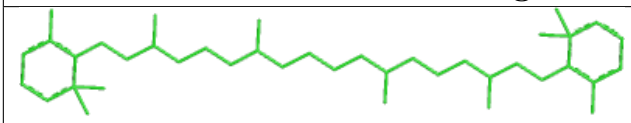


Torsions

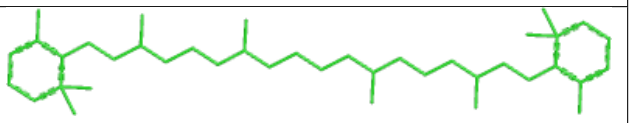


Rings

**Ligand BCR A2 848**



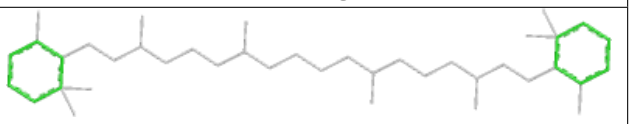
Bond lengths



Bond angles

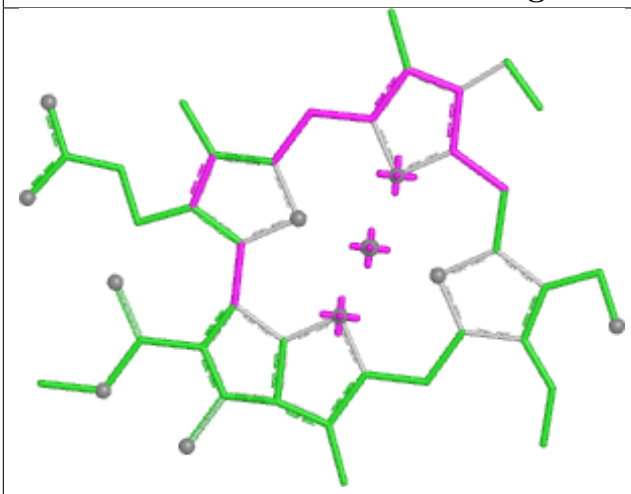


Torsions

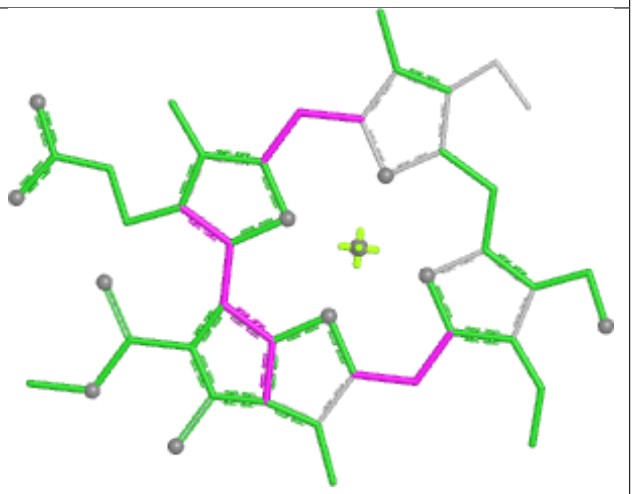


Rings

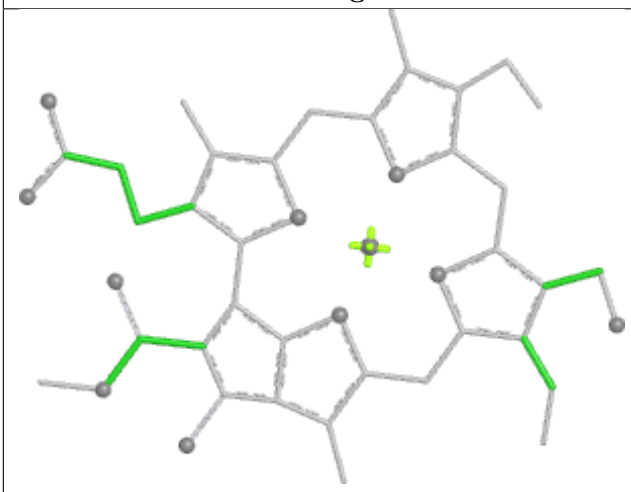
## Ligand CHL 1 606



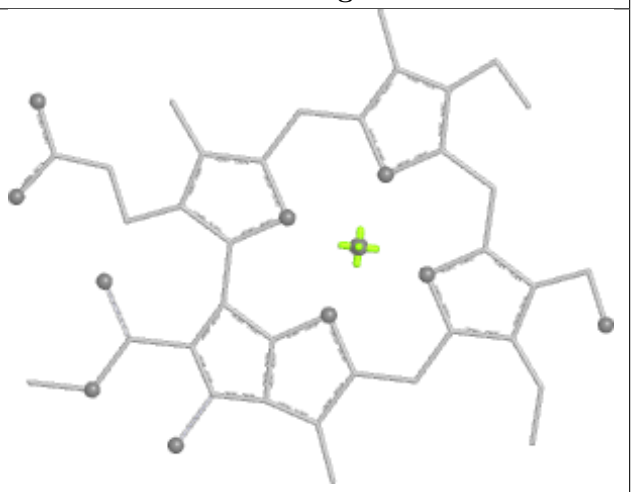
Bond lengths



Bond angles

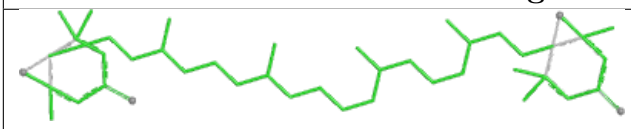


Torsions

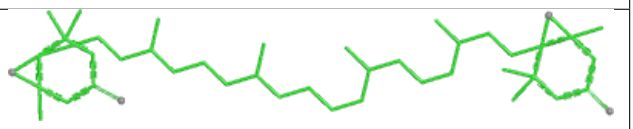


Rings

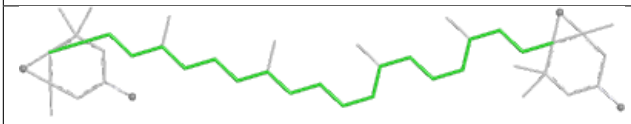
## Ligand XAT 6 624



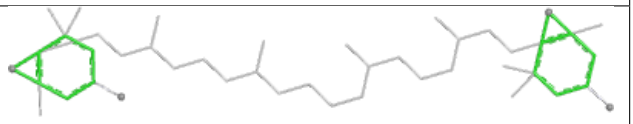
Bond lengths



Bond angles

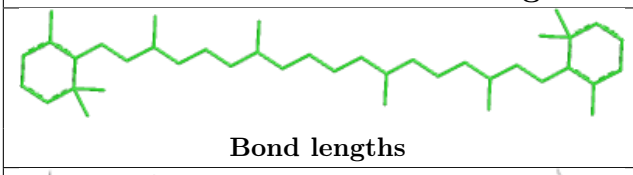


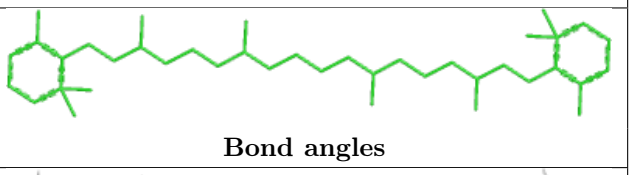
Torsions

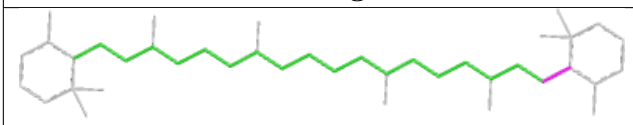


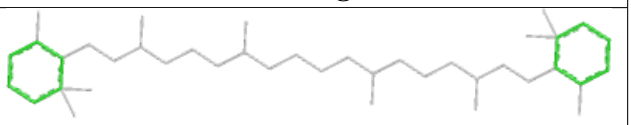
Rings

## Ligand BCR B 846


Bond lengths


Bond angles

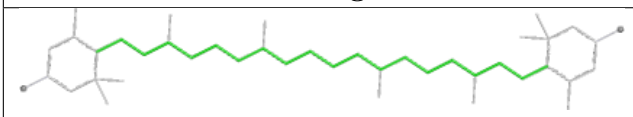

Torsions

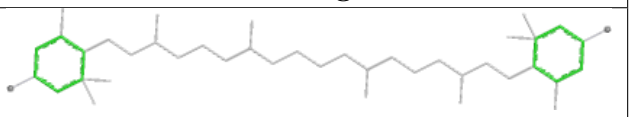

Rings

## Ligand LUT 9 617

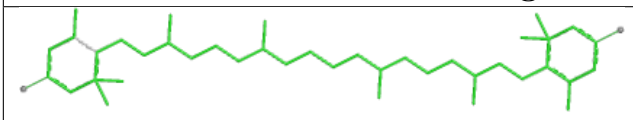

Bond lengths

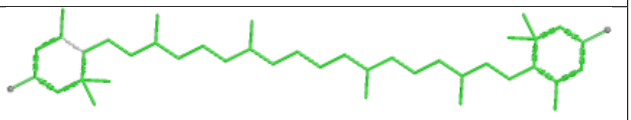

Bond angles

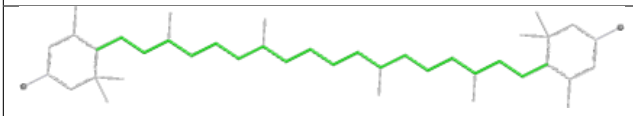

Torsions

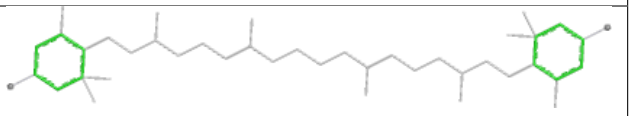

Rings

## Ligand LUT 92 617

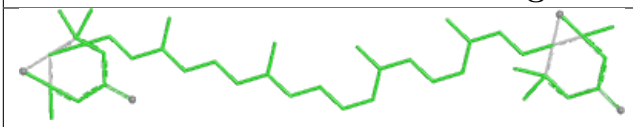

Bond lengths

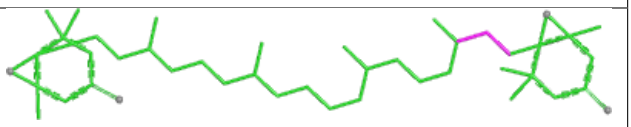

Bond angles

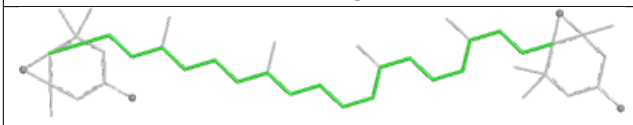

Torsions

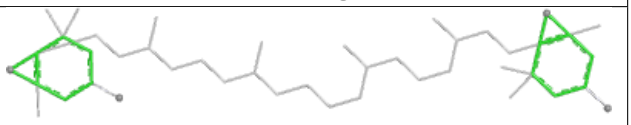

Rings

## Ligand XAT 1 618

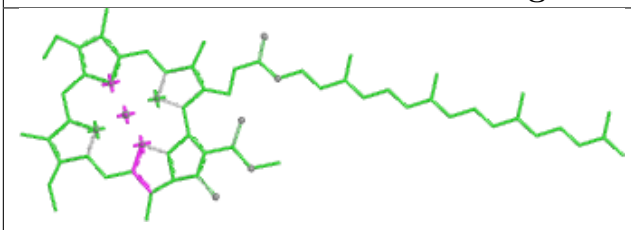

Bond lengths


Bond angles

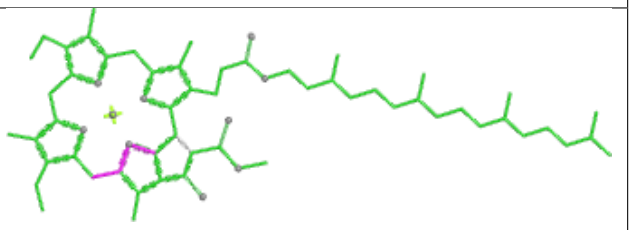

Torsions


Rings

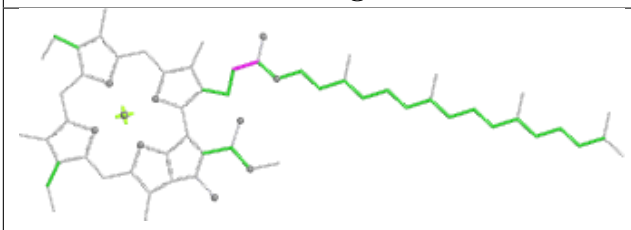
## Ligand CLA 7 613



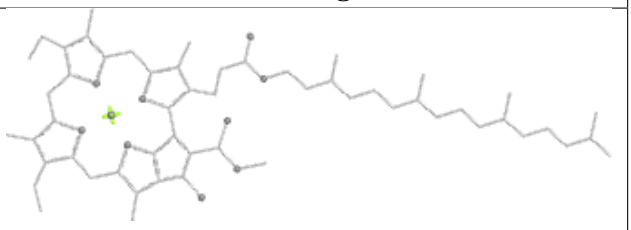
Bond lengths



Bond angles

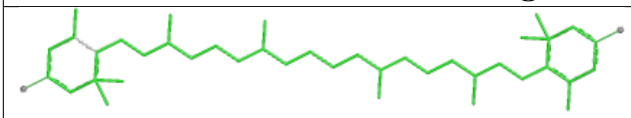


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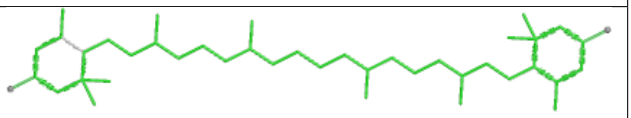


Rings

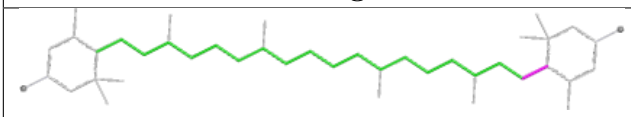
## Ligand LUT 72 621



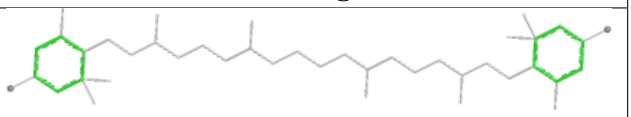
Bond lengths



Bond angles

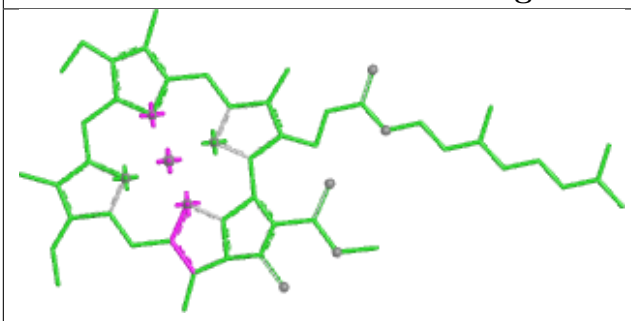


Torsions

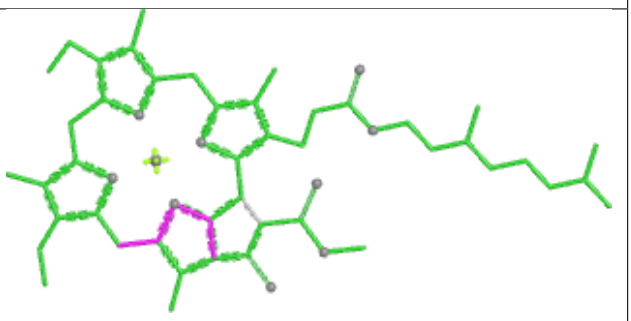


Rings

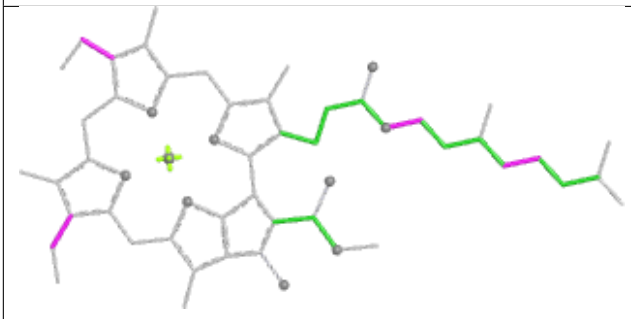
## Ligand CLA A2 825



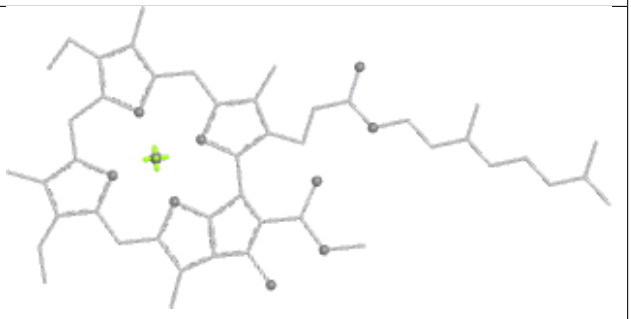
Bond lengths



Bond angles

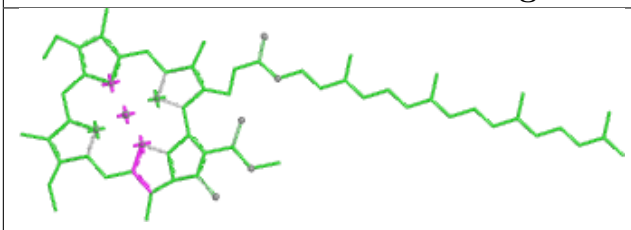


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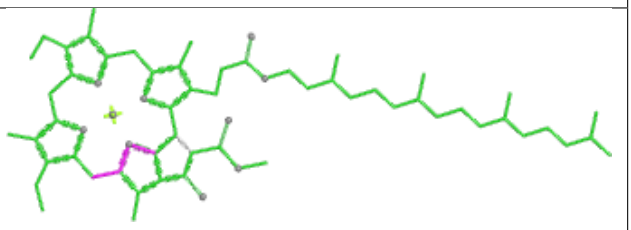


Rings

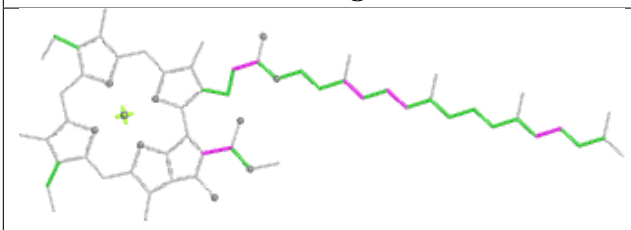
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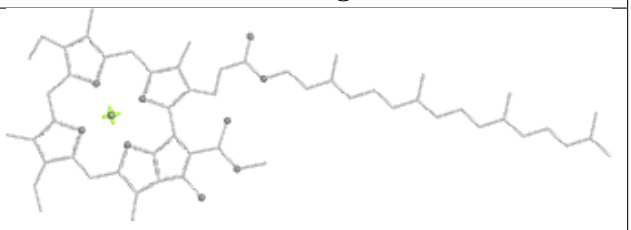
Bond lengths



Bond angles

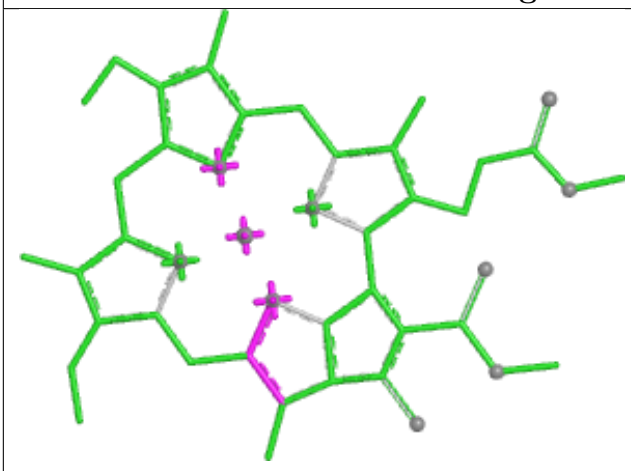


Torsions

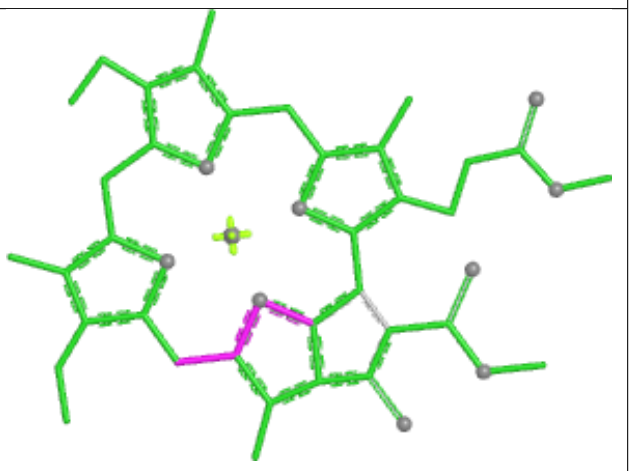


Rings

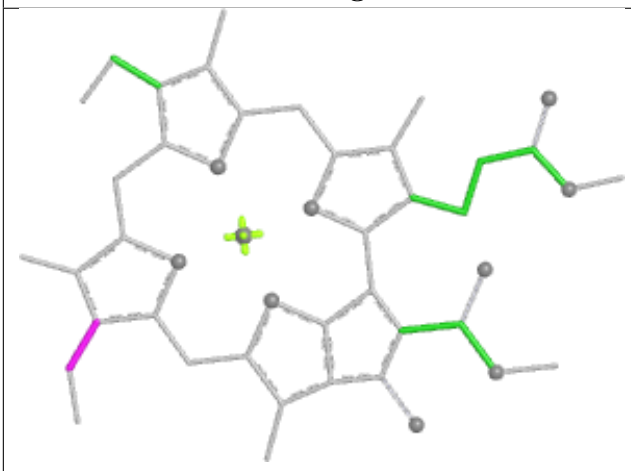
## Ligand CLA 32 617



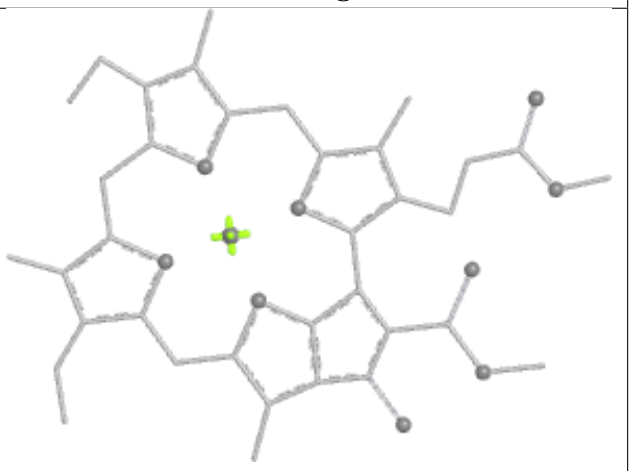
Bond lengths



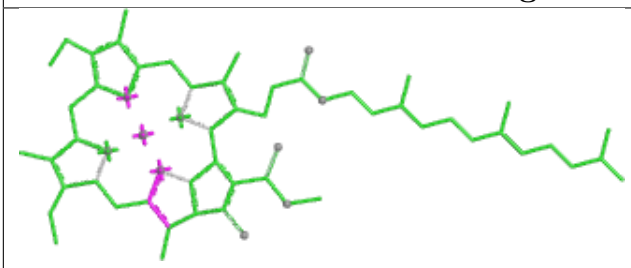
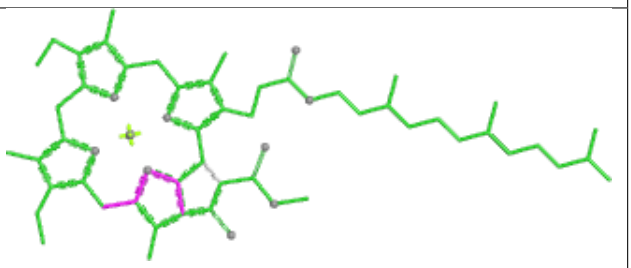
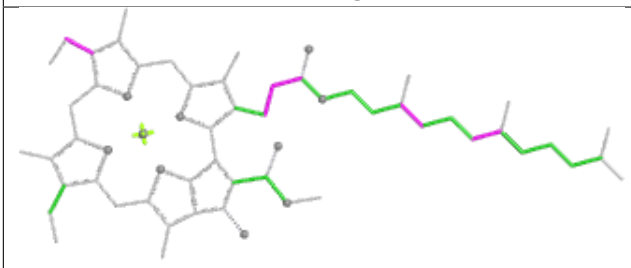
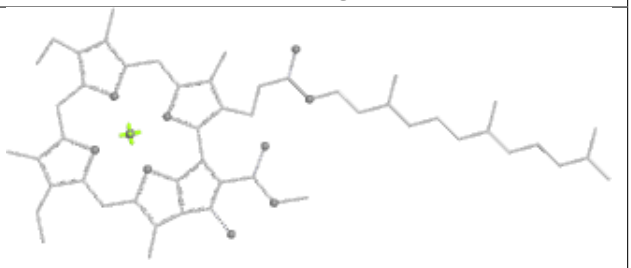
Bond angles

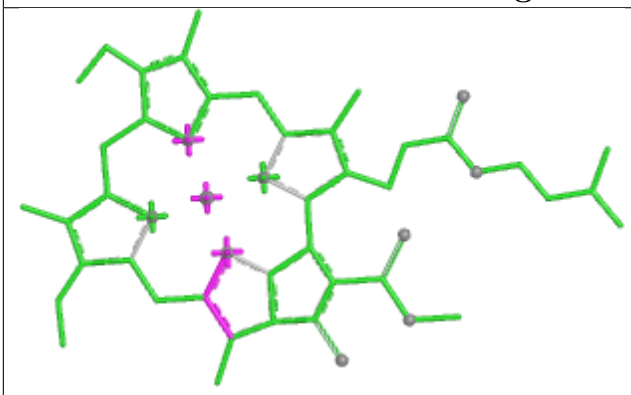
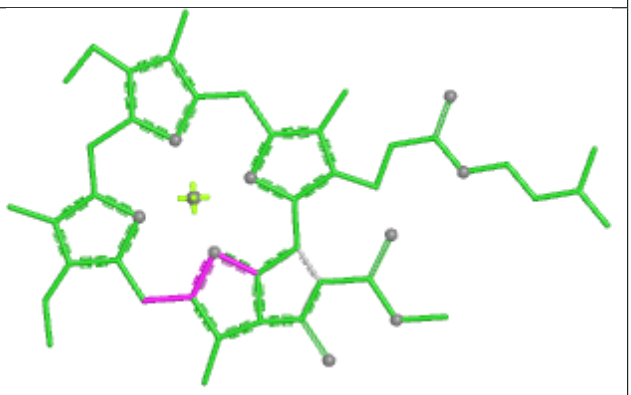
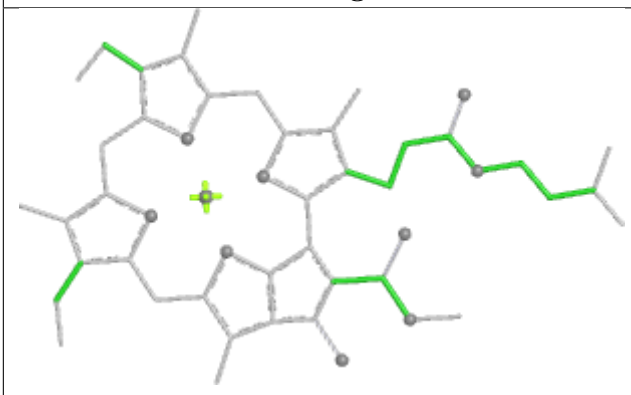
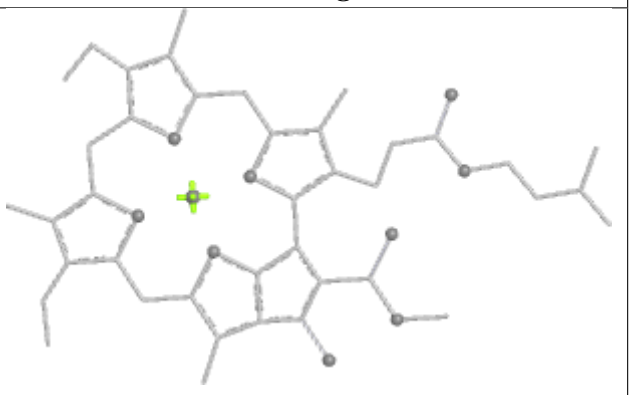


Torsions

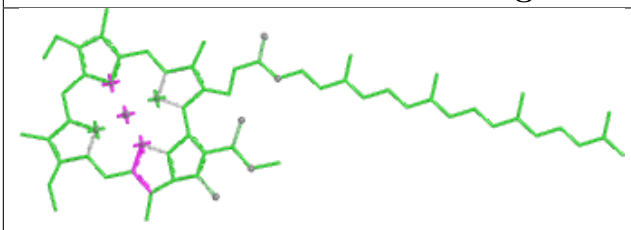


Rings

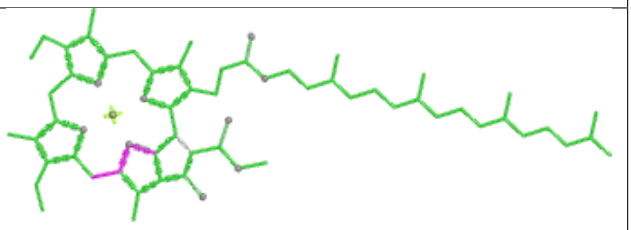
| Ligand CLA 12 614 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA A2 808 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

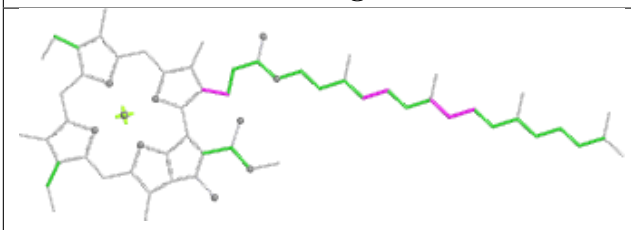
**Ligand CLA B2 827**



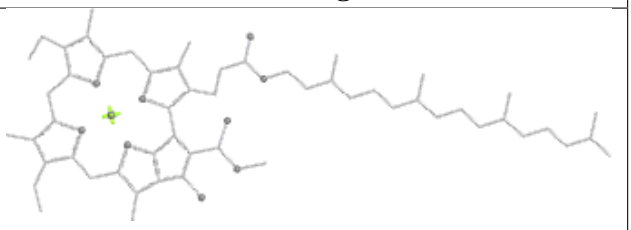
Bond lengths



Bond angles

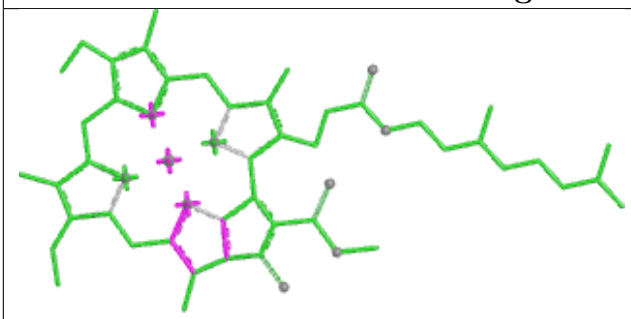


Torsions

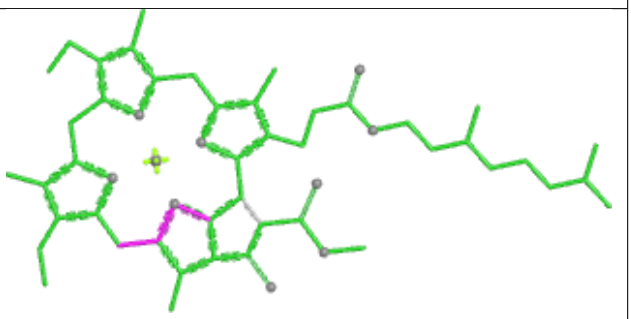


Rings

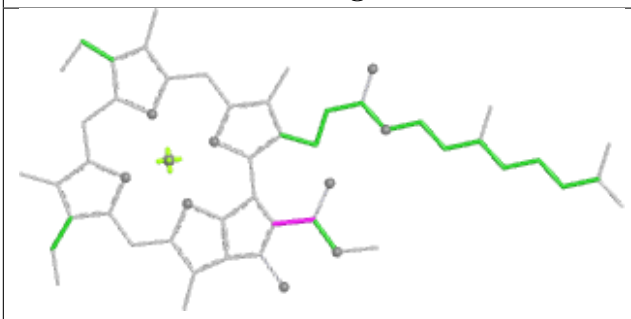
**Ligand CLA A2 805**



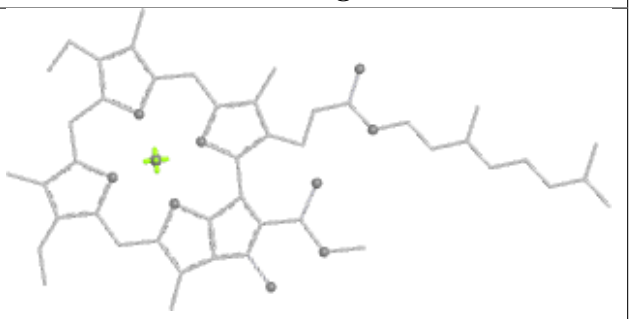
Bond lengths



Bond angles

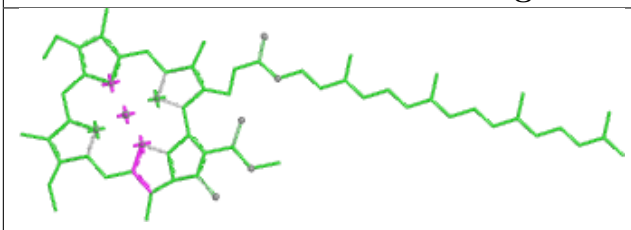


Torsions

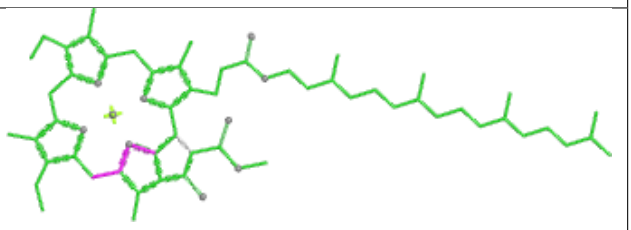


Rings

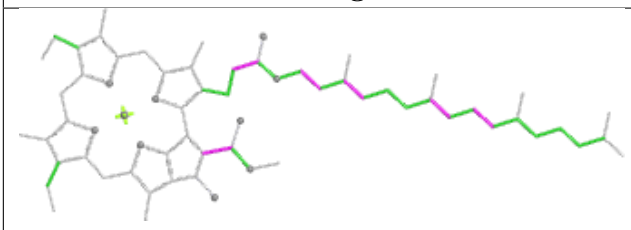
## Ligand CLA A2 826



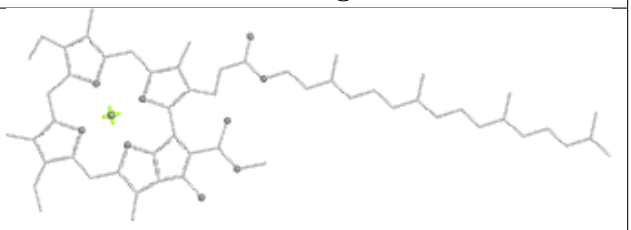
Bond lengths



Bond angles

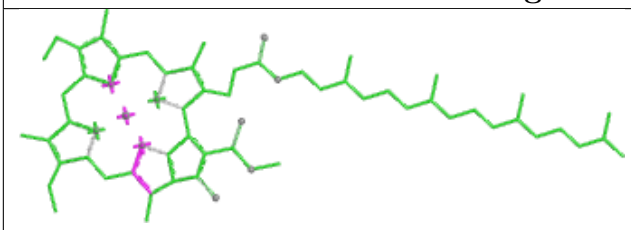


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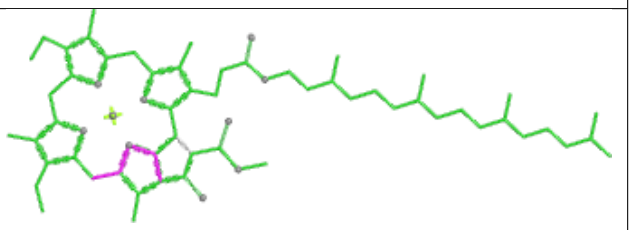


Rings

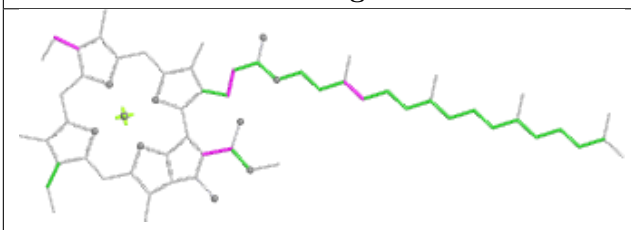
## Ligand CLA B 839



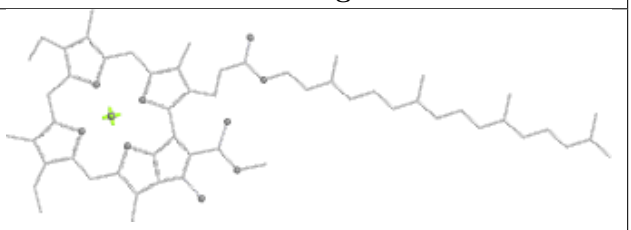
Bond lengths



Bond angles

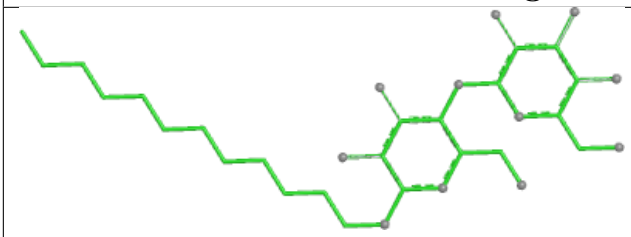


Torsions

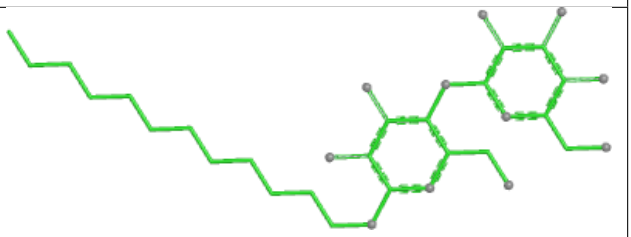


Rings

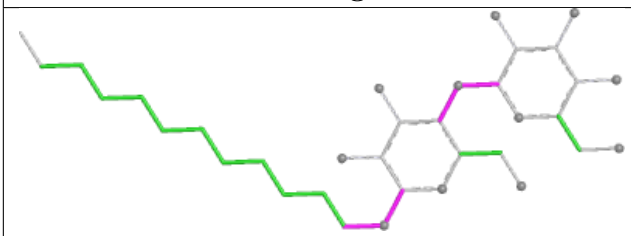
## Ligand LMU 1 621



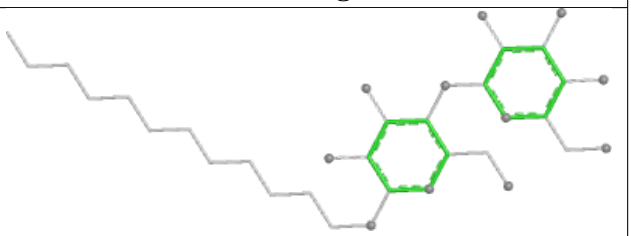
Bond lengths



Bond angles

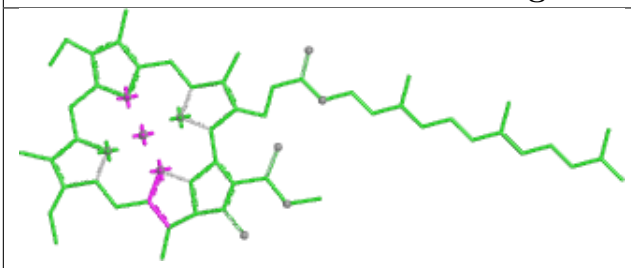


Torsions

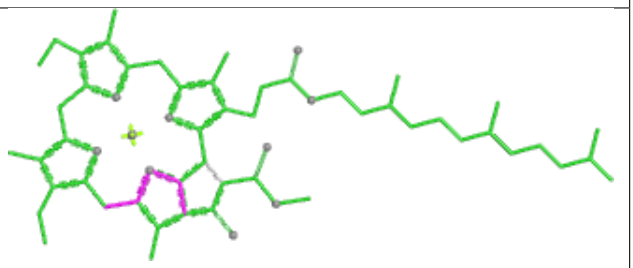


Rings

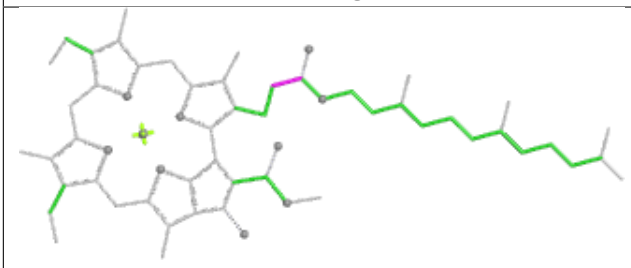
## Ligand CLA 8 604



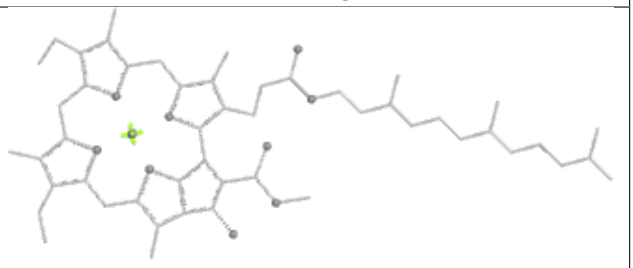
Bond lengths



Bond angles

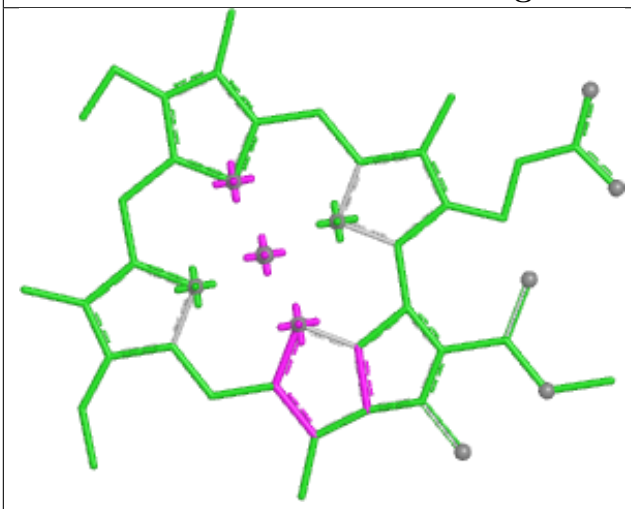


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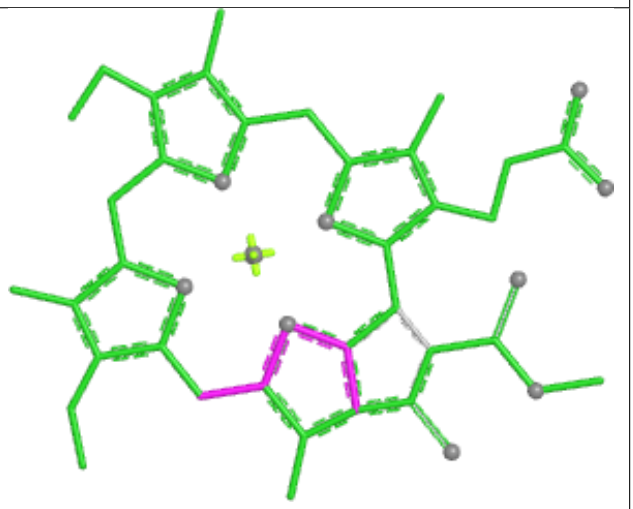


Rings

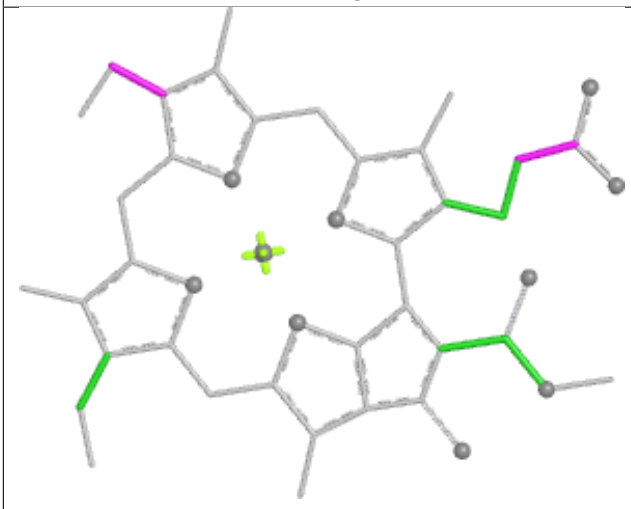
## Ligand CLA A2 824



Bond lengths



Bond angles

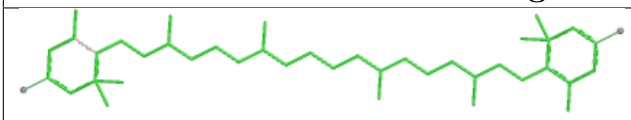


Torsions

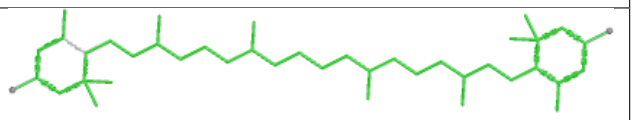


Rings

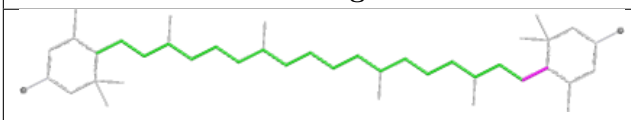
## Ligand LUT 1 619



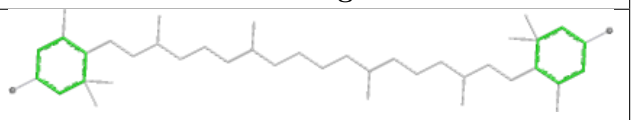
Bond lengths



Bond angles

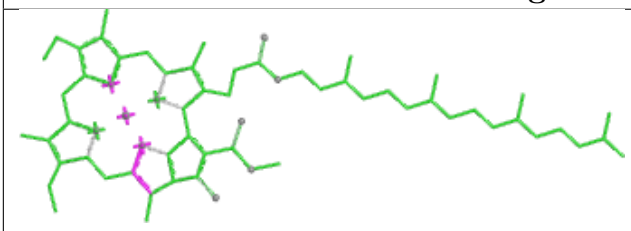


Torsions

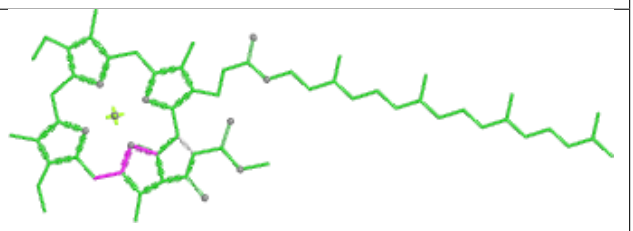


Rings

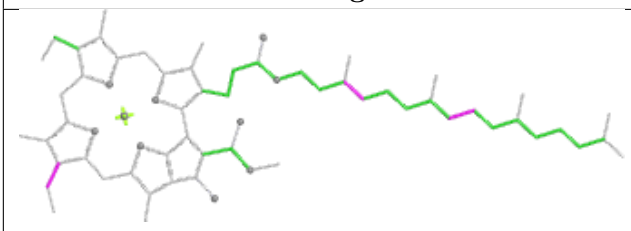
## Ligand CLA 3 603



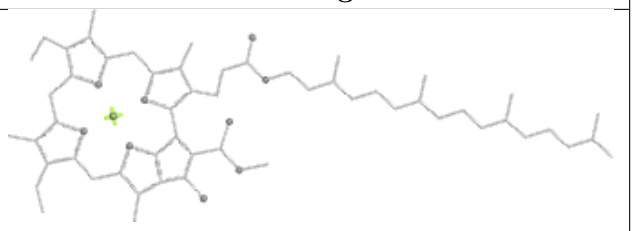
Bond lengths



Bond angles

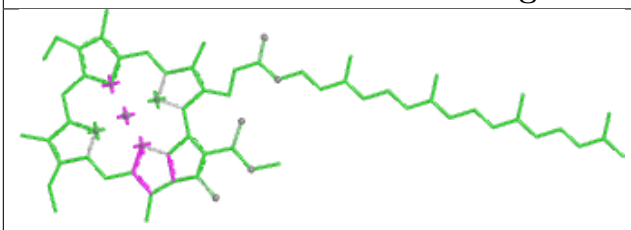


Torsions

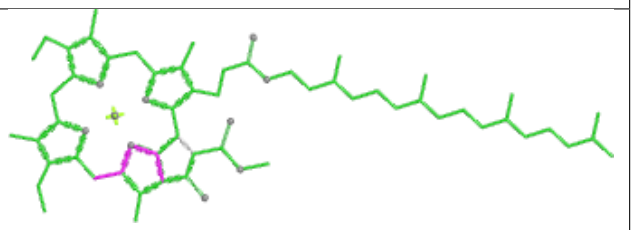


Rings

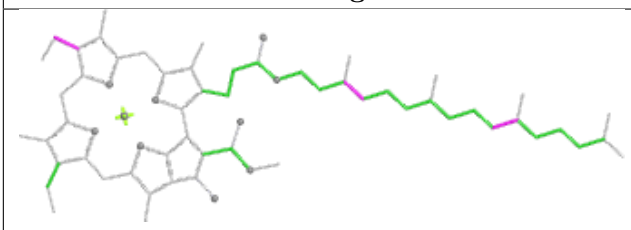
## Ligand CLA 12 613



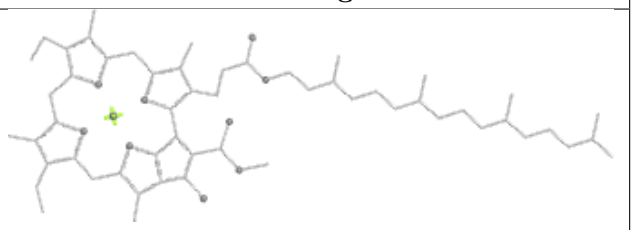
Bond lengths



Bond angles

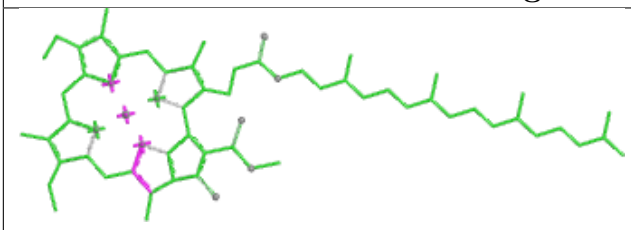


Torsions

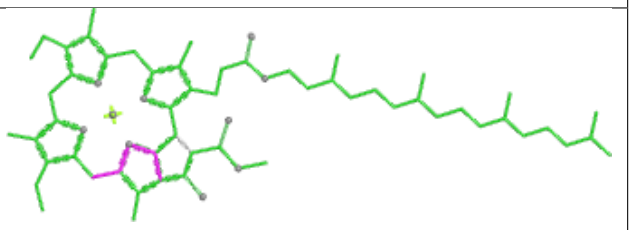


Rings

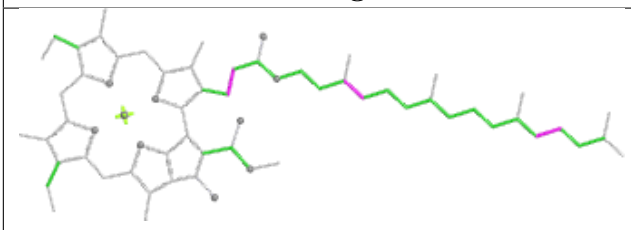
## Ligand CLA A 830



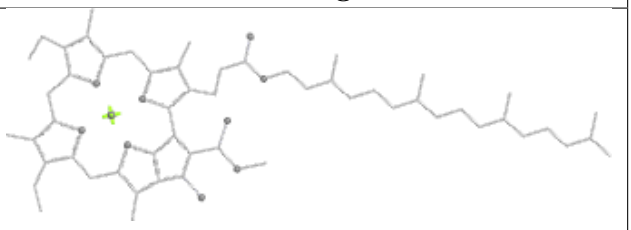
Bond lengths



Bond angles

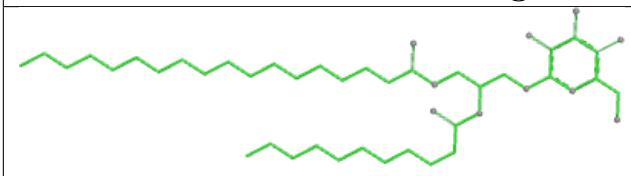


Torsions

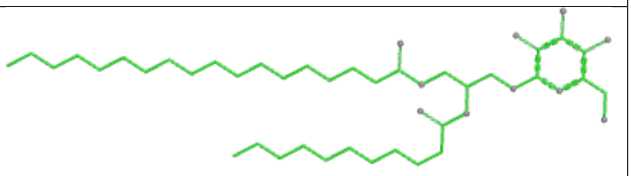


Rings

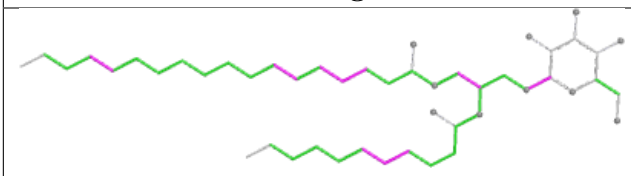
## Ligand LMG A2 859



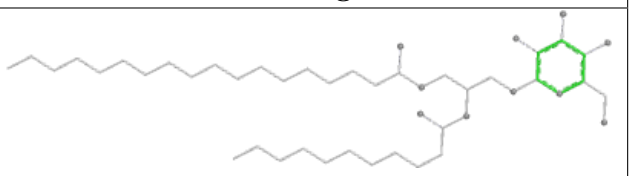
Bond lengths



Bond angles

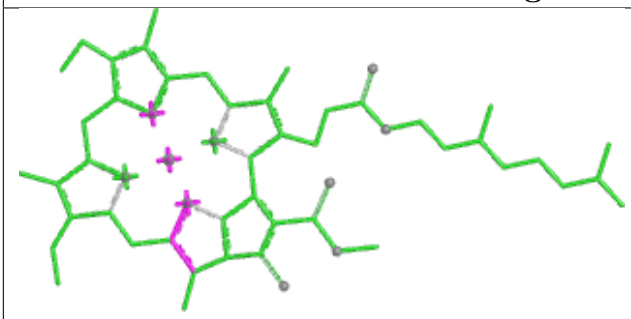


Torsions

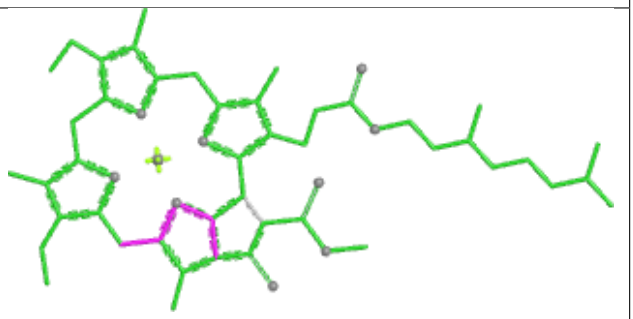


Rings

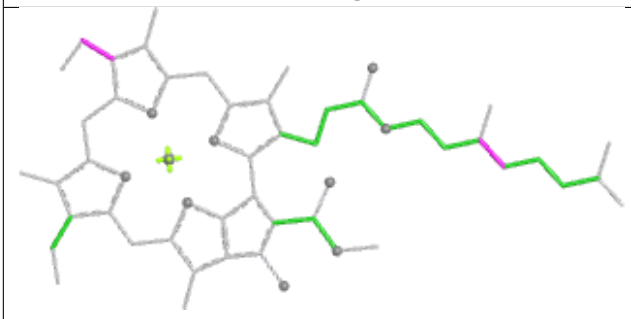
**Ligand CLA B 807**



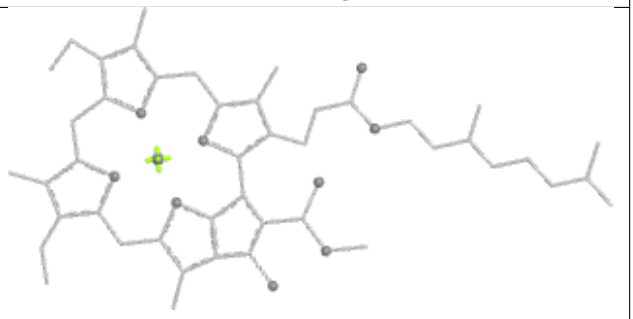
**Bond lengths**



**Bond angles**

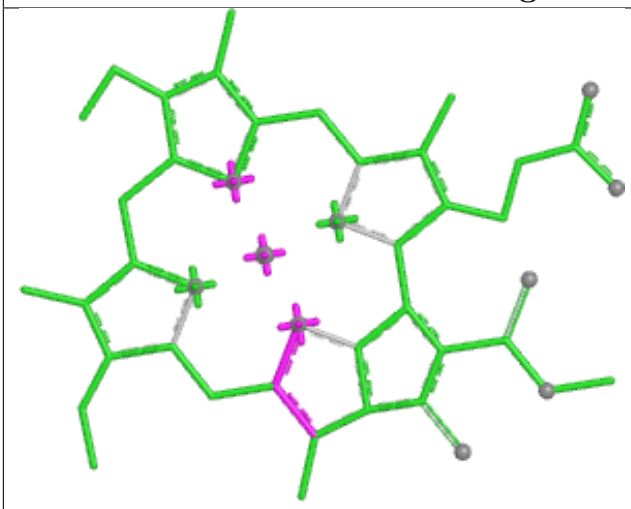


**Torsions**

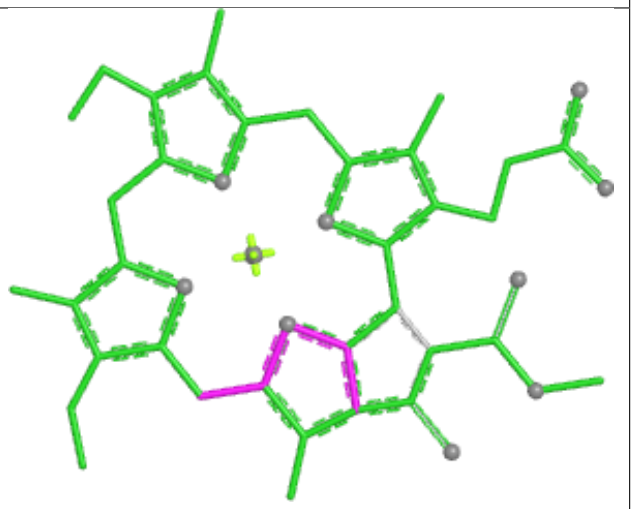


**Rings**

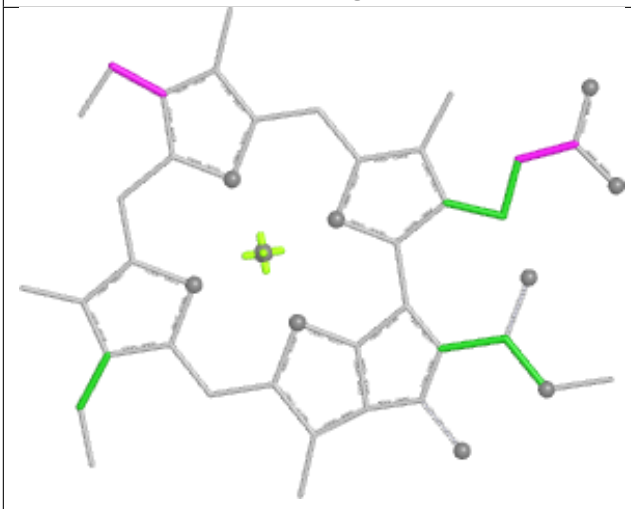
## Ligand CLA 92 614



Bond lengths



Bond angles

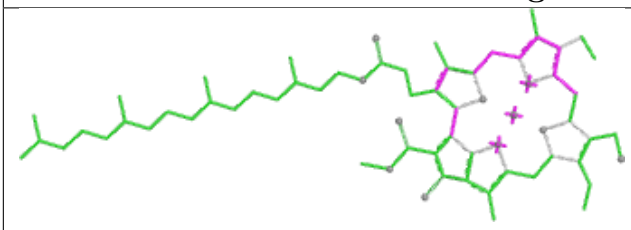


Torsions

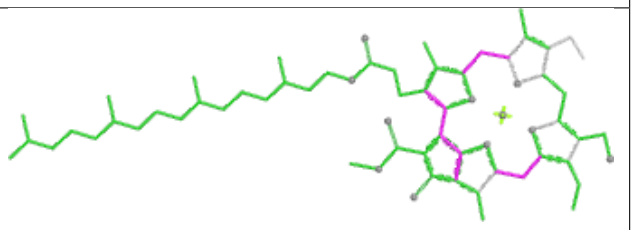


Rings

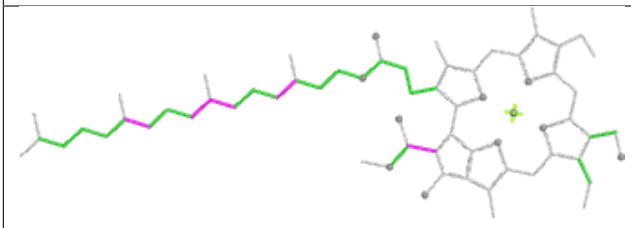
## Ligand CHL 1 601



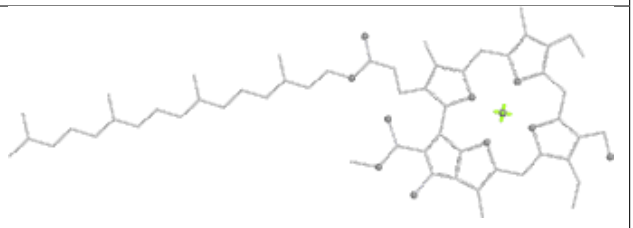
Bond lengths



Bond angles

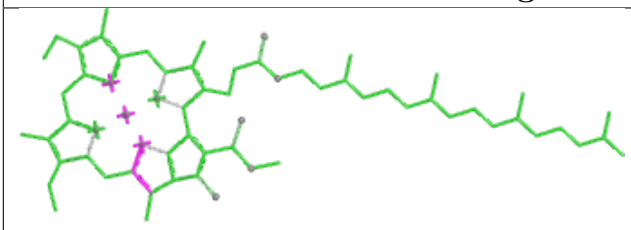


Torsions

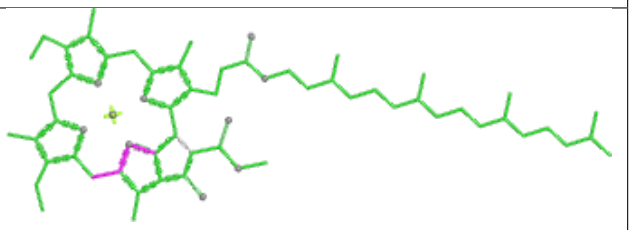


Rings

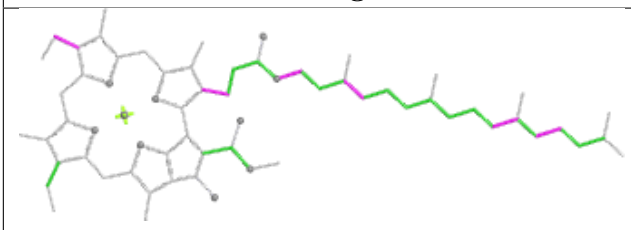
## Ligand CLA Z2 609



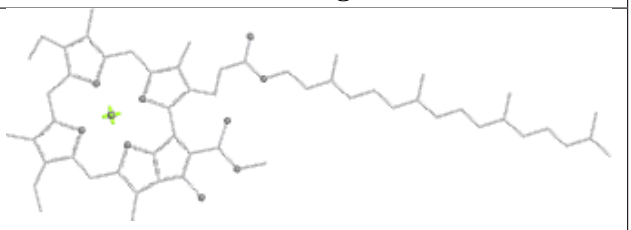
Bond lengths



Bond angles

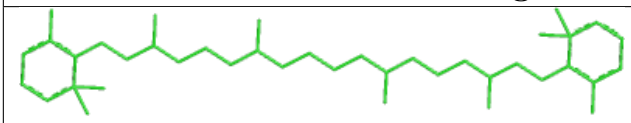


Torsions

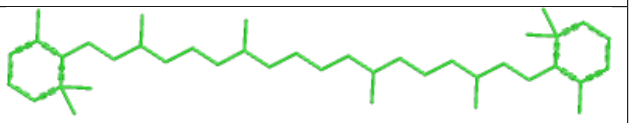


Rings

## Ligand BCR K2 202



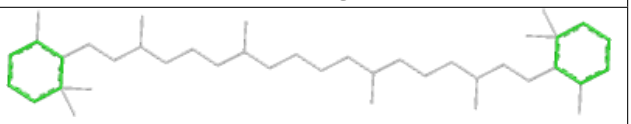
Bond lengths



Bond angles

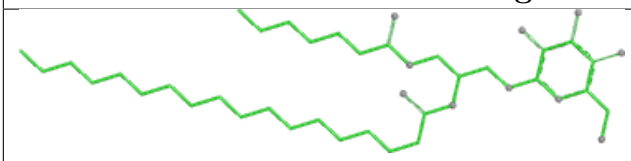


Torsions

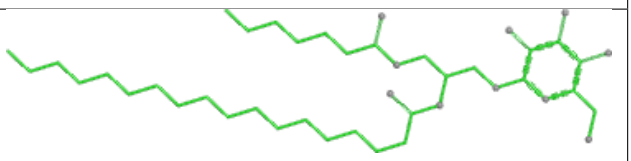


Rings

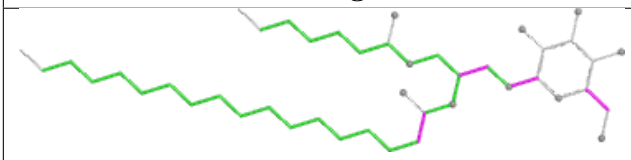
## Ligand LMG 92 620



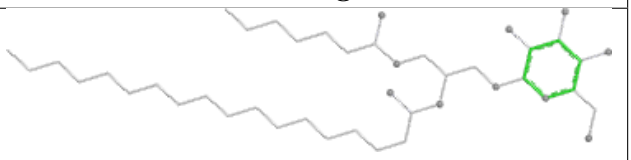
Bond lengths



Bond angles

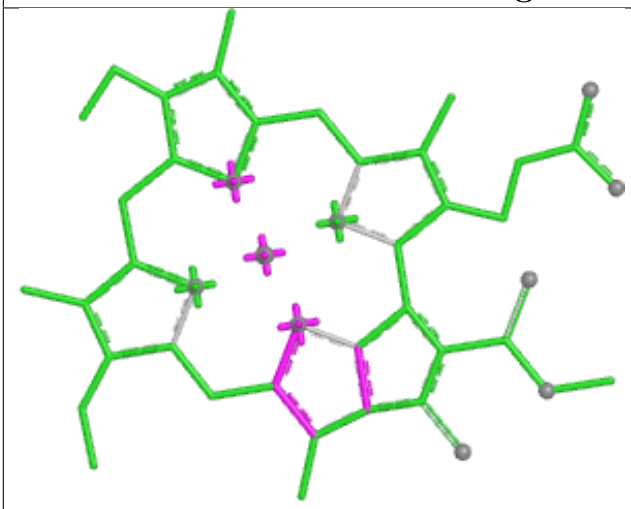


Torsions

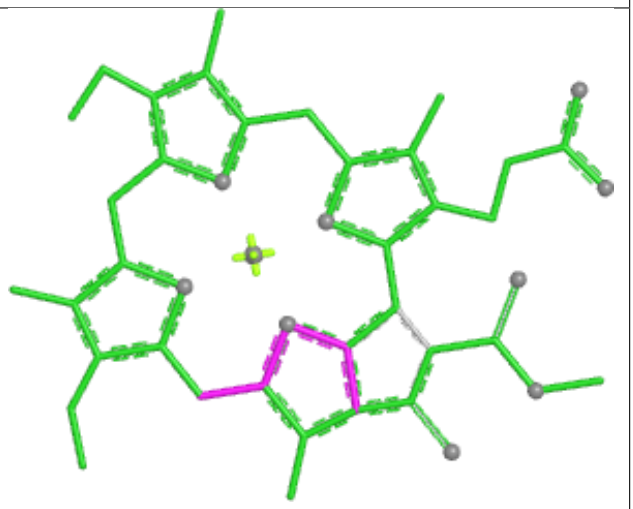


Rings

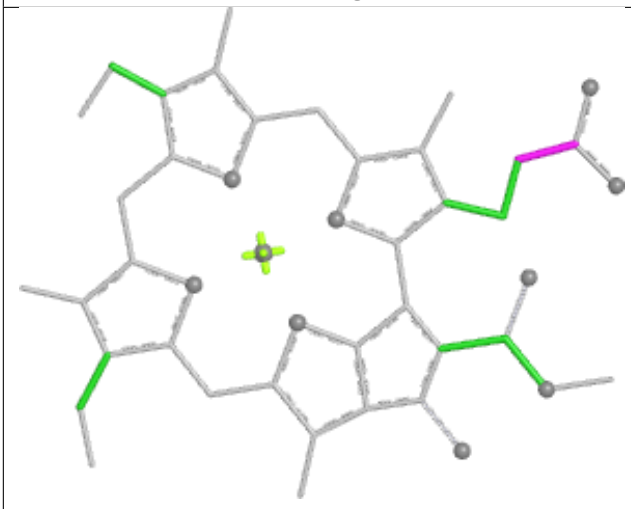
## Ligand CLA B2 835



Bond lengths



Bond angles

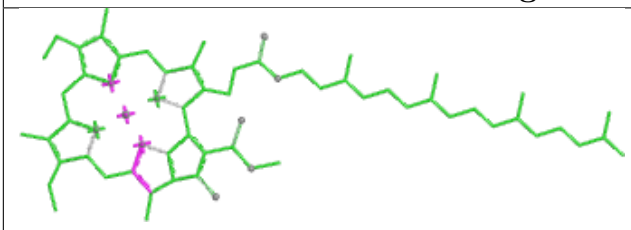


Torsions

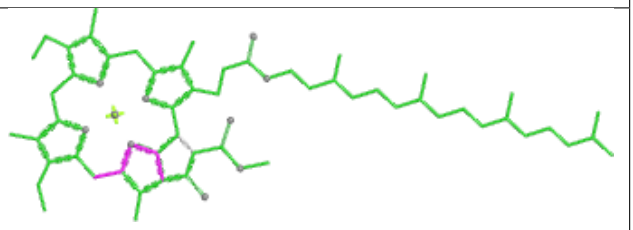


Rings

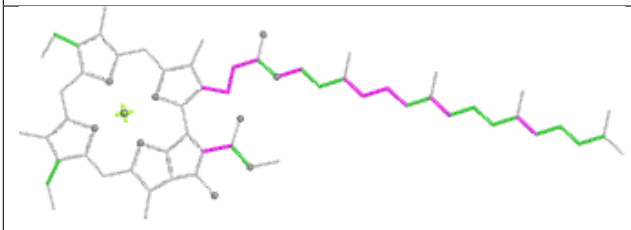
## Ligand CLA 52 603



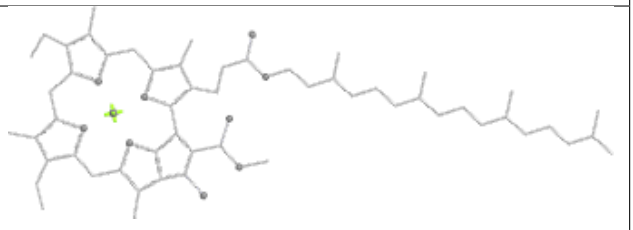
Bond lengths



Bond angles

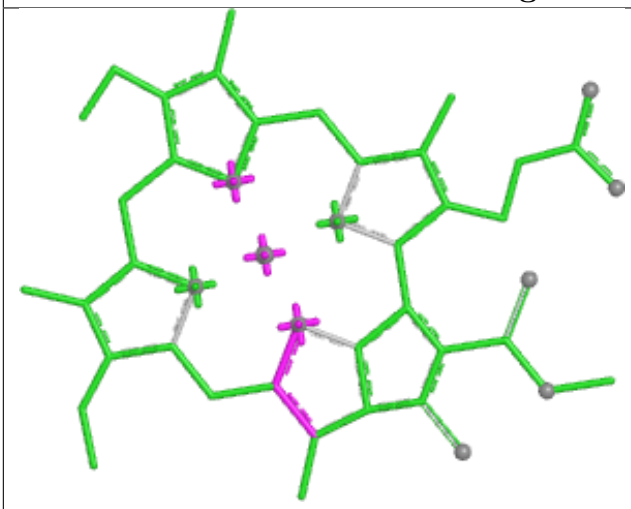


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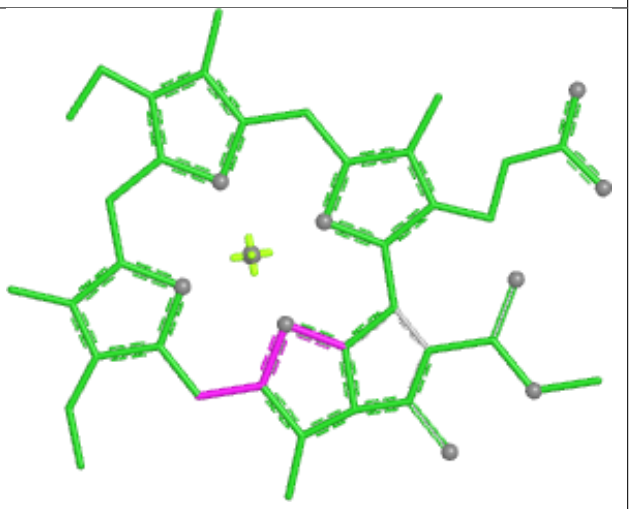


Rings

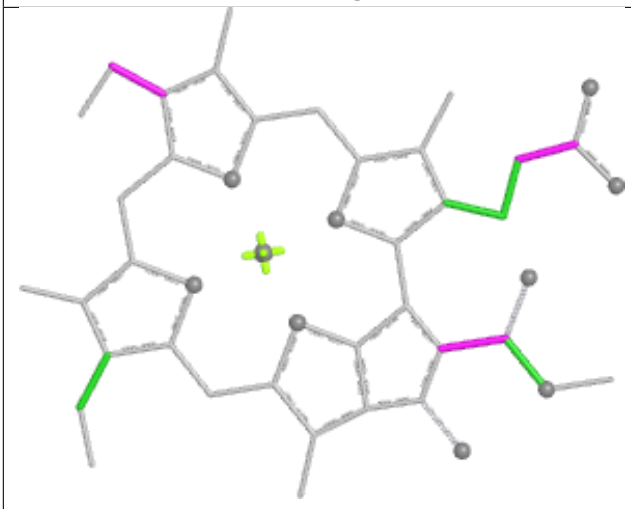
## Ligand CLA 52 612



Bond lengths



Bond angles

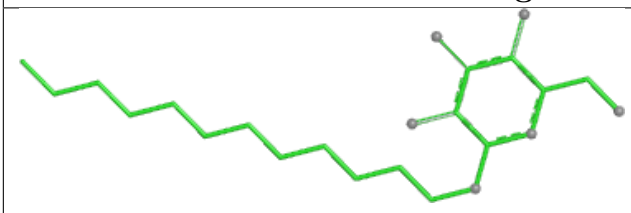


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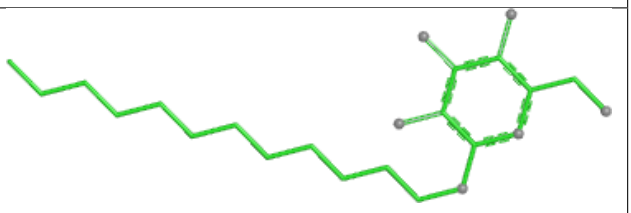


Rings

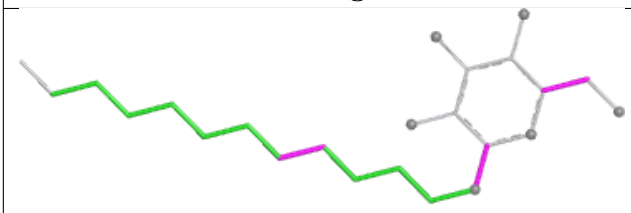
## Ligand LMU 62 631



Bond lengths



Bond angles

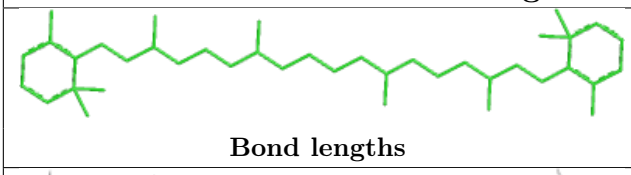


Torsions

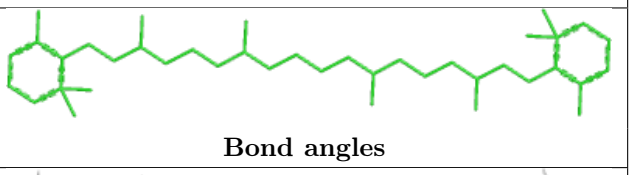


Rings

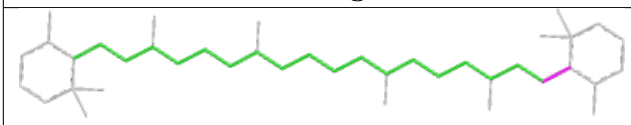
## Ligand BCR B 847



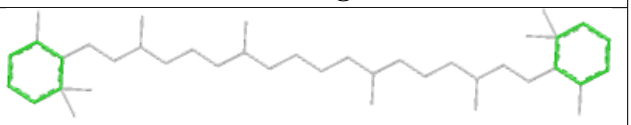
Bond lengths



Bond angles

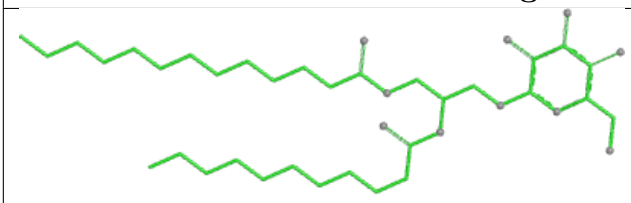


Torsions

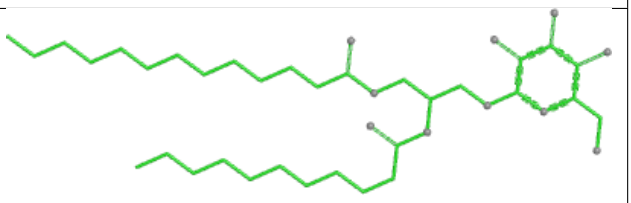


Rings

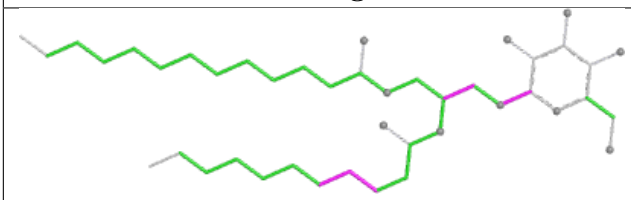
## Ligand LMG B 852



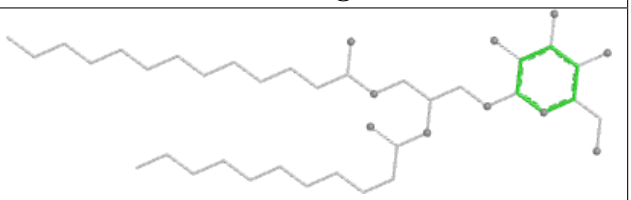
Bond lengths



Bond angles

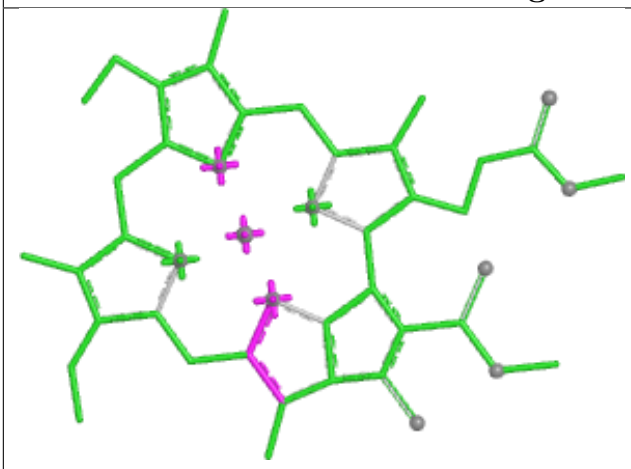


Torsions

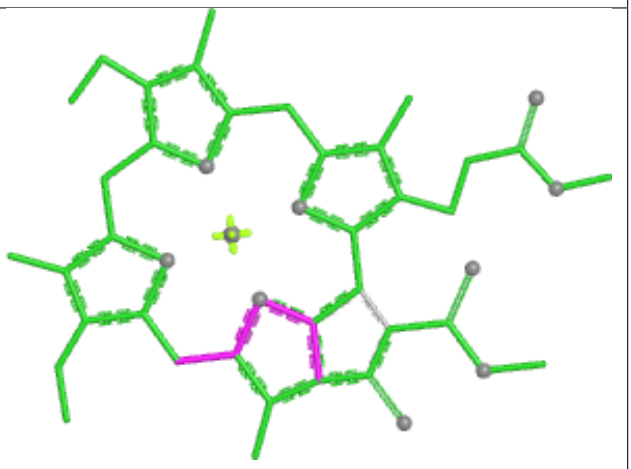


Rings

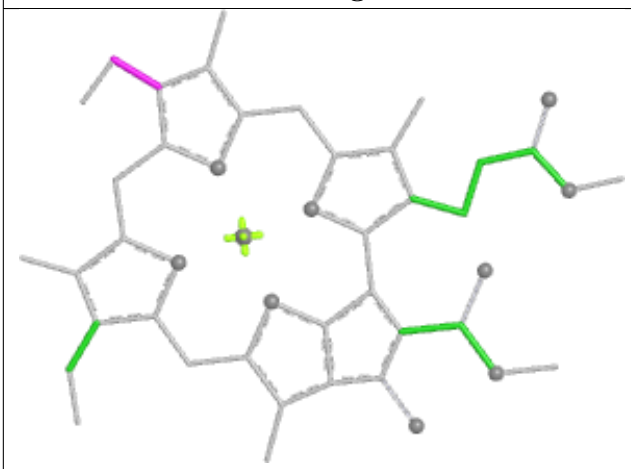
**Ligand CLA 9 601**



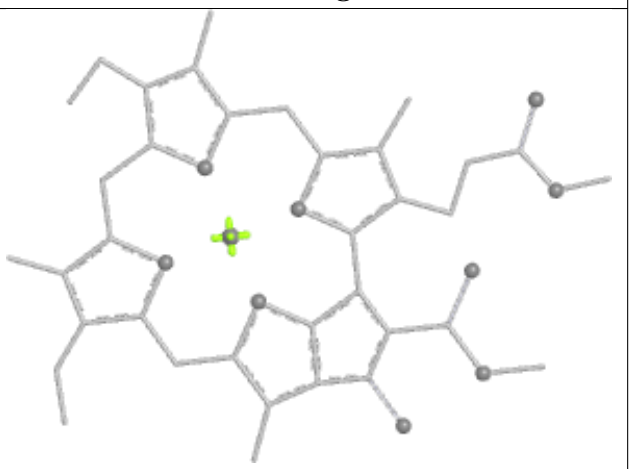
**Bond lengths**



**Bond angles**

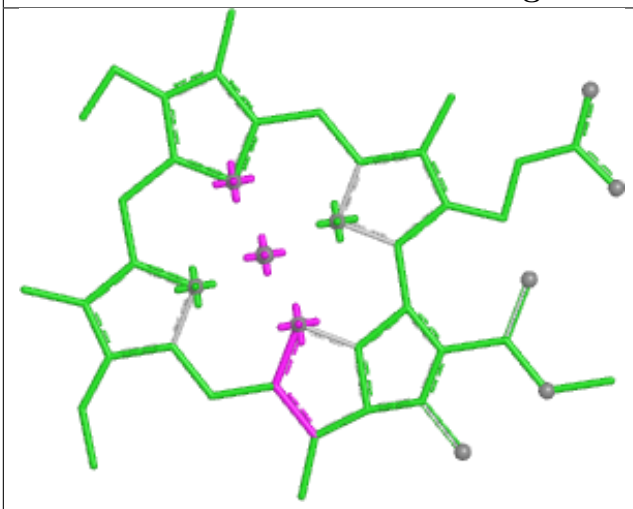


**Torsions**

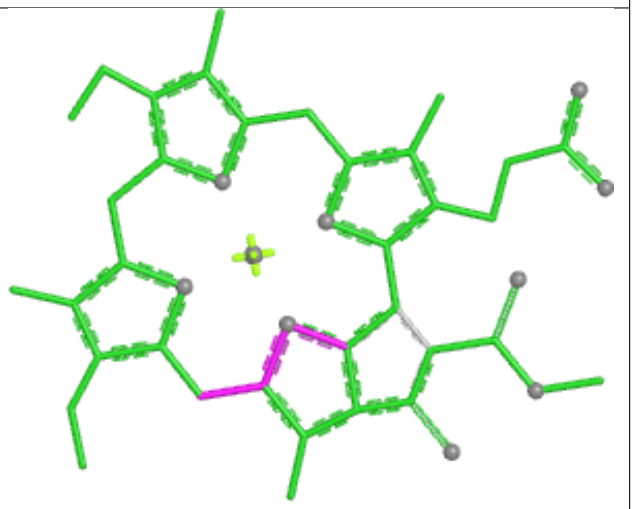


**Rings**

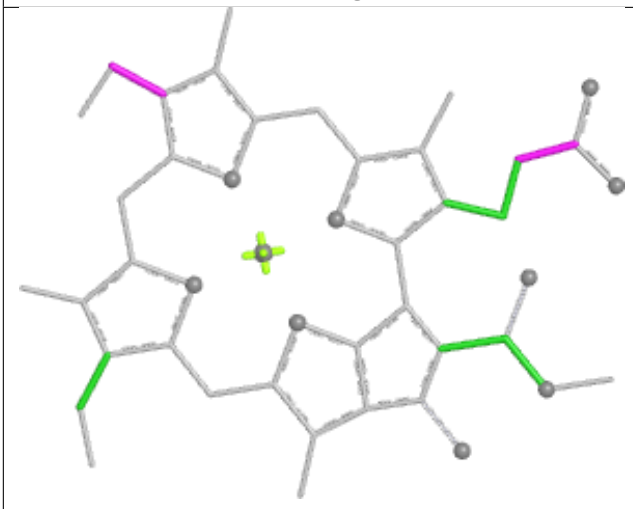
## Ligand CLA K 206



Bond lengths



Bond angles

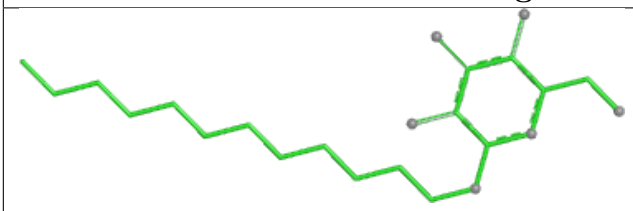


Torsions

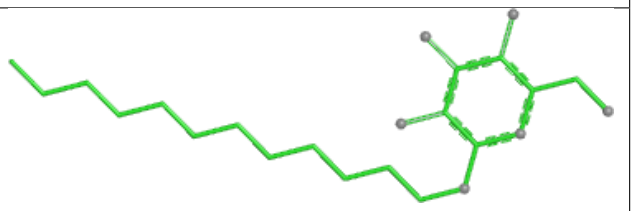


Rings

## Ligand LMU 62 630



Bond lengths



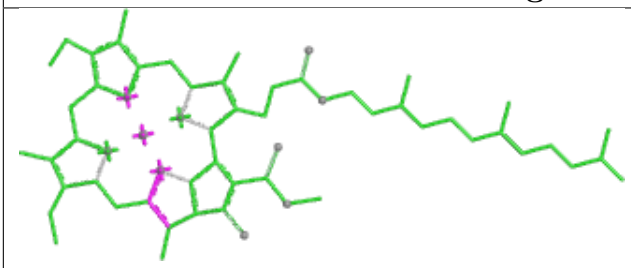
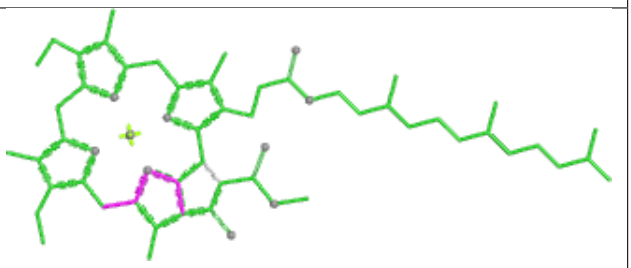
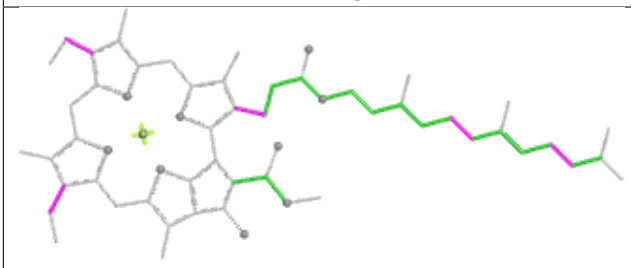
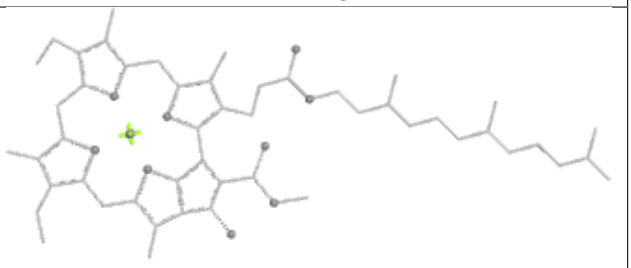
Bond angles

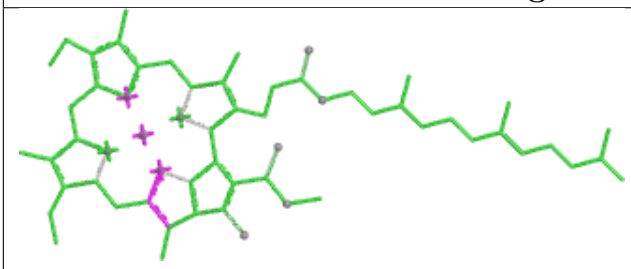
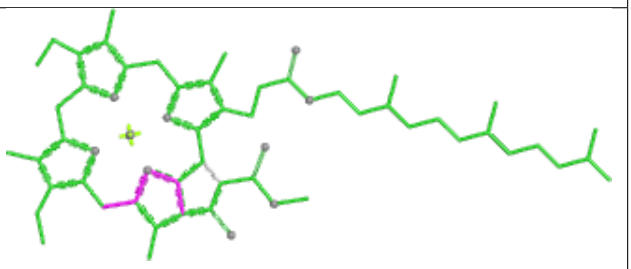
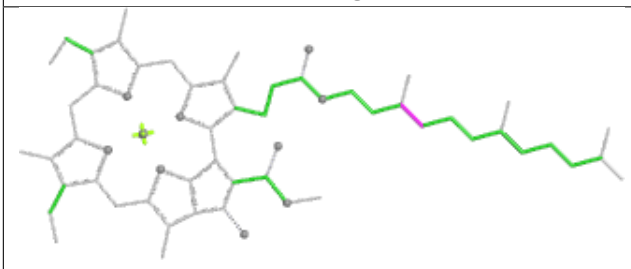
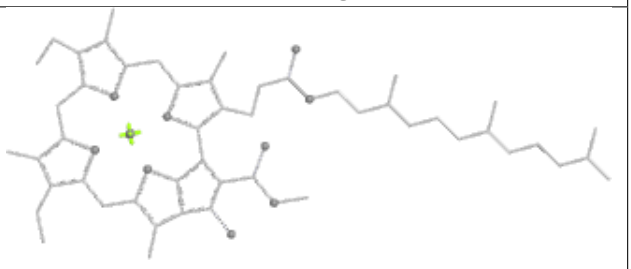


Torsions

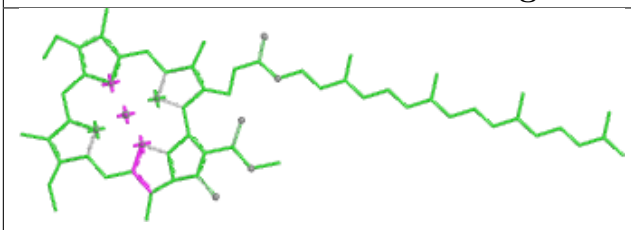


Rings

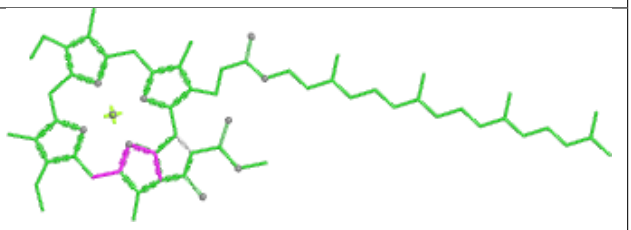
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|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 5 610 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

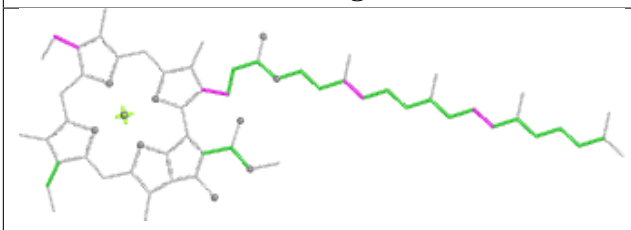
## Ligand CLA 92 611



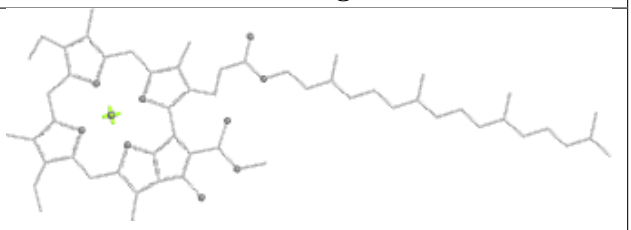
Bond lengths



Bond angles

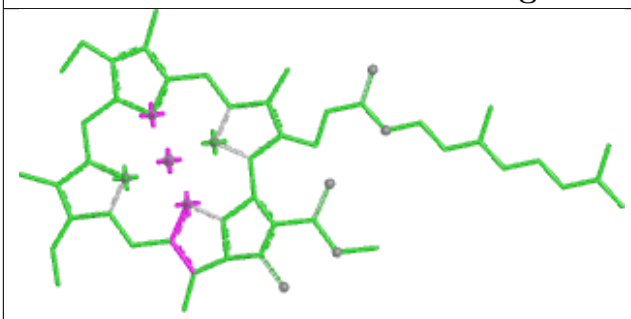


Torsions

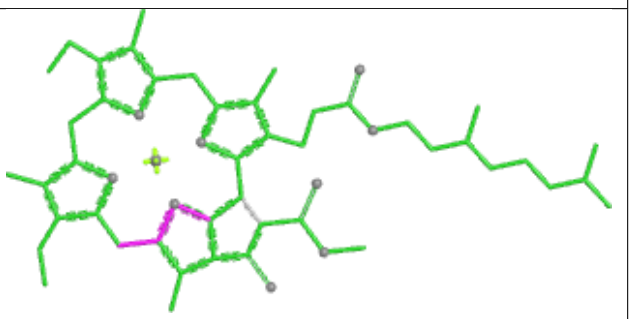


Rings

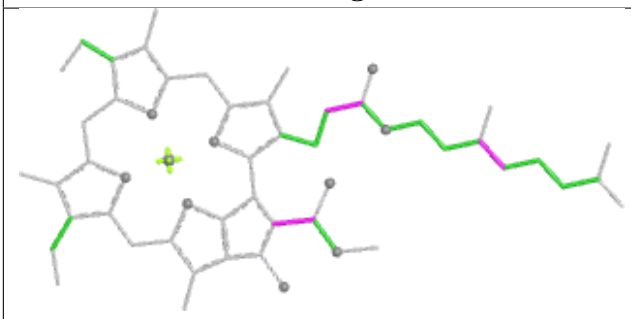
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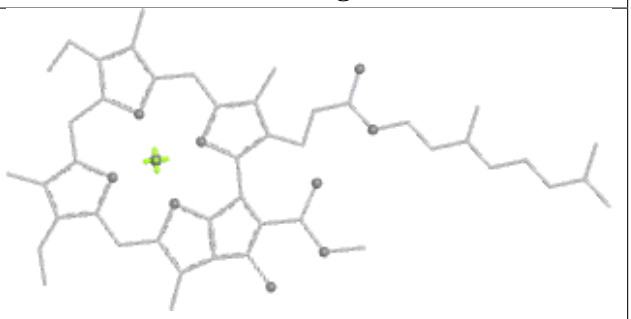
Bond lengths



Bond angles

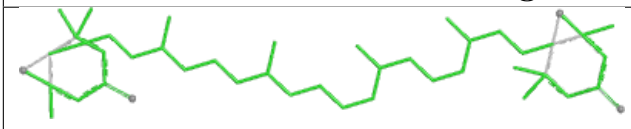


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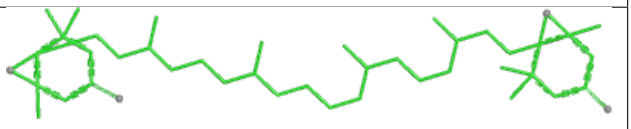


Rings

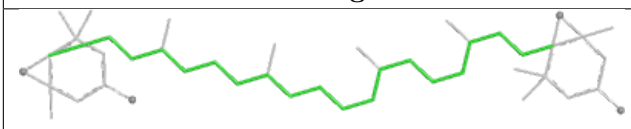
## Ligand XAT 42 620



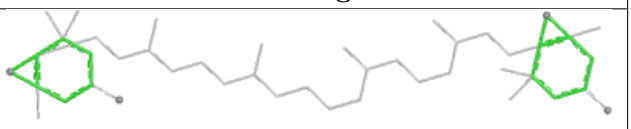
Bond lengths



Bond angles

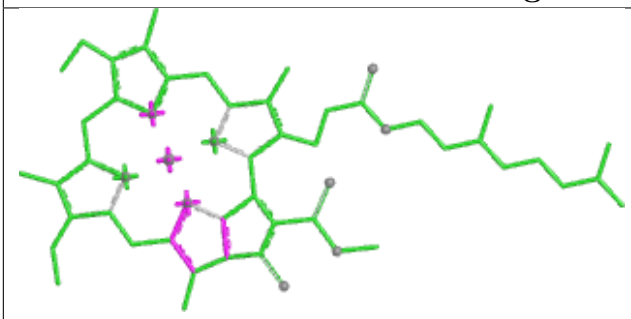


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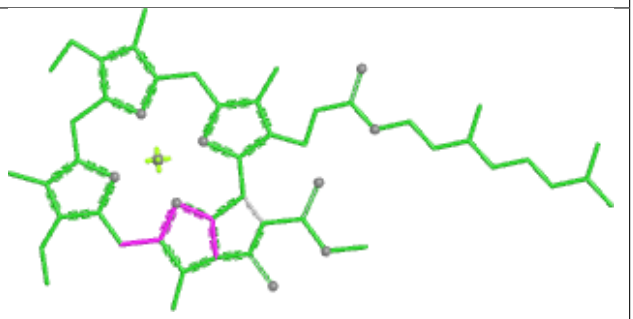


Rings

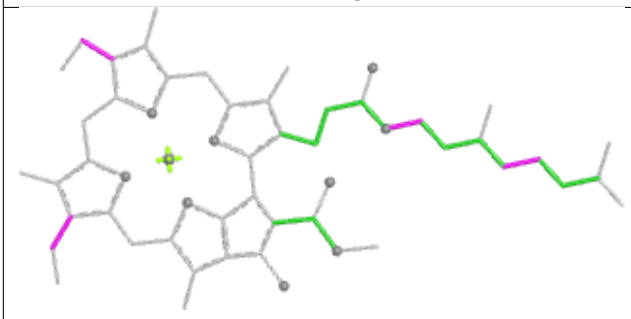
## Ligand CLA A 825



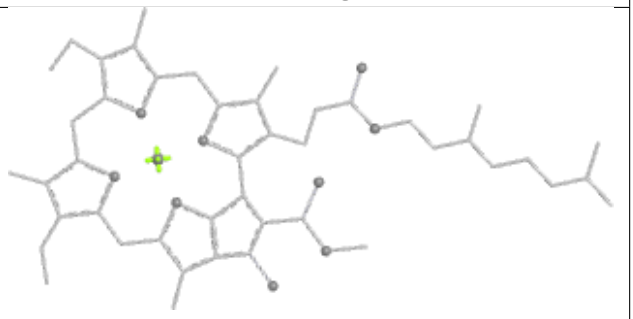
Bond lengths



Bond angles

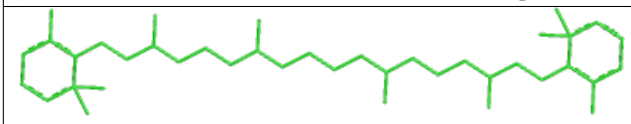


Torsions

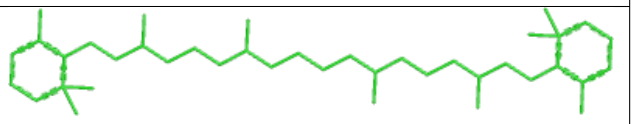


Rings

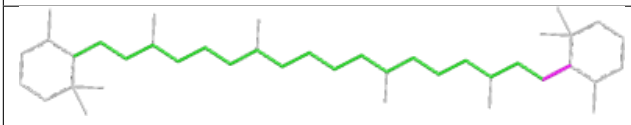
## Ligand BCR B2 846



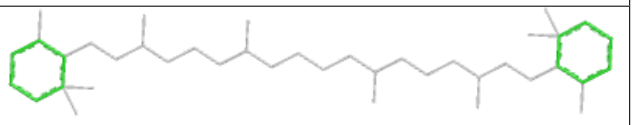
Bond lengths



Bond angles

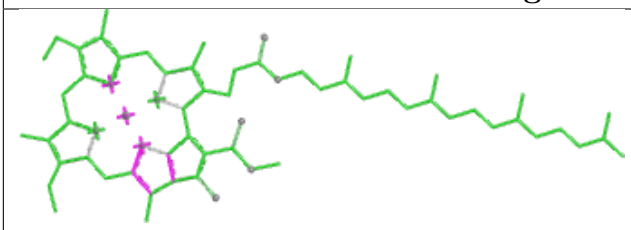


Torsions

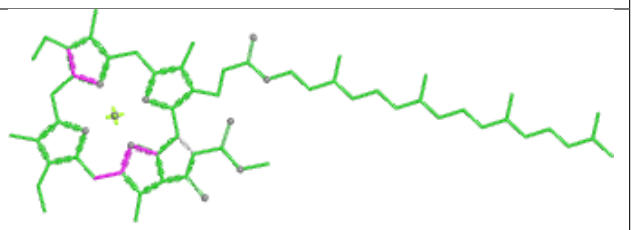


Rings

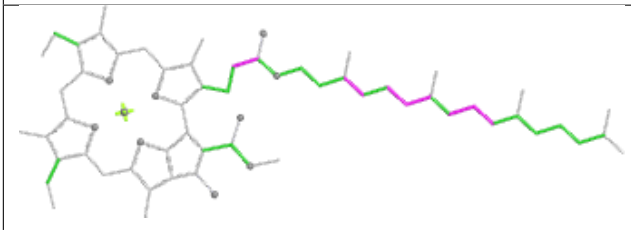
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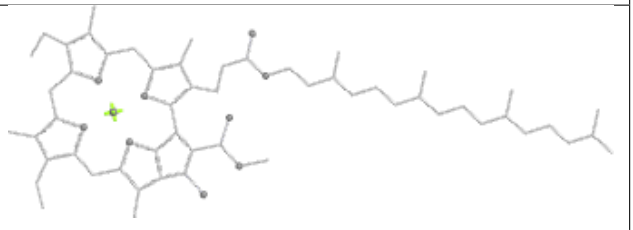
Bond lengths



Bond angles

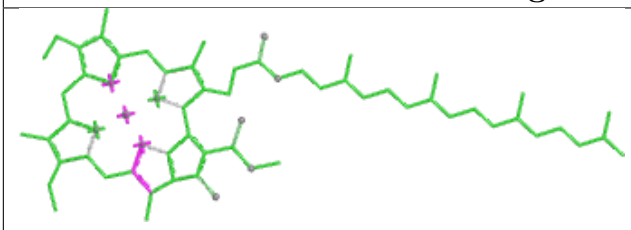


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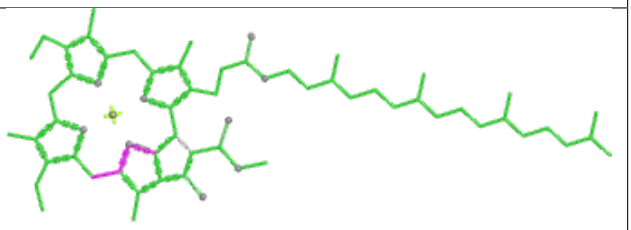


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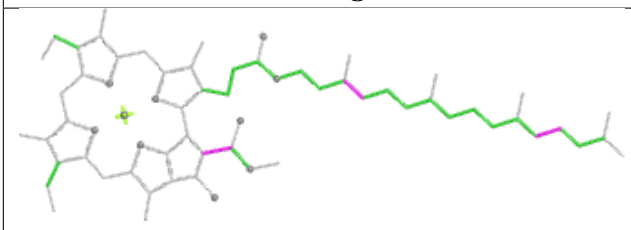
## Ligand CLA 9 612



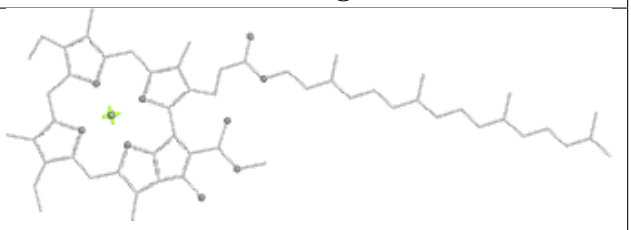
Bond lengths



Bond angles

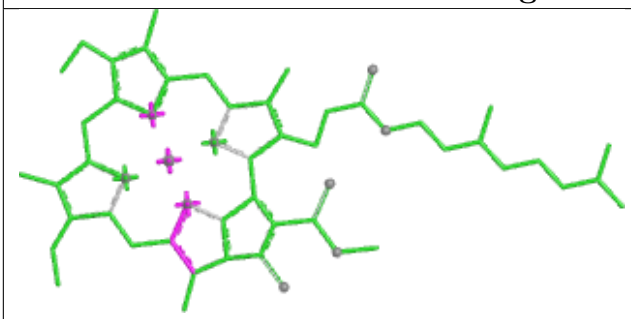


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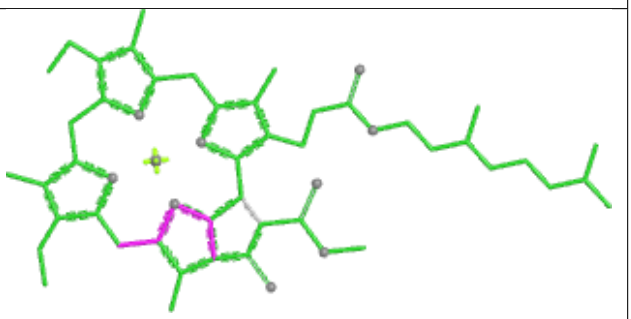


Rings

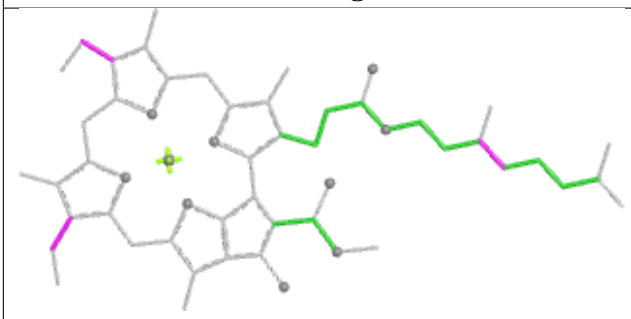
## Ligand CLA 32 607



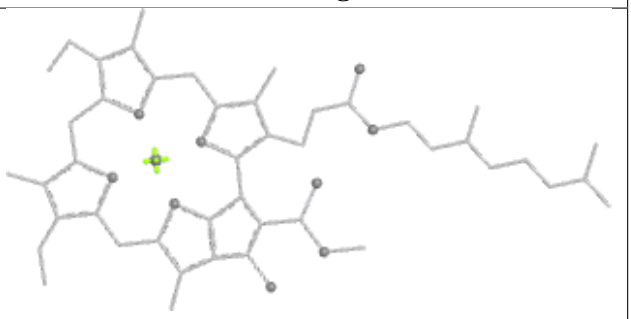
Bond lengths



Bond angles



Torsions

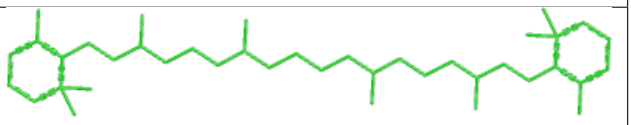


Rings

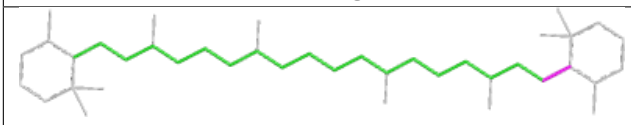
## Ligand BCR 7 623



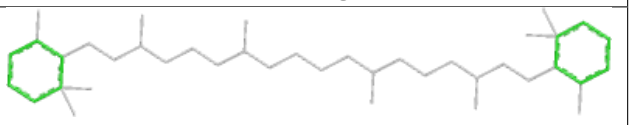
Bond lengths



Bond angles

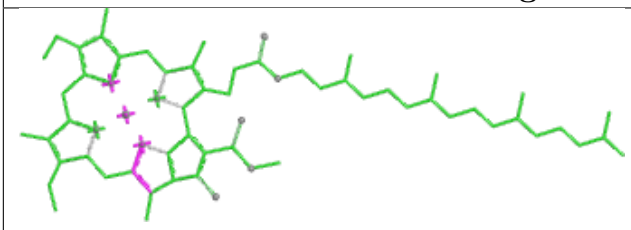


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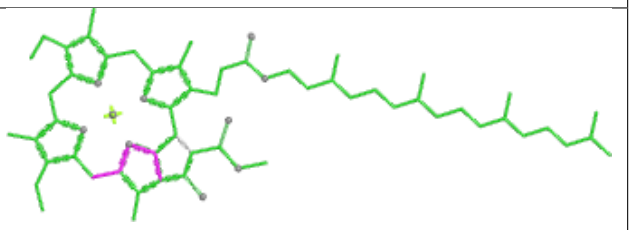


Rings

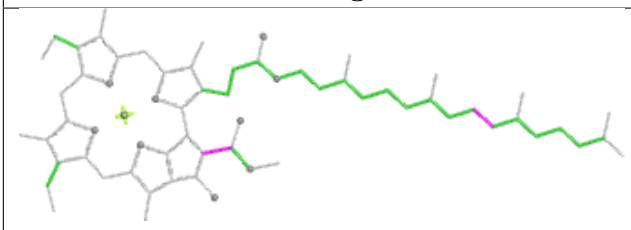
## Ligand CLA 12 608



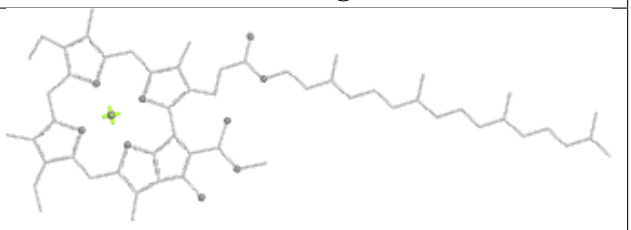
Bond lengths



Bond angles

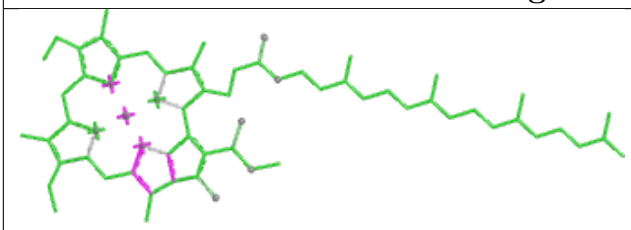


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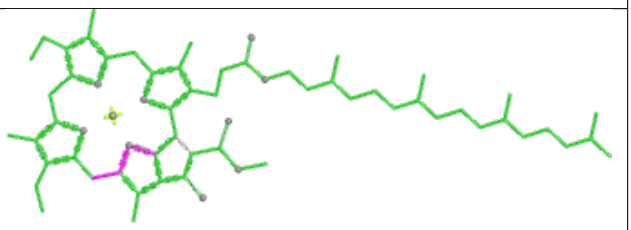


Rings

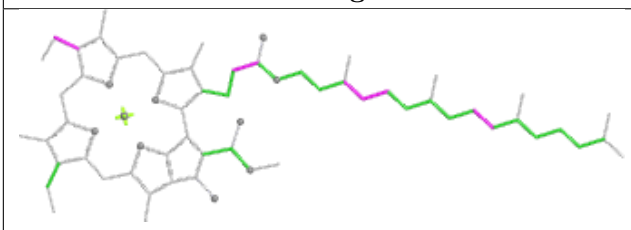
## Ligand CLA 4 603



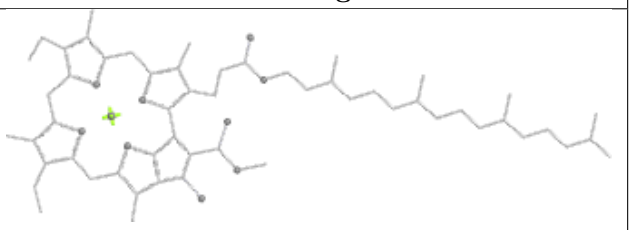
Bond lengths



Bond angles

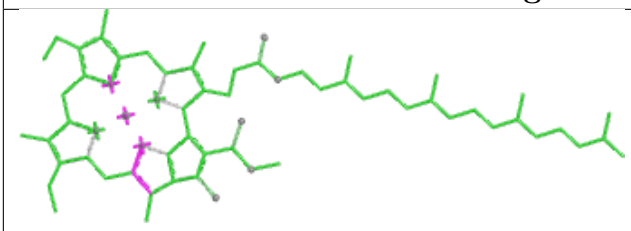


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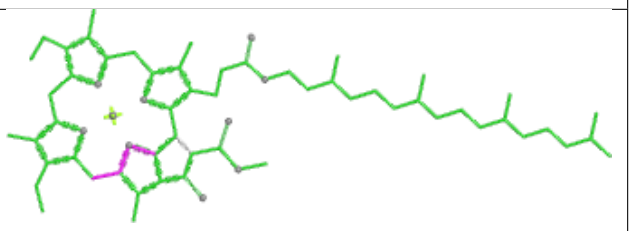


Rings

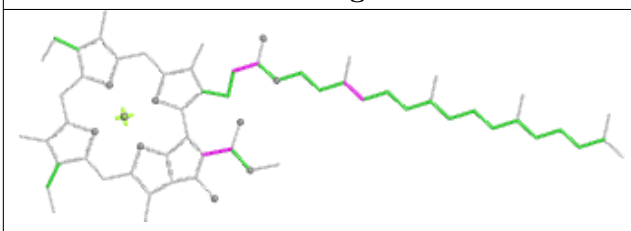
## Ligand CLA A 814



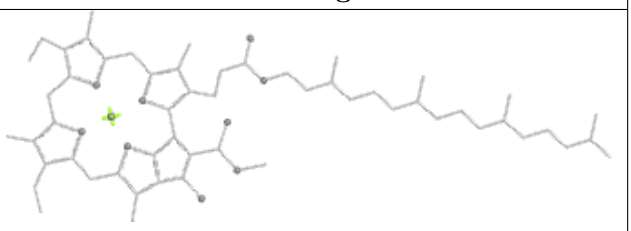
Bond lengths



Bond angles

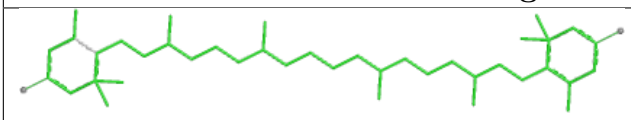


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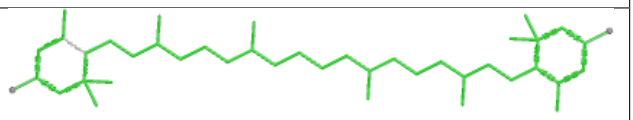


Rings

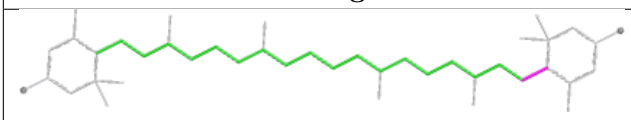
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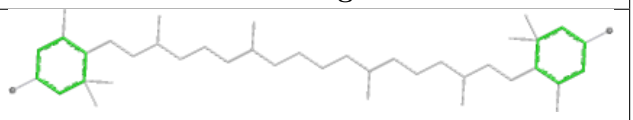
Bond lengths



Bond angles

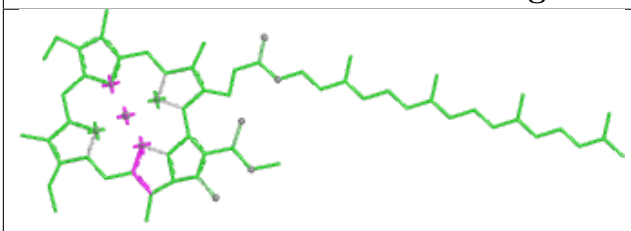


Torsions

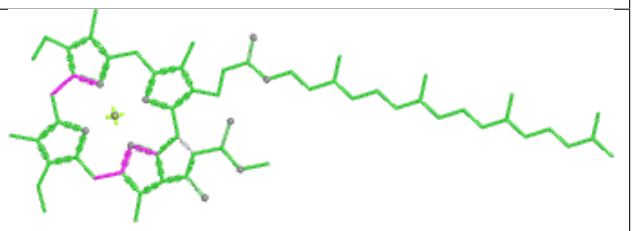


Rings

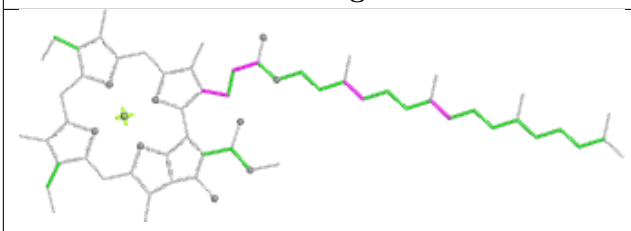
## Ligand CLA 3 615



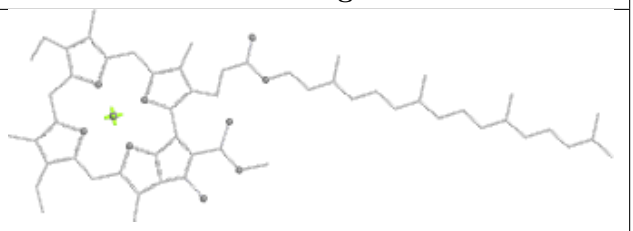
Bond lengths



Bond angles

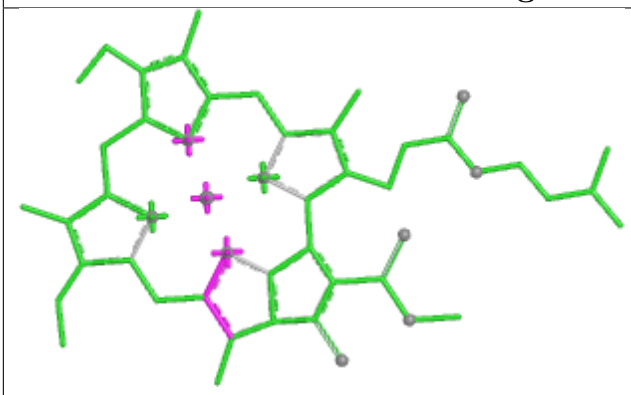


Torsions

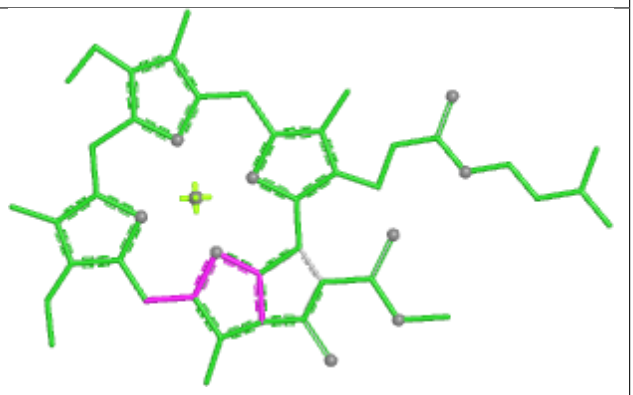


Rings

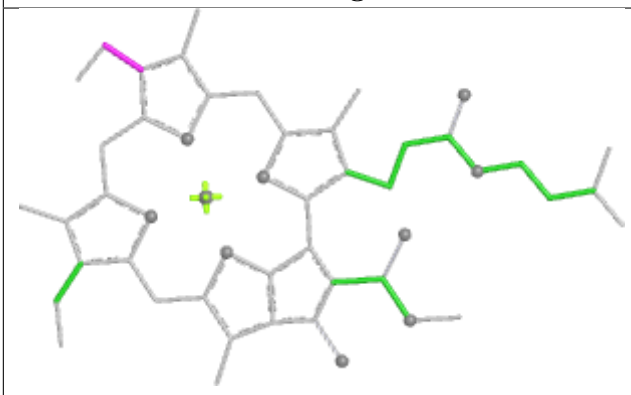
## Ligand CLA Z2 608



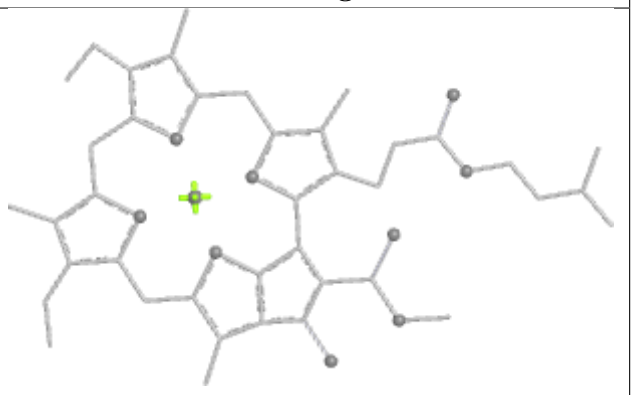
Bond lengths



Bond angles

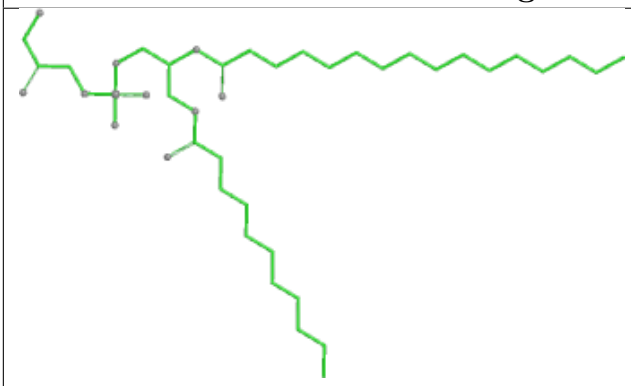


Torsions

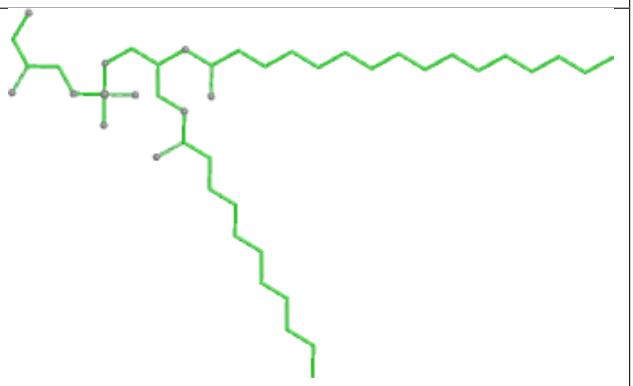


Rings

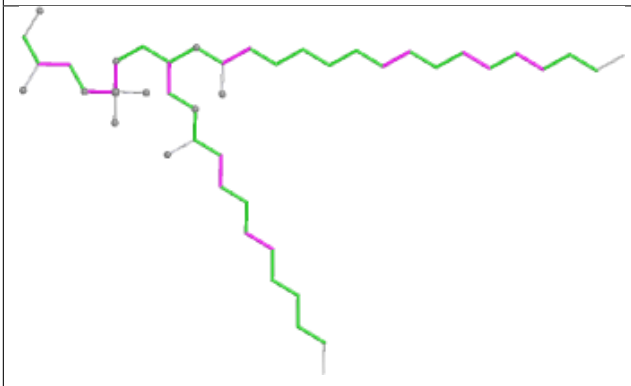
## Ligand LHG 82 620



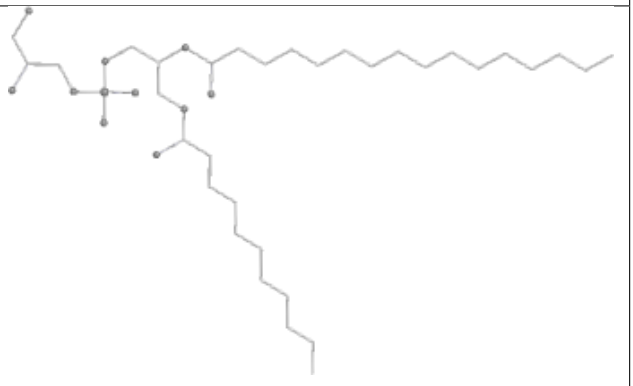
Bond lengths



Bond angles

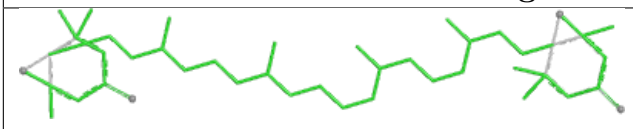


Torsions

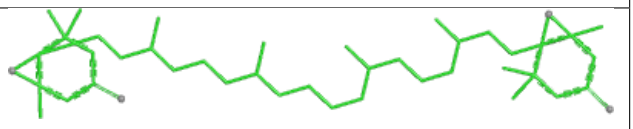


Rings

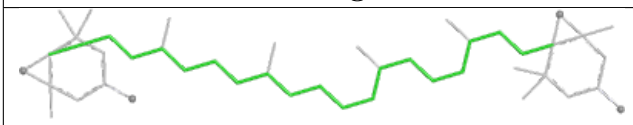
## Ligand XAT 52 624



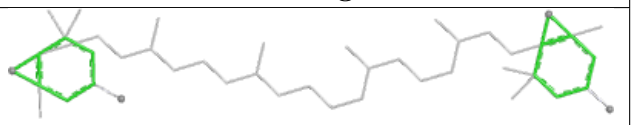
Bond lengths



Bond angles

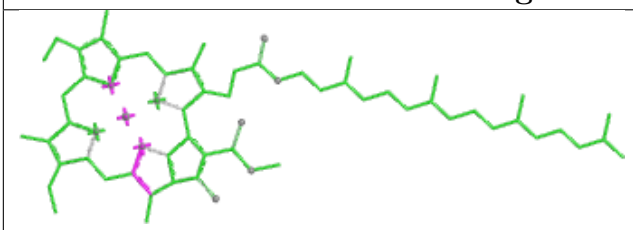


Torsions

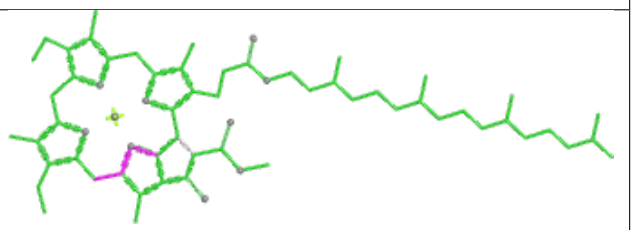


Rings

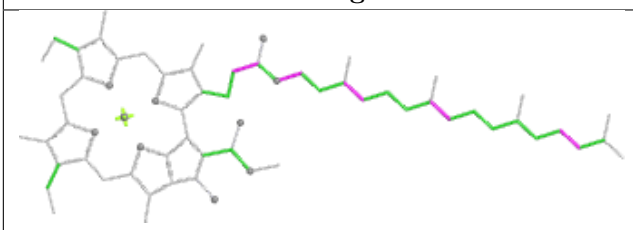
## Ligand CLA B2 811



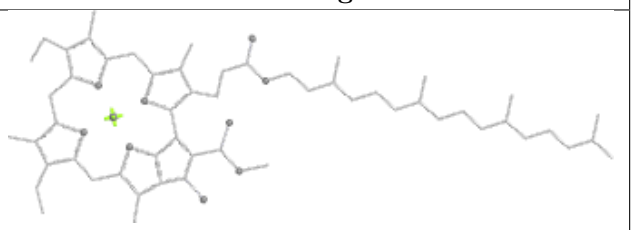
Bond lengths



Bond angles

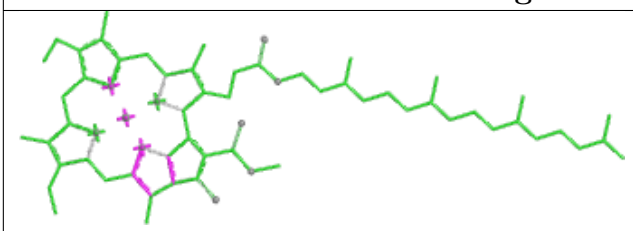


Torsions

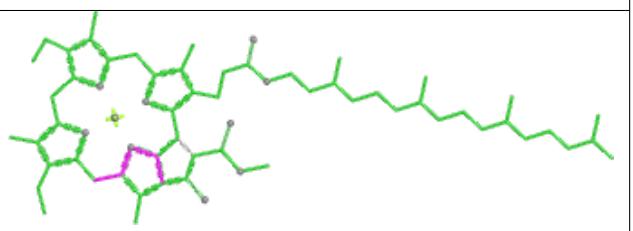


Rings

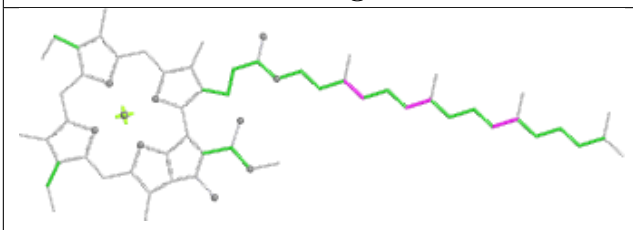
## Ligand CLA A2 820



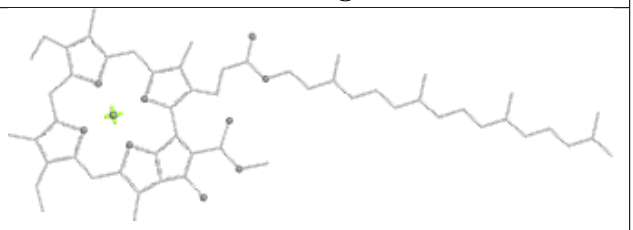
Bond lengths



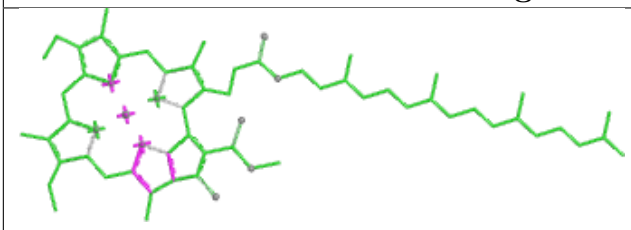
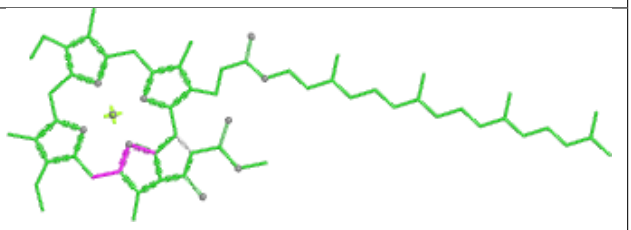
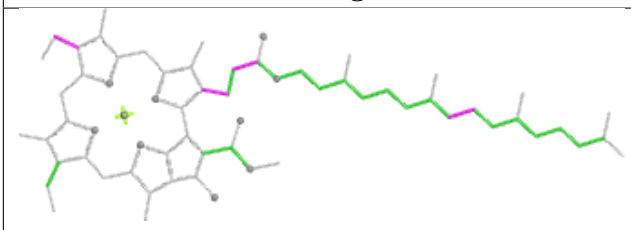
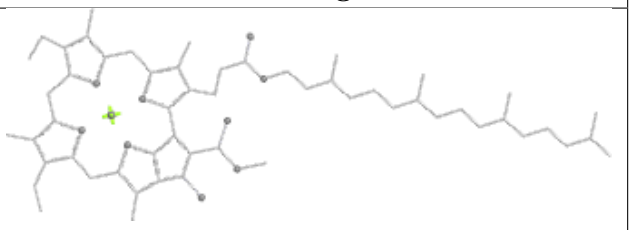
Bond angles

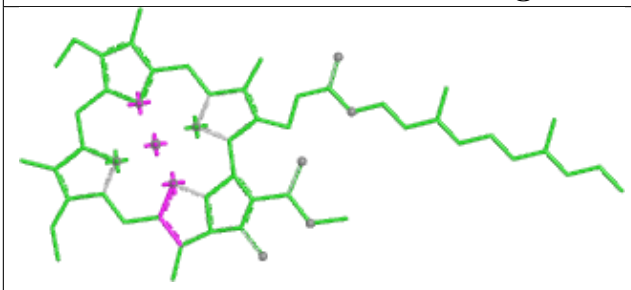
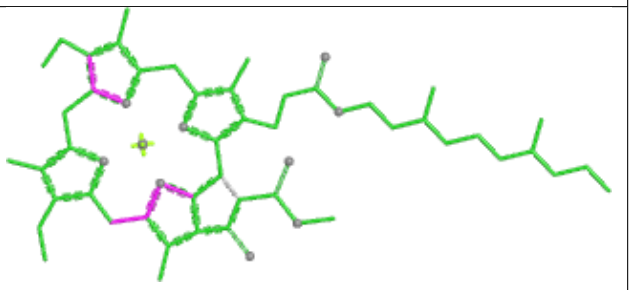
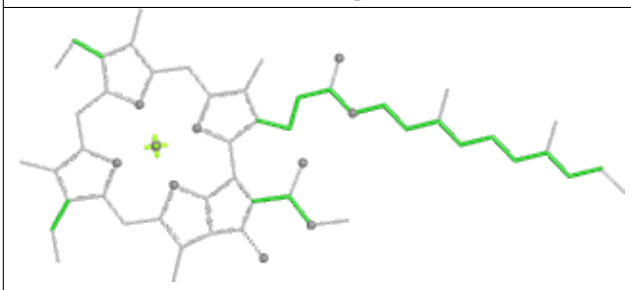
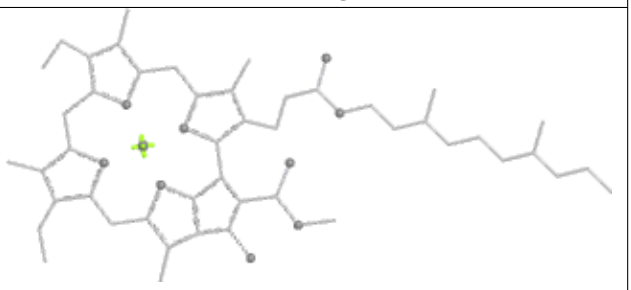


Torsions

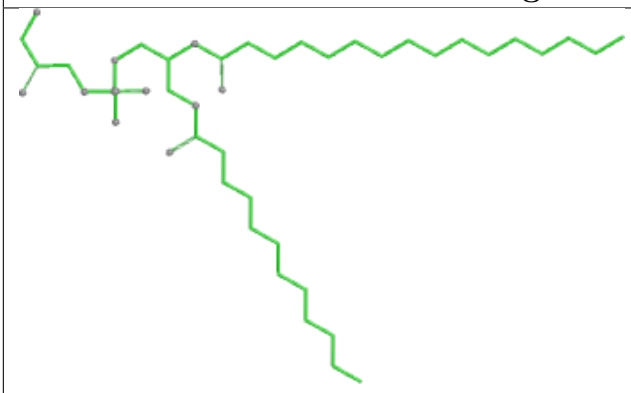


Rings

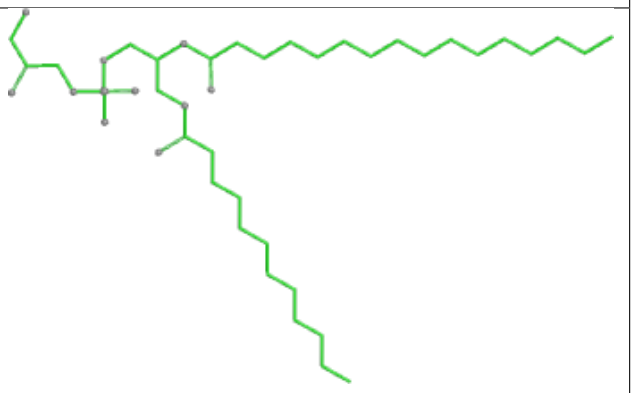
| Ligand CLA A2 836 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA A2 837 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

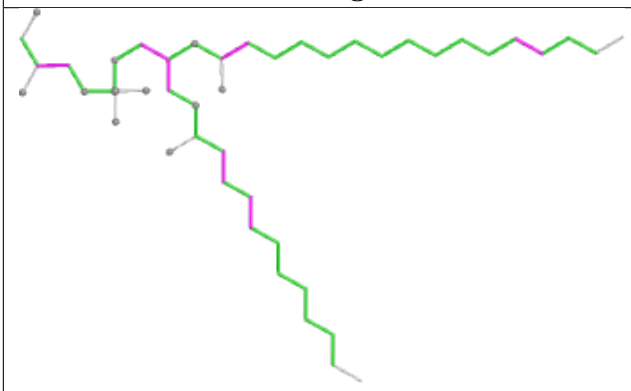
## Ligand LHG B 851



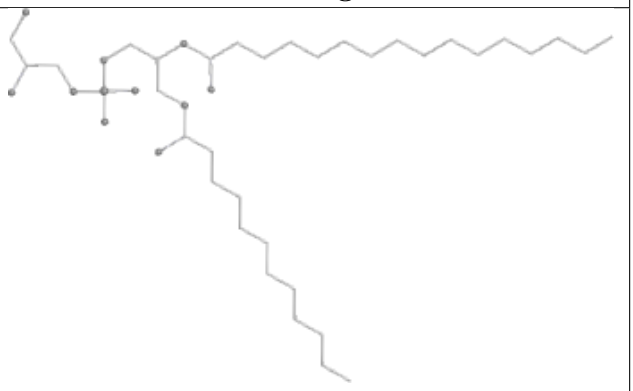
Bond lengths



Bond angles

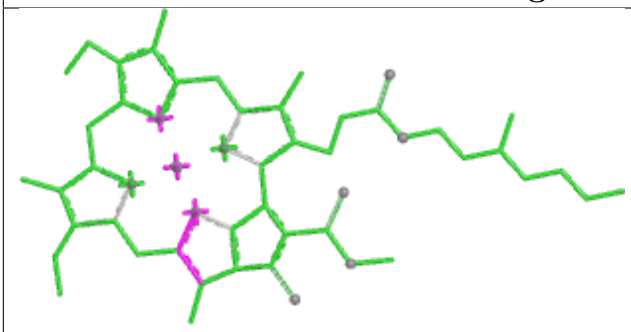


Torsions

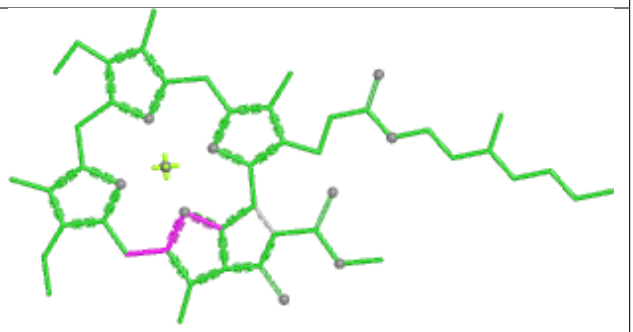


Rings

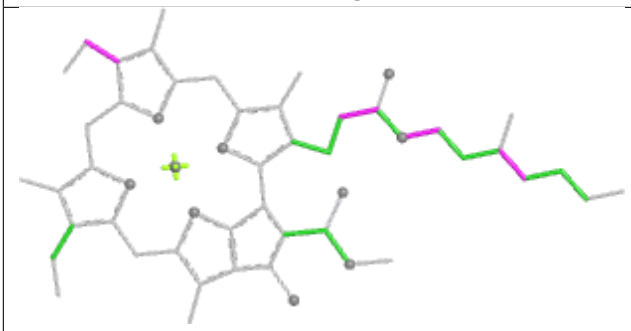
## Ligand CLA 5 616



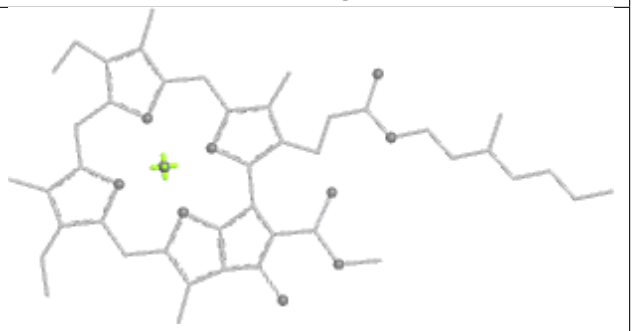
Bond lengths



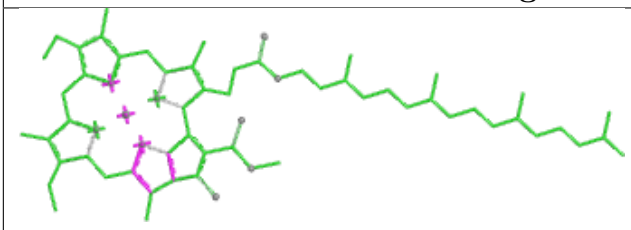
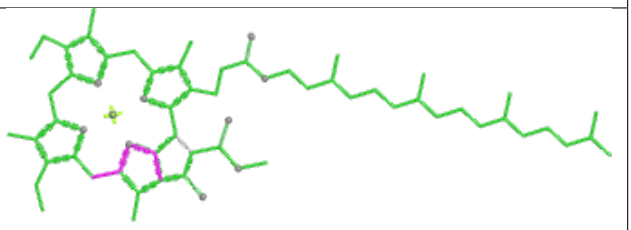
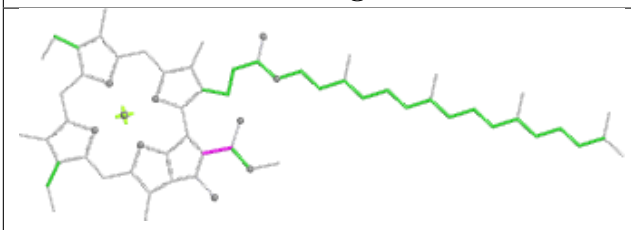
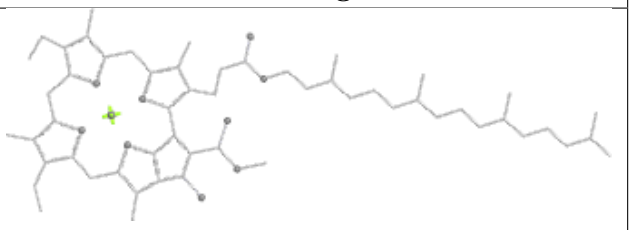
Bond angles

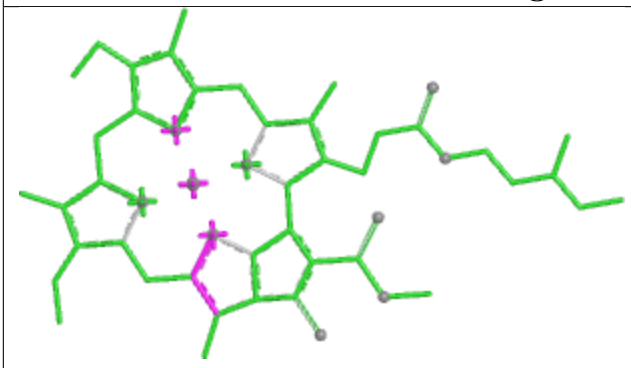
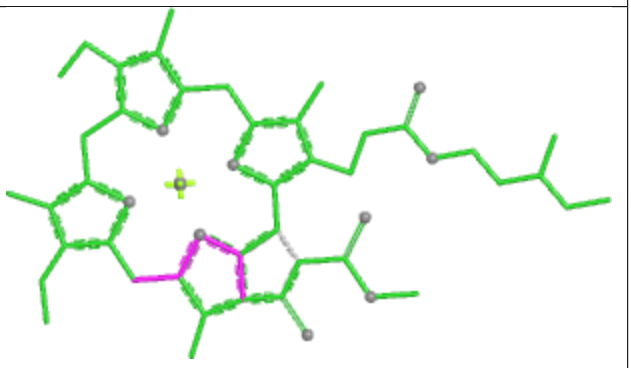
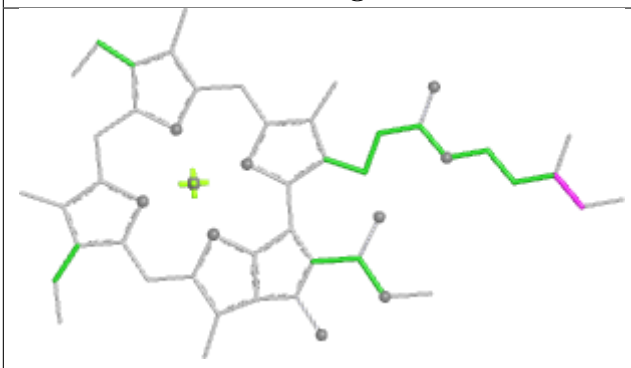
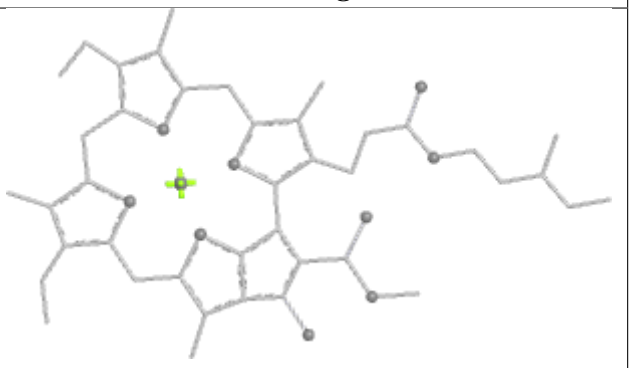


Torsions

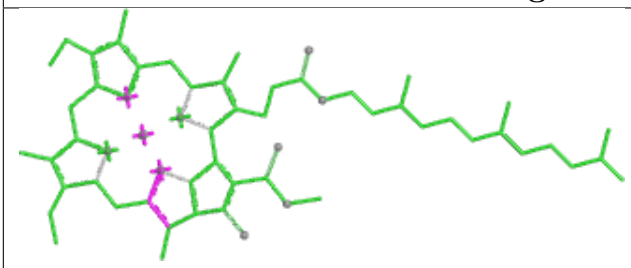


Rings

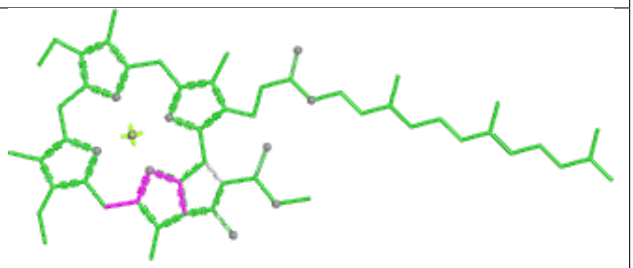
| Ligand CLA 72 602 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 7 604 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

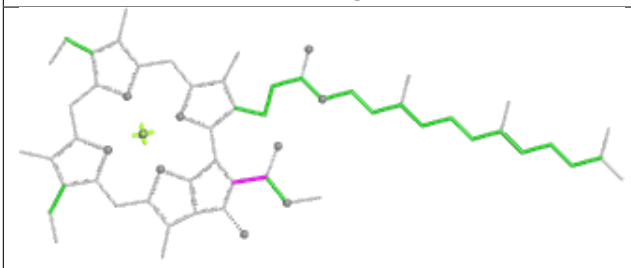
## Ligand CLA 4 602



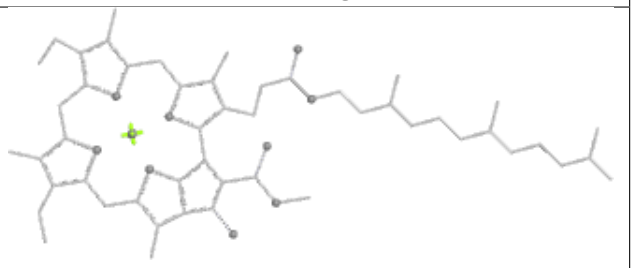
Bond lengths



Bond angles

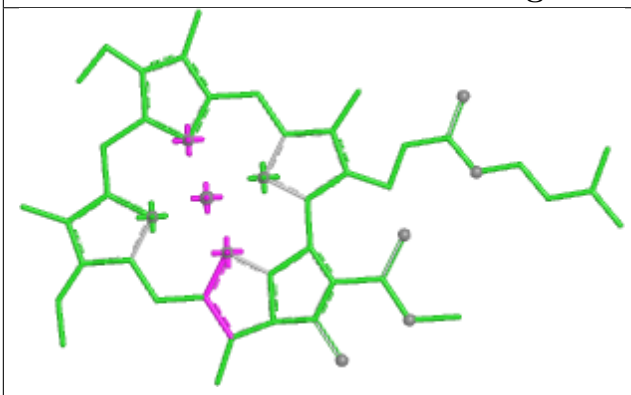


Torsions

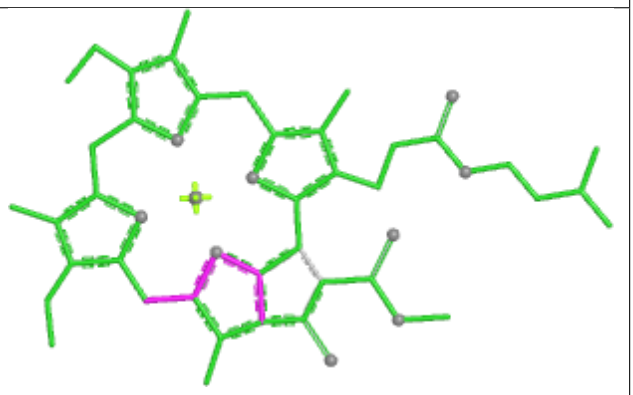


Rings

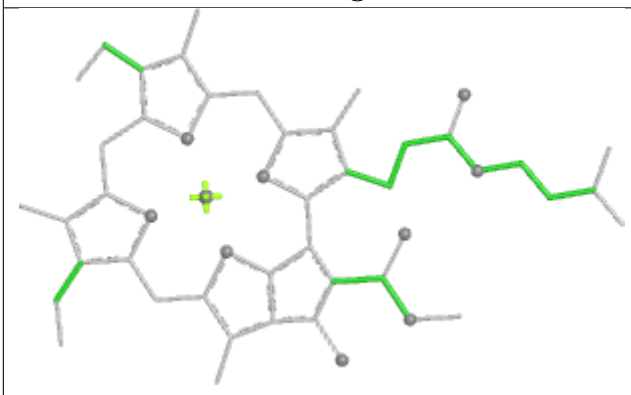
## Ligand CLA Z 614



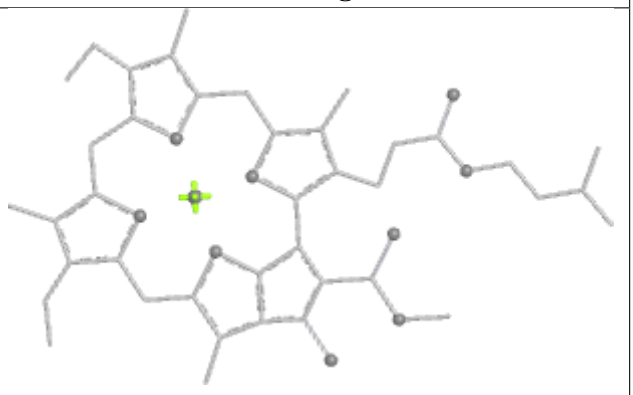
Bond lengths



Bond angles

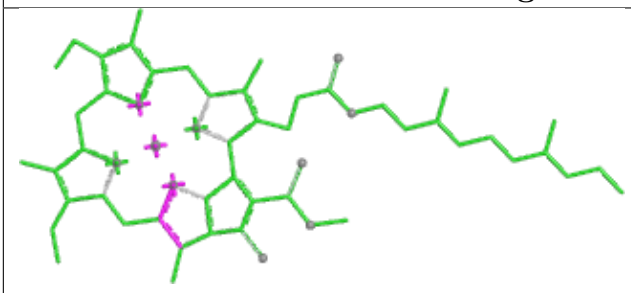


Torsions

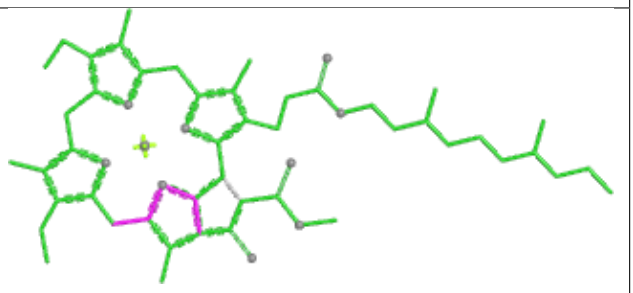


Rings

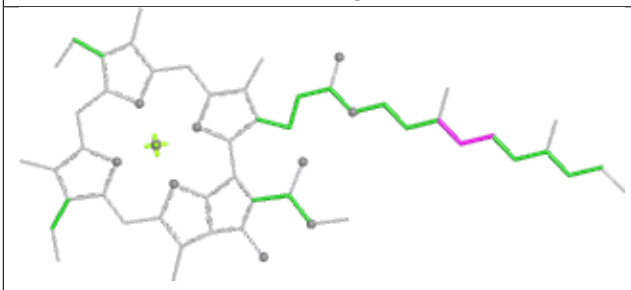
## Ligand CLA Z2 604



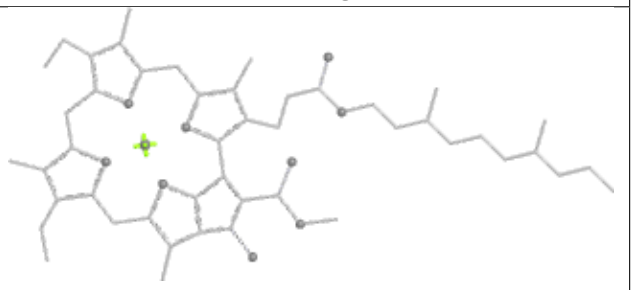
Bond lengths



Bond angles

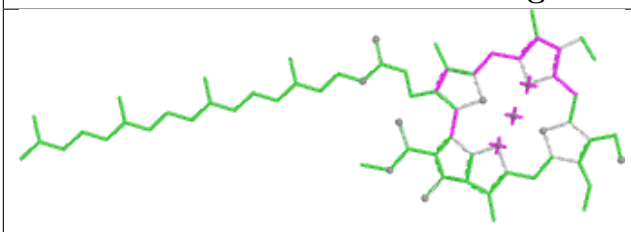


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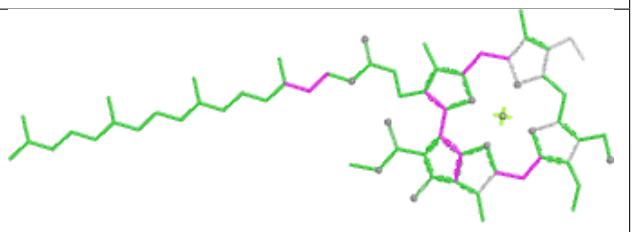


Rings

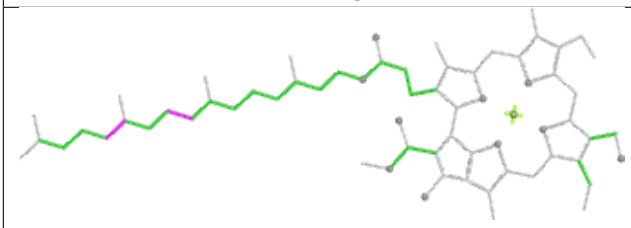
## Ligand CHL 6 616



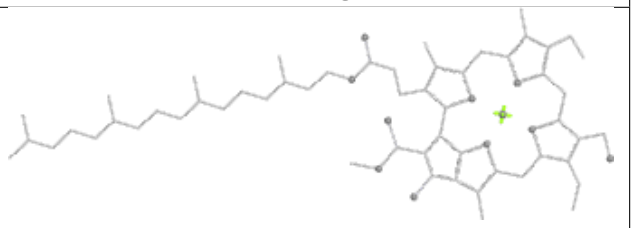
Bond lengths



Bond angles

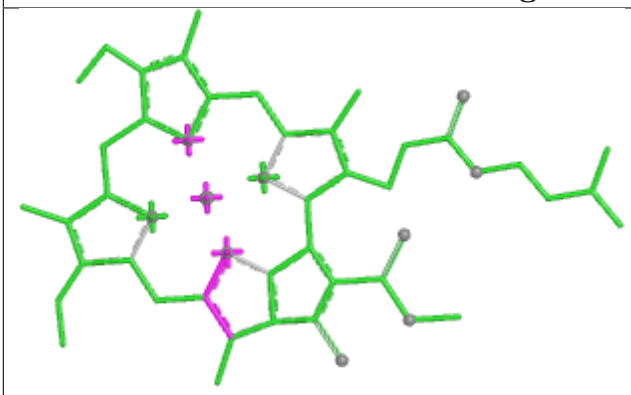


Torsions

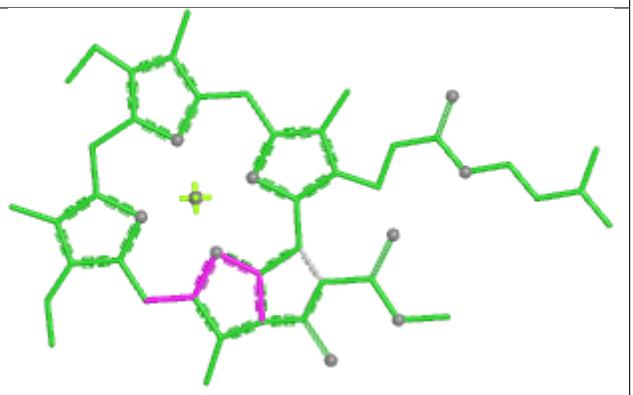


Rings

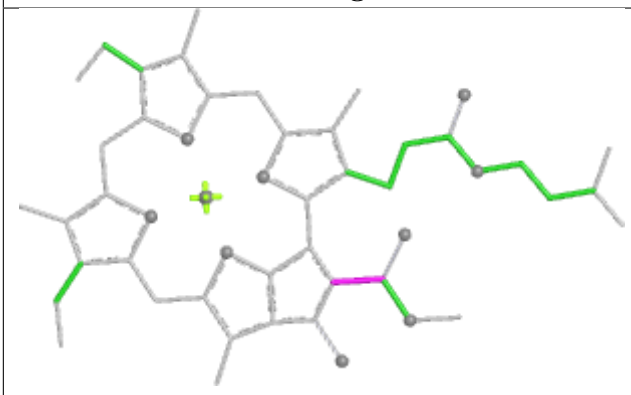
## Ligand CLA 42 604



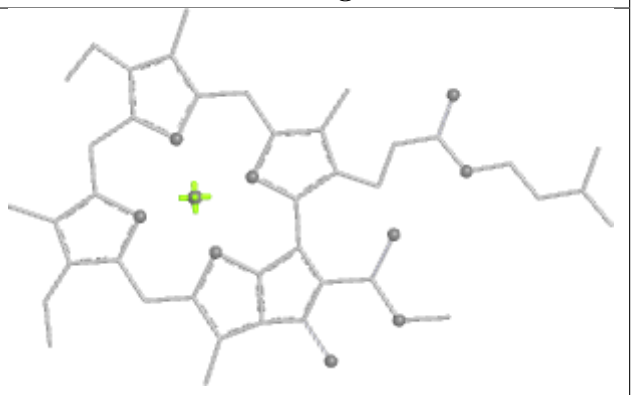
Bond lengths



Bond angles

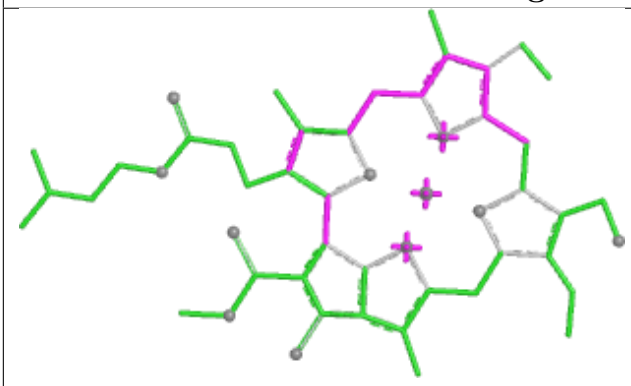


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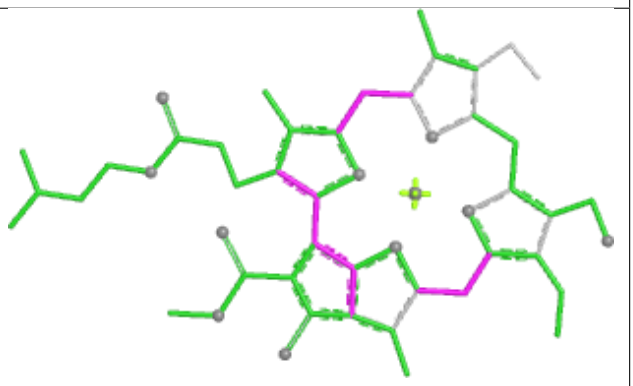


Rings

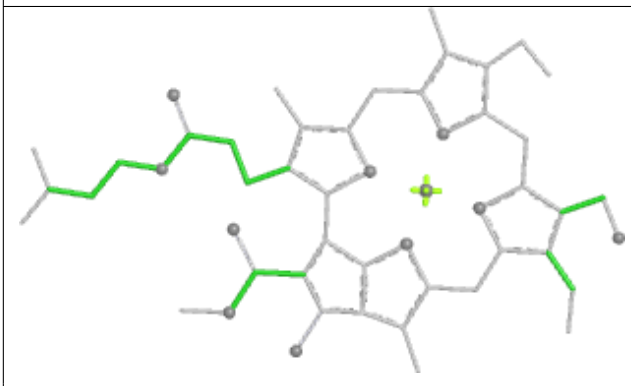
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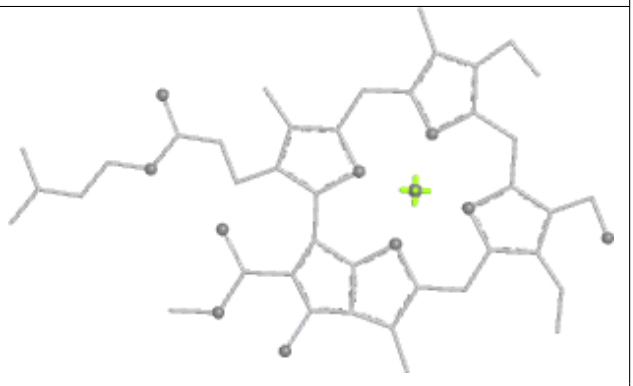
Bond lengths



Bond angles

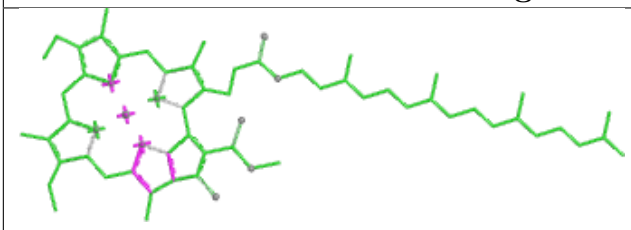


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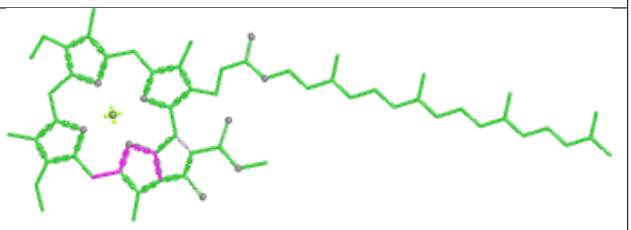


Rings

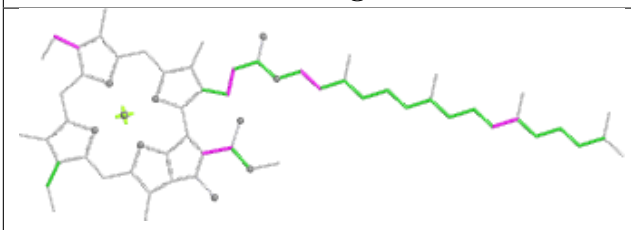
## Ligand CLA A2 823



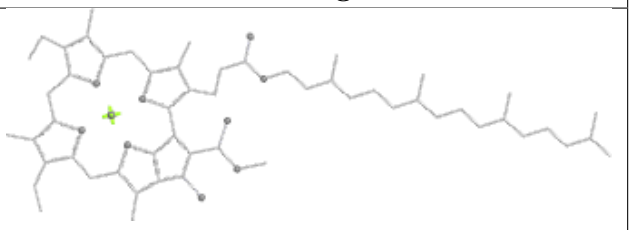
Bond lengths



Bond angles

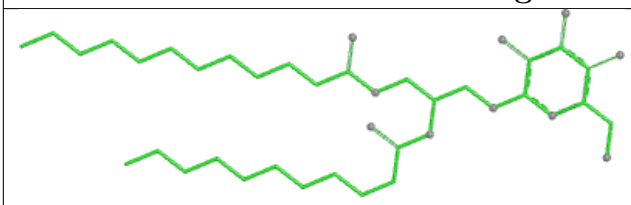


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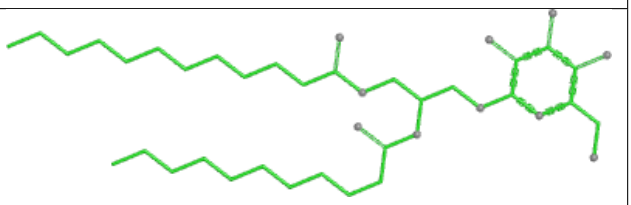


Rings

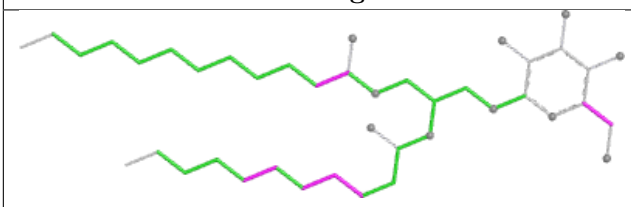
## Ligand LMG 12 628



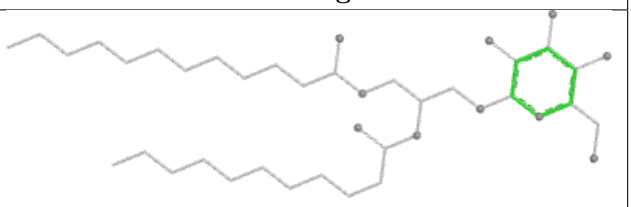
Bond lengths



Bond angles

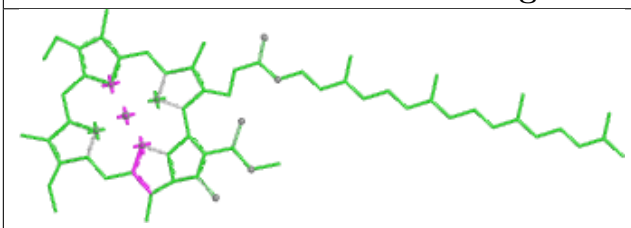


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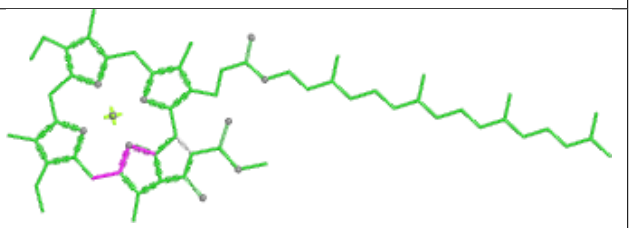


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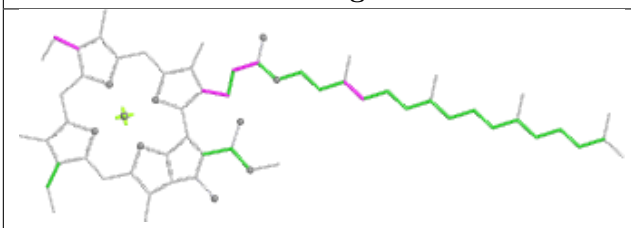
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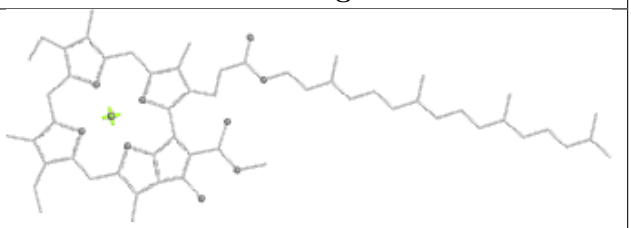
Bond lengths



Bond angles

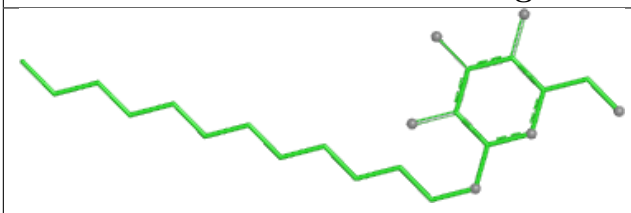


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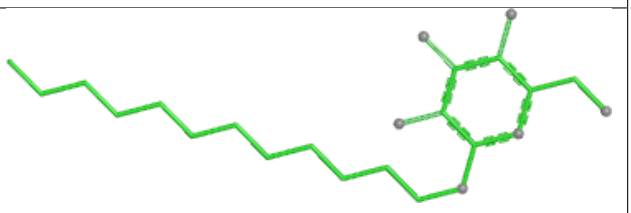


Rings

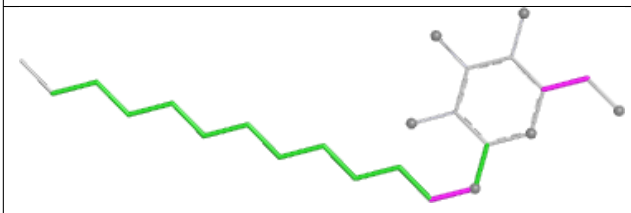
## Ligand LMU 82 625



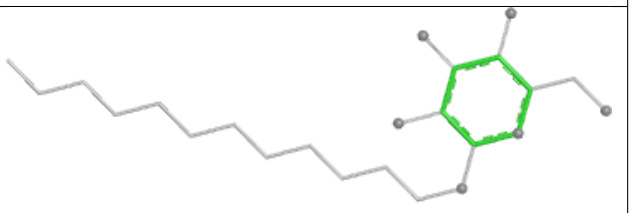
Bond lengths



Bond angles

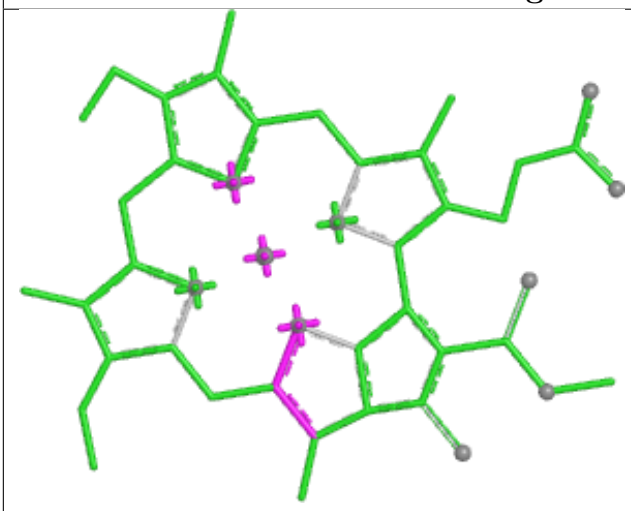


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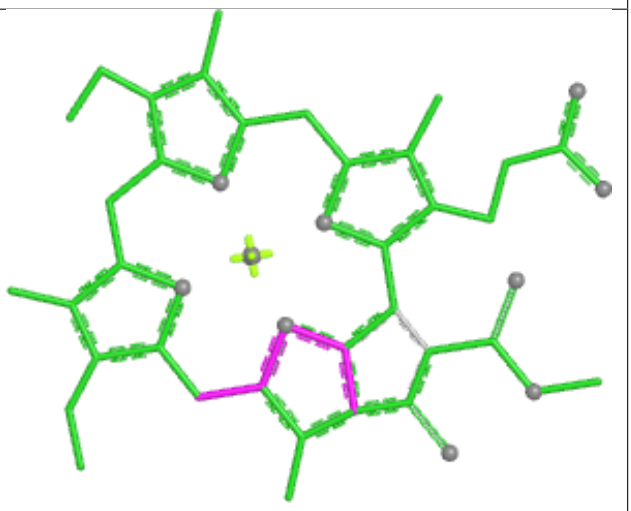


Rings

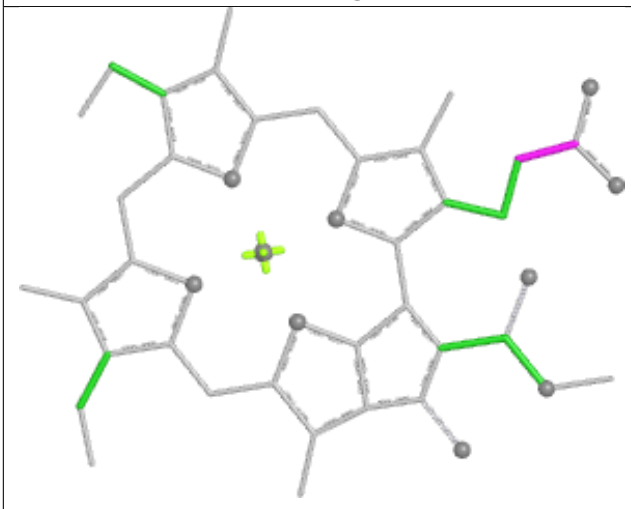
## Ligand CLA F 303



Bond lengths



Bond angles

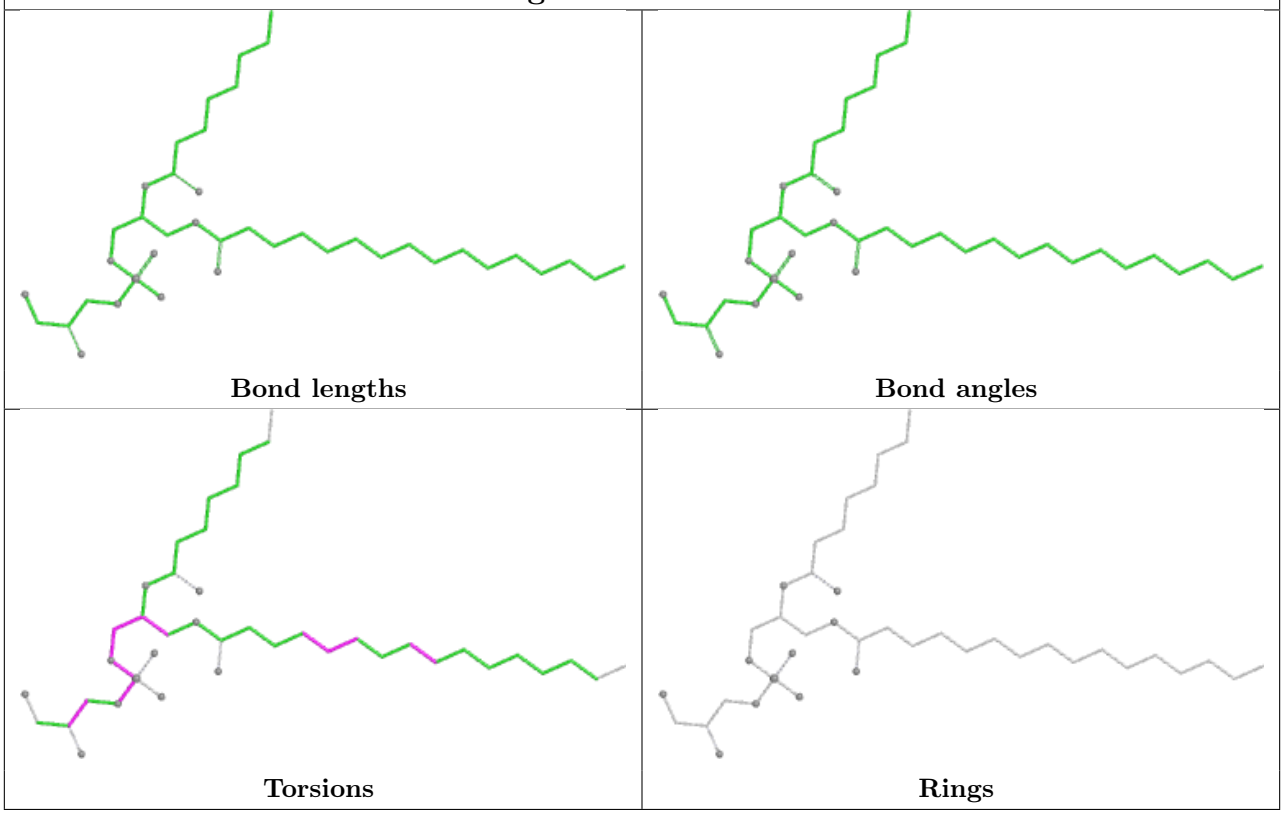


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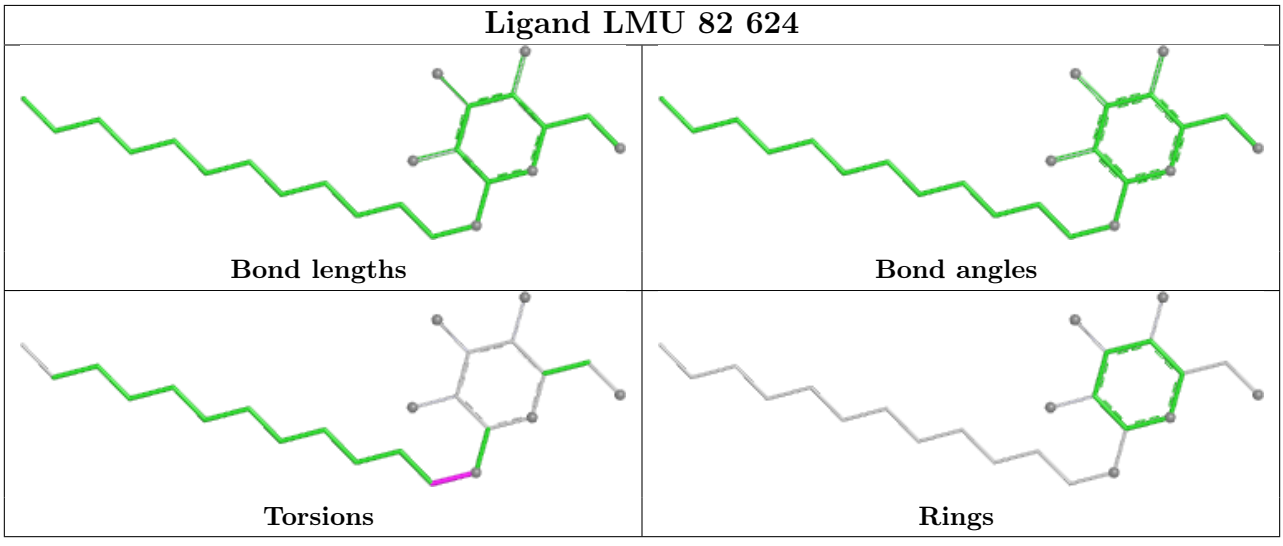


Rings

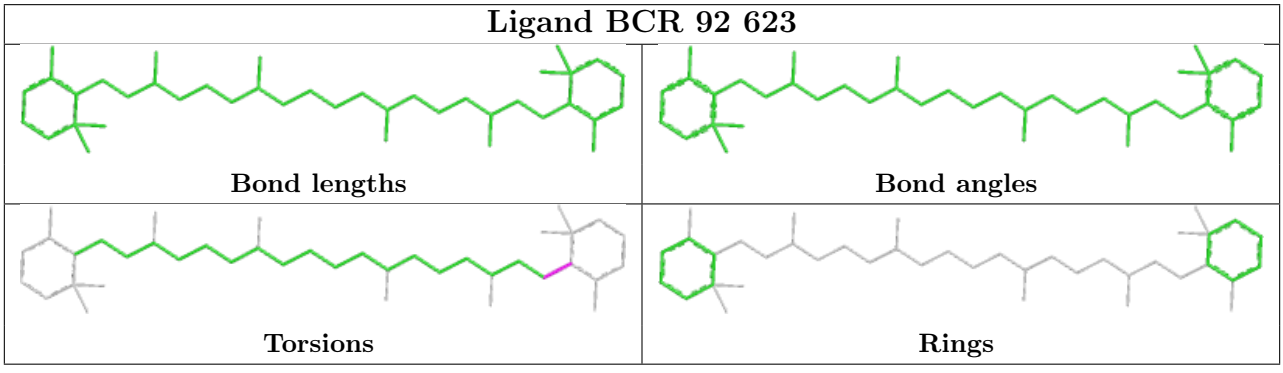
## Ligand LHG 9 622



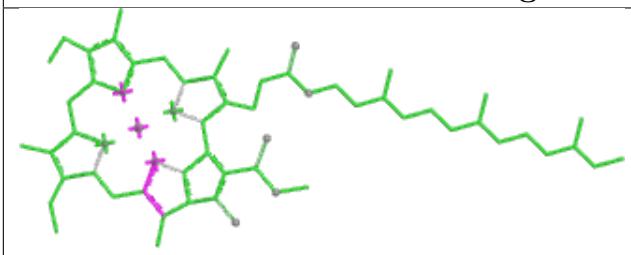

## Ligand LMU 82 624



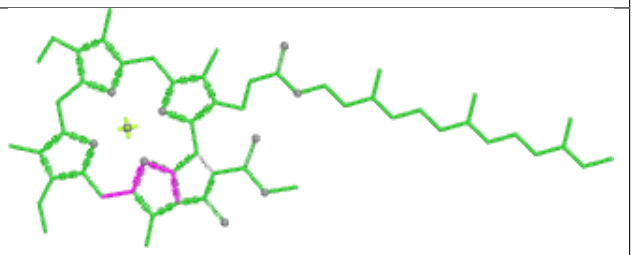

## Ligand BCR 92 623



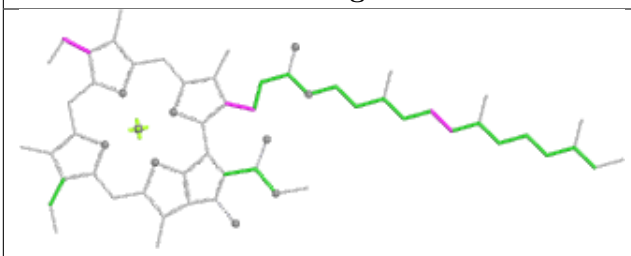
## Ligand CLA 12 611



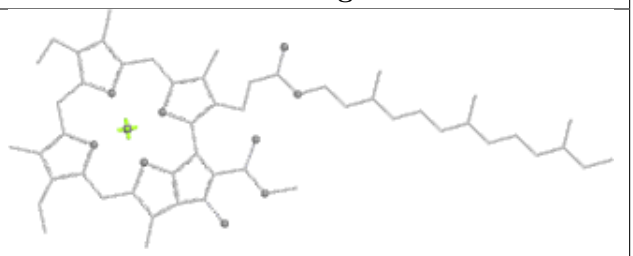
Bond lengths



Bond angles

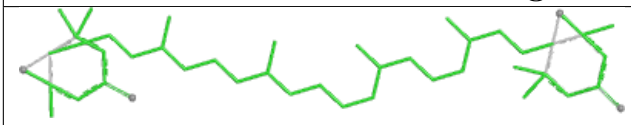


Torsions

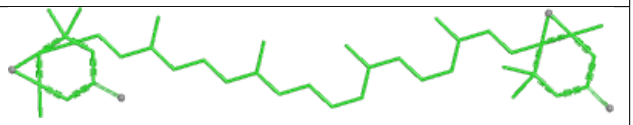


Rings

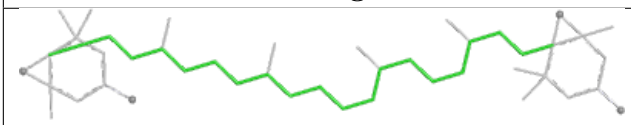
## Ligand XAT 4 620



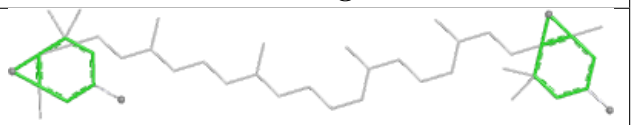
Bond lengths



Bond angles

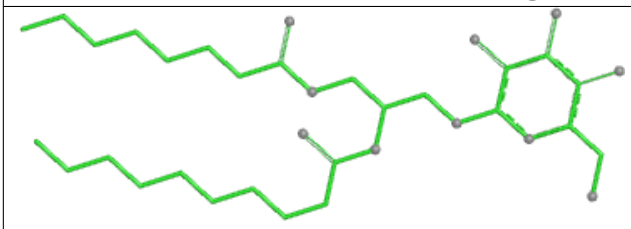


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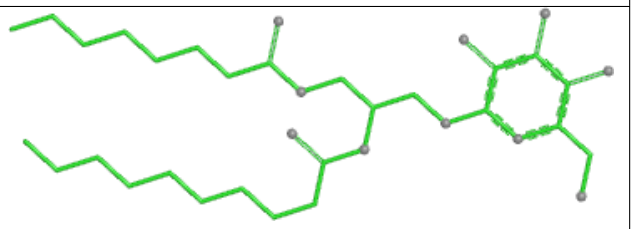


Rings

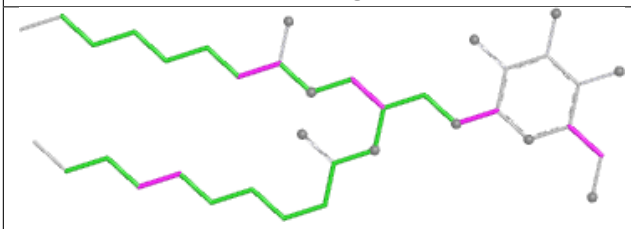
## Ligand LMG 7 626



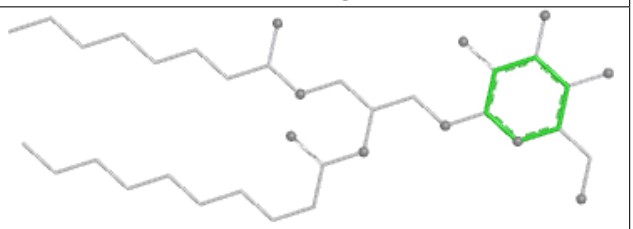
Bond lengths



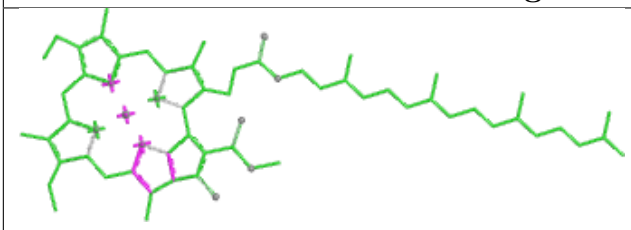
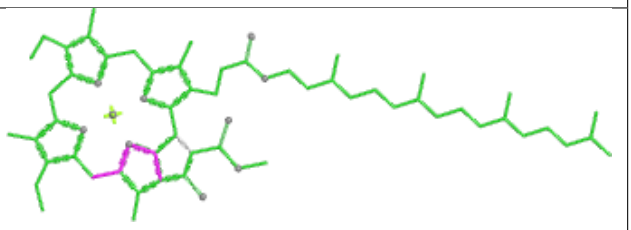
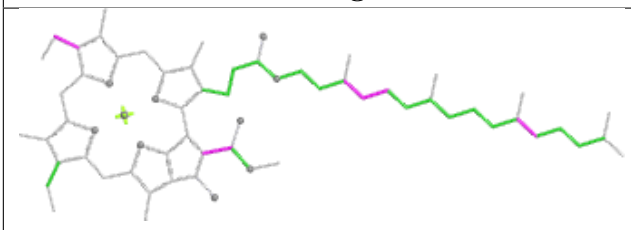
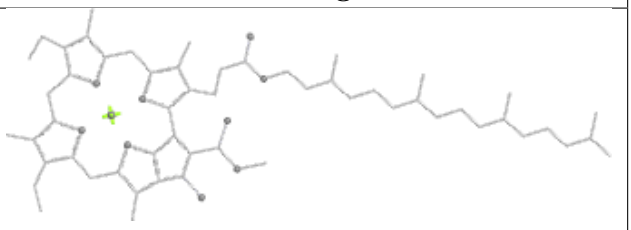
Bond angles

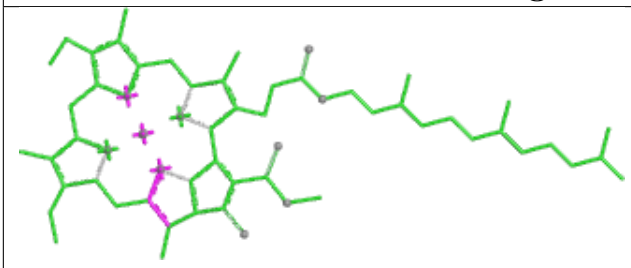
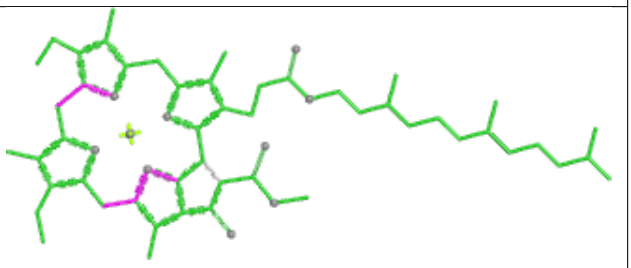
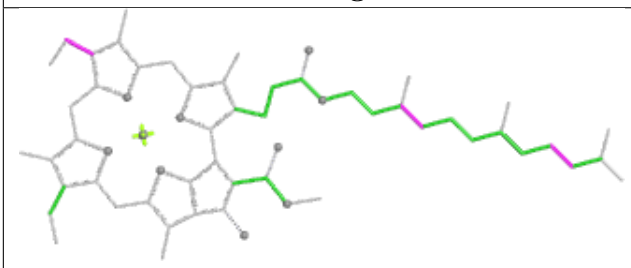
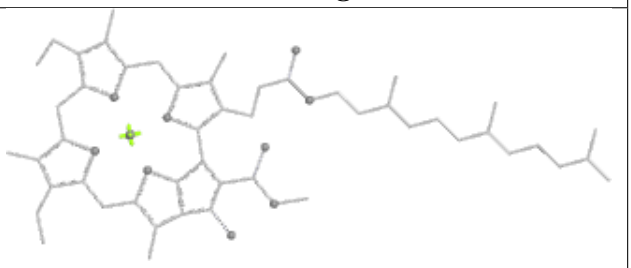


Torsions

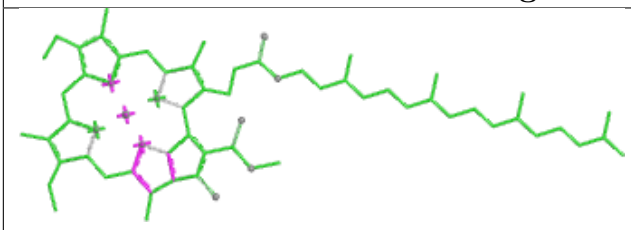


Rings

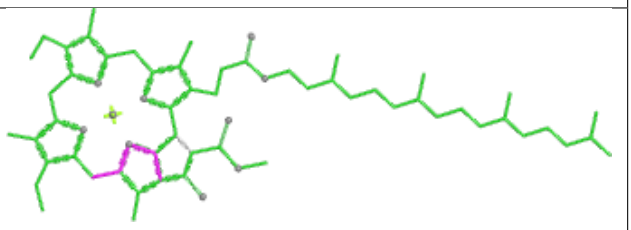
| Ligand CLA B 808 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 3 613 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

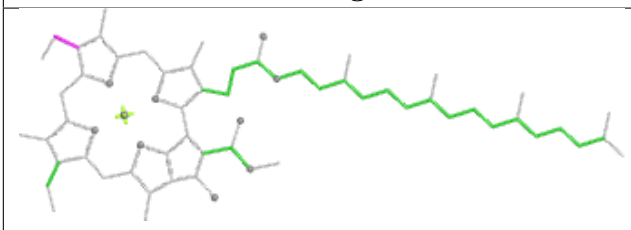
## Ligand CLA 12 610



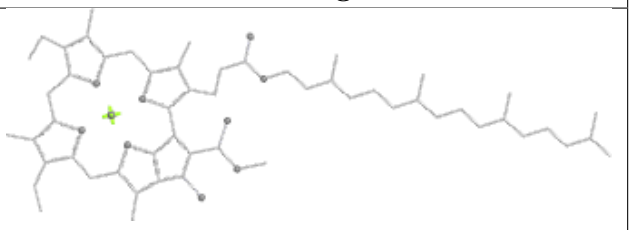
Bond lengths



Bond angles

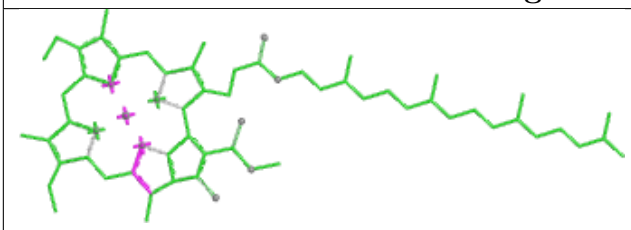


Torsions

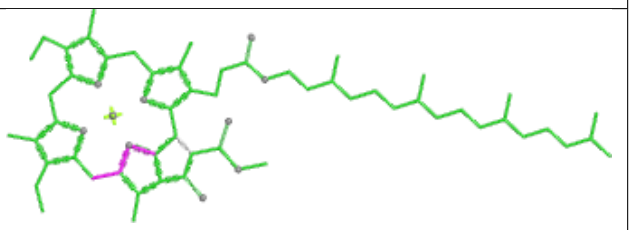


Rings

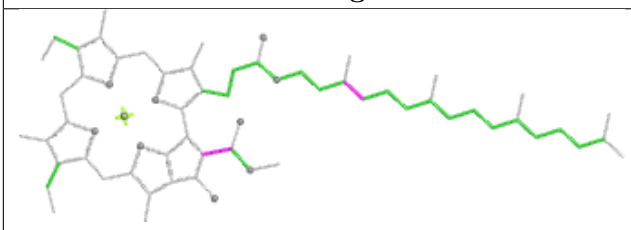
## Ligand CLA B 815



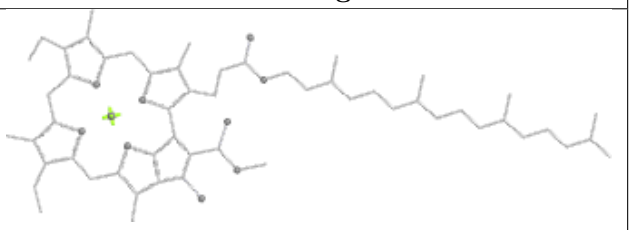
Bond lengths



Bond angles

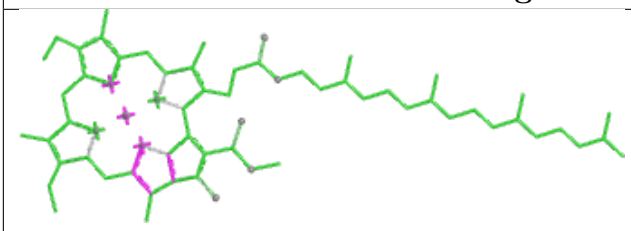


Torsions

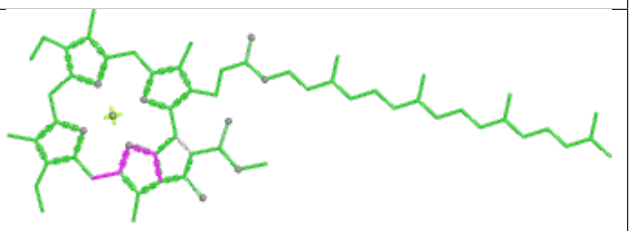


Rings

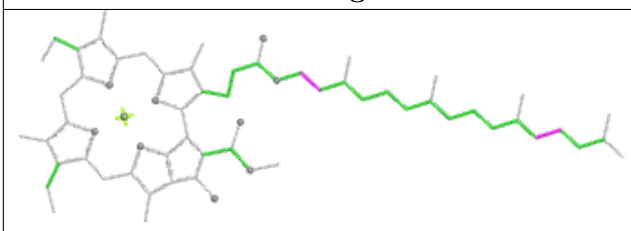
## Ligand CLA A2 827



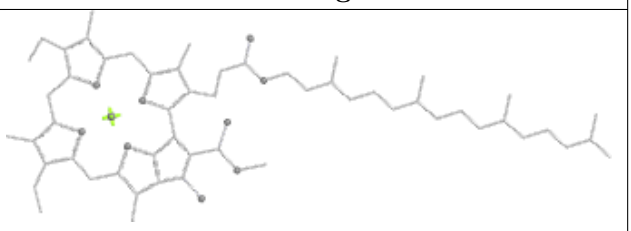
Bond lengths



Bond angles

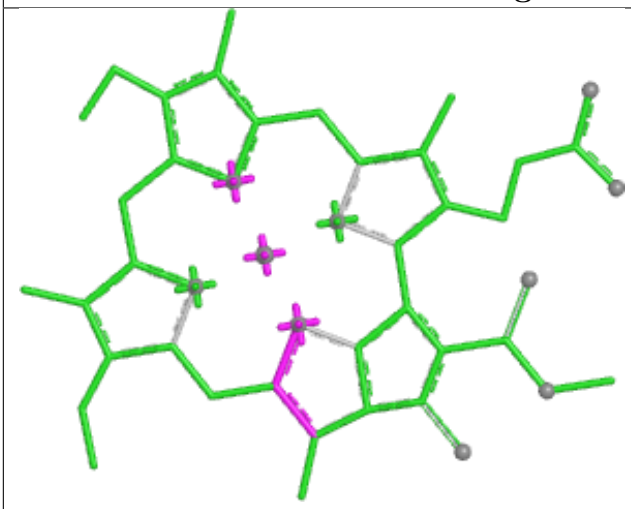


Torsions

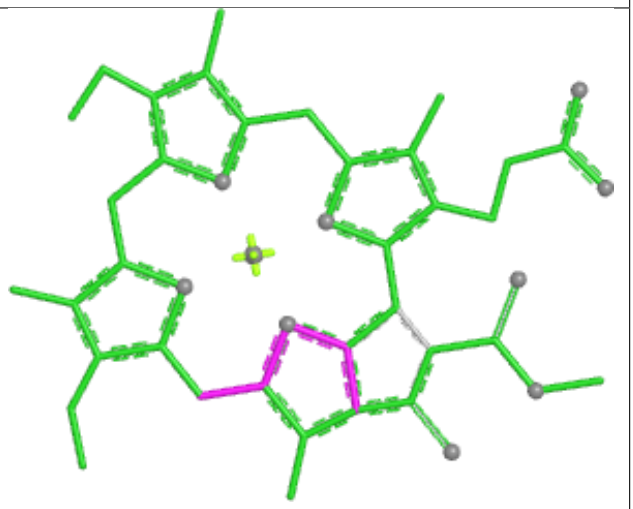


Rings

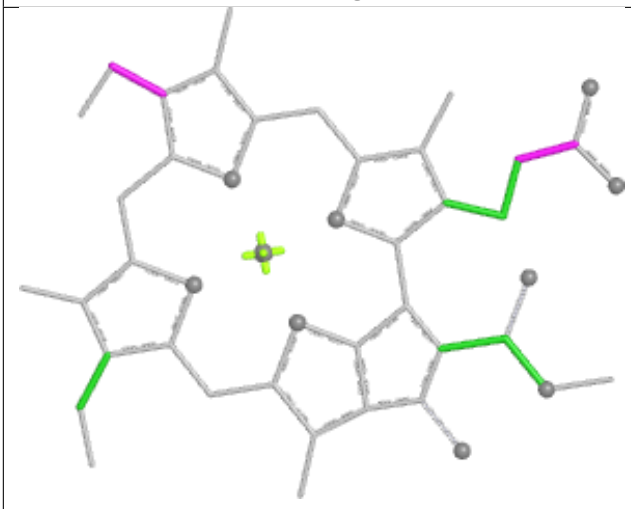
## Ligand CLA K2 206



Bond lengths



Bond angles

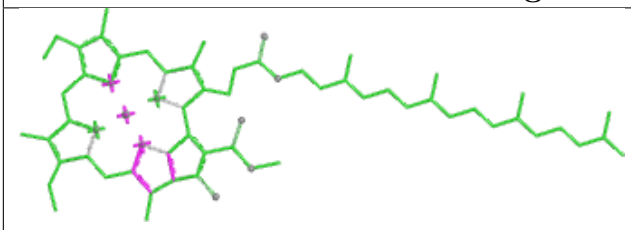


Torsions

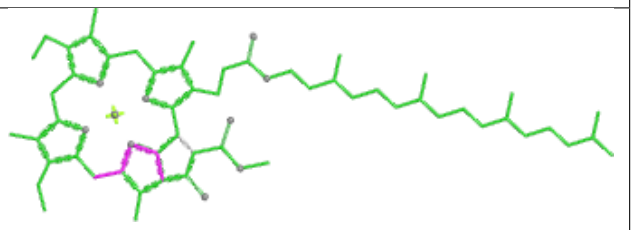


Rings

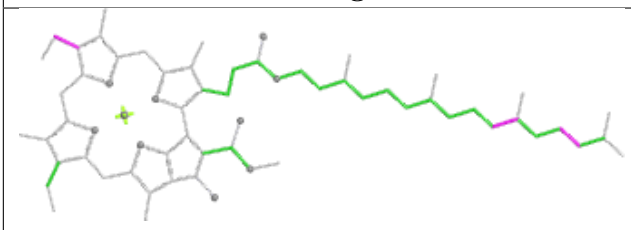
## Ligand CLA B 832



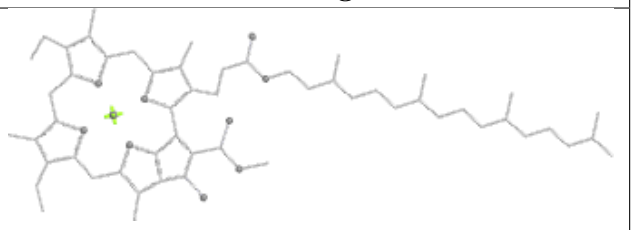
Bond lengths



Bond angles

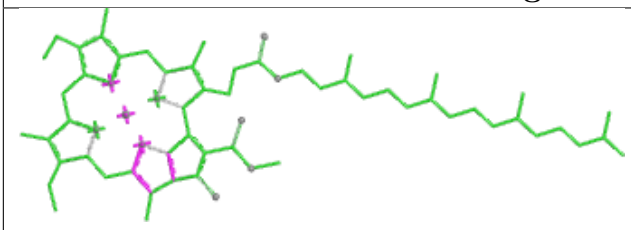


Torsions

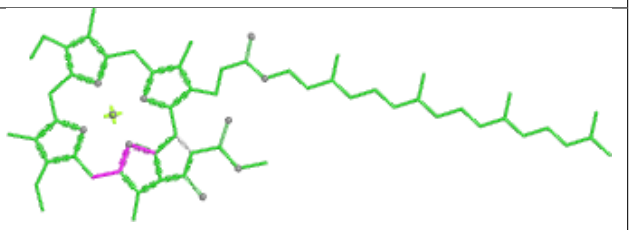


Rings

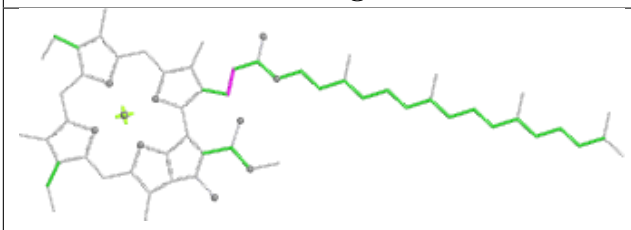
## Ligand CLA A 854



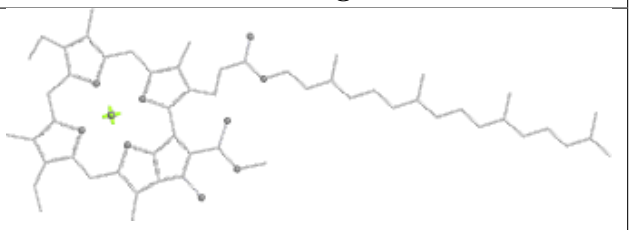
Bond lengths



Bond angles

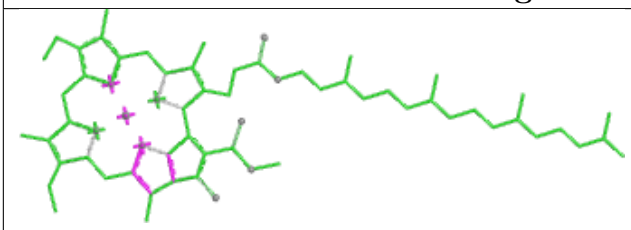


Torsions

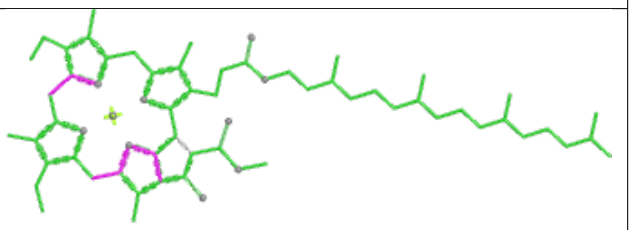


Rings

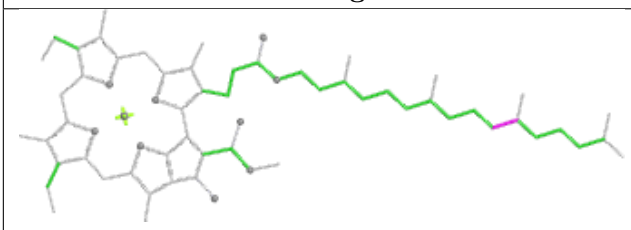
## Ligand CLA A2 839



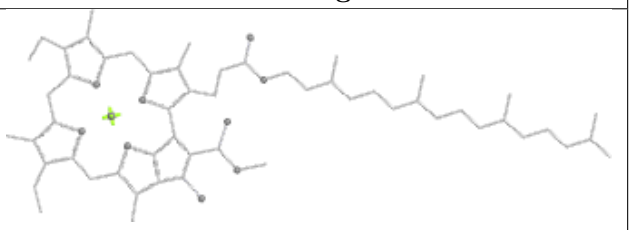
Bond lengths



Bond angles

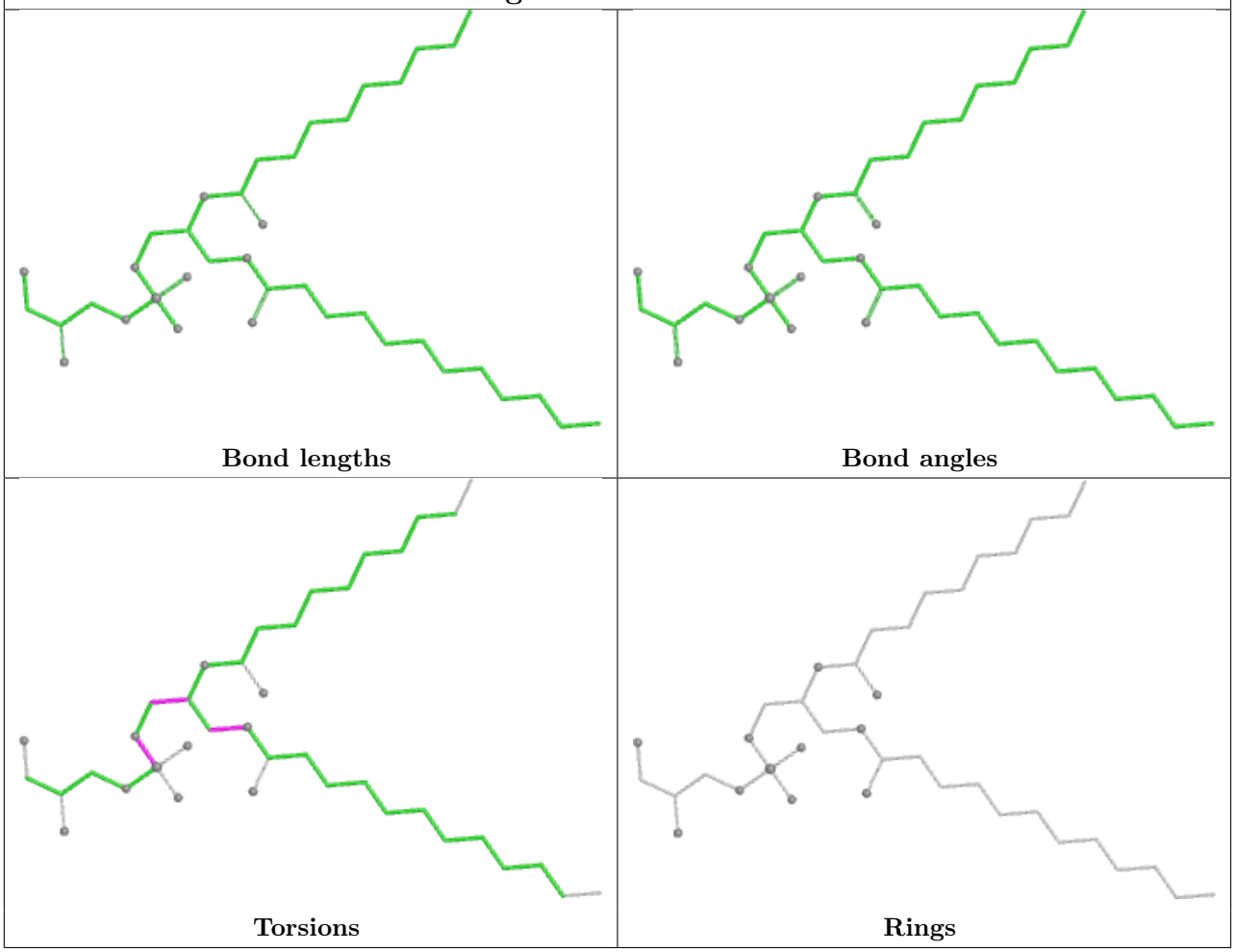


Torsions

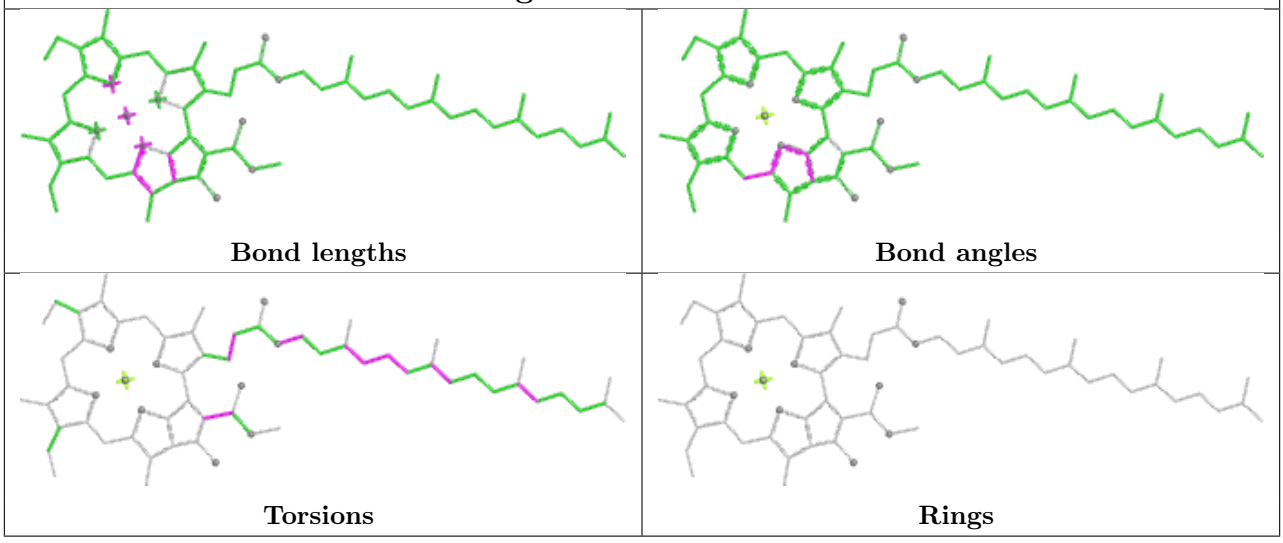


Rings

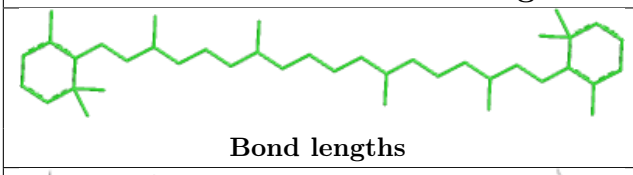
## Ligand LHG Z 620



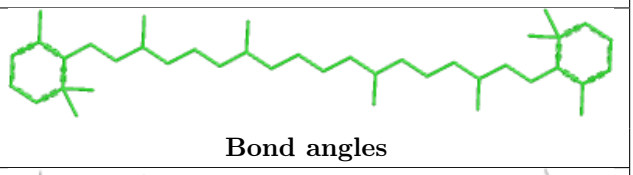

## Ligand CLA A2 806



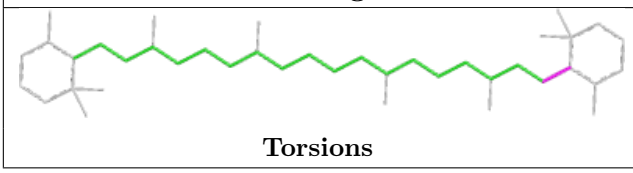
## Ligand BCR J2 102



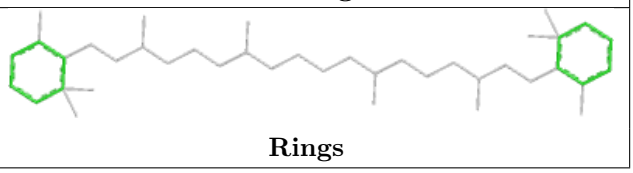
Bond lengths



Bond angles

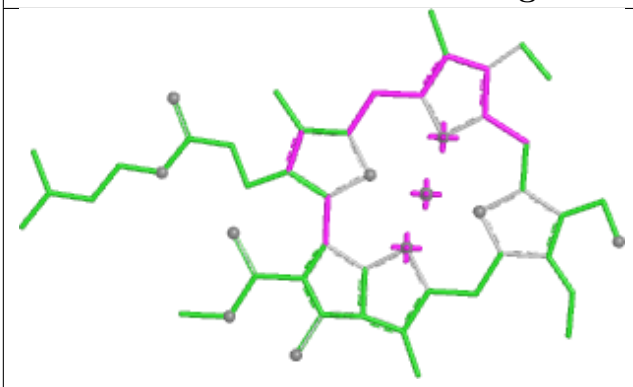


Torsions

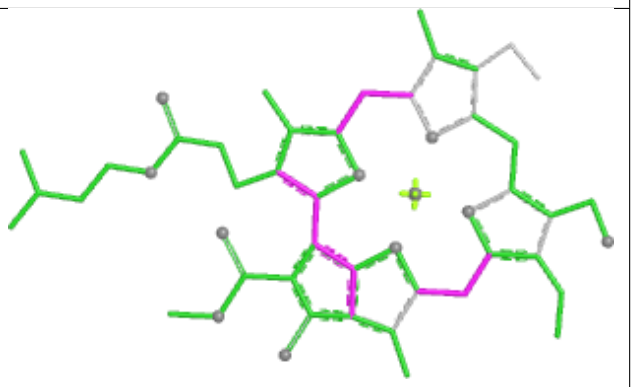


Rings

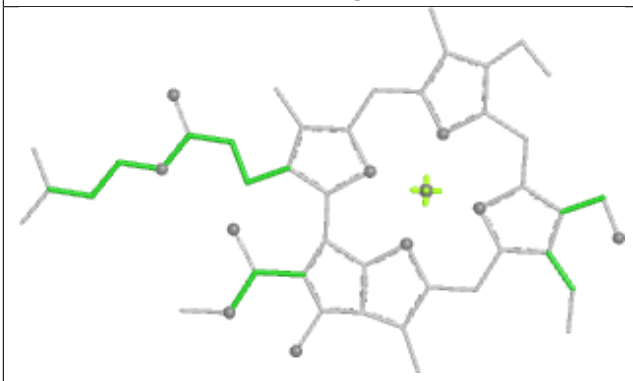
## Ligand CHL 52 608



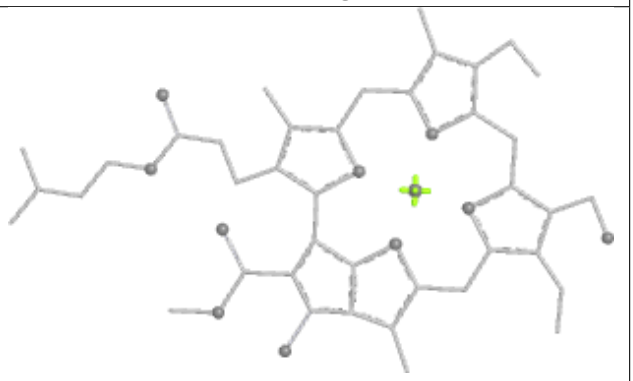
Bond lengths



Bond angles

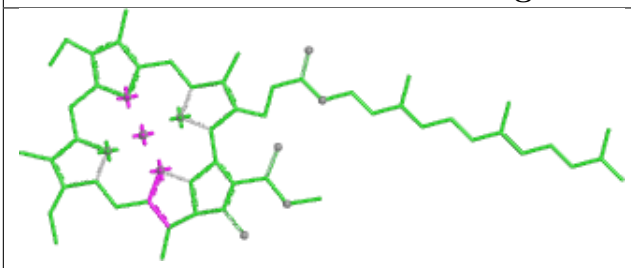


Torsions

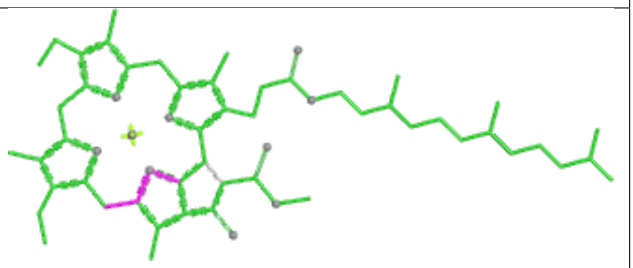


Rings

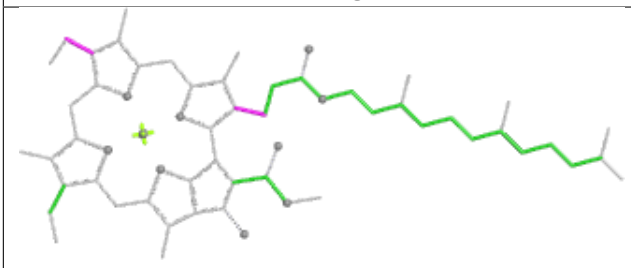
**Ligand CLA A2 819**



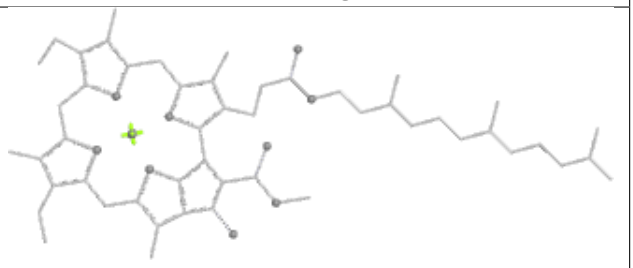
Bond lengths



Bond angles

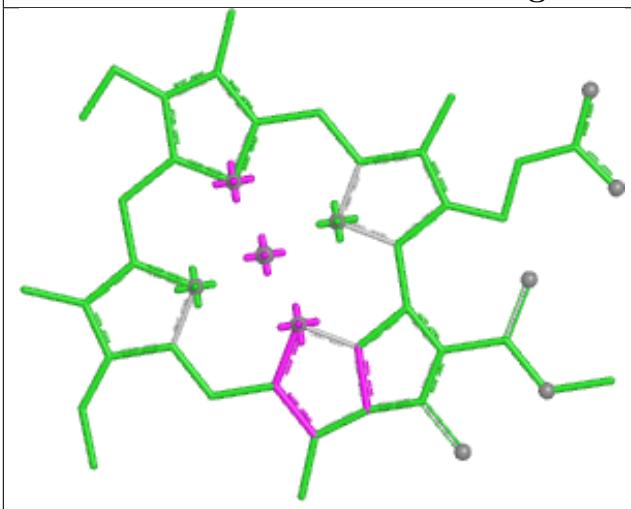


Torsions

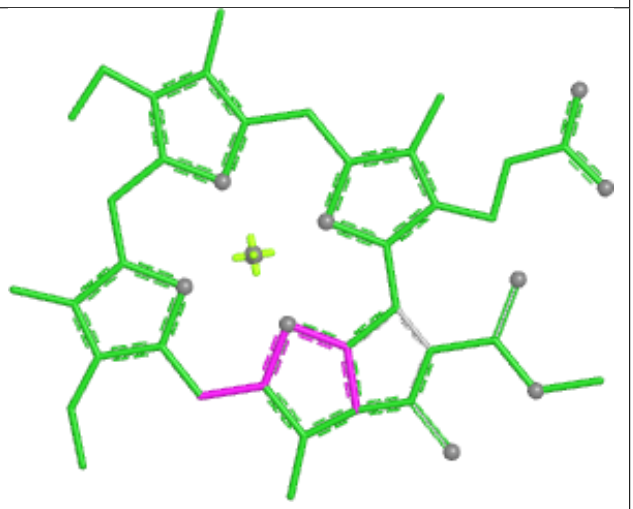


Rings

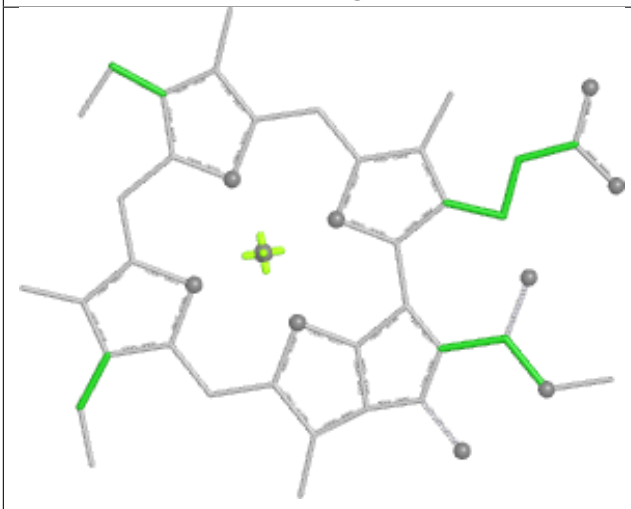
**Ligand CLA 8 616**



Bond lengths



Bond angles

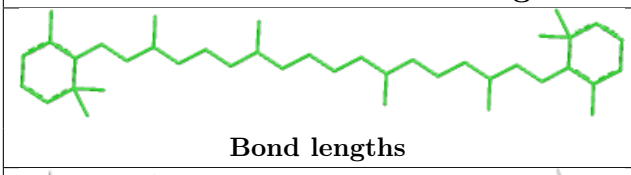


Torsions

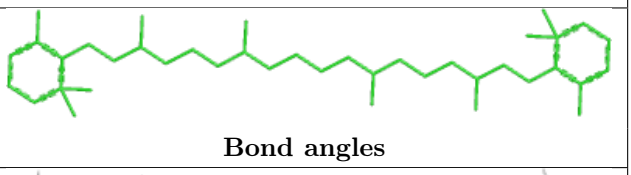


Rings

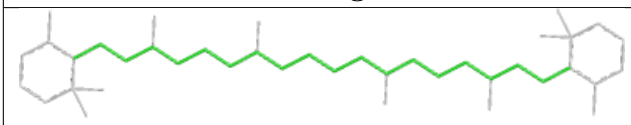
## Ligand BCR A2 849



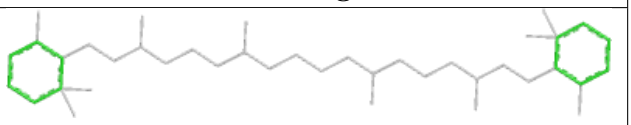
Bond lengths



Bond angles



Torsions

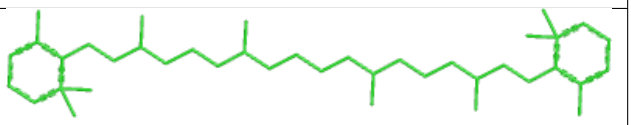


Rings

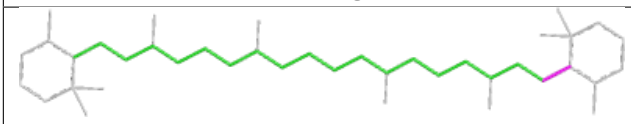
## Ligand BCR A2 851



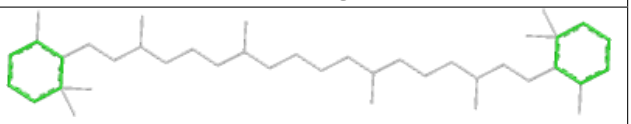
Bond lengths



Bond angles

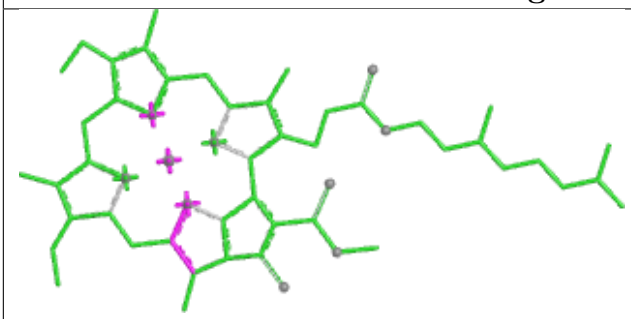


Torsions

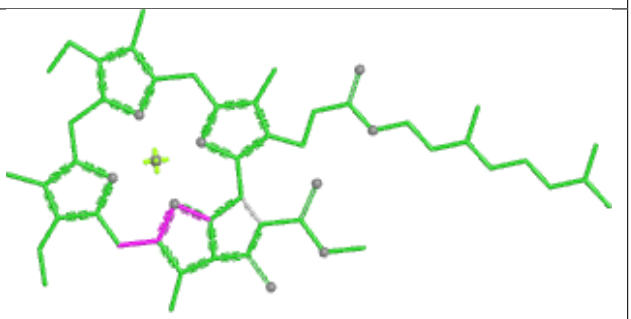


Rings

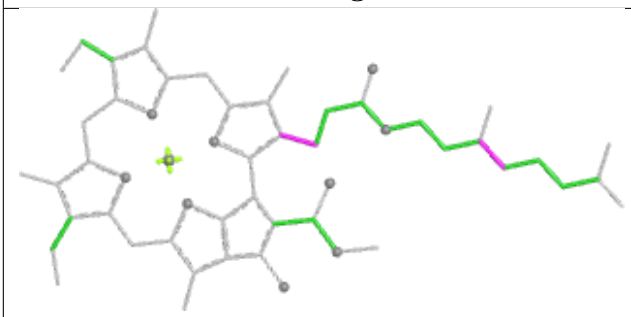
## Ligand CLA J 101



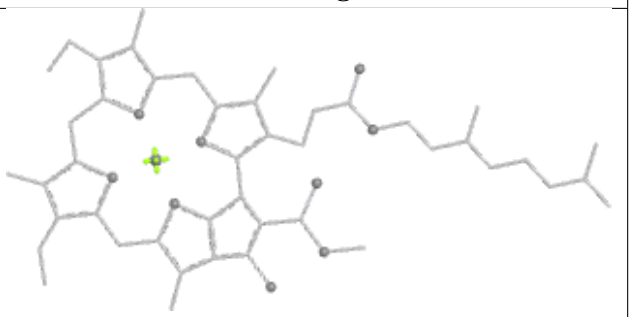
Bond lengths



Bond angles

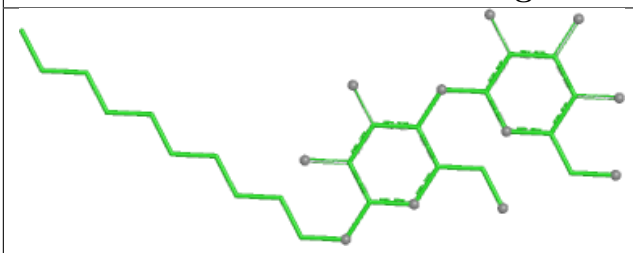


Torsions

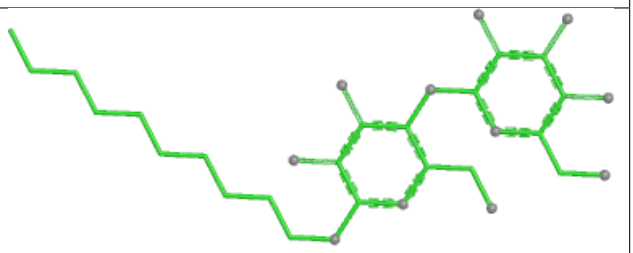


Rings

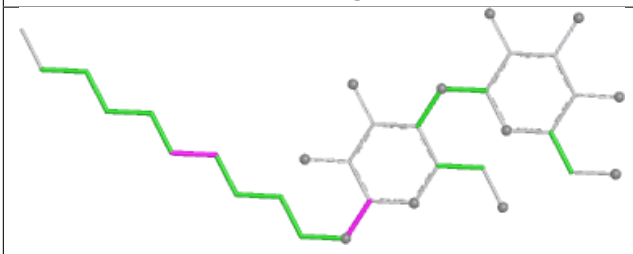
**Ligand LMU 42 625**



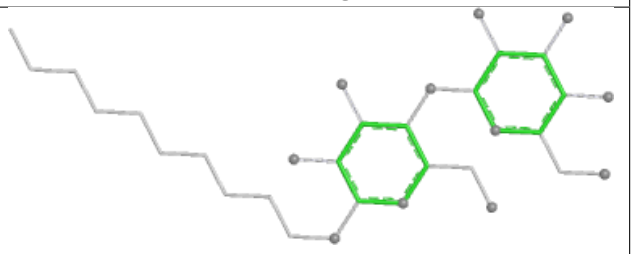
**Bond lengths**



**Bond angles**

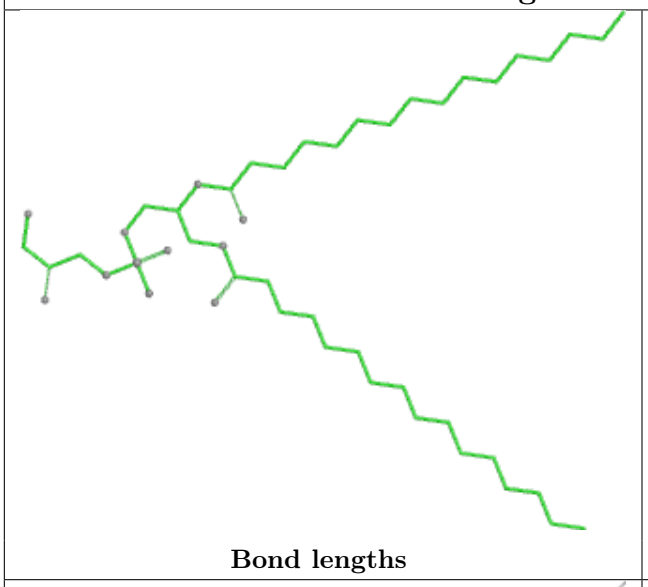


**Torsions**

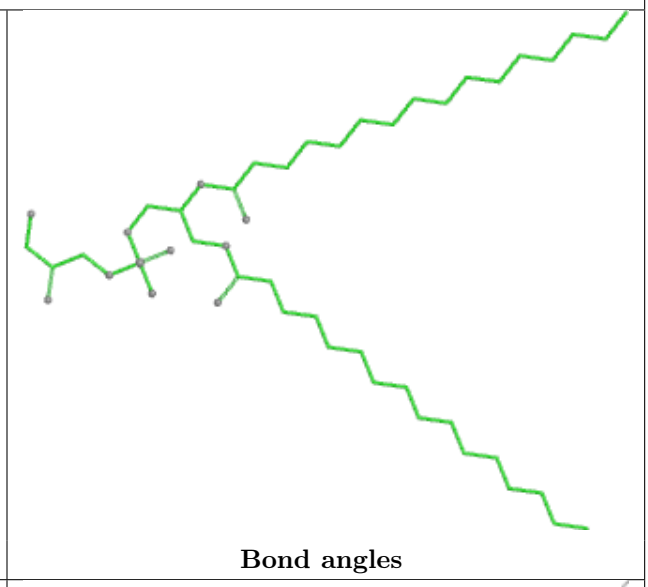


**Rings**

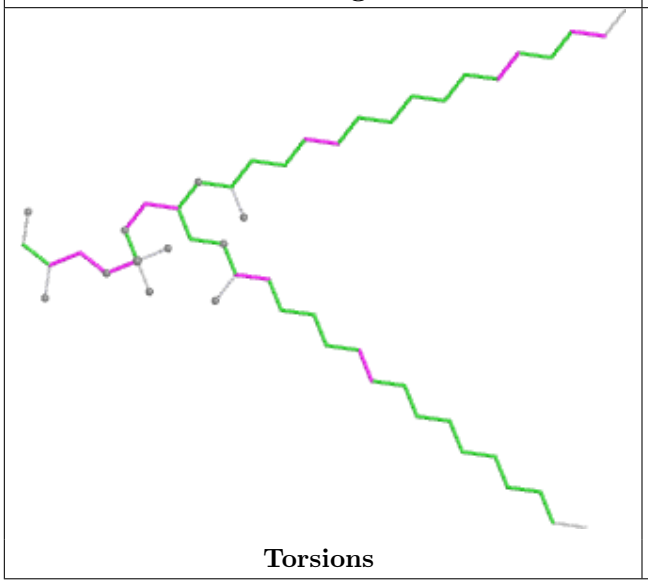
**Ligand LHG 42 622**



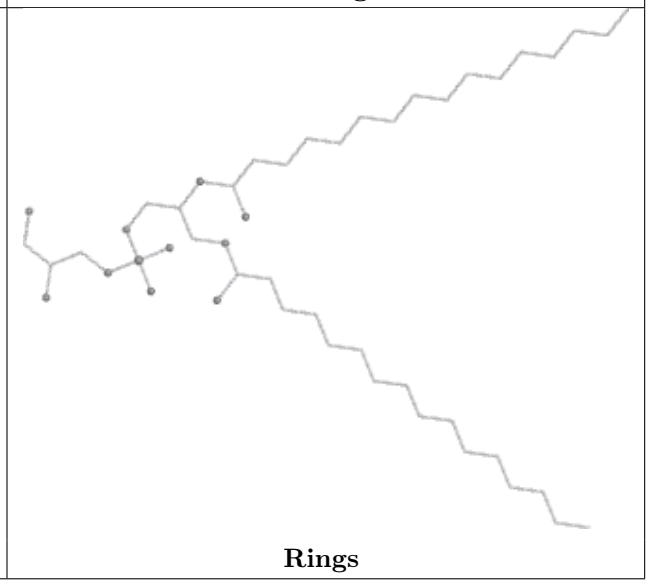
**Bond lengths**



**Bond angles**

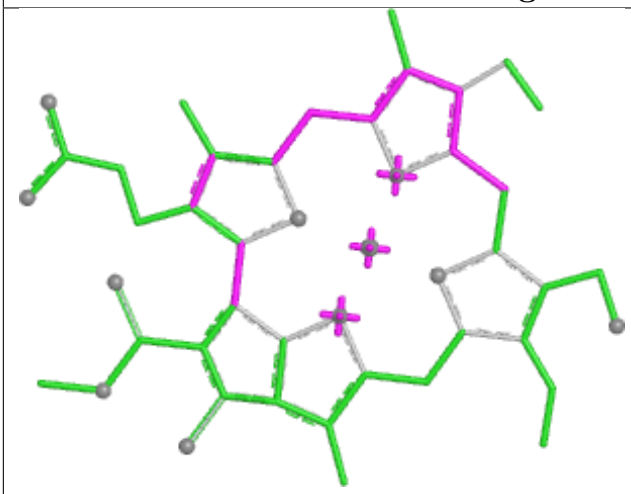


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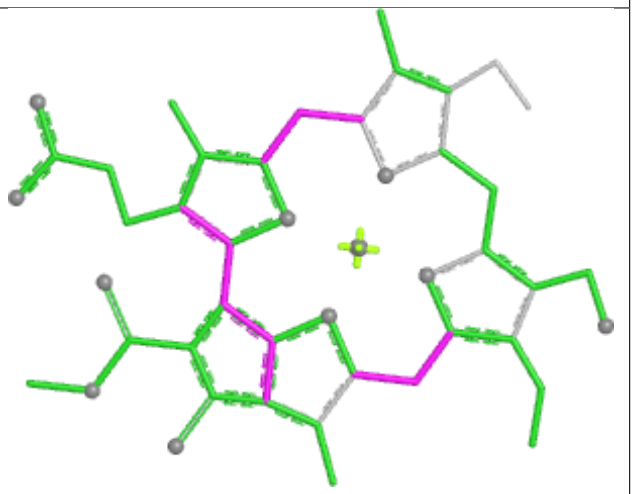


**Rings**

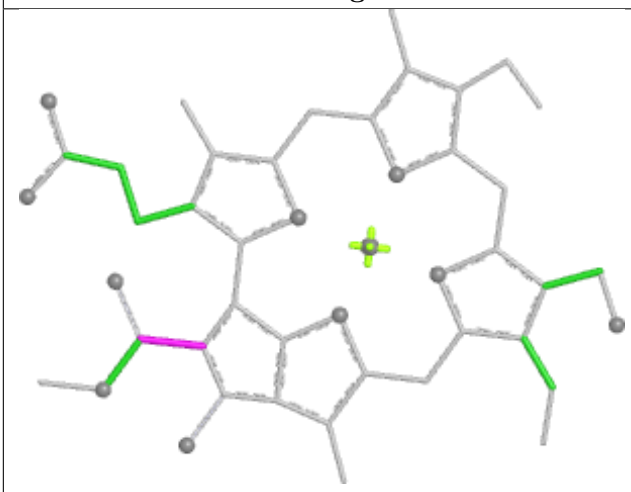
## Ligand CHL 12 607



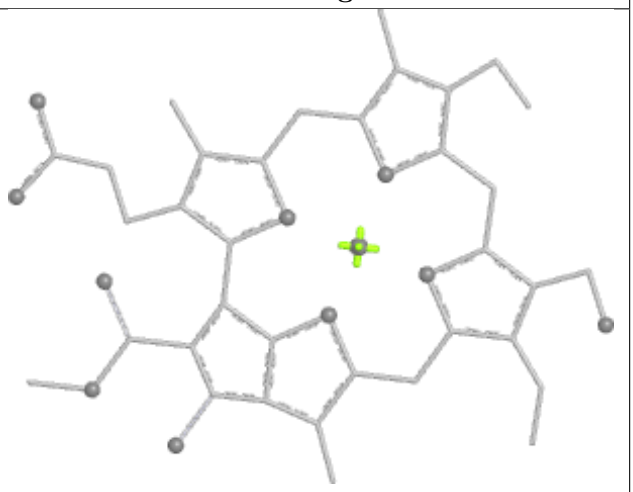
Bond lengths



Bond angles

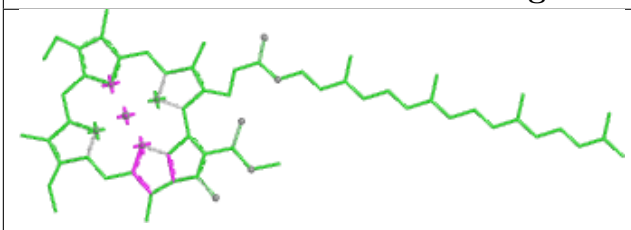


Torsions

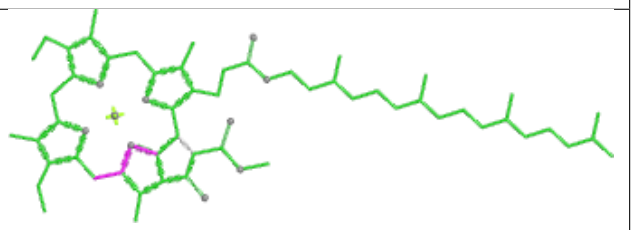


Rings

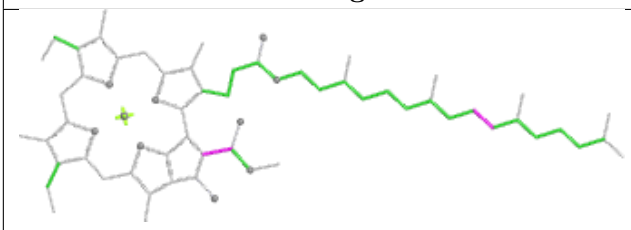
## Ligand CLA 1 608



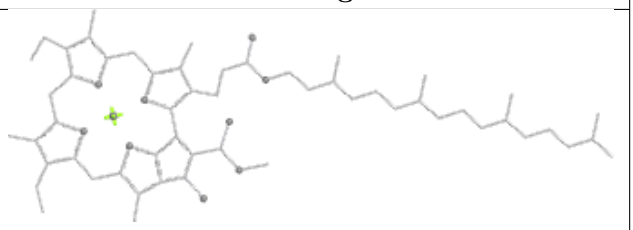
Bond lengths



Bond angles

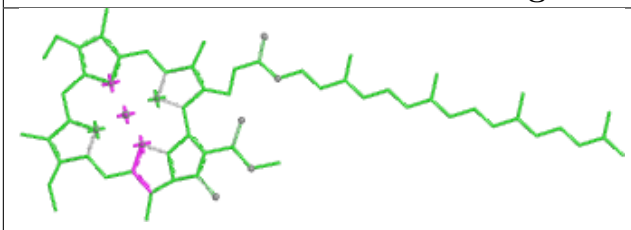


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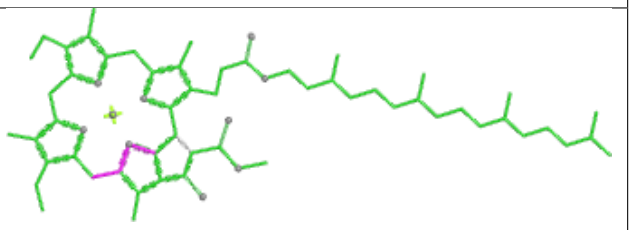


Rings

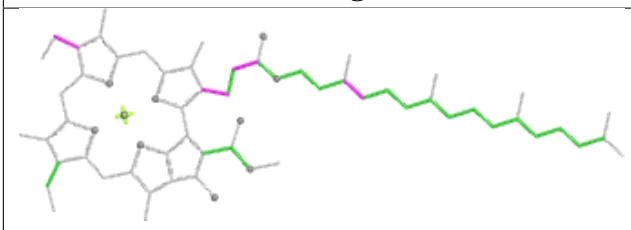
## Ligand CLA 4 613



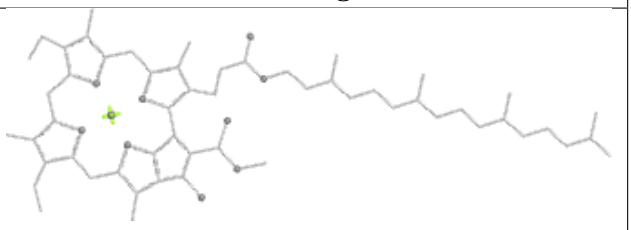
Bond lengths



Bond angles

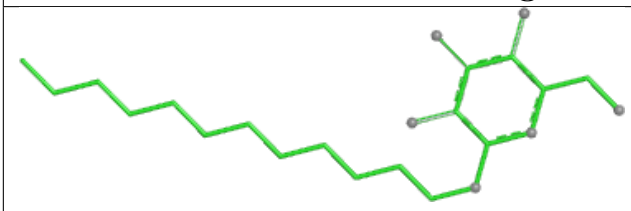


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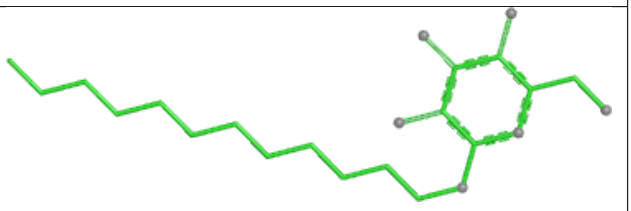


Rings

## Ligand LMU G 206



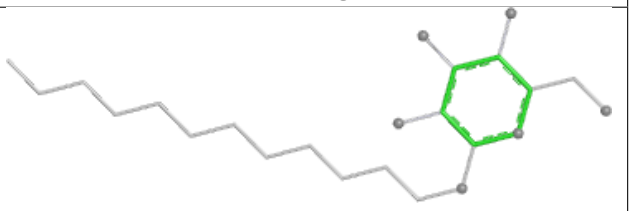
Bond lengths



Bond angles

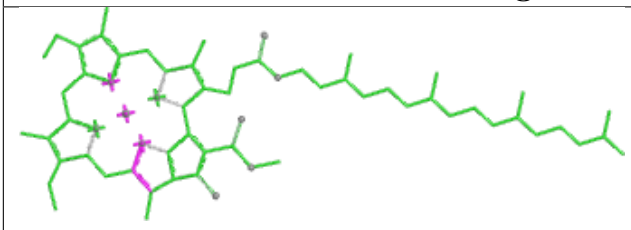


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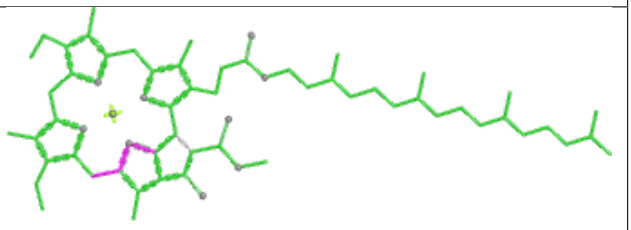


Rings

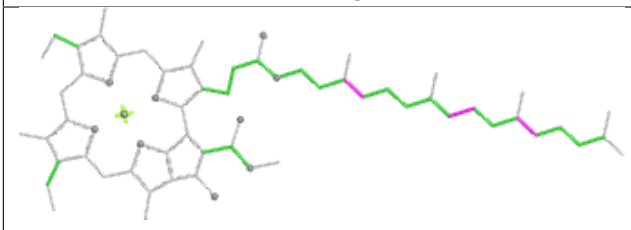
## Ligand CLA A2 828



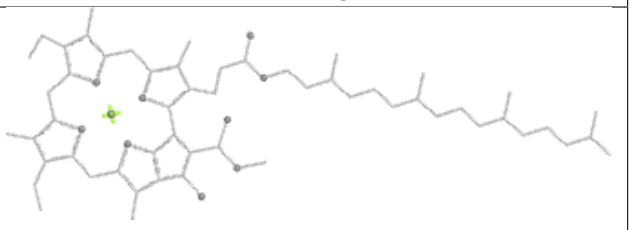
Bond lengths



Bond angles

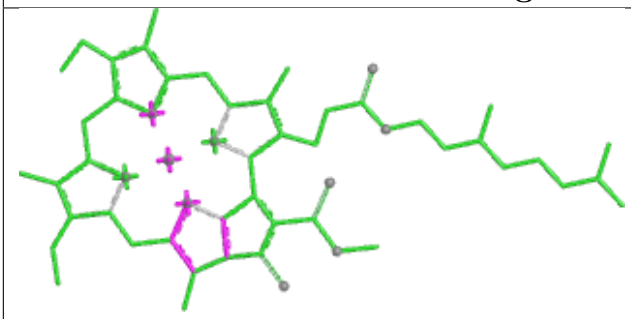


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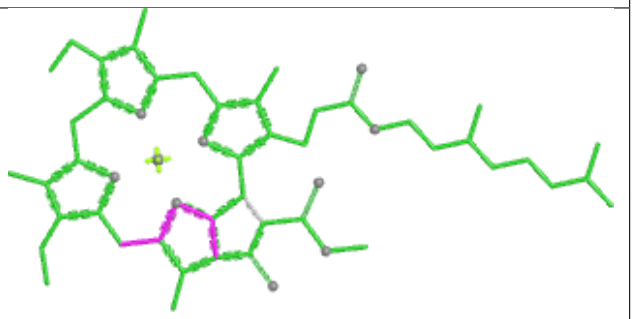


Rings

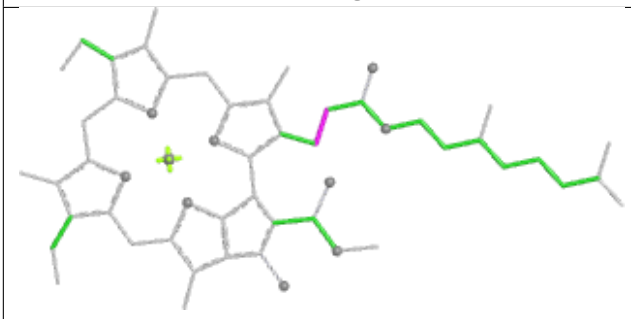
## Ligand CLA B2 831



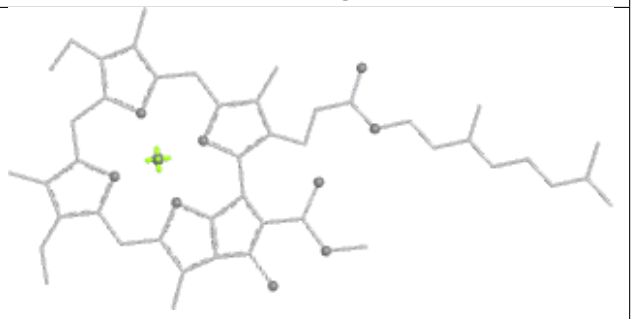
Bond lengths



Bond angles

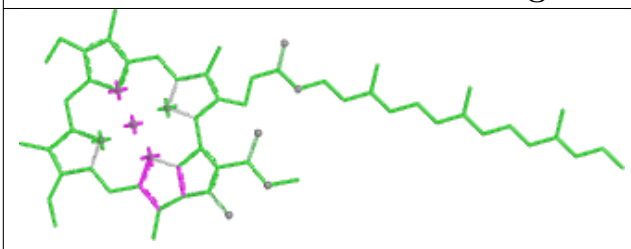


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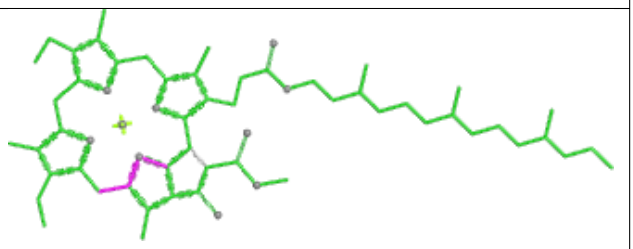


Rings

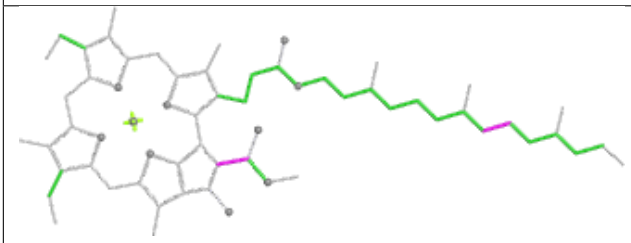
## Ligand CLA 8 602



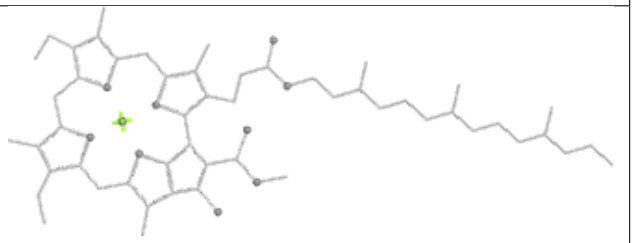
Bond lengths



Bond angles

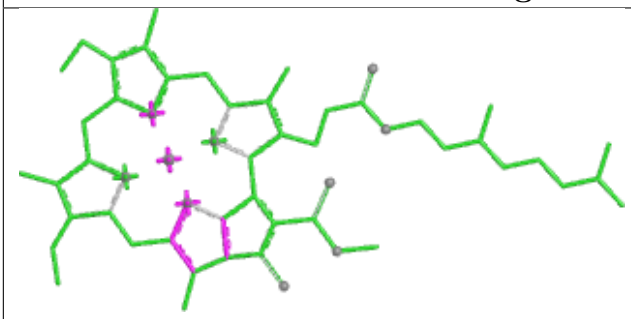


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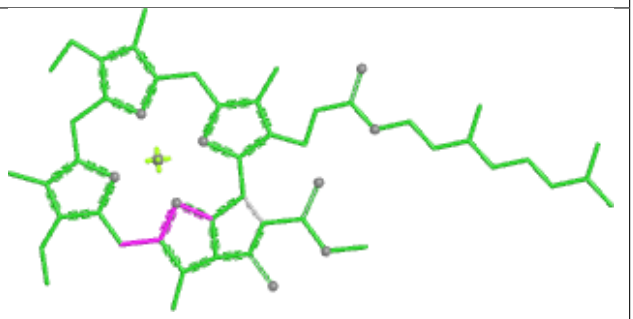


Rings

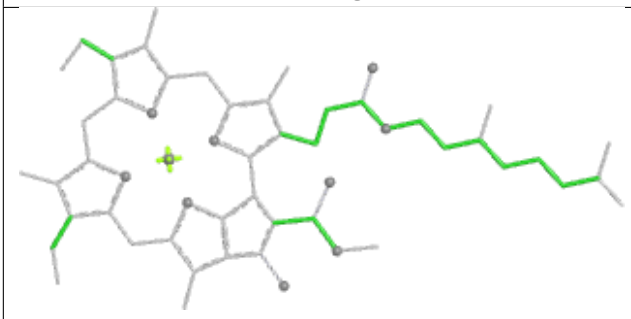
## Ligand CLA A2 832



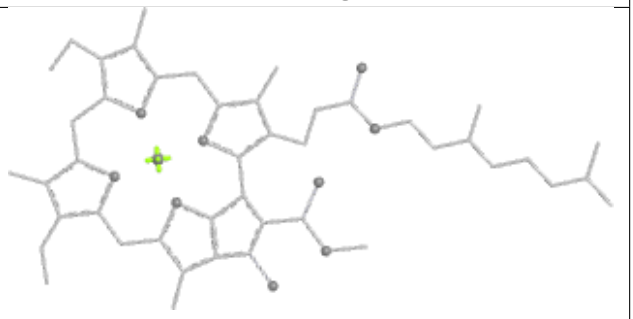
Bond lengths



Bond angles

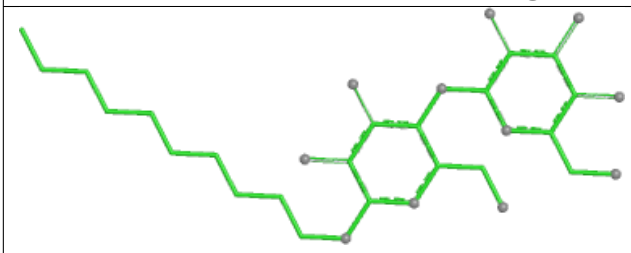


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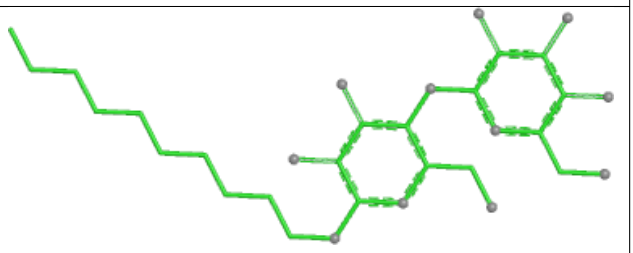


Rings

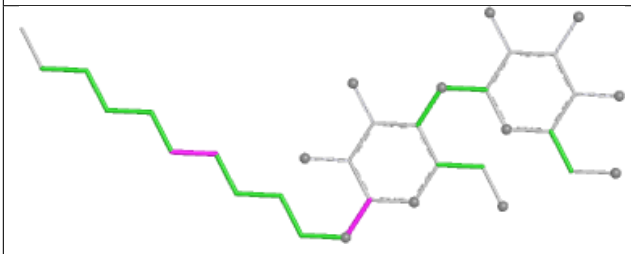
## Ligand LMU 4 625



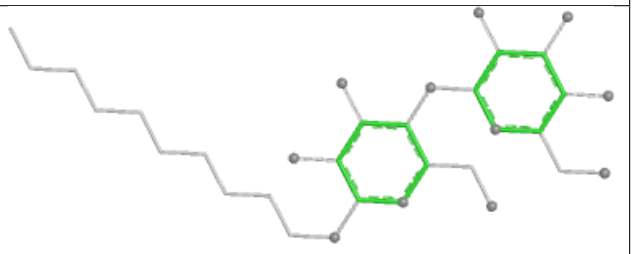
Bond lengths



Bond angles



Torsions



Rings

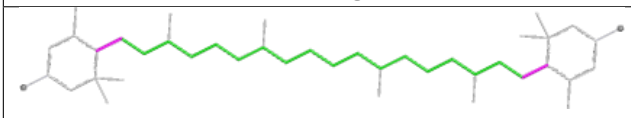
## Ligand LUT 5 626



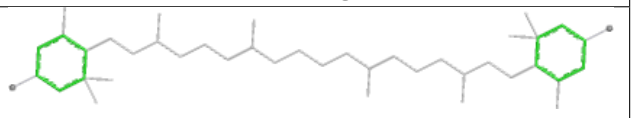
Bond lengths



Bond angles

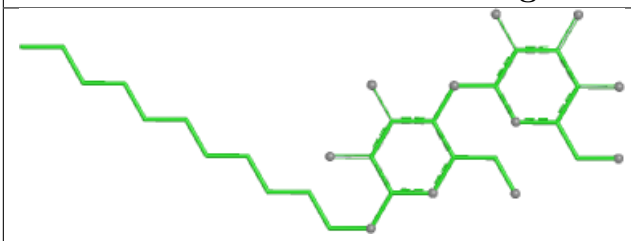


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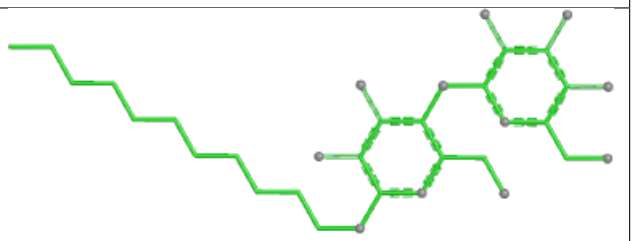


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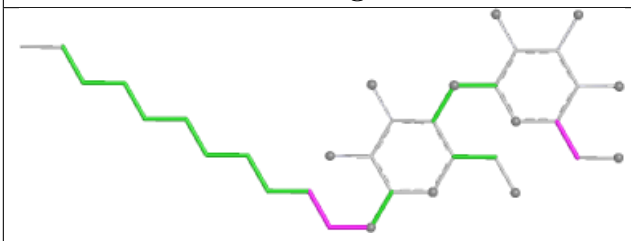
## Ligand LMU A 857



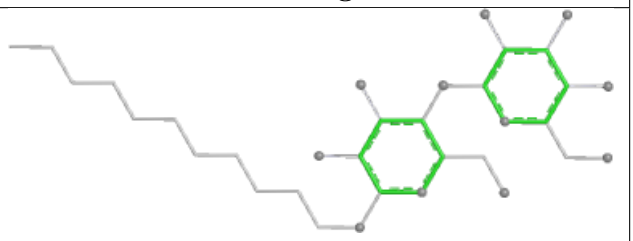
Bond lengths



Bond angles

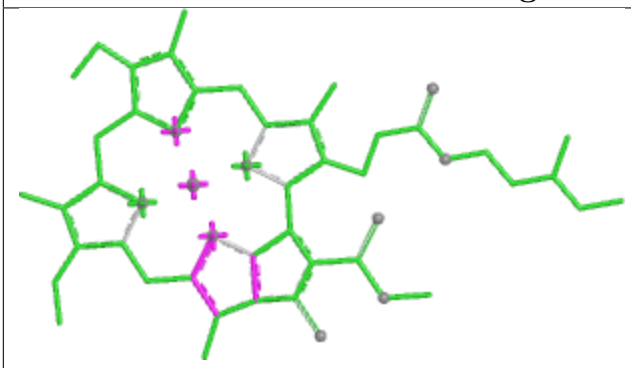


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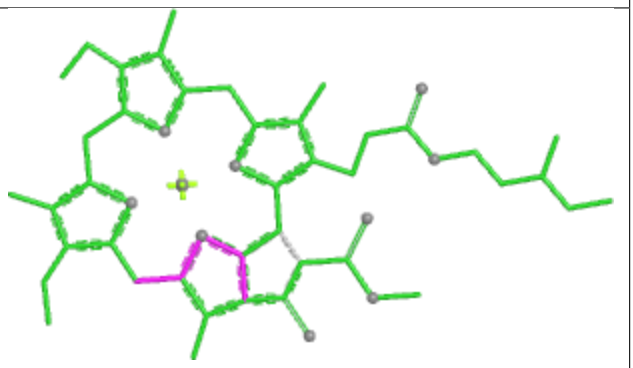


Rings

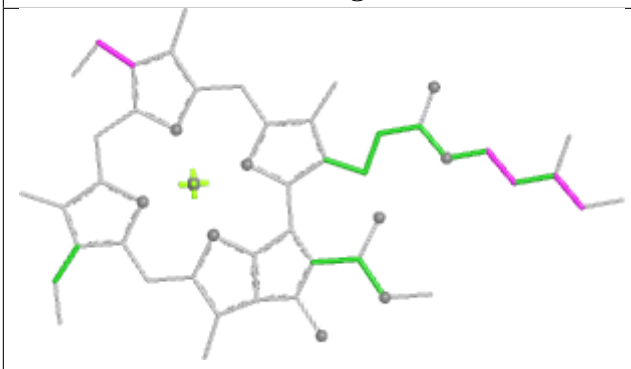
## Ligand CLA 92 609



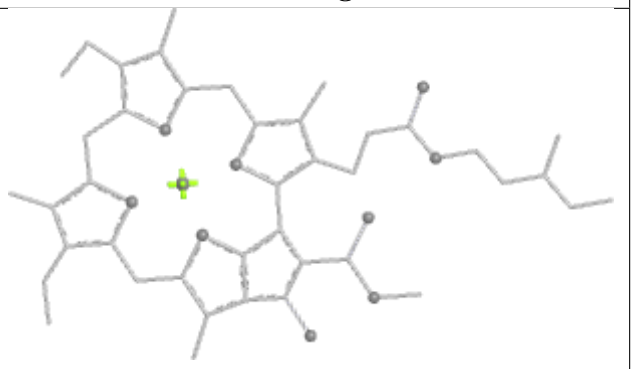
Bond lengths



Bond angles

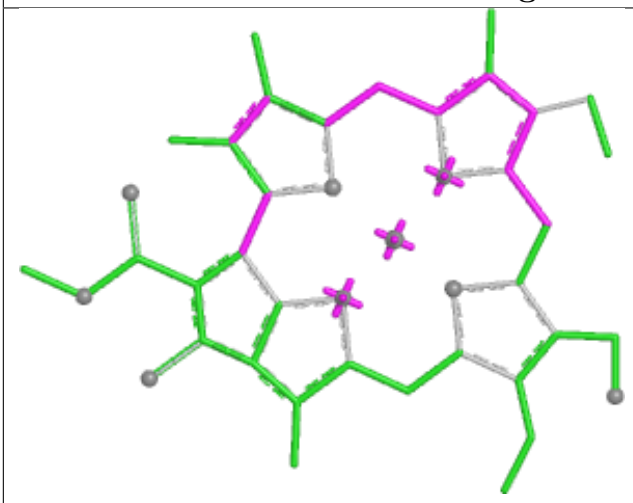


Torsions



Rings

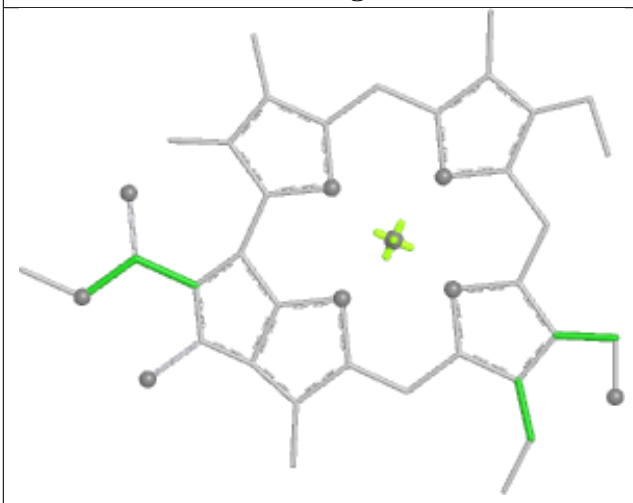
## Ligand CHL 92 606



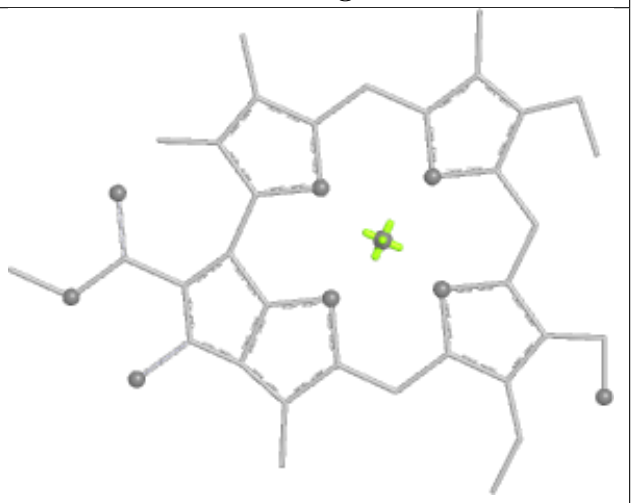
Bond lengths



Bond angles

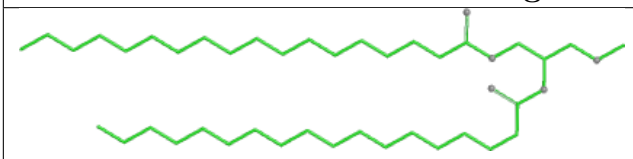


Torsions

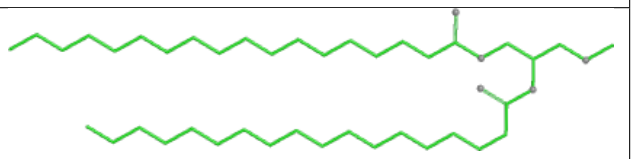


Rings

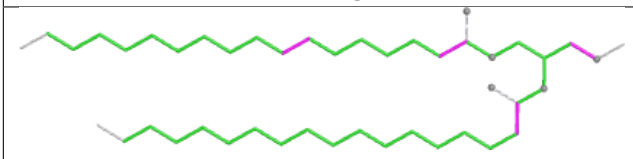
## Ligand LMG 3 722



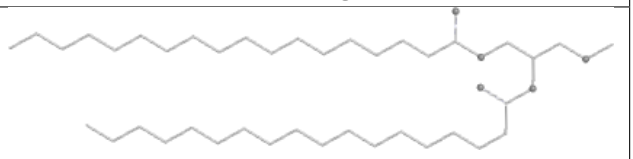
Bond lengths



Bond angles

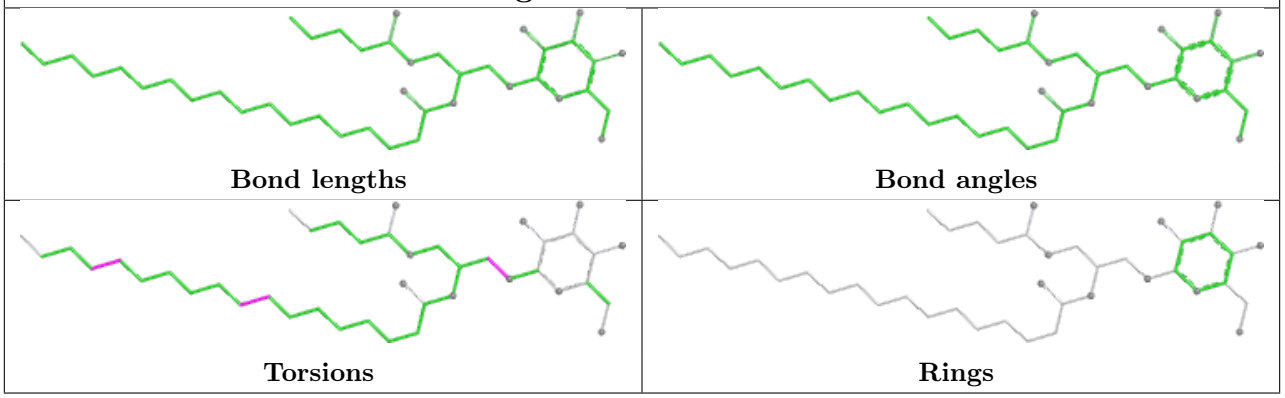


Torsions

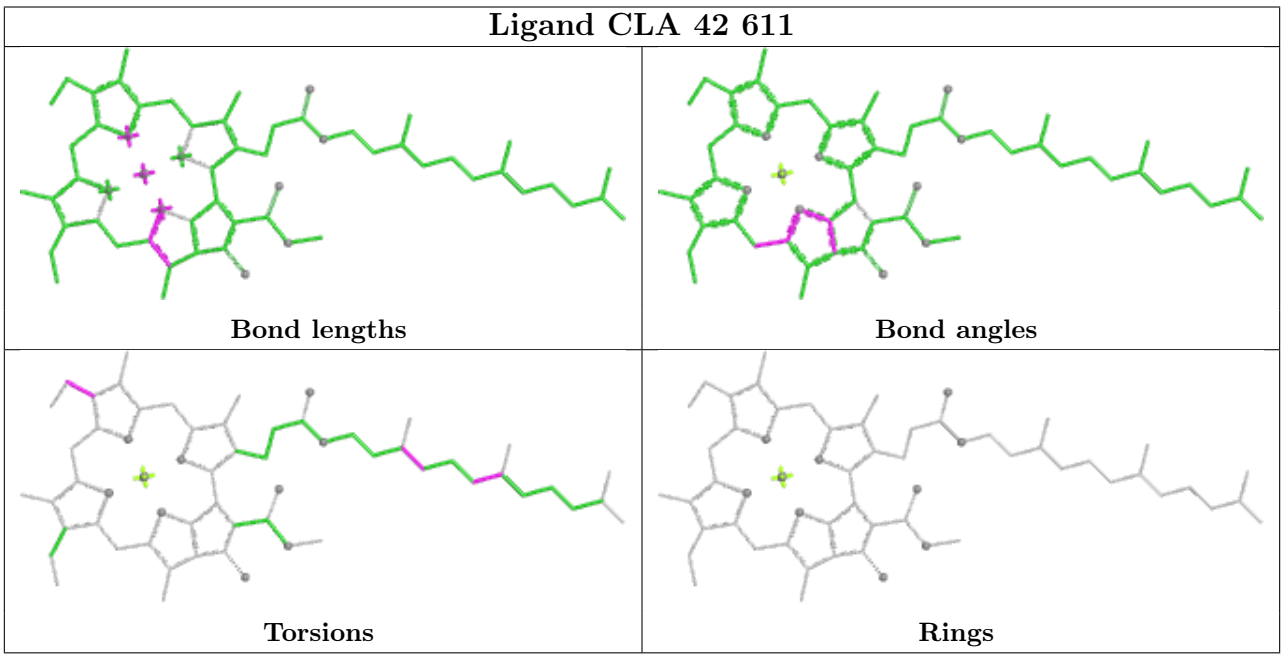


Rings

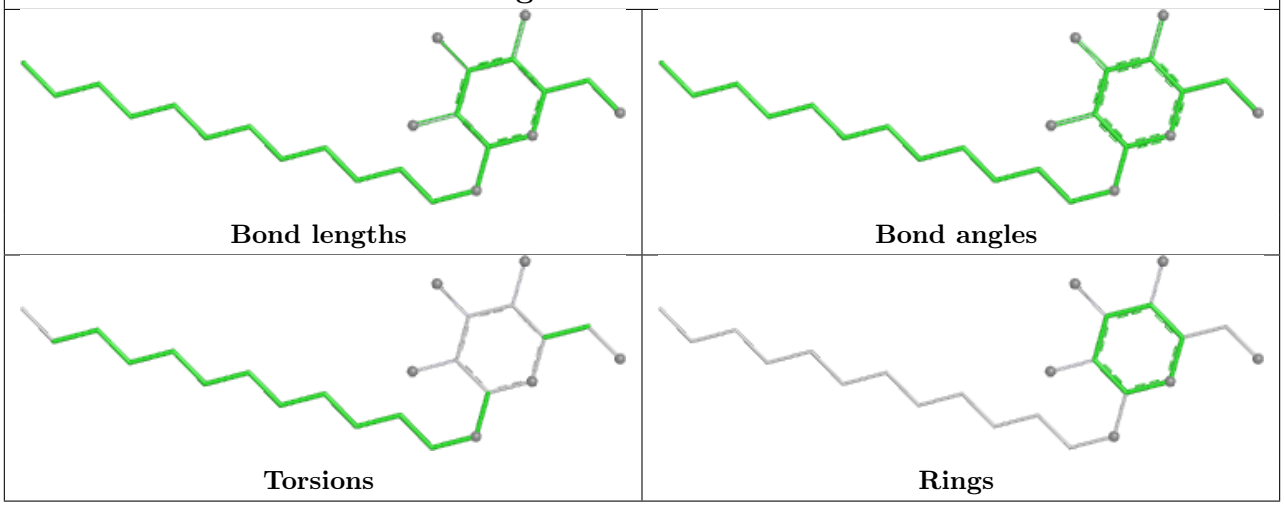
## Ligand LMG J2 103



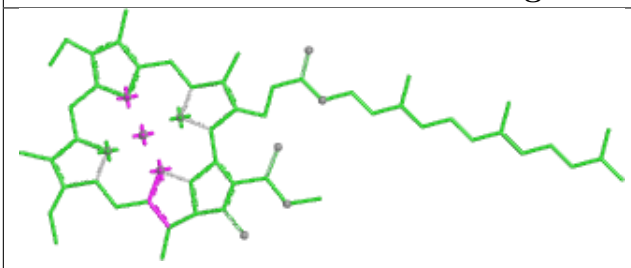

## Ligand CLA 42 611



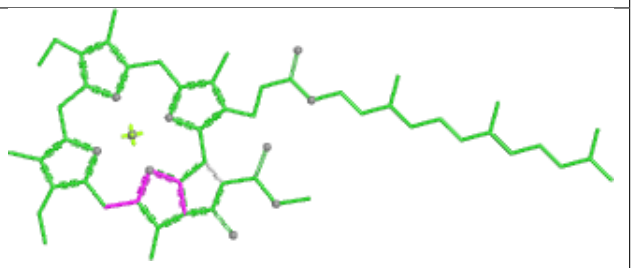

## Ligand LMU 12 626



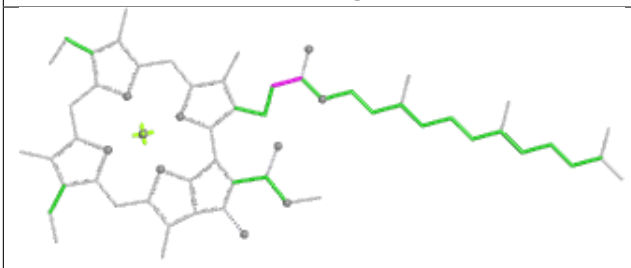
## Ligand CLA B 814



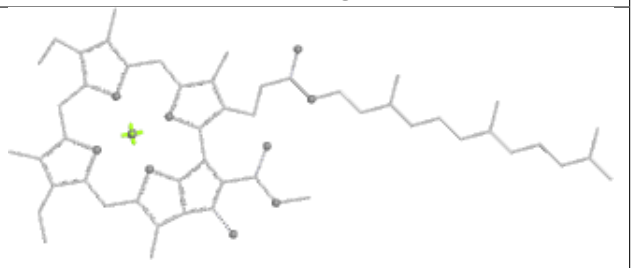
Bond lengths



Bond angles

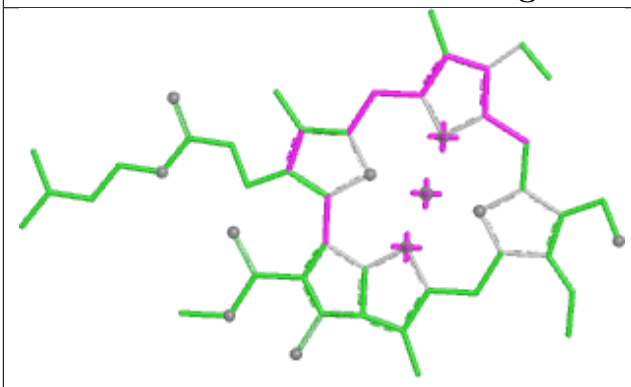


Torsions

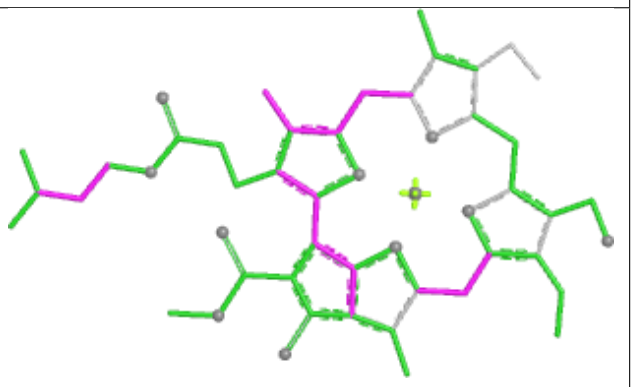


Rings

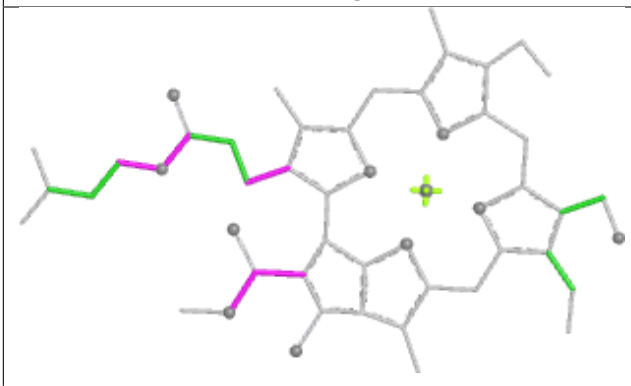
## Ligand CHL 92 607



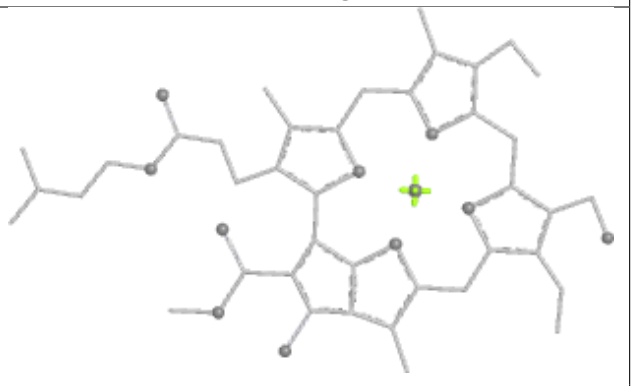
Bond lengths



Bond angles

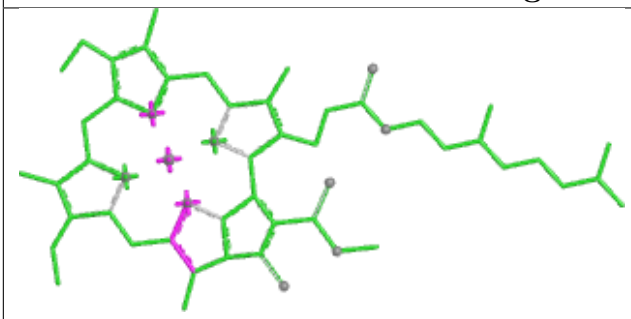


Torsions

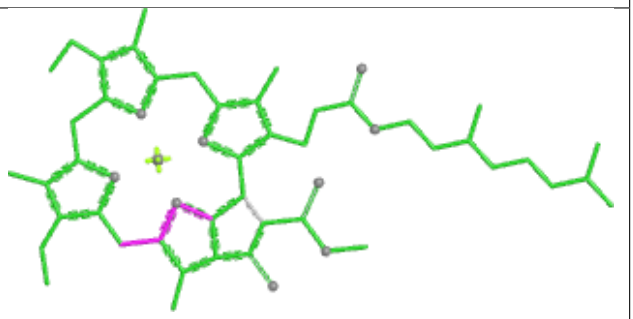


Rings

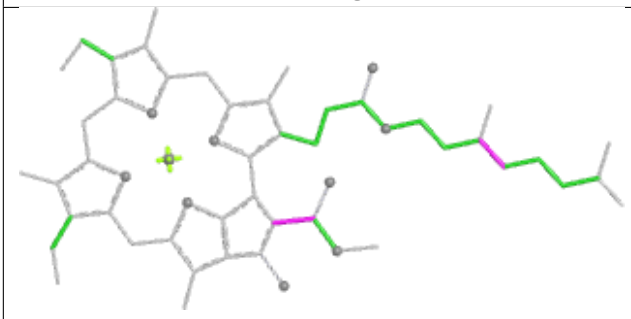
## Ligand CLA A 817



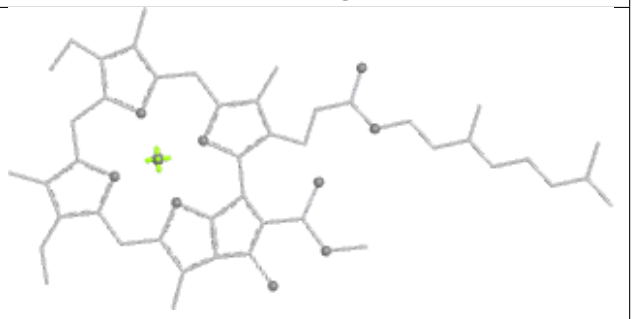
Bond lengths



Bond angles

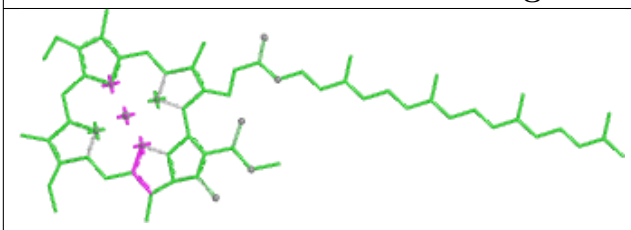


Torsions

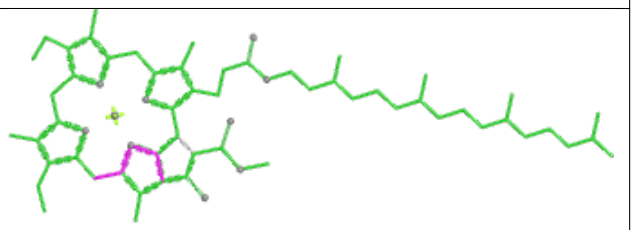


Rings

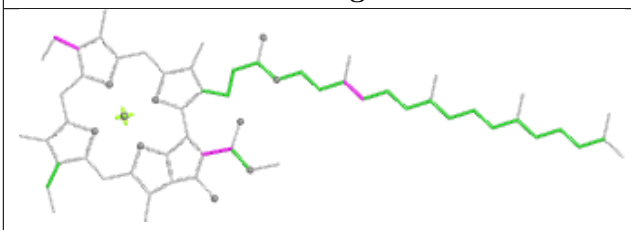
## Ligand CLA A 835



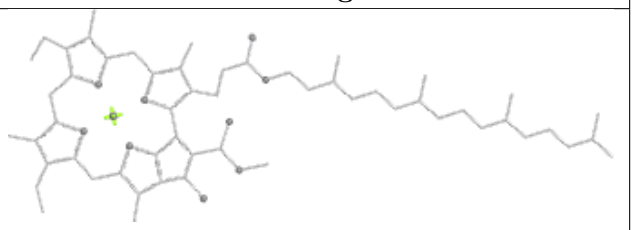
Bond lengths



Bond angles

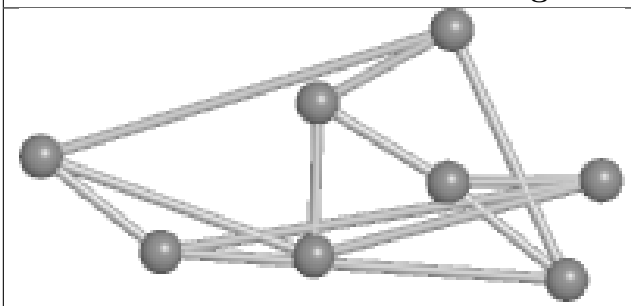


Torsions

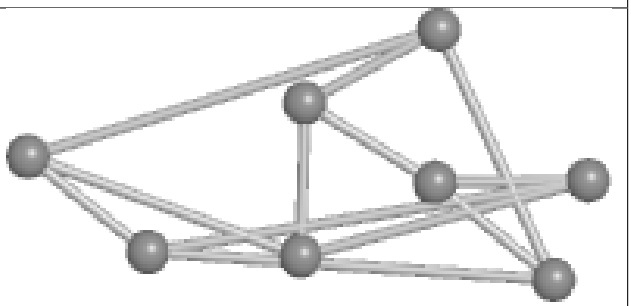


Rings

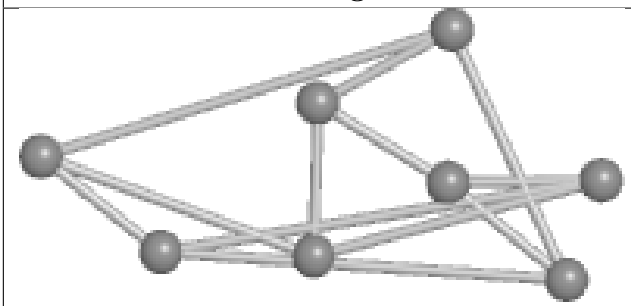
## Ligand SF4 A 853



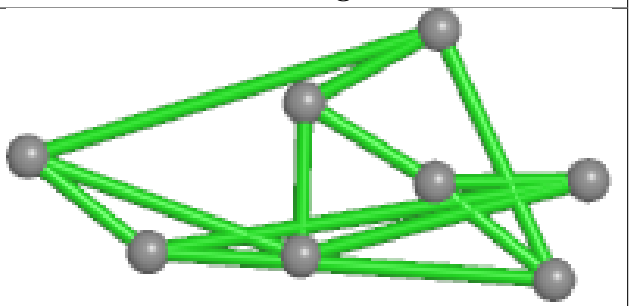
Bond lengths



Bond angles

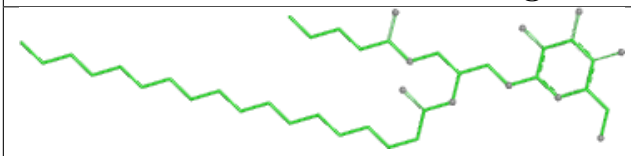


Torsions

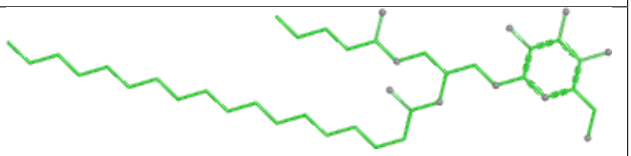


Rings

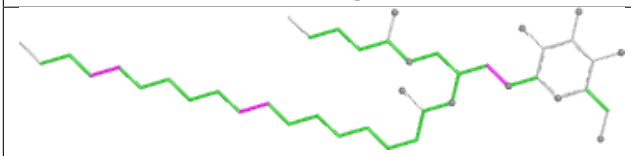
## Ligand LMG J 103



Bond lengths



Bond angles

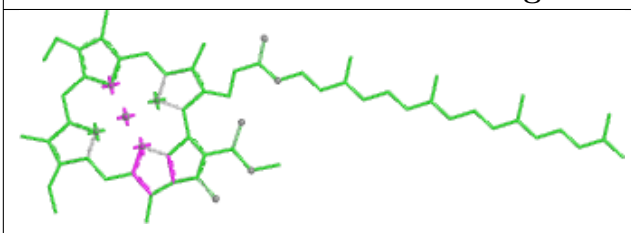


Torsions

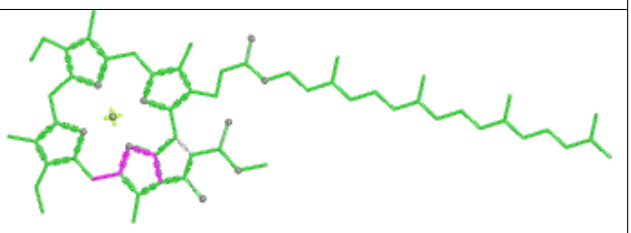


Rings

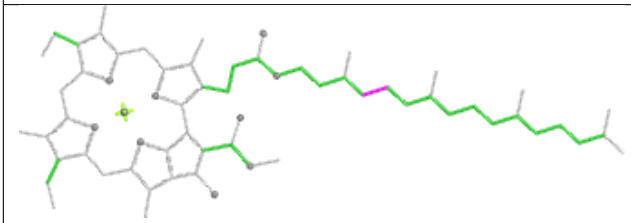
## Ligand CLA A 833



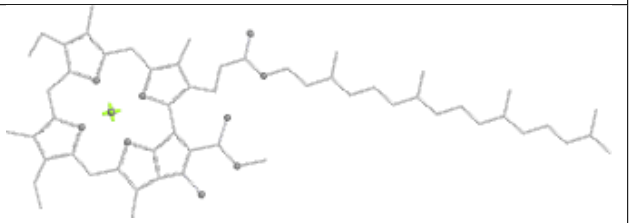
Bond lengths



Bond angles

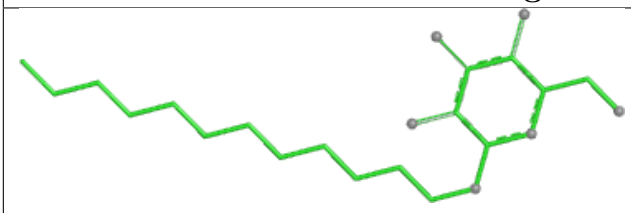


Torsions

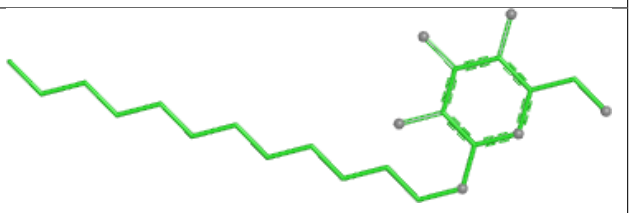


Rings

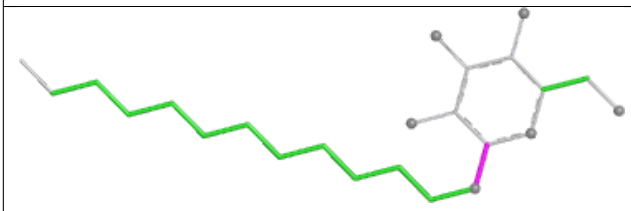
## Ligand LMU 6 628



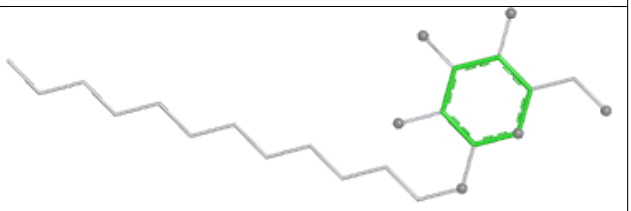
Bond lengths



Bond angles

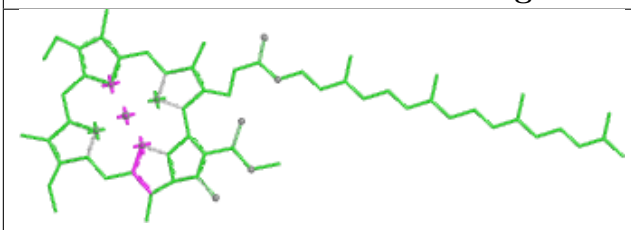


Torsions

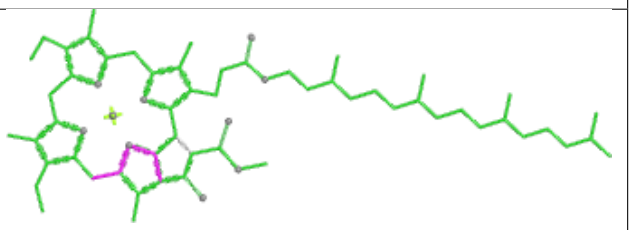


Rings

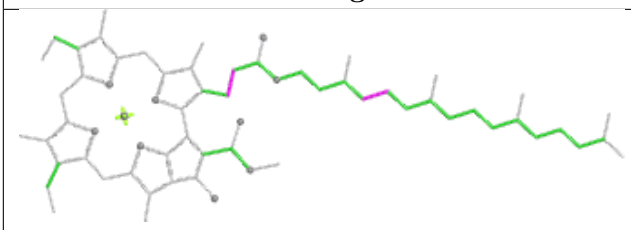
## Ligand CLA A2 818



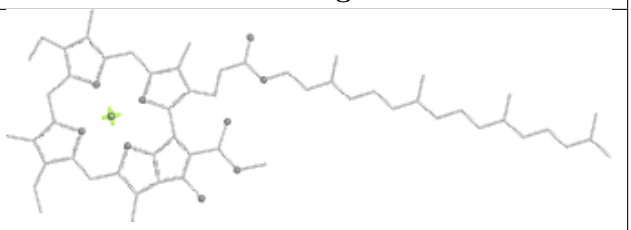
Bond lengths



Bond angles

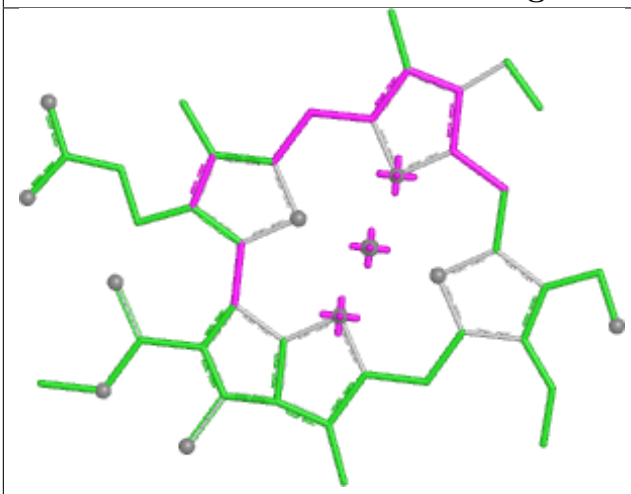


Torsions

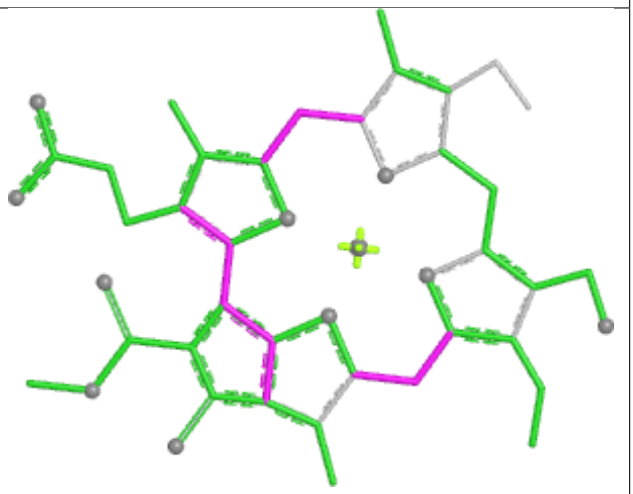


Rings

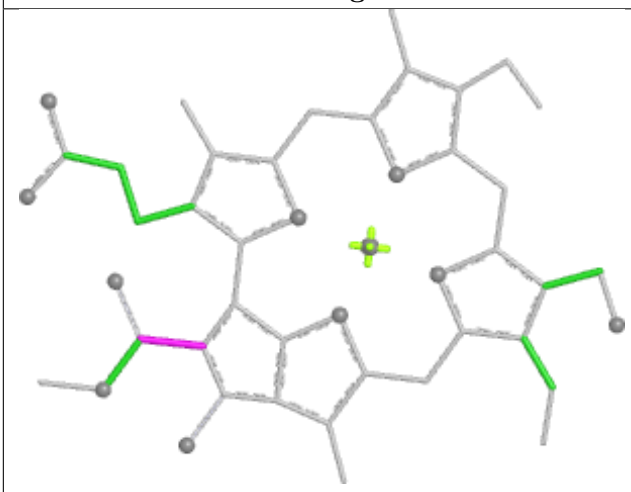
**Ligand CHL 1 607**



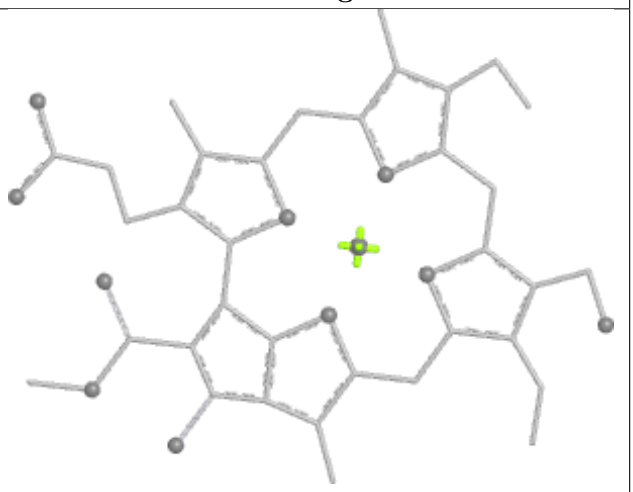
**Bond lengths**



**Bond angles**

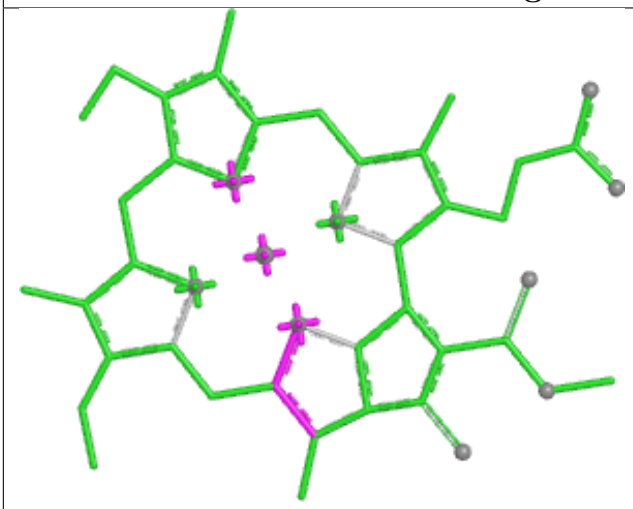


**Torsions**

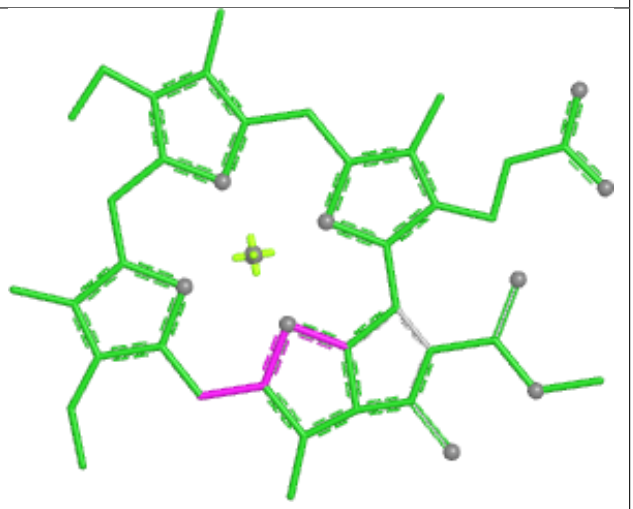


**Rings**

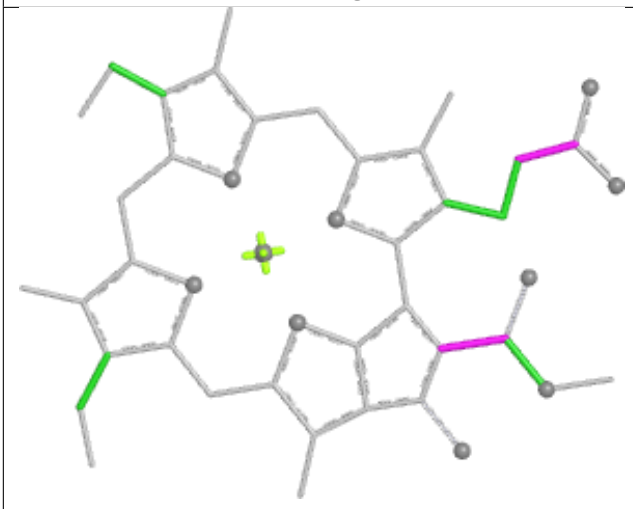
## Ligand CLA B 804



Bond lengths



Bond angles

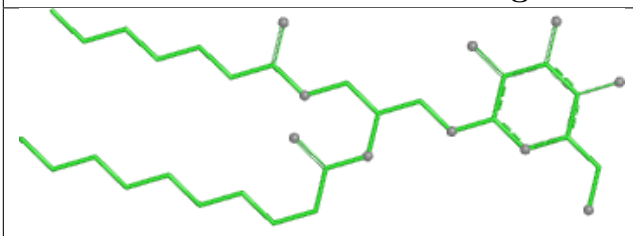


Torsions

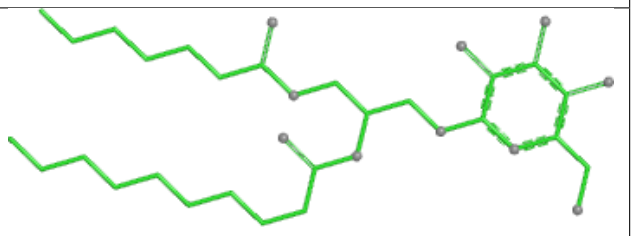


Rings

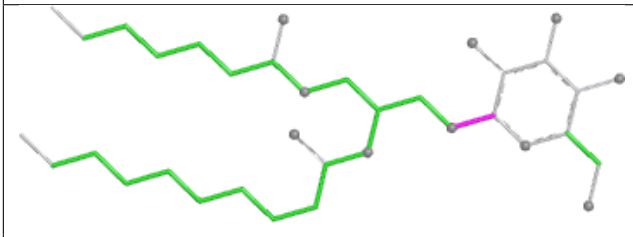
## Ligand LMG B2 854



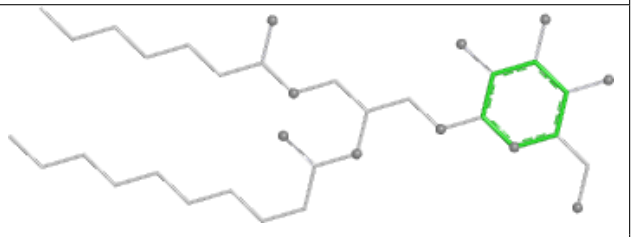
Bond lengths



Bond angles

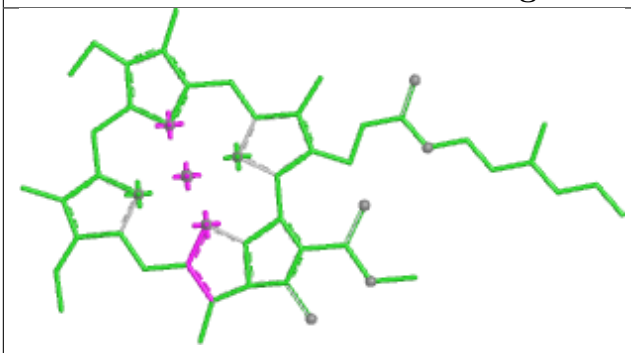


Torsions

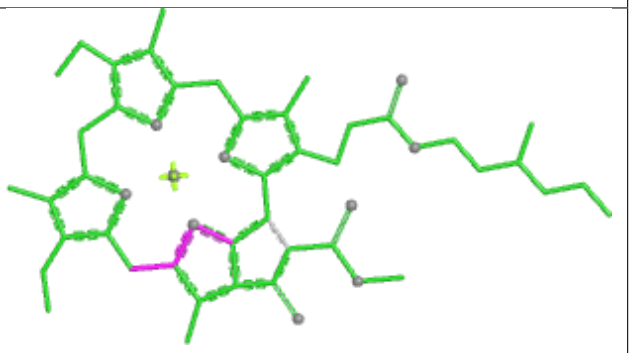


Rings

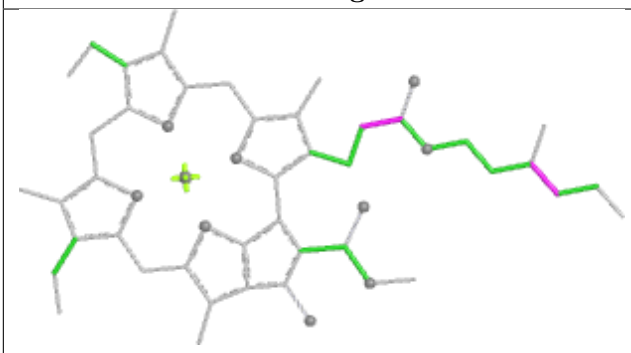
## Ligand CLA 72 612



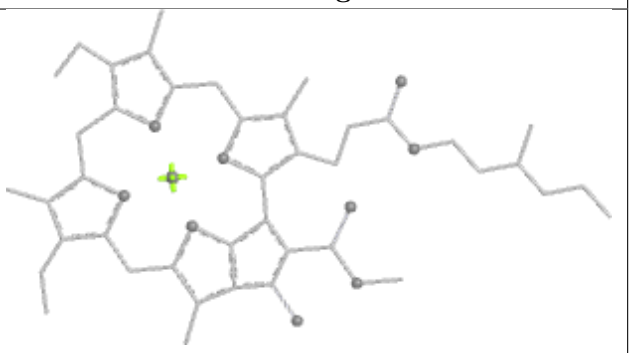
Bond lengths



Bond angles

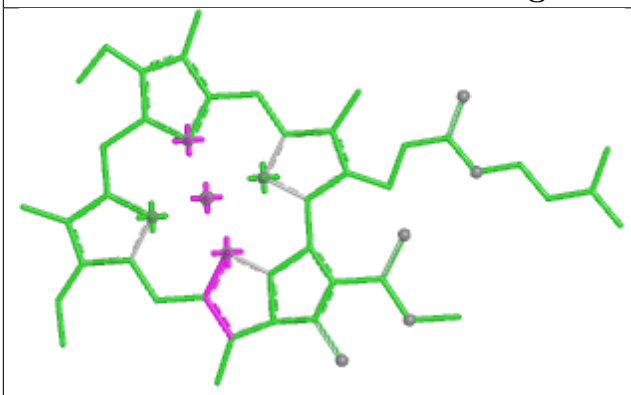


Torsions

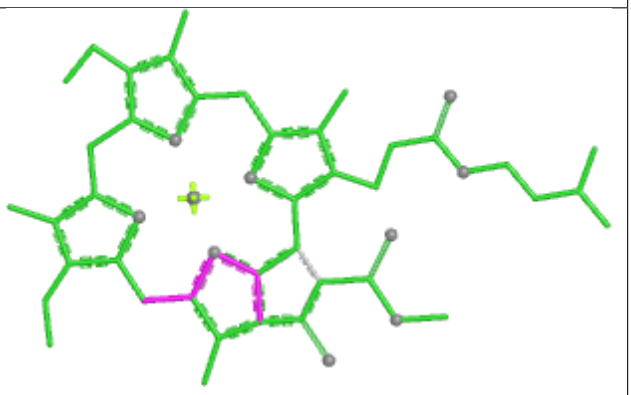


Rings

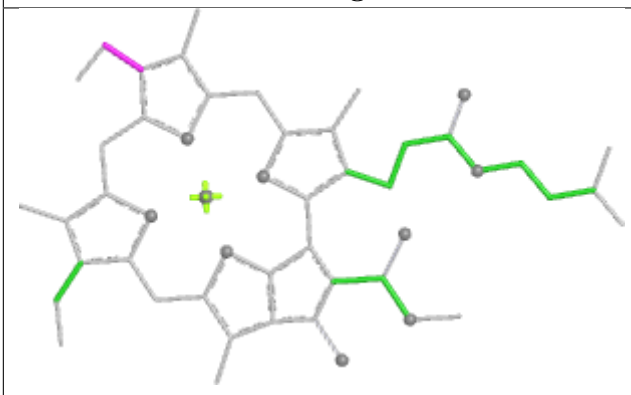
## Ligand CLA 6 614



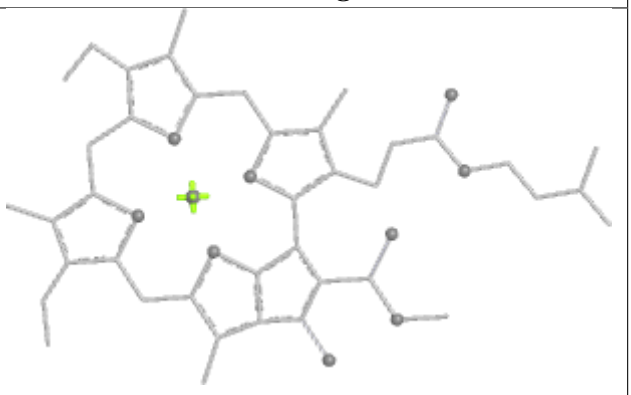
Bond lengths



Bond angles

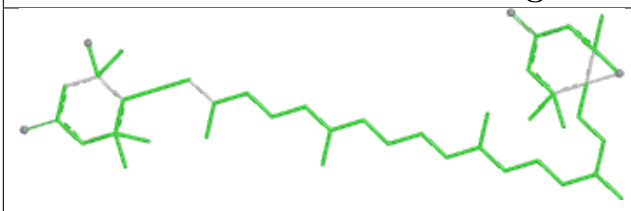


Torsions

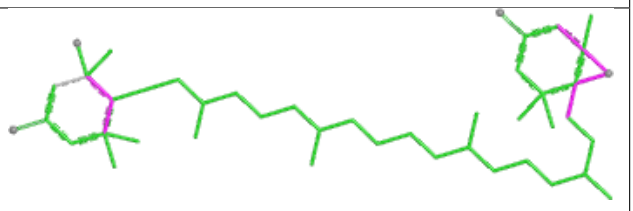


Rings

## Ligand NEX 6 625



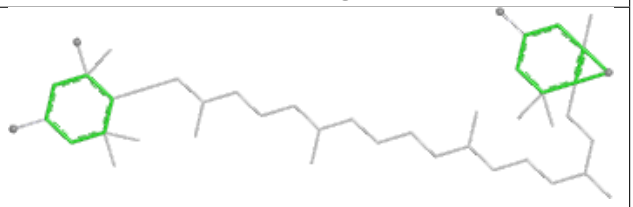
Bond lengths



Bond angles



Torsions

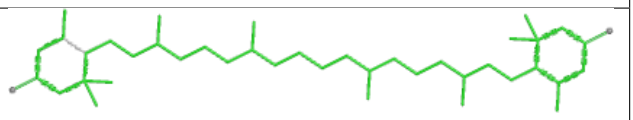


Rings

## Ligand LUT A 856



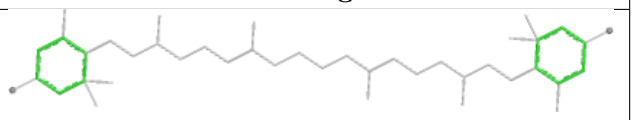
Bond lengths



Bond angles



Torsions



Rings

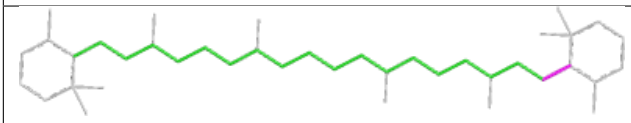
## Ligand BCR 32 718



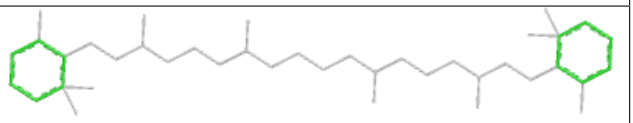
Bond lengths



Bond angles

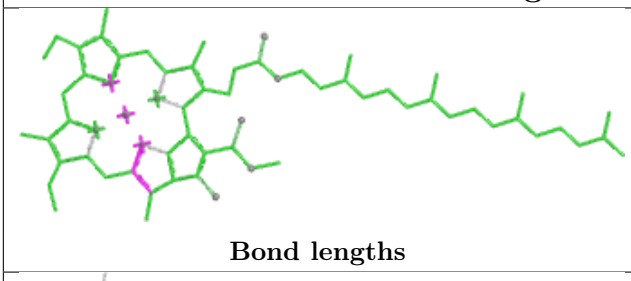


Torsions

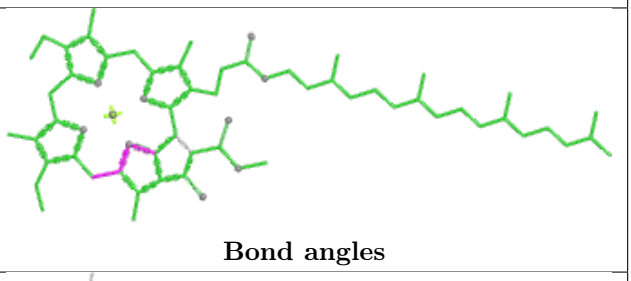


Rings

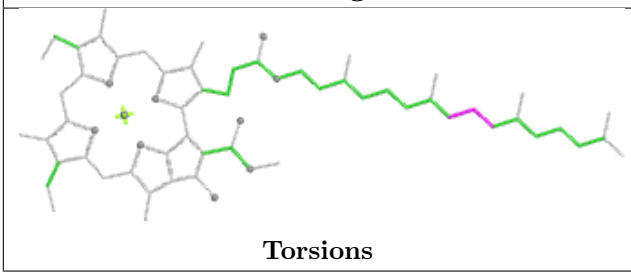
## Ligand CLA B 803



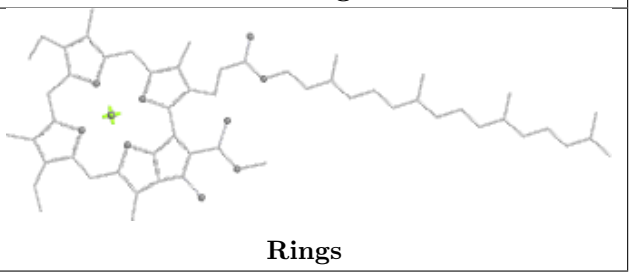
Bond lengths



Bond angles

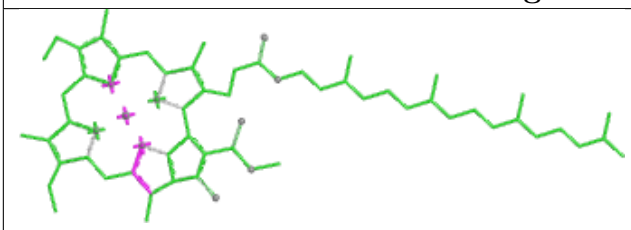


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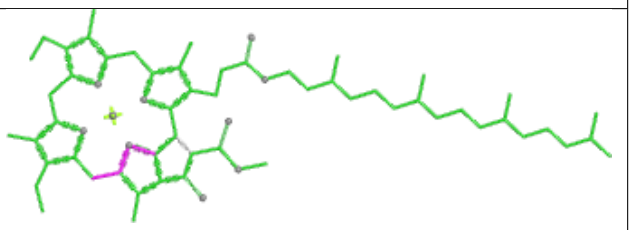


Rings

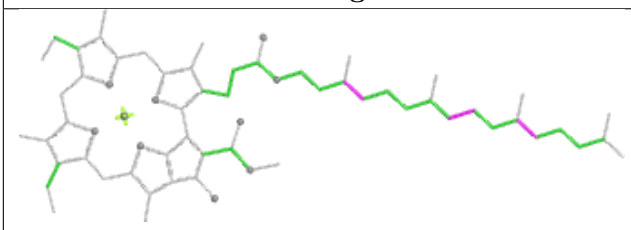
## Ligand CLA A 828



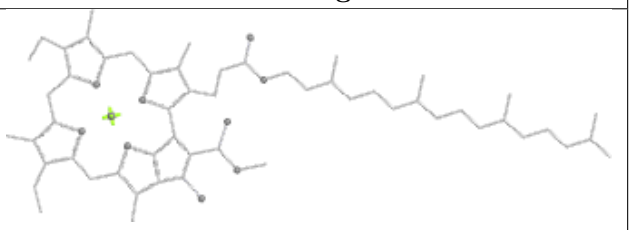
Bond lengths



Bond angles

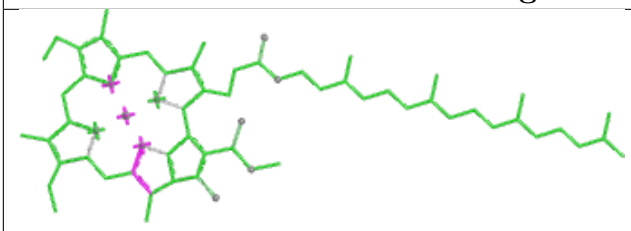


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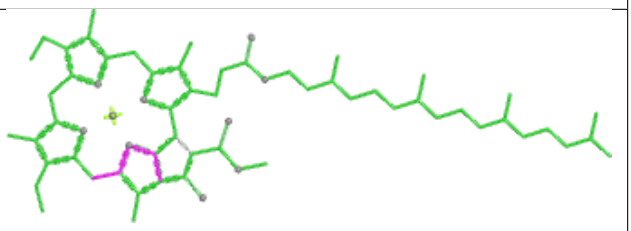


Rings

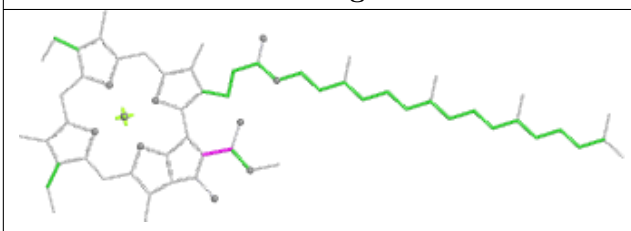
## Ligand CLA 62 602



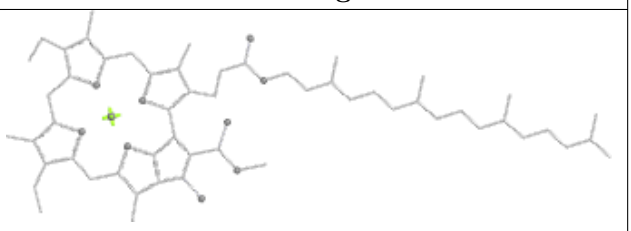
Bond lengths



Bond angles

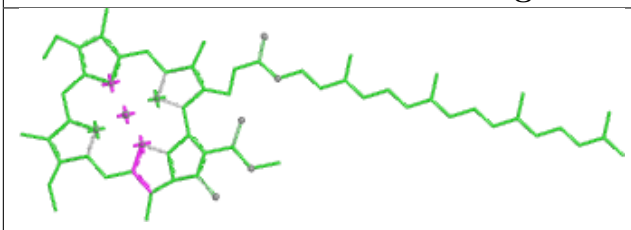


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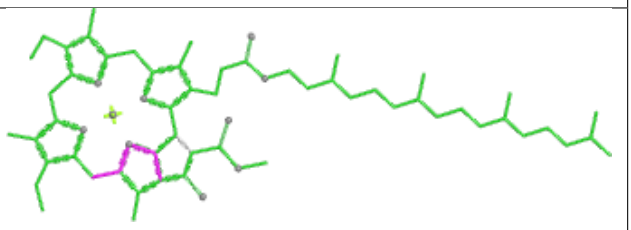


Rings

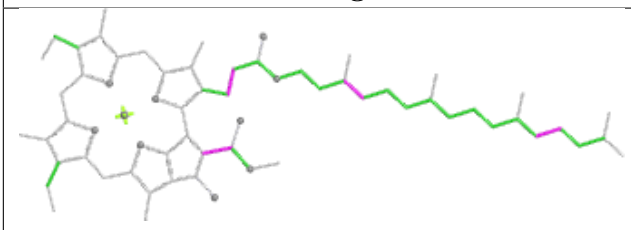
## Ligand CLA A2 830



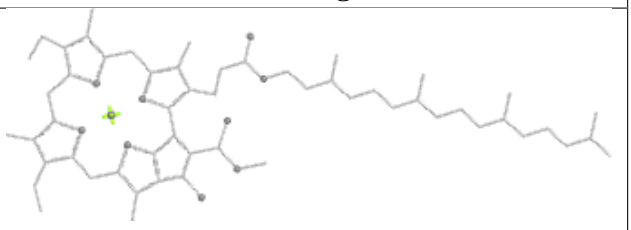
Bond lengths



Bond angles

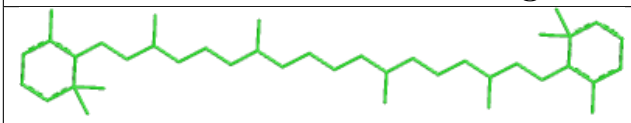


Torsions

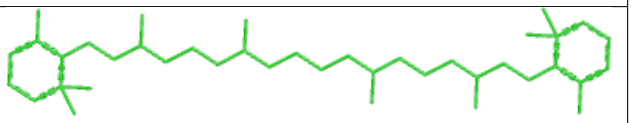


Rings

## Ligand BCR G 205



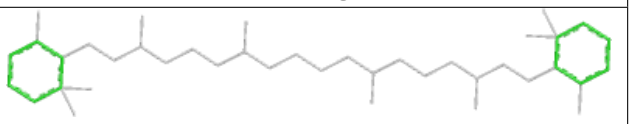
Bond lengths



Bond angles

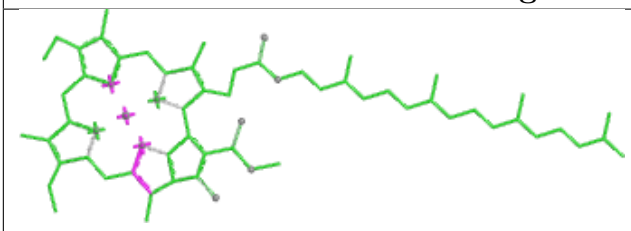


Torsions

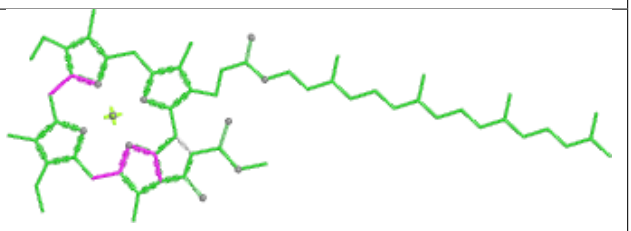


Rings

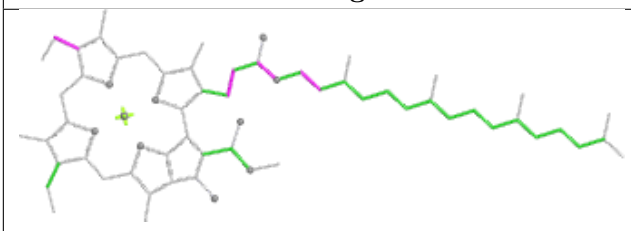
## Ligand CLA 92 613



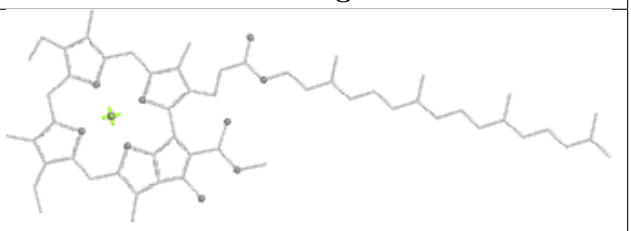
Bond lengths



Bond angles

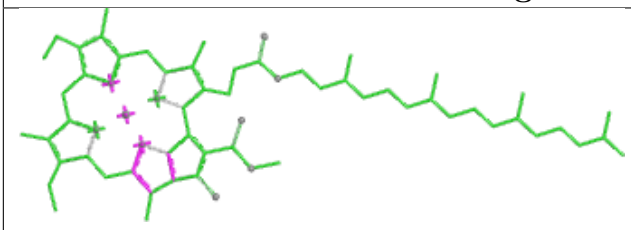


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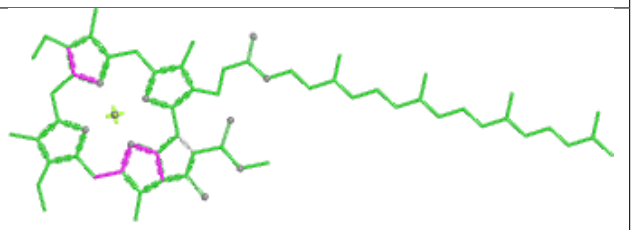


Rings

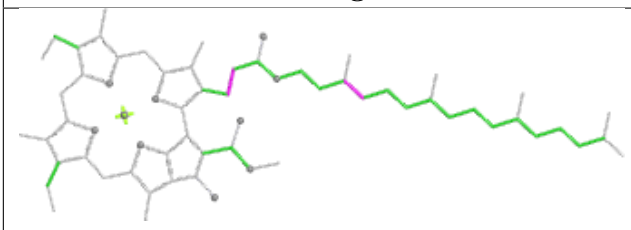
## Ligand CLA A2 803



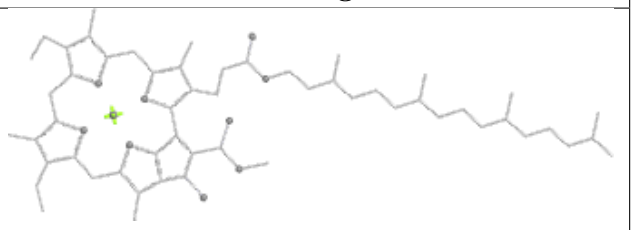
Bond lengths



Bond angles

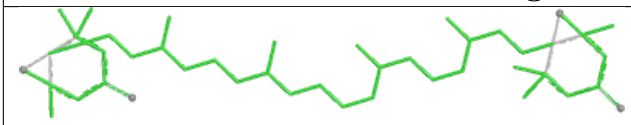


Torsions

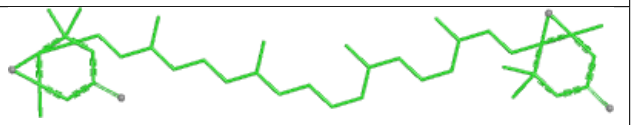


Rings

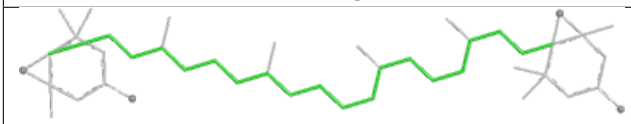
## Ligand XAT Z 618



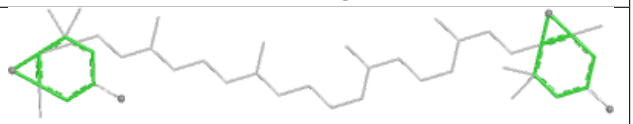
Bond lengths



Bond angles

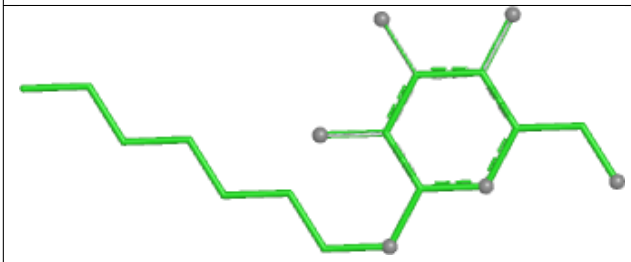


Torsions

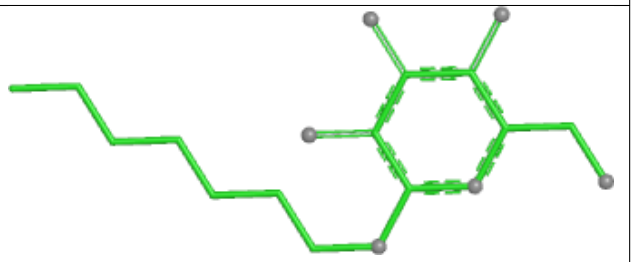


Rings

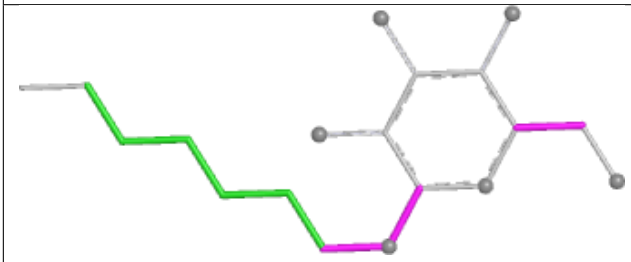
## Ligand LMU 1 622



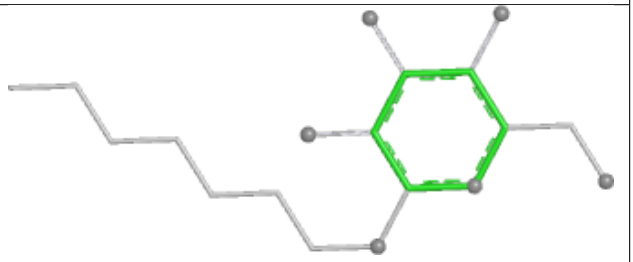
Bond lengths



Bond angles

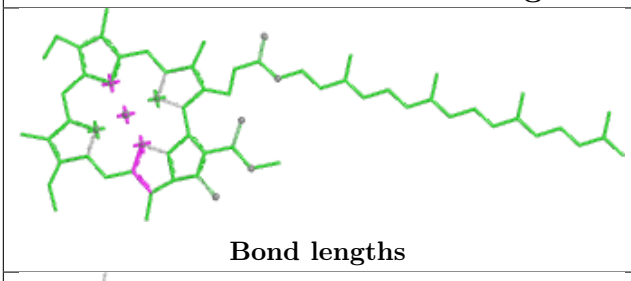


Torsions

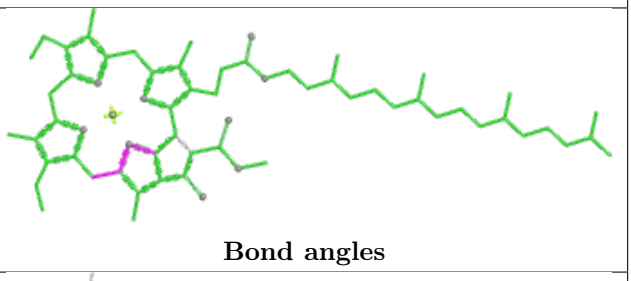


Rings

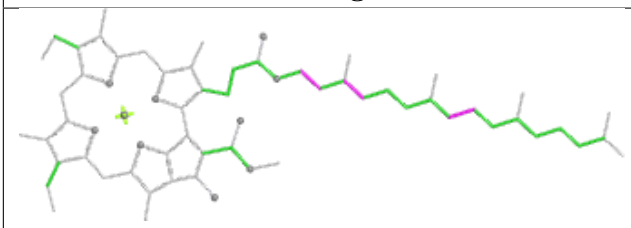
## Ligand CLA B 824



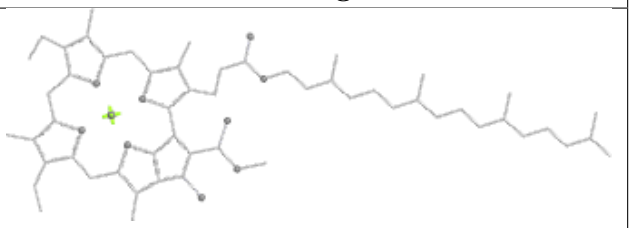
Bond lengths



Bond angles

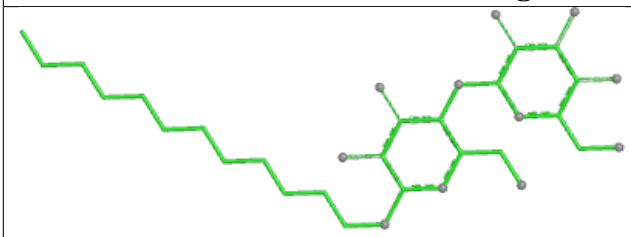


Torsions

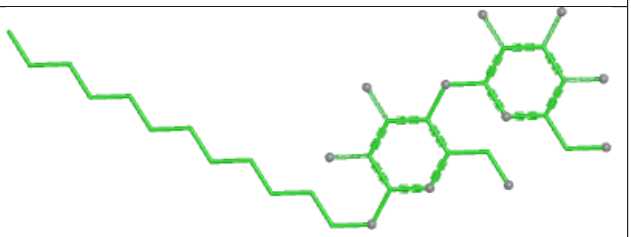


Rings

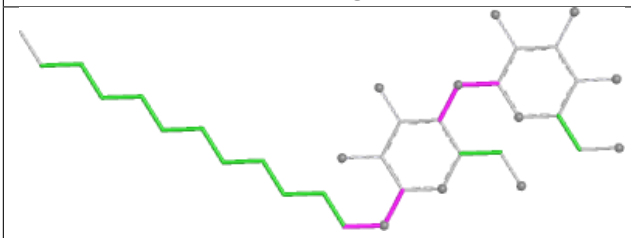
## Ligand LMU 12 621



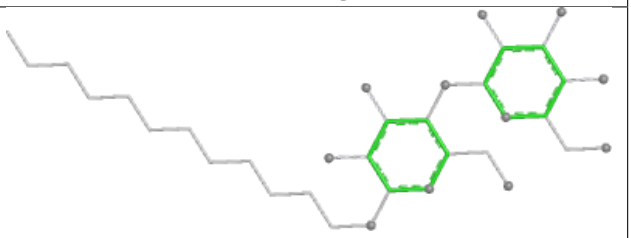
Bond lengths



Bond angles

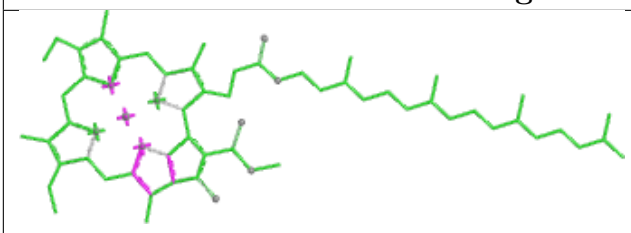


Torsions

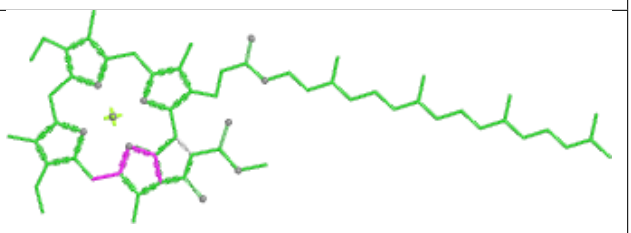


Rings

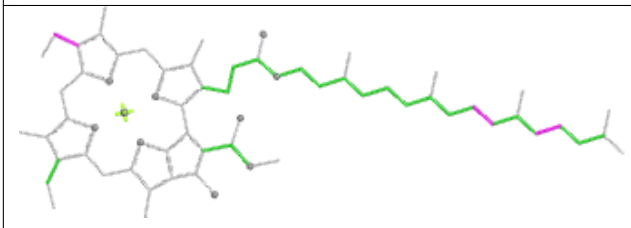
## Ligand CLA B2 818



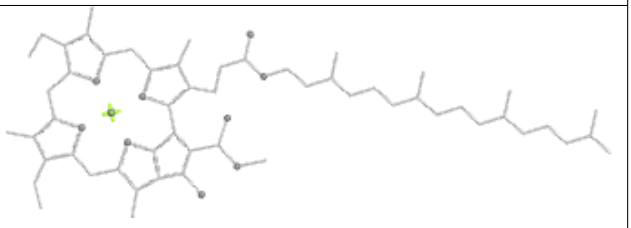
Bond lengths



Bond angles

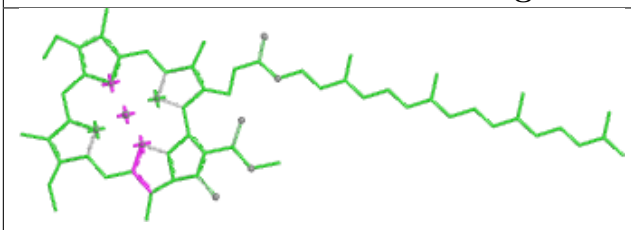


Torsions

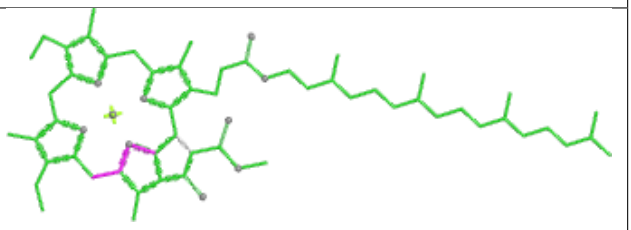


Rings

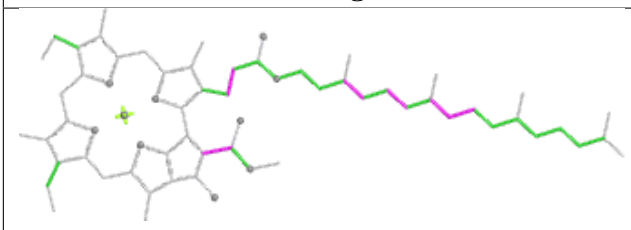
## Ligand CLA A2 810



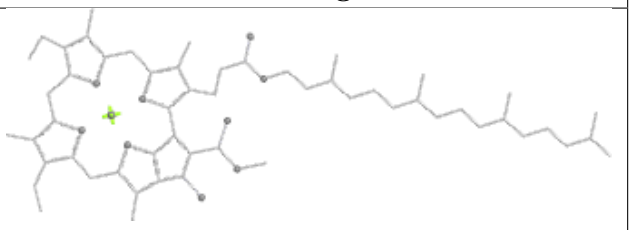
Bond lengths



Bond angles

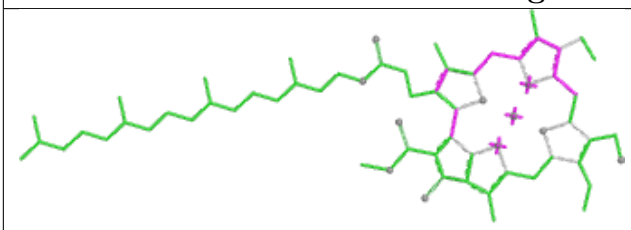


Torsions

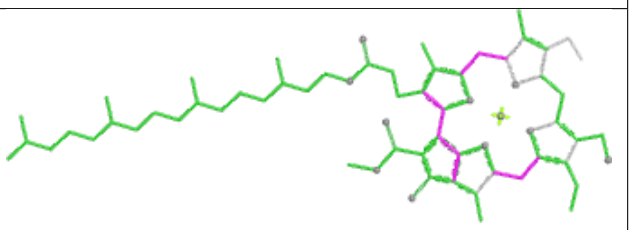


Rings

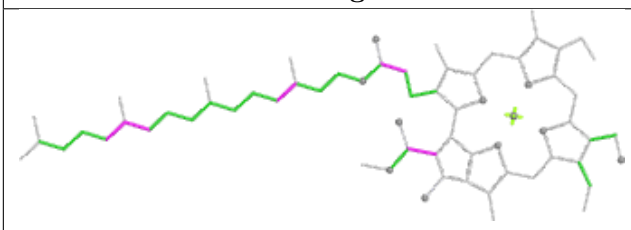
## Ligand CHL 8 601



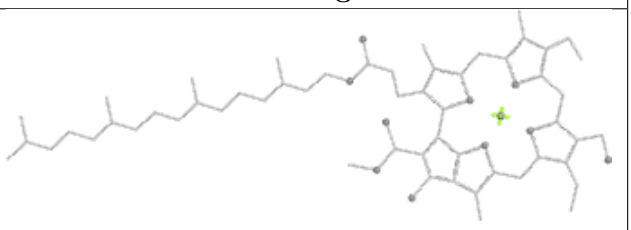
Bond lengths



Bond angles

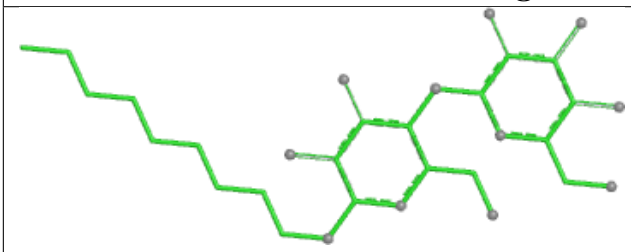


Torsions

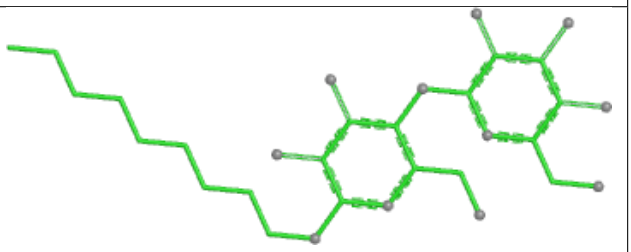


Rings

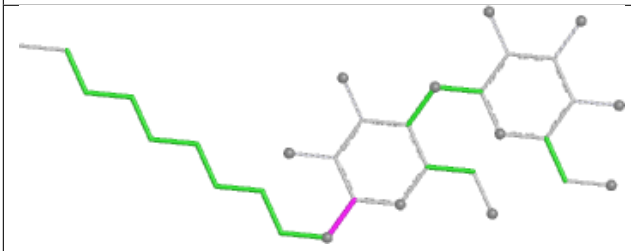
## Ligand LMU 72 627



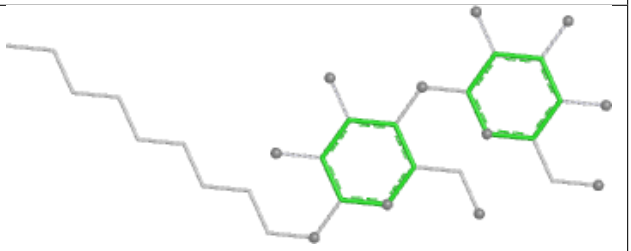
Bond lengths



Bond angles

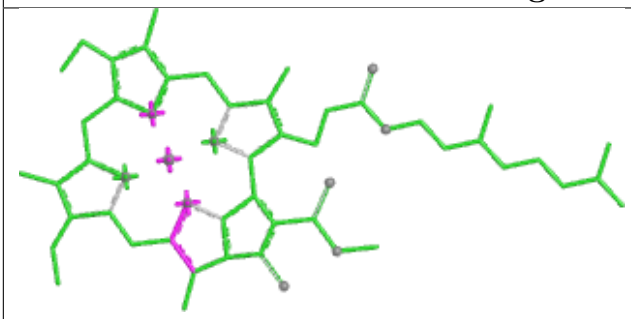


Torsions

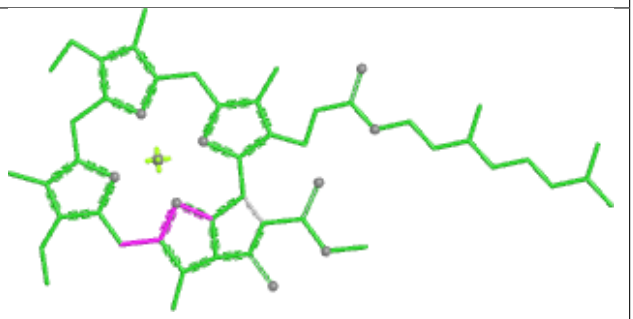


Rings

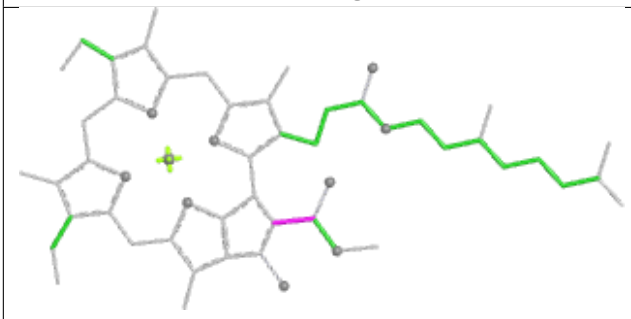
**Ligand CLA 6 622**



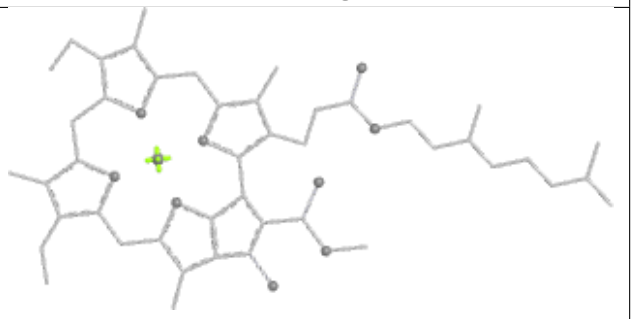
Bond lengths



Bond angles

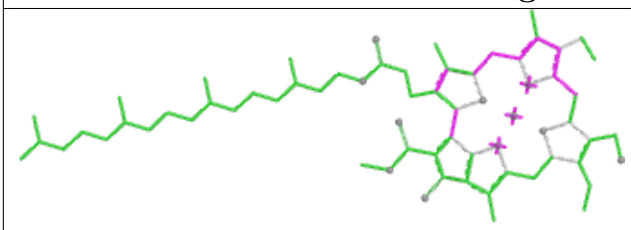


Torsions

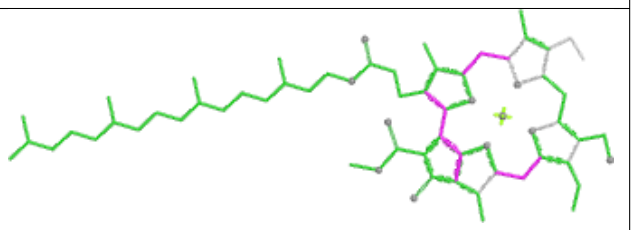


Rings

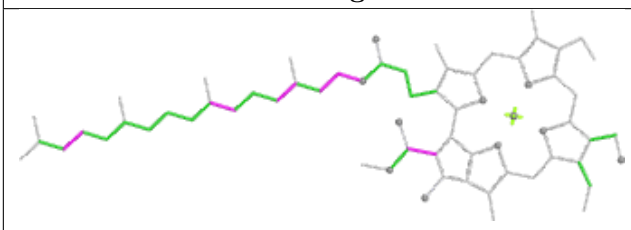
**Ligand CHL 82 607**



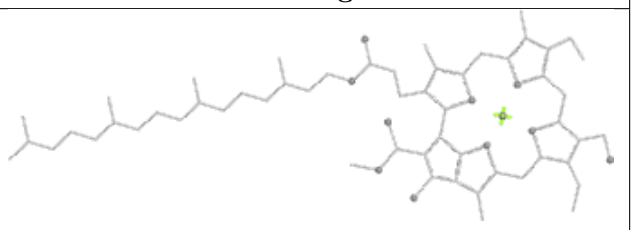
Bond lengths



Bond angles

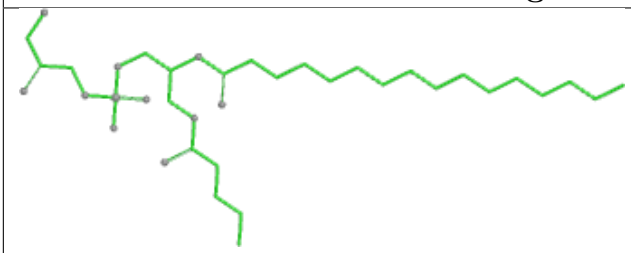


Torsions

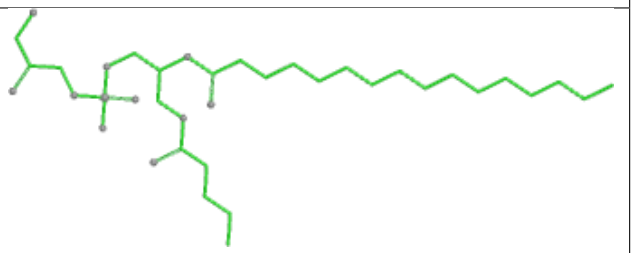


Rings

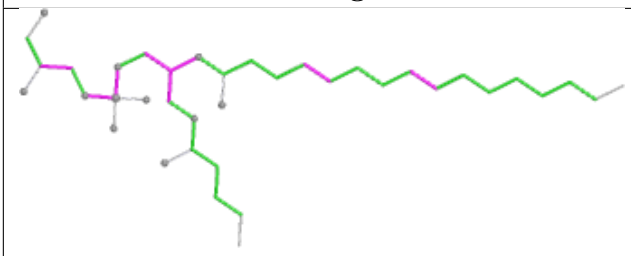
**Ligand LHG 4 623**



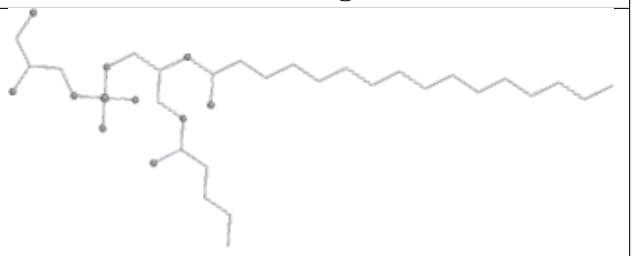
Bond lengths



Bond angles

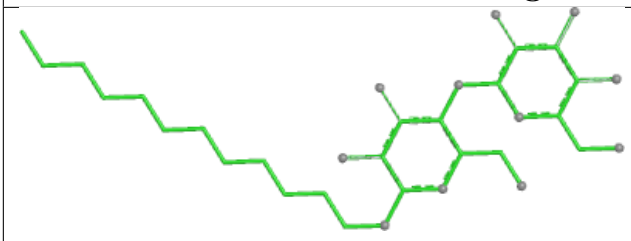


Torsions

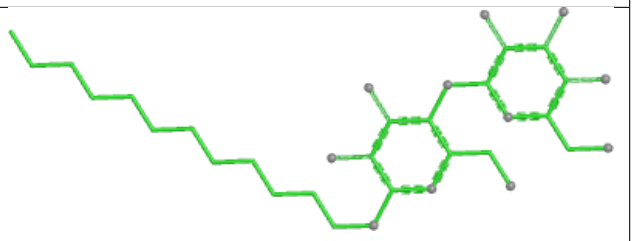


Rings

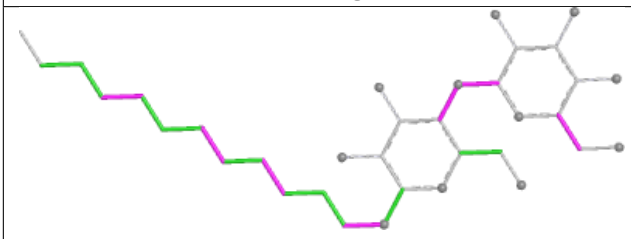
**Ligand LMU 8 627**



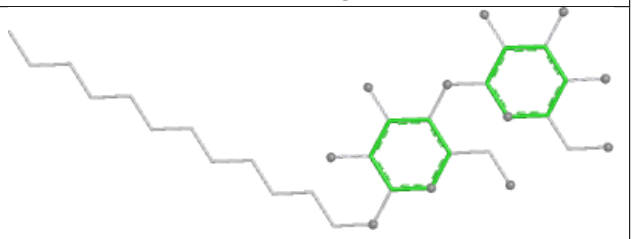
Bond lengths



Bond angles

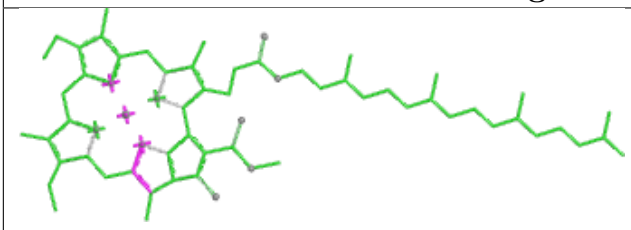


Torsions

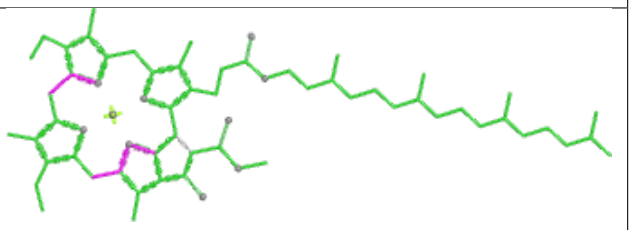


Rings

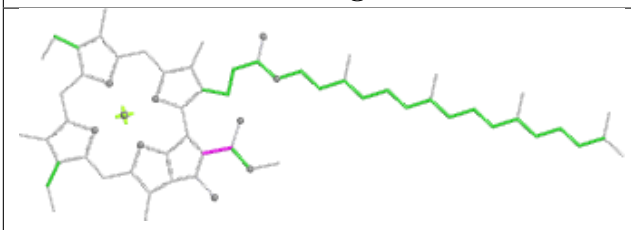
## Ligand CLA 5 602



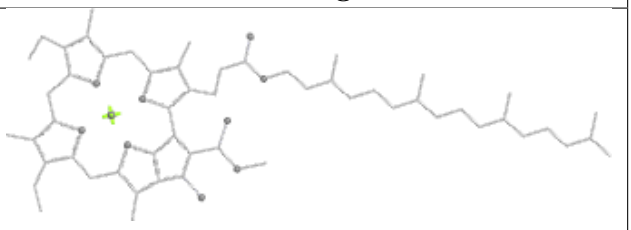
Bond lengths



Bond angles

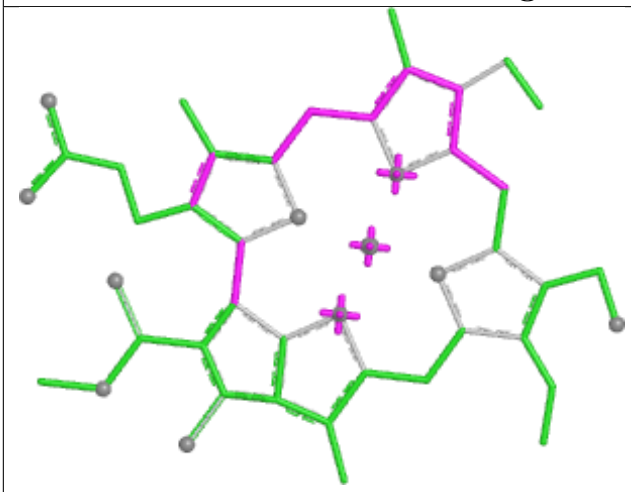


Torsions

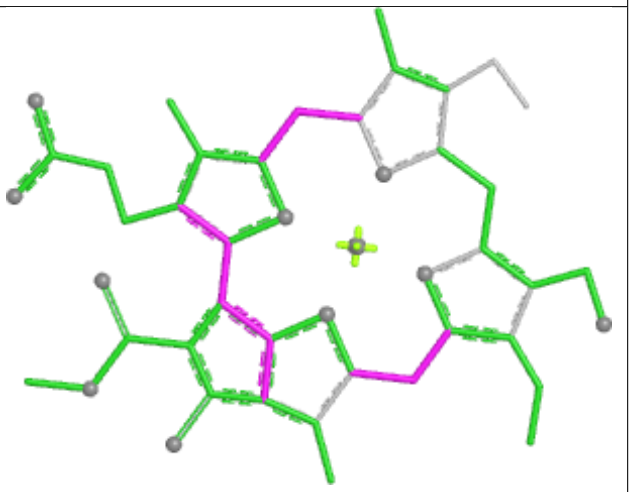


Rings

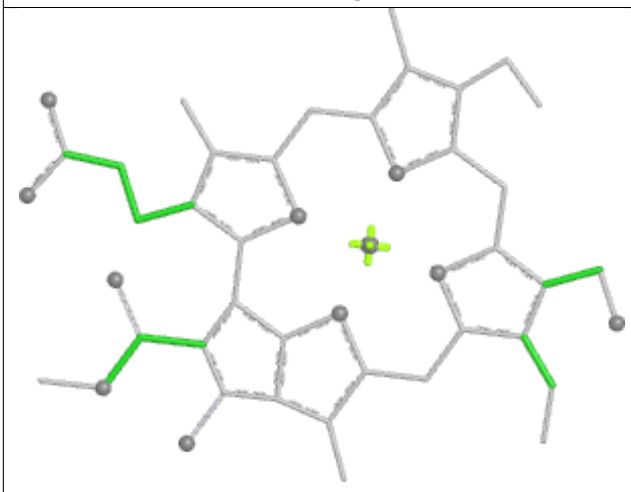
## Ligand CHL 42 618



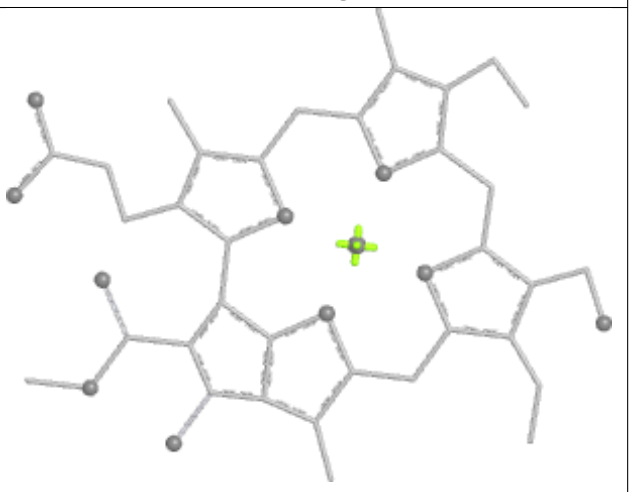
Bond lengths



Bond angles

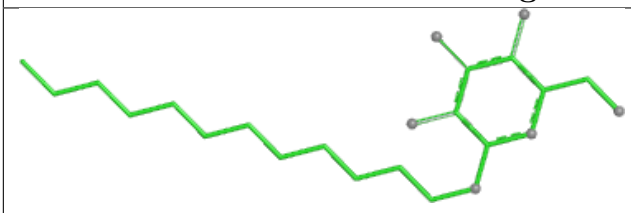


Torsions

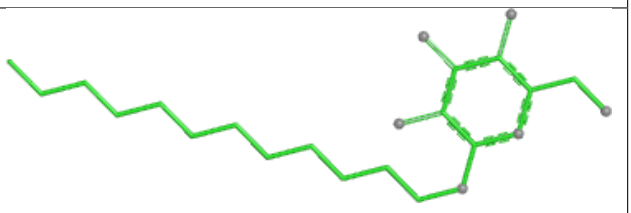


Rings

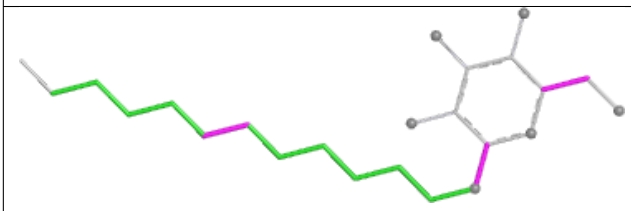
## Ligand LMU A 864



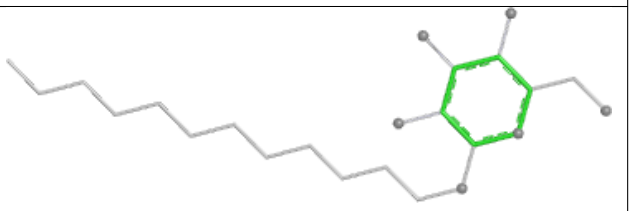
Bond lengths



Bond angles

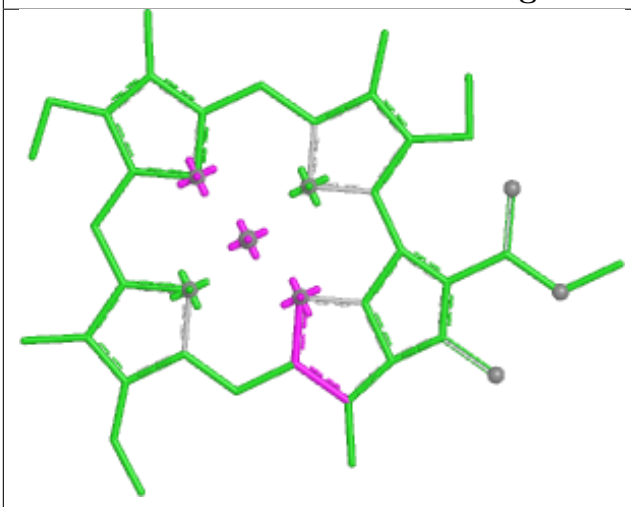


Torsions

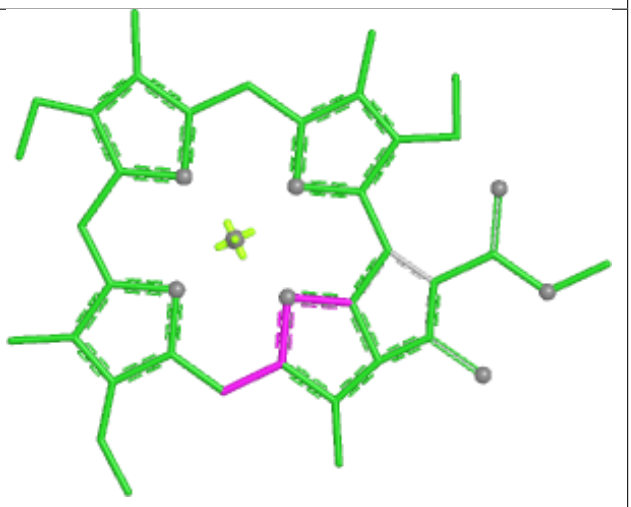


Rings

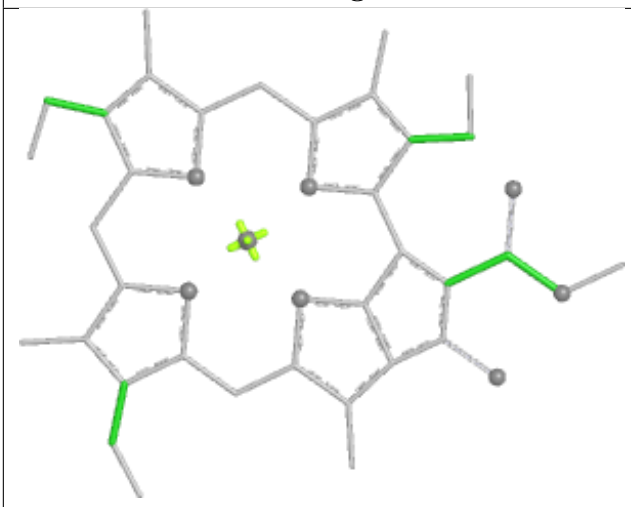
## Ligand CLA 32 606



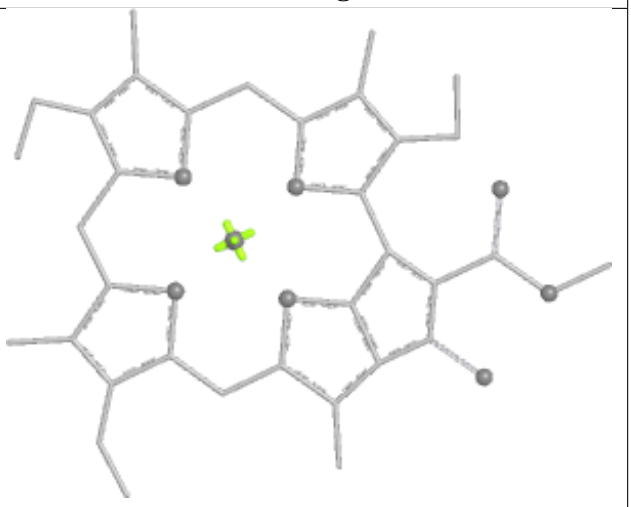
Bond lengths



Bond angles

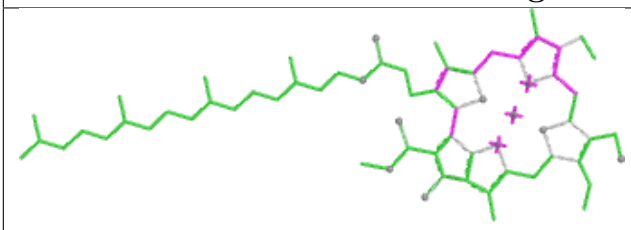


Torsions

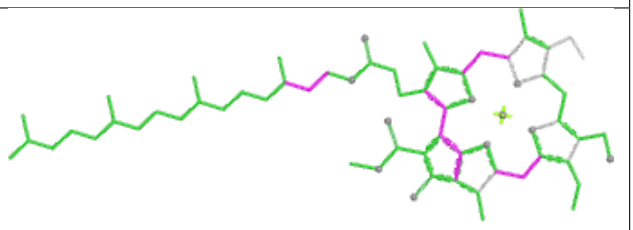


Rings

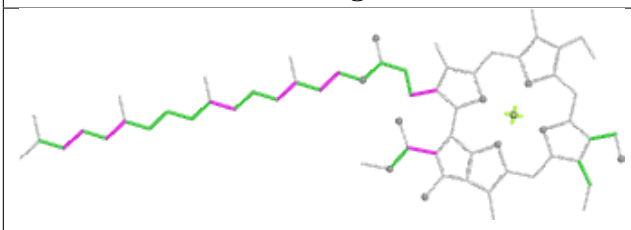
## Ligand CHL 6 607



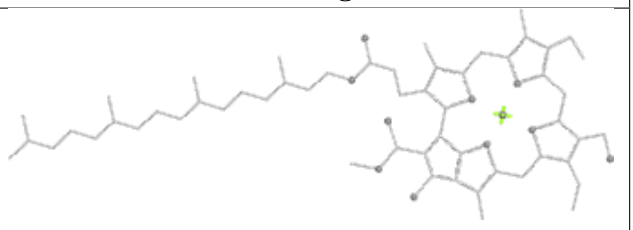
Bond lengths



Bond angles

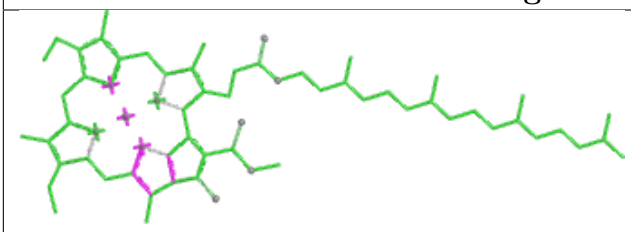


Torsions

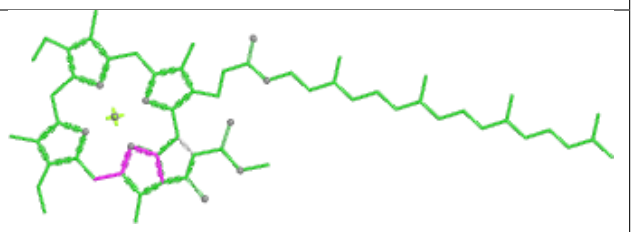


Rings

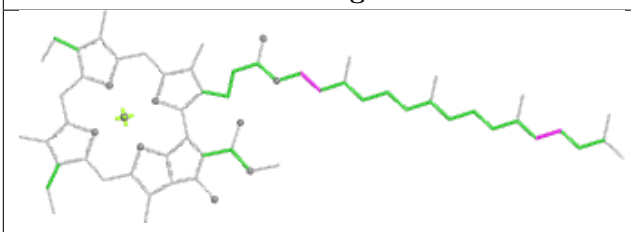
## Ligand CLA A 827



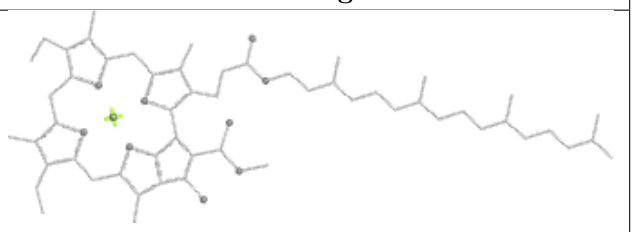
Bond lengths



Bond angles

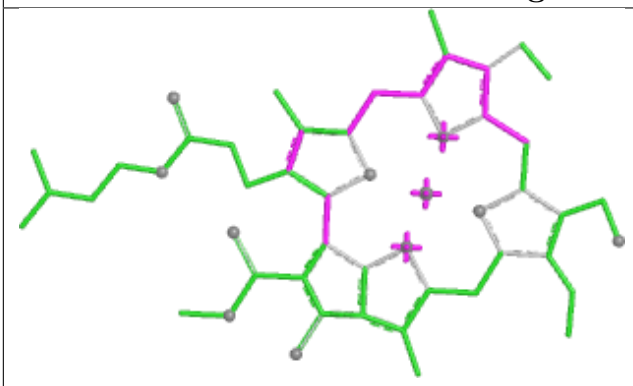


Torsions

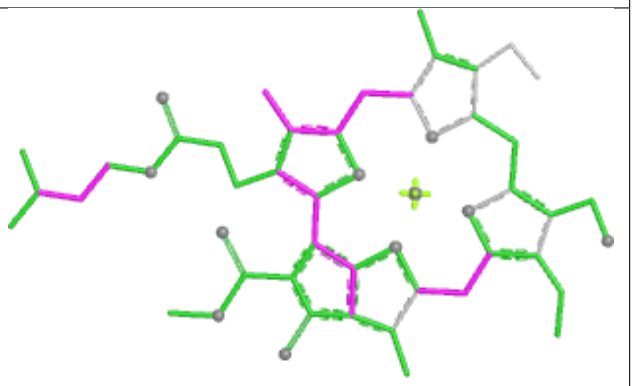


Rings

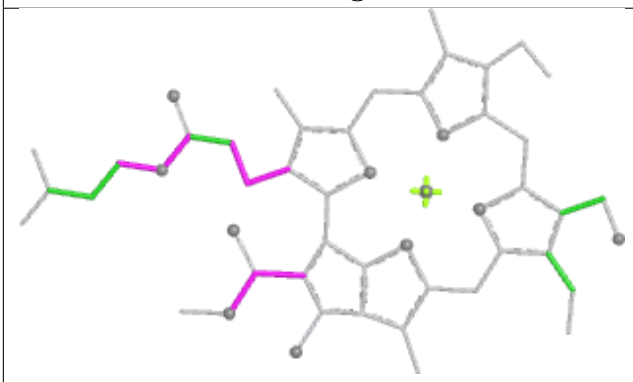
## Ligand CHL 9 607



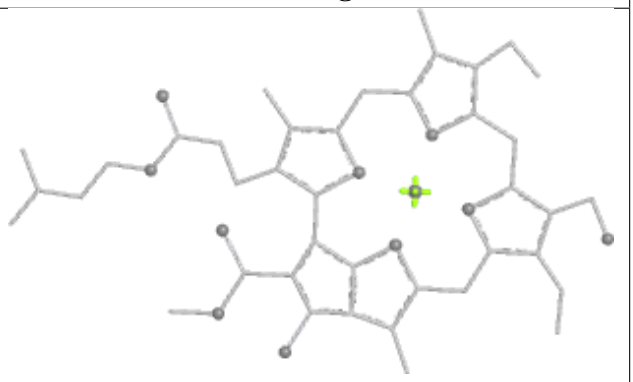
Bond lengths



Bond angles



Torsions



Rings

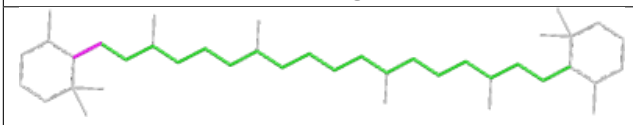
## Ligand BCR G2 205



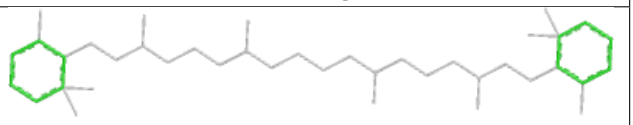
Bond lengths



Bond angles

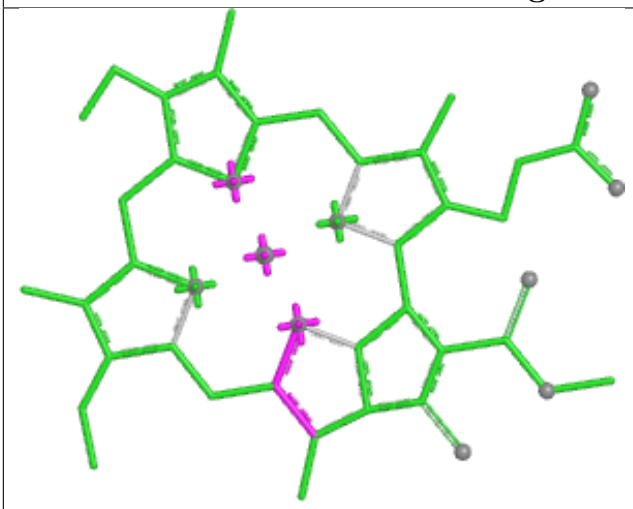


Torsions

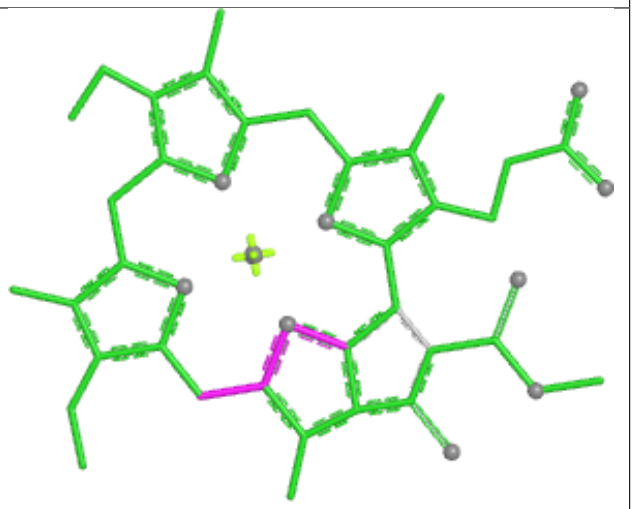


Rings

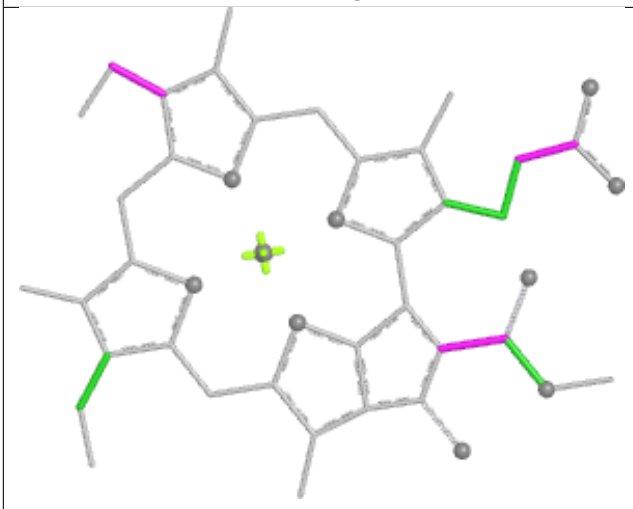
## Ligand CLA 5 612



Bond lengths



Bond angles

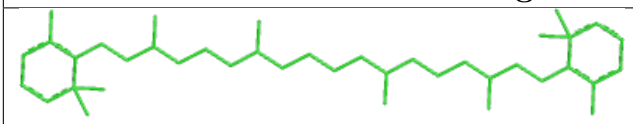


Torsions

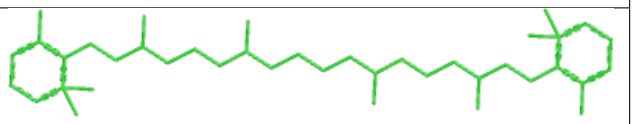


Rings

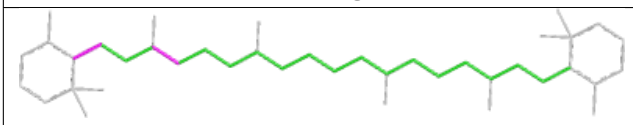
## Ligand BCR L2 201



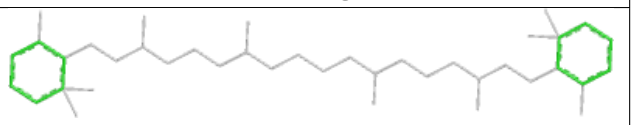
Bond lengths



Bond angles

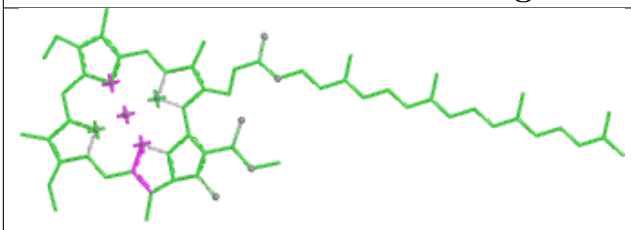


Torsions

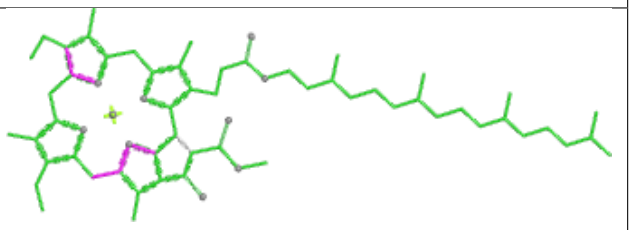


Rings

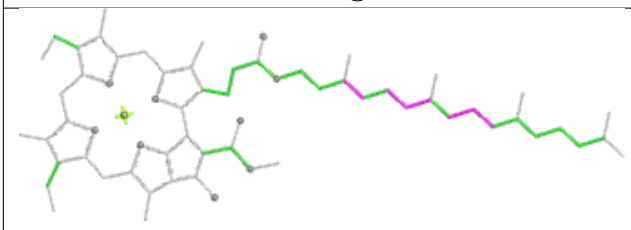
## Ligand CLA A2 829



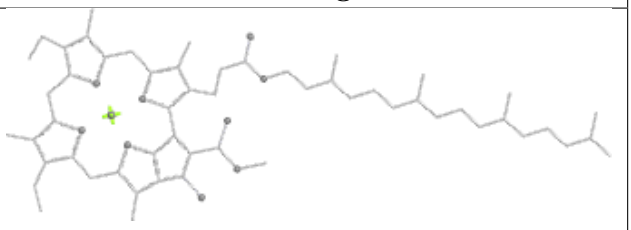
Bond lengths



Bond angles

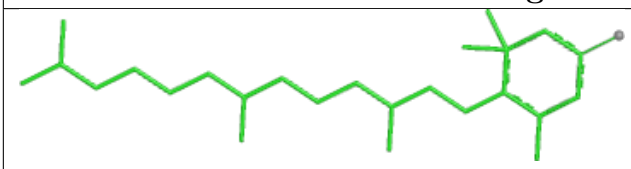


Torsions

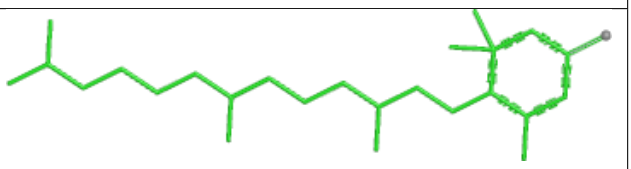


Rings

## Ligand LUT Z 619



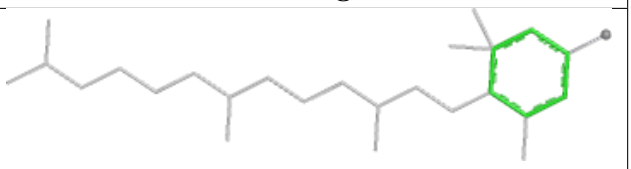
Bond lengths



Bond angles

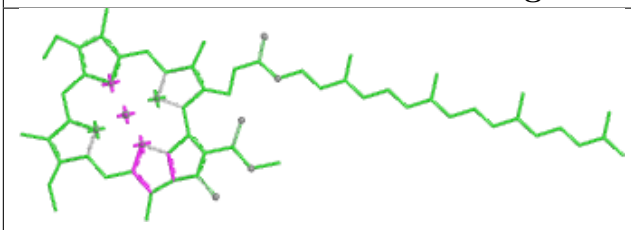


Torsions

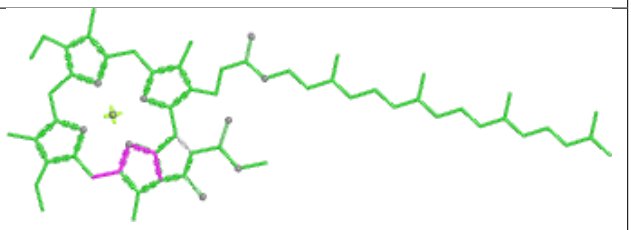


Rings

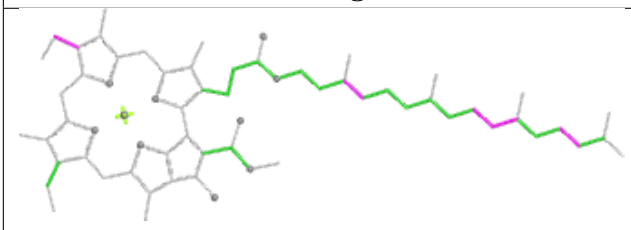
## Ligand CLA B 840



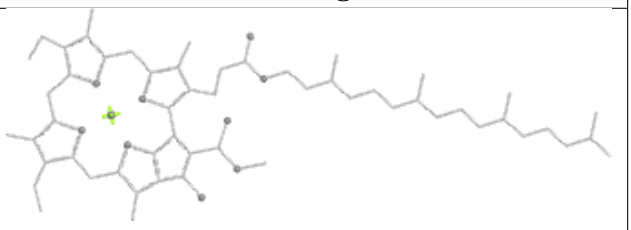
Bond lengths



Bond angles

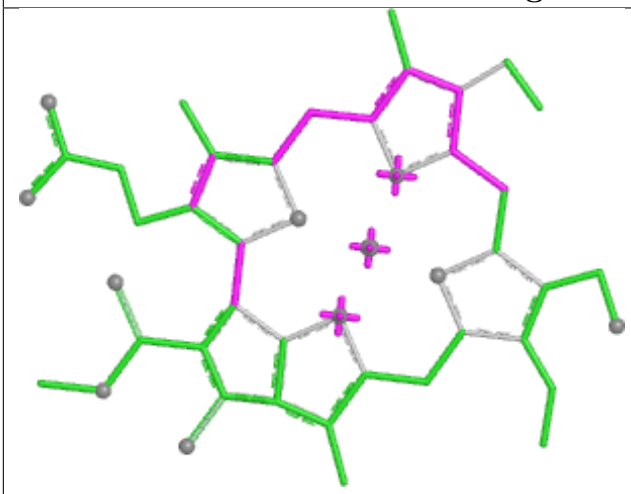


Torsions

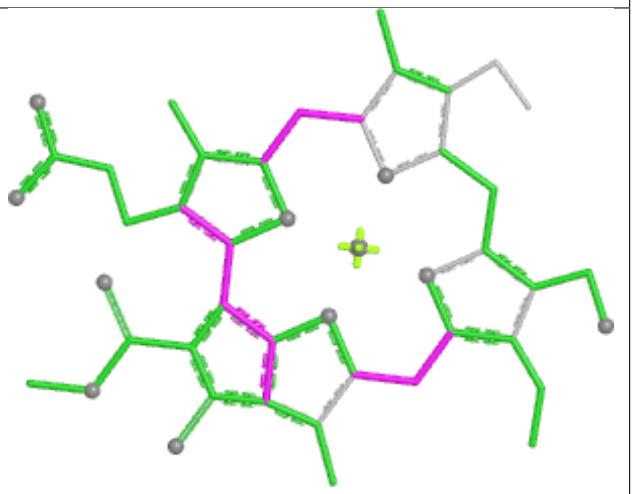


Rings

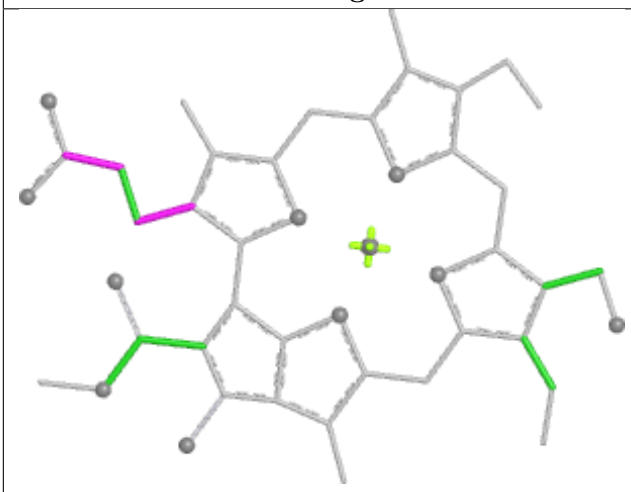
**Ligand CHL Z 606**



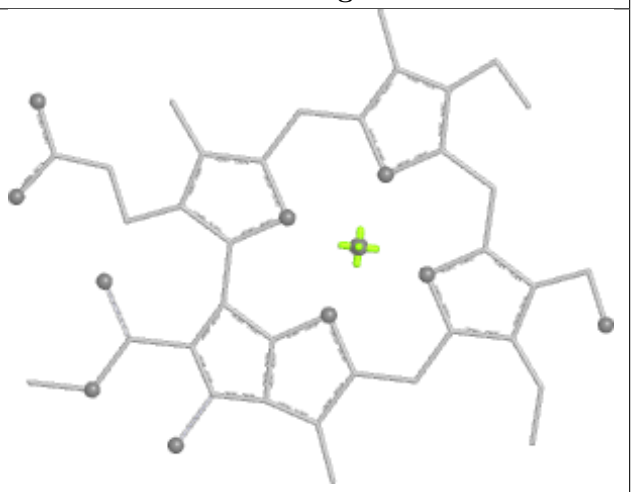
**Bond lengths**



**Bond angles**

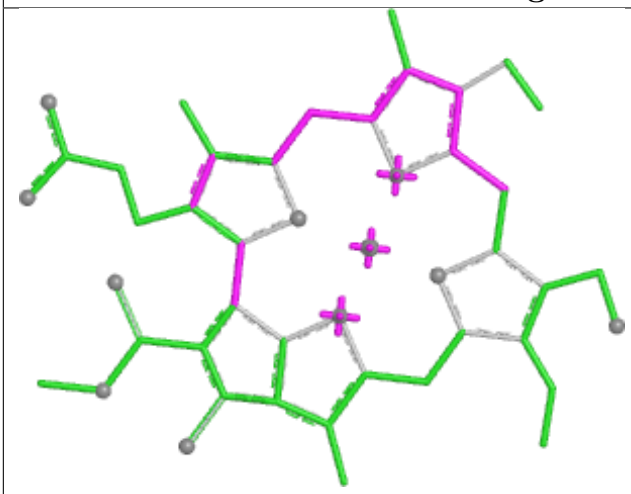


**Torsions**

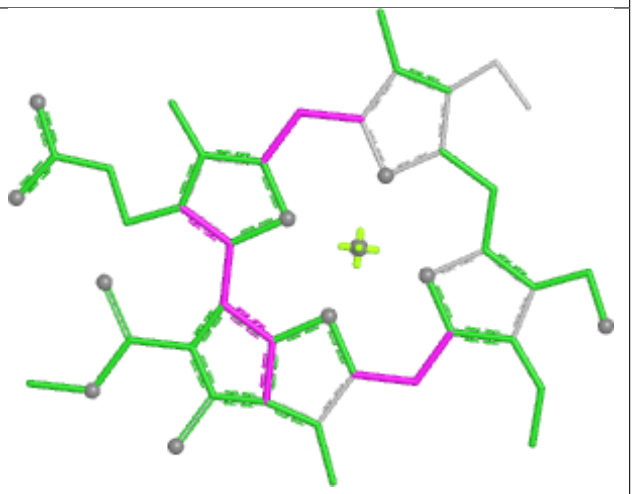


**Rings**

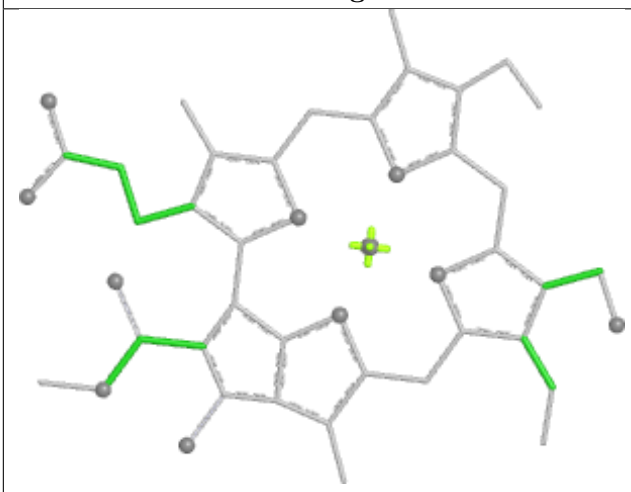
## Ligand CHL 4 618



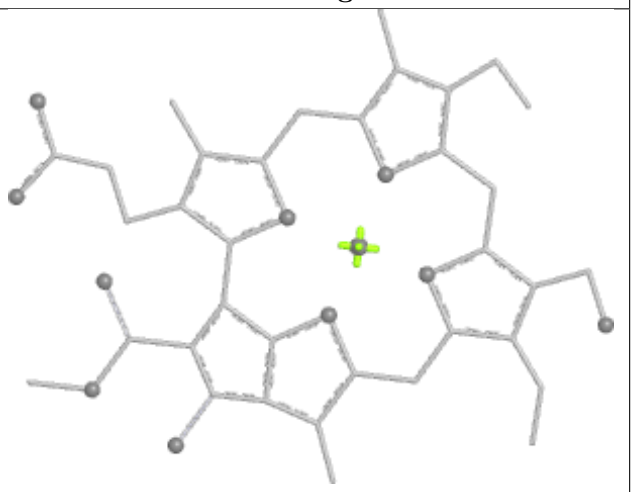
Bond lengths



Bond angles



Torsions

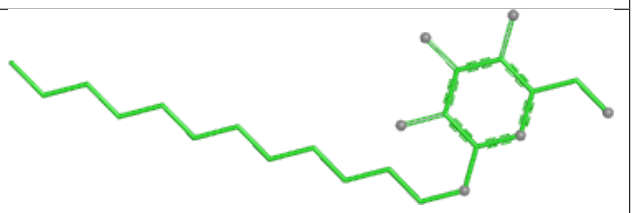


Rings

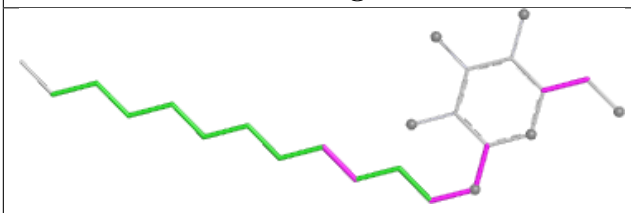
## Ligand LMU 1 625



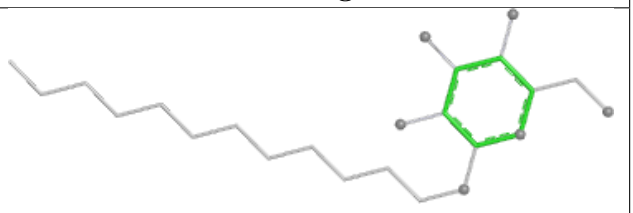
Bond lengths



Bond angles

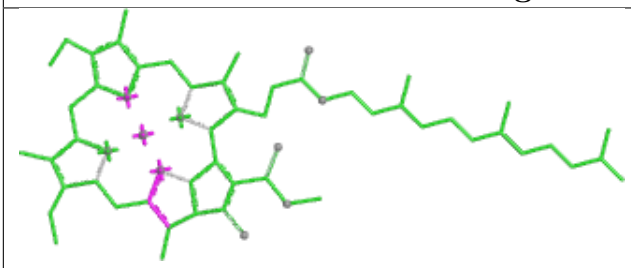


Torsions

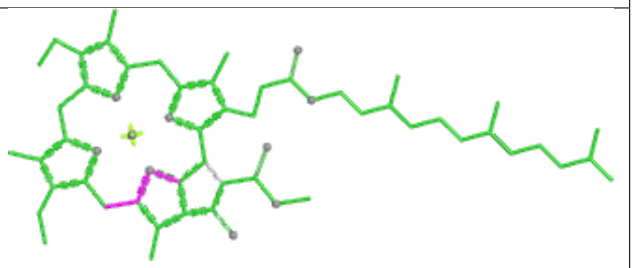


Rings

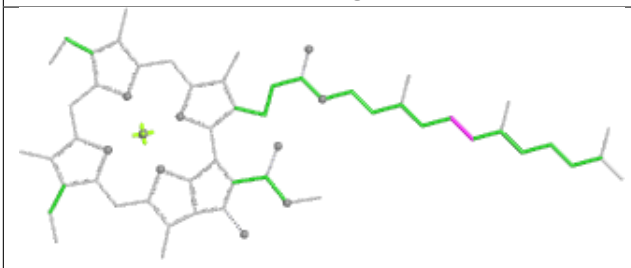
## Ligand CLA K2 203



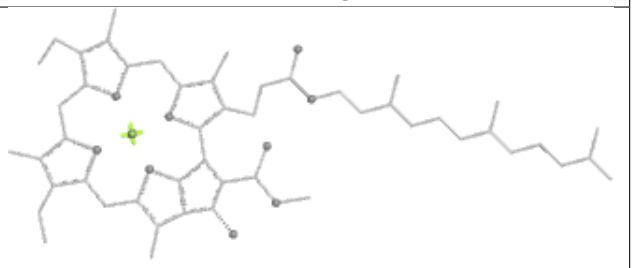
Bond lengths



Bond angles

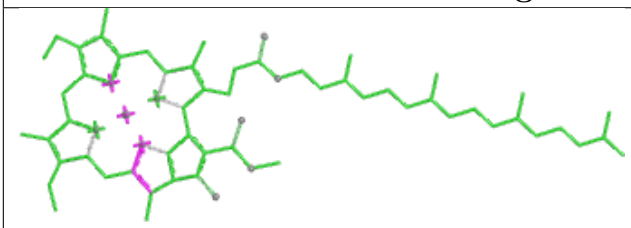


Torsions

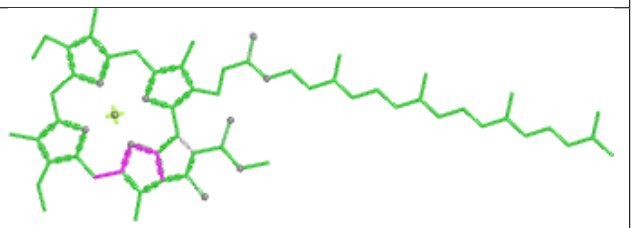


Rings

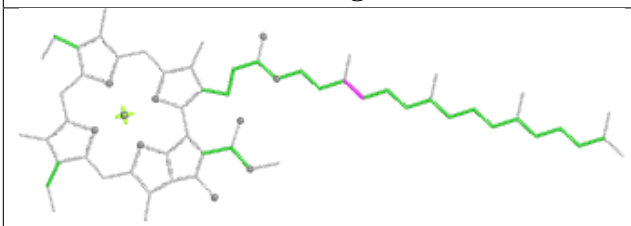
## Ligand CLA B2 810



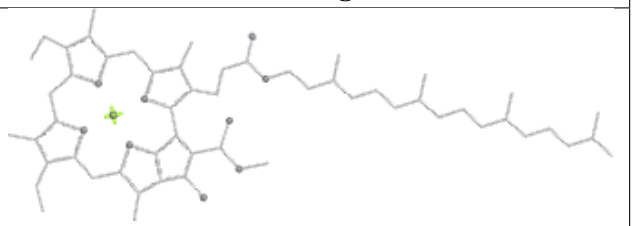
Bond lengths



Bond angles



Torsions



Rings

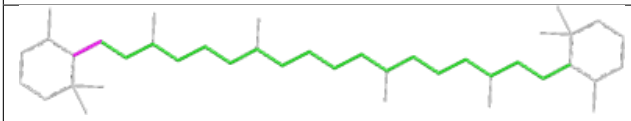
## Ligand BCR B 848



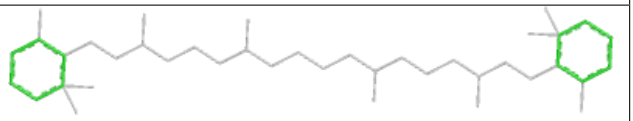
Bond lengths



Bond angles

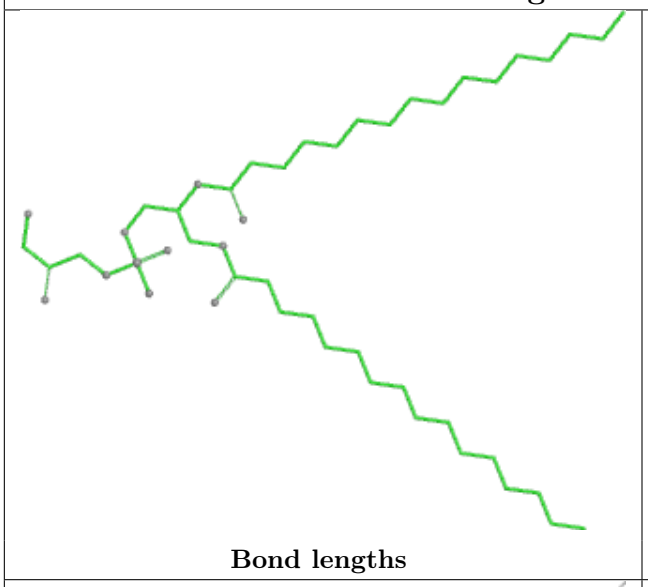


Torsions

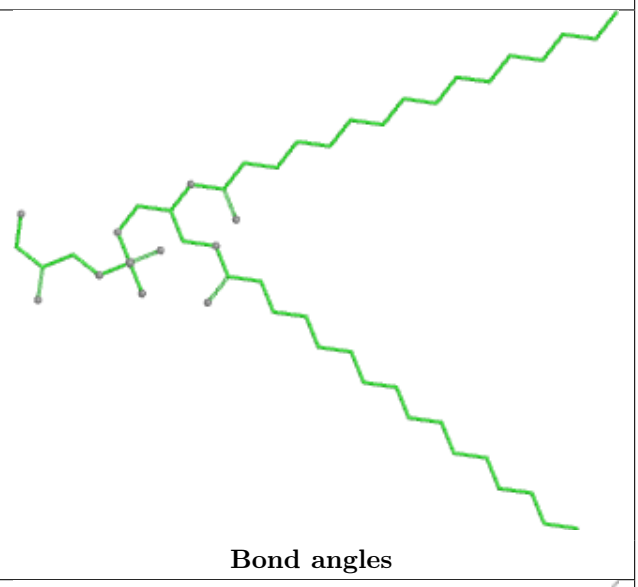


Rings

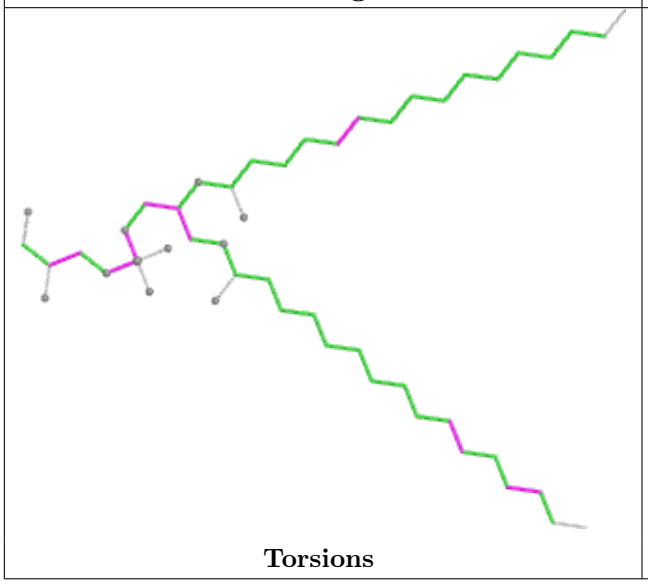
## Ligand LHG 7 625



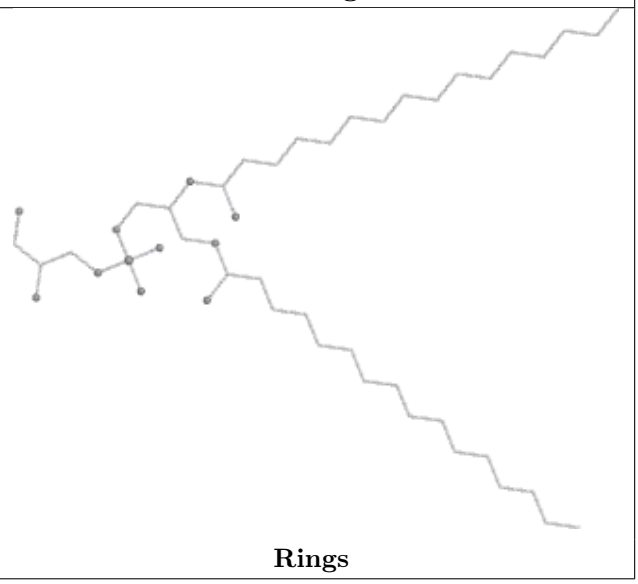
Bond lengths



Bond angles

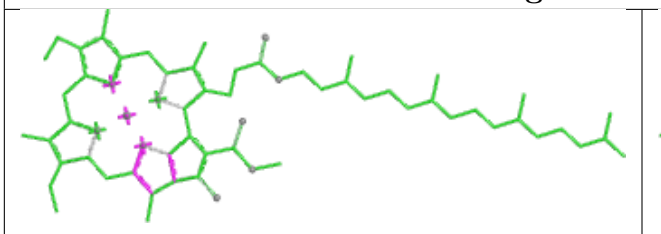


Torsions

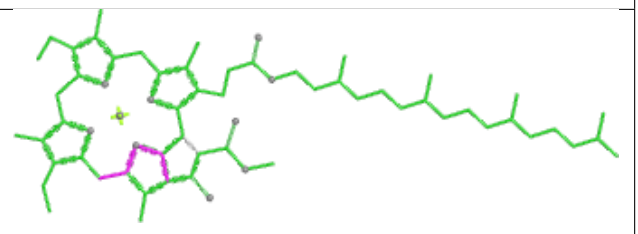


Rings

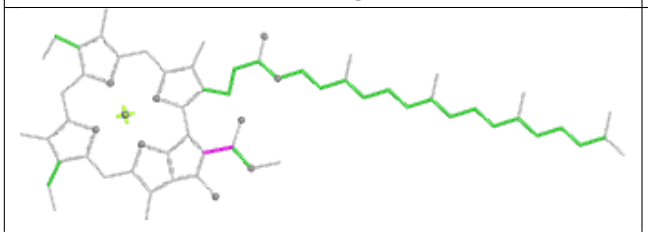
## Ligand CLA B 825



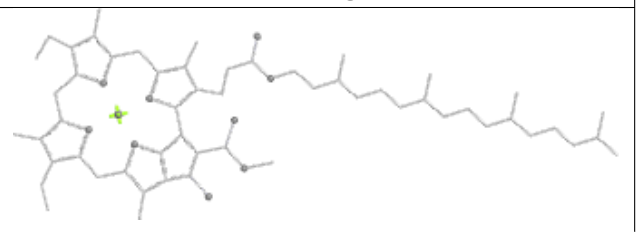
Bond lengths



Bond angles

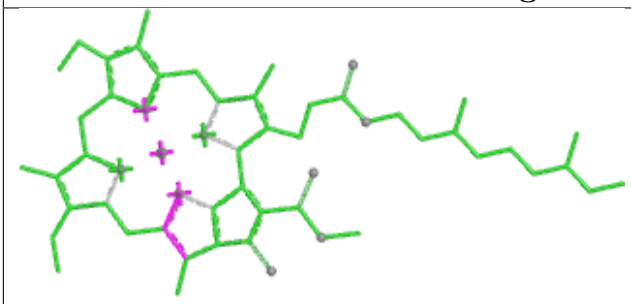


Torsions

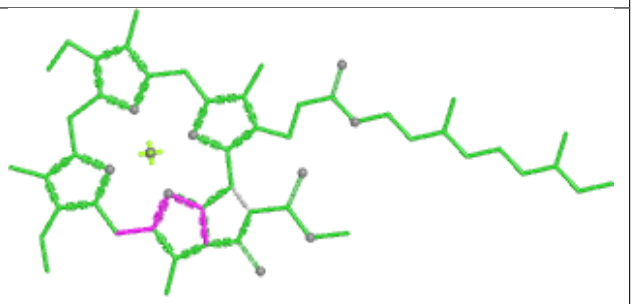


Rings

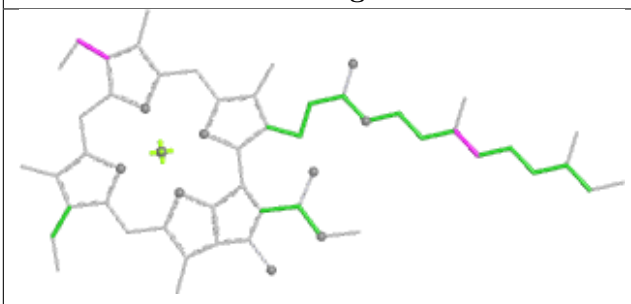
## Ligand CLA 52 613



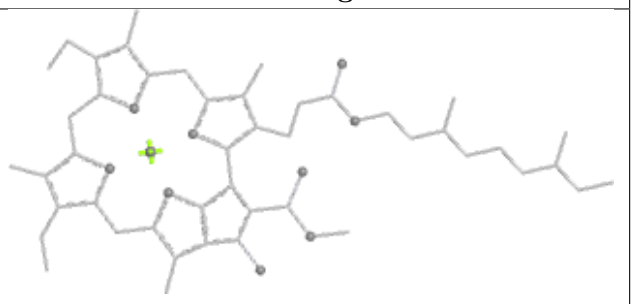
Bond lengths



Bond angles

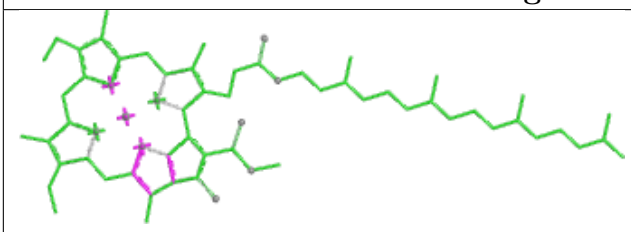


Torsions

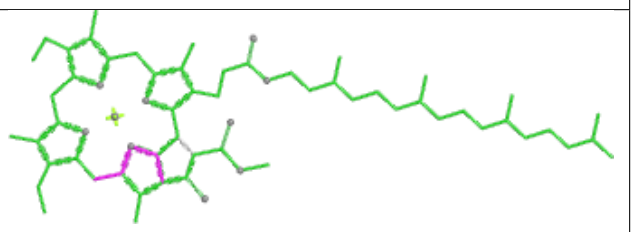


Rings

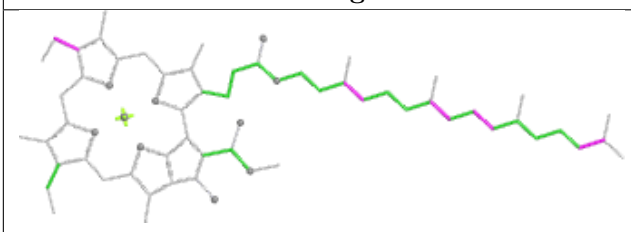
## Ligand CLA A 841



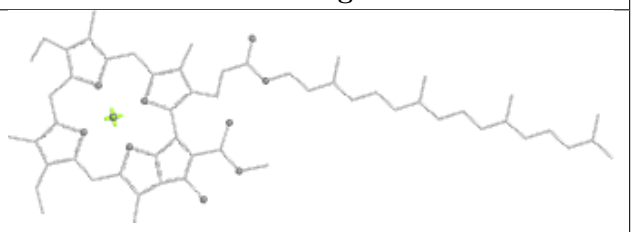
Bond lengths



Bond angles



Torsions

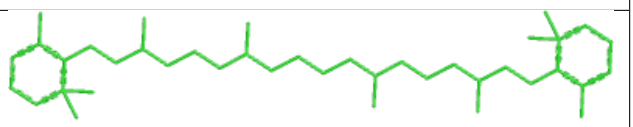


Rings

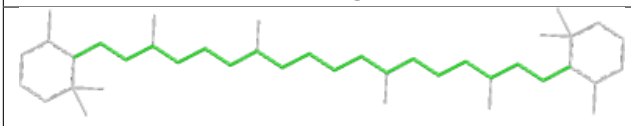
## Ligand BCR I2 172



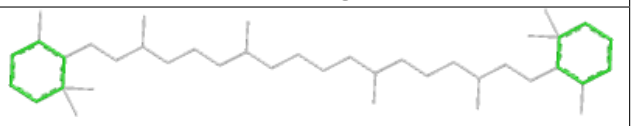
Bond lengths



Bond angles

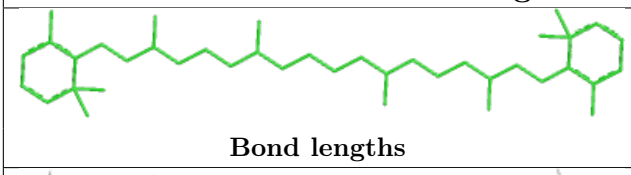


Torsions

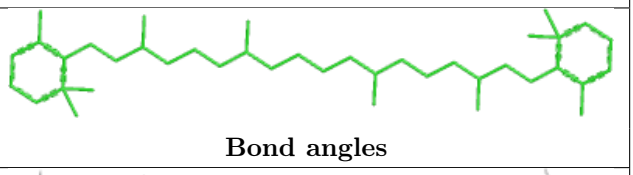


Rings

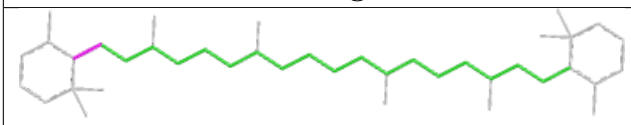
## Ligand BCR B2 848



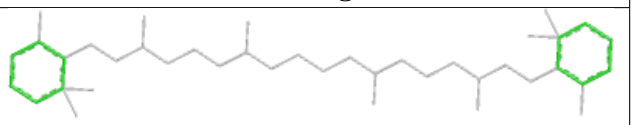
Bond lengths



Bond angles

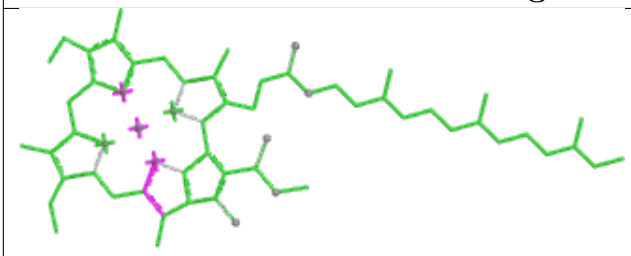


Torsions

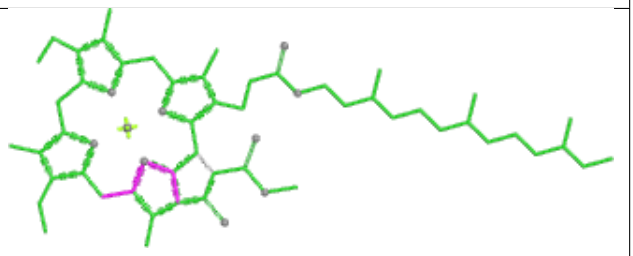


Rings

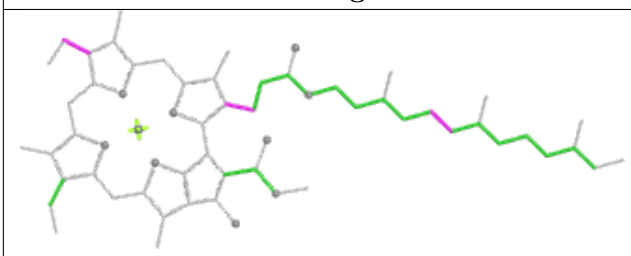
## Ligand CLA 1 611



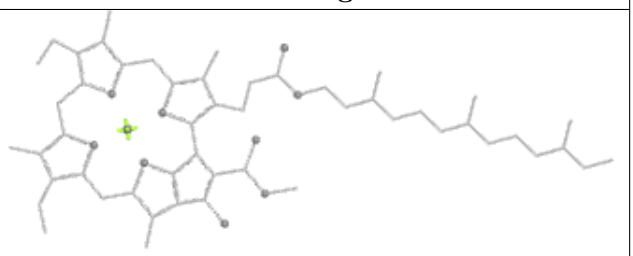
Bond lengths



Bond angles

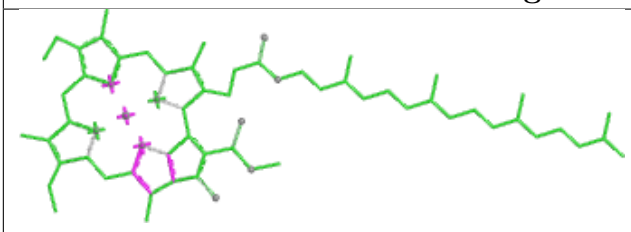


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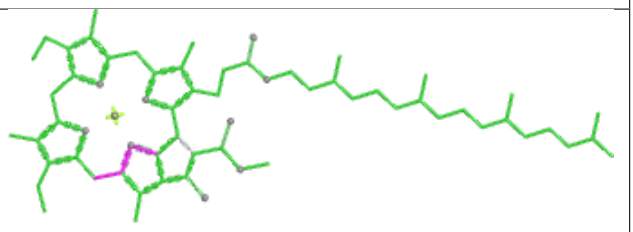


Rings

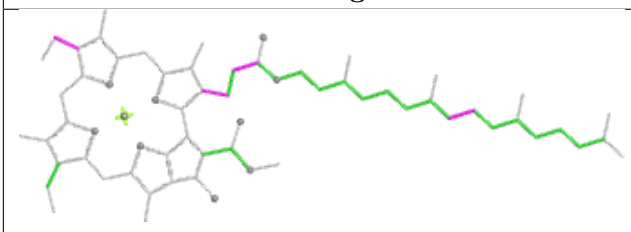
## Ligand CLA A 836



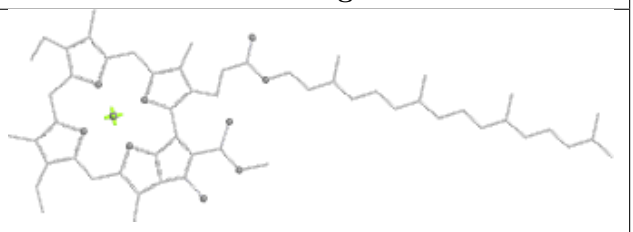
Bond lengths



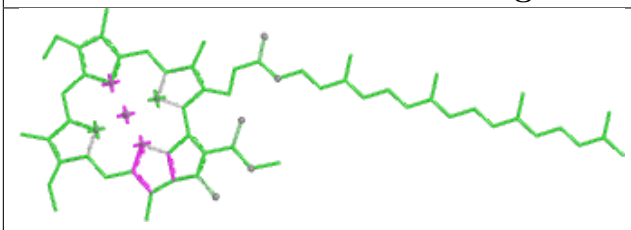
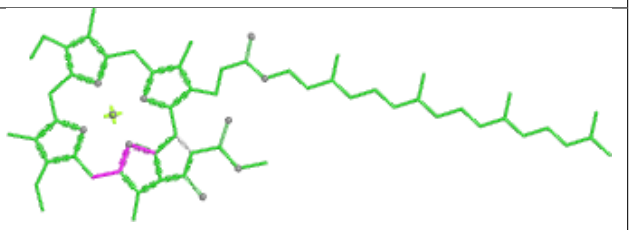
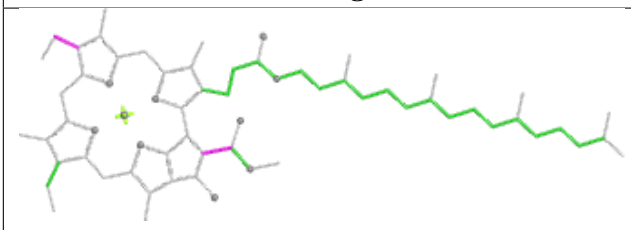
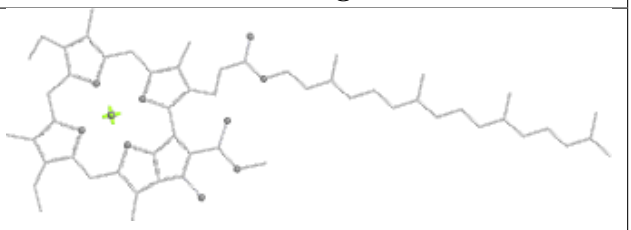
Bond angles

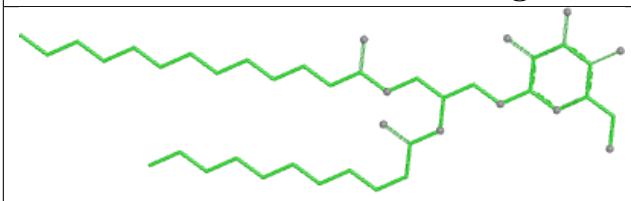
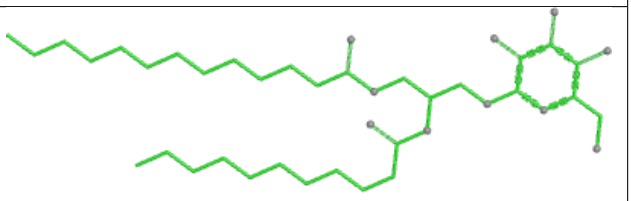
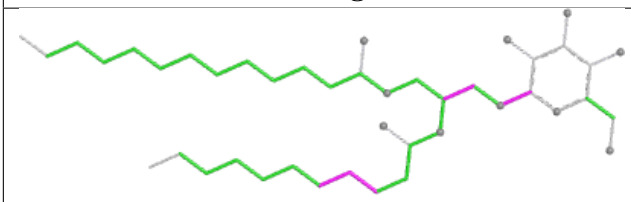
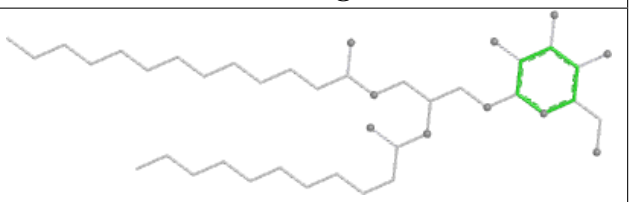


Torsions

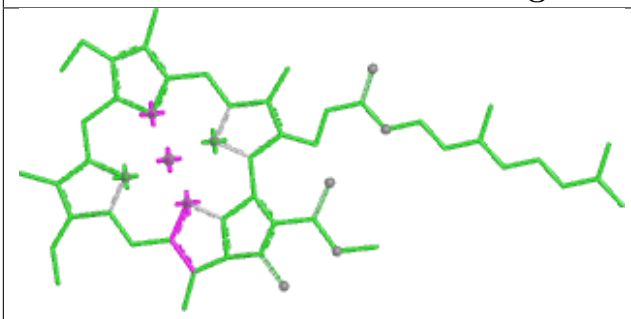


Rings

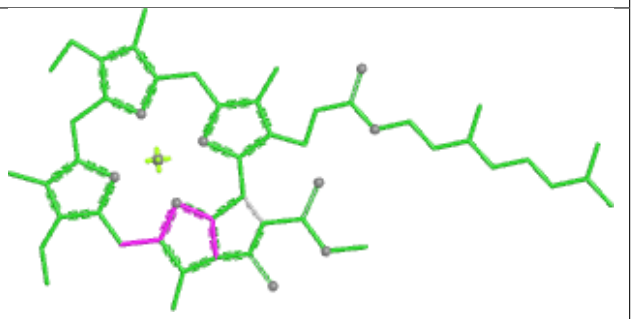
| Ligand CLA A2 842 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand LMG B2 852 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

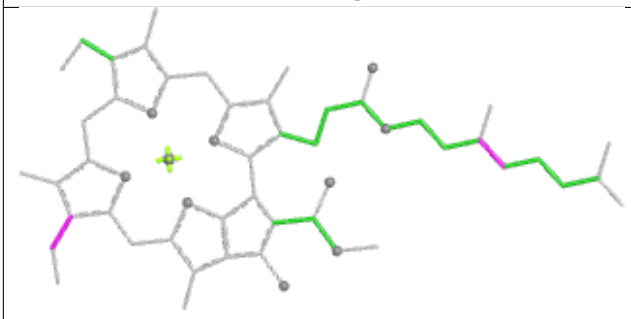
## Ligand CLA 3 607



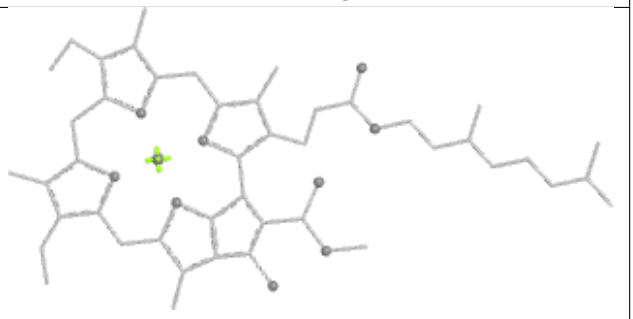
Bond lengths



Bond angles

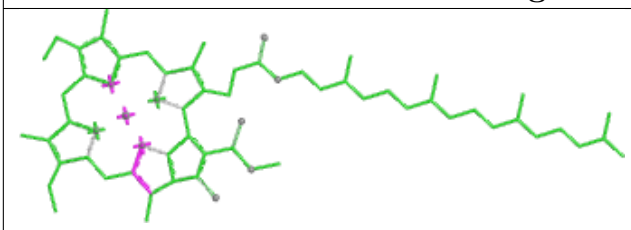


Torsions

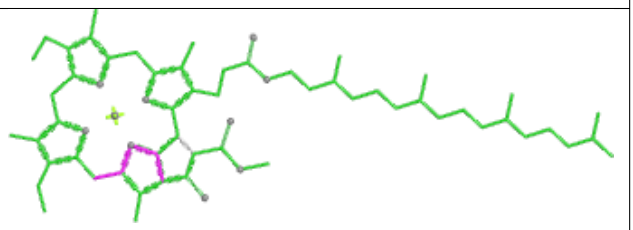


Rings

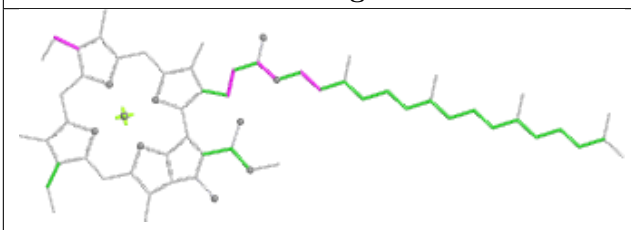
## Ligand CLA 9 613



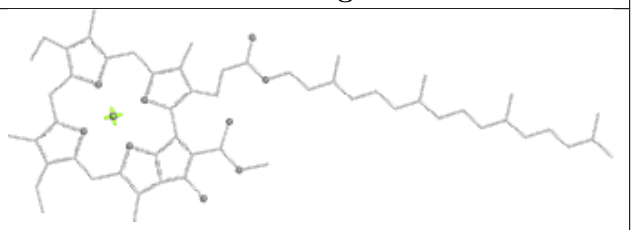
Bond lengths



Bond angles



Torsions



Rings

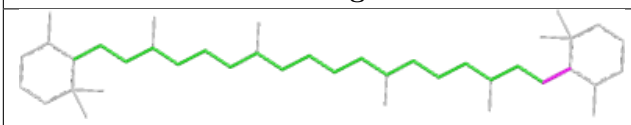
## Ligand BCR J 102



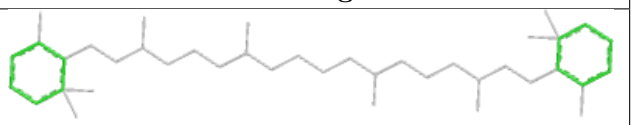
Bond lengths



Bond angles

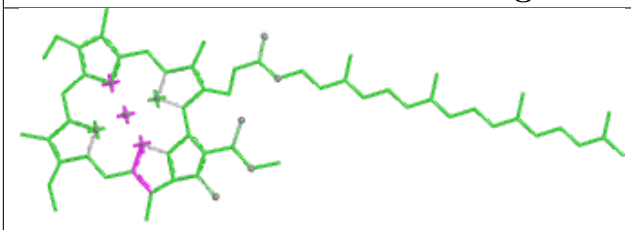


Torsions

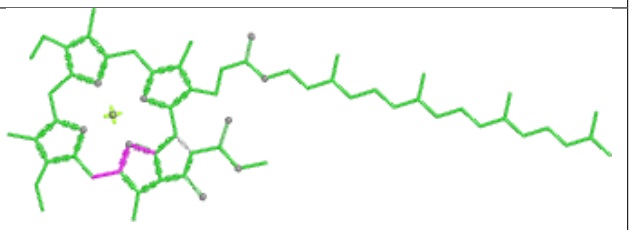


Rings

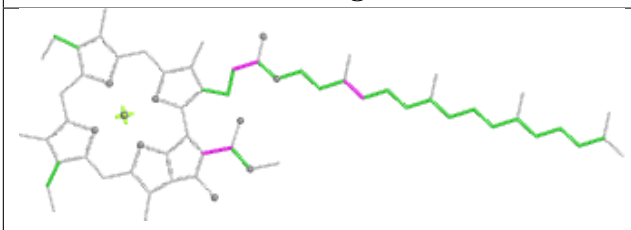
## Ligand CLA A2 814



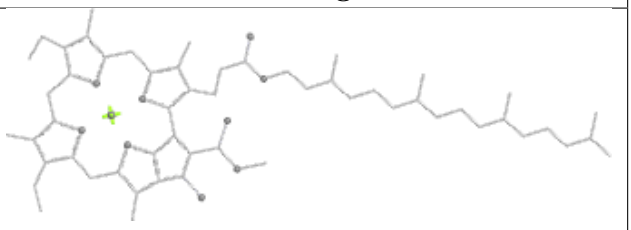
Bond lengths



Bond angles

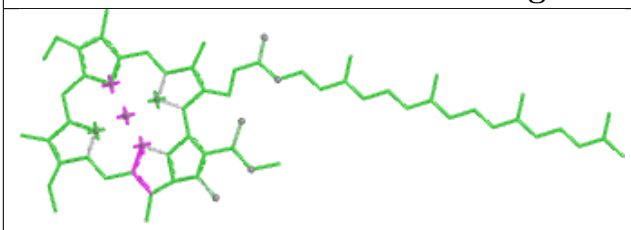


Torsions

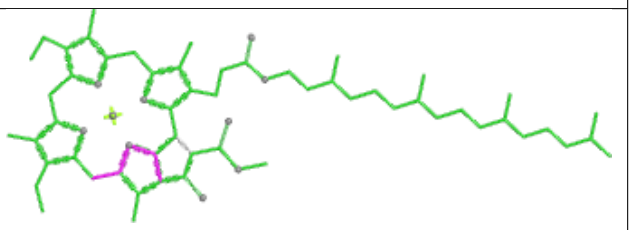


Rings

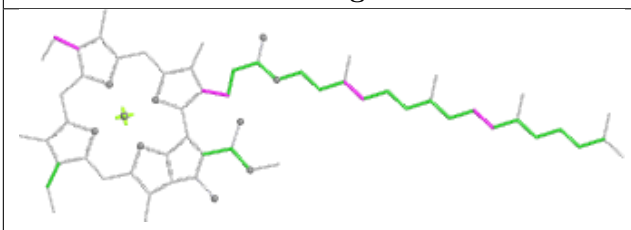
## Ligand CLA 9 611



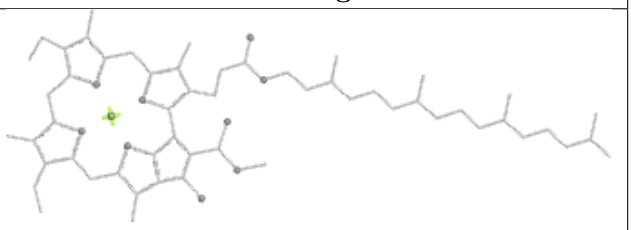
Bond lengths



Bond angles

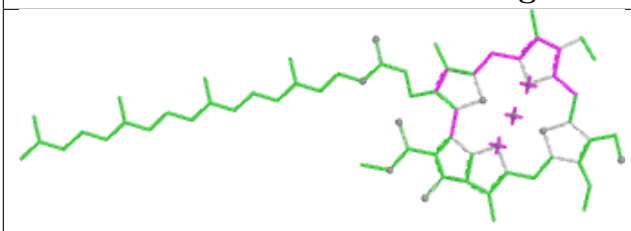


Torsions

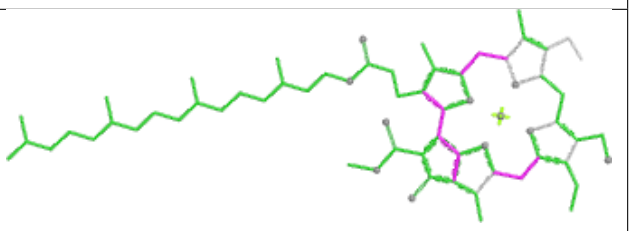


Rings

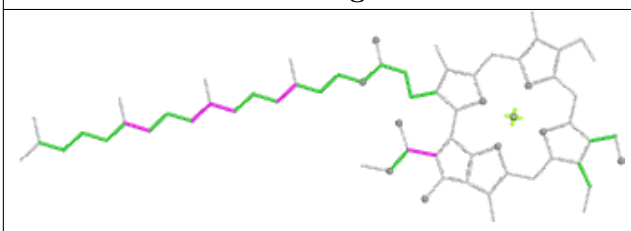
## Ligand CHL 12 601



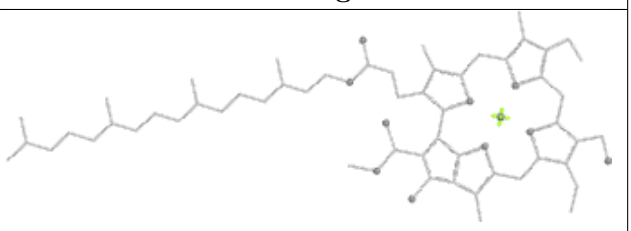
Bond lengths



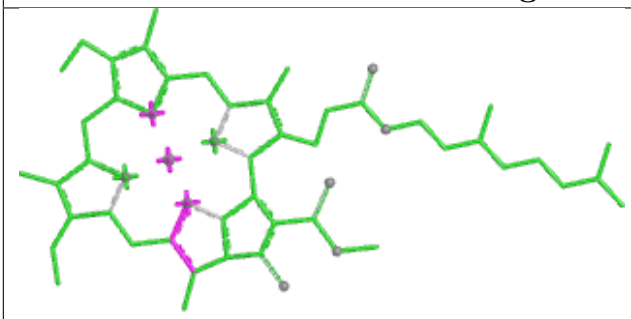
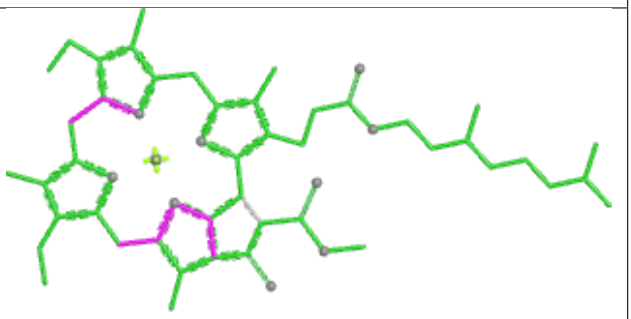
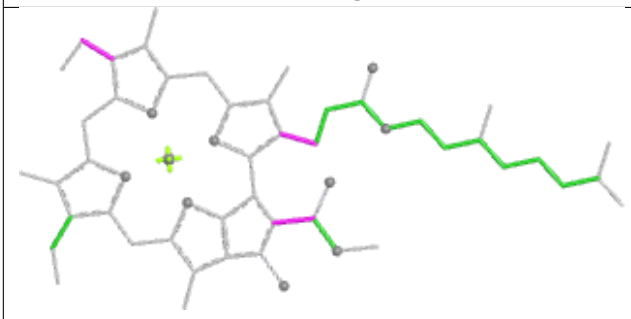
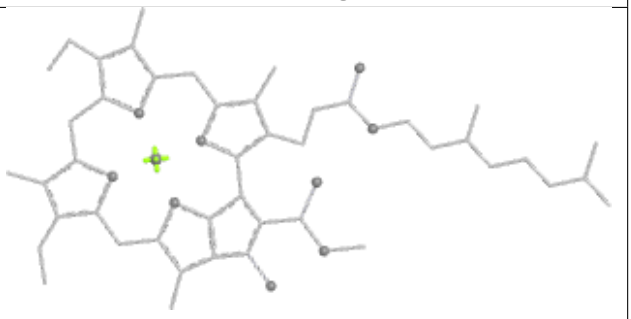
Bond angles

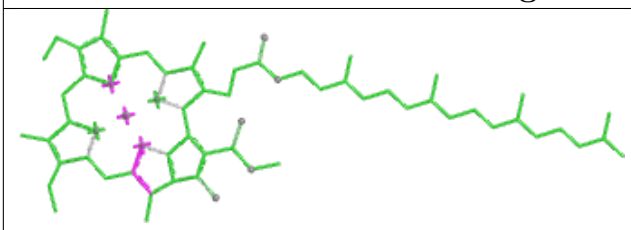
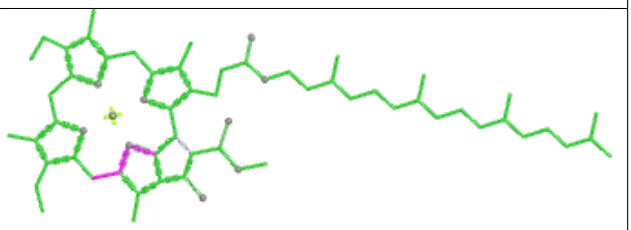
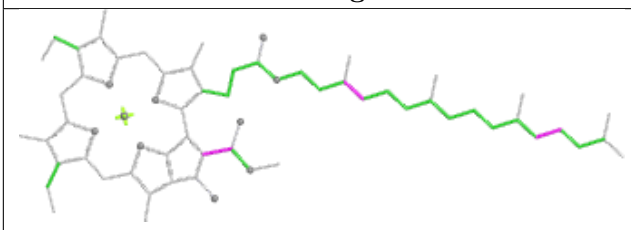
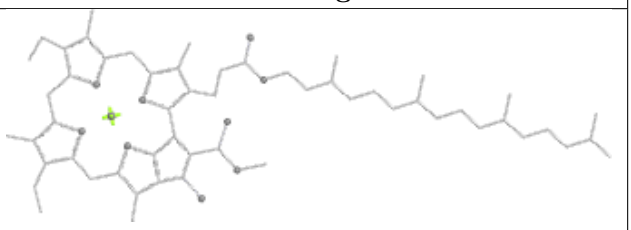


Torsions

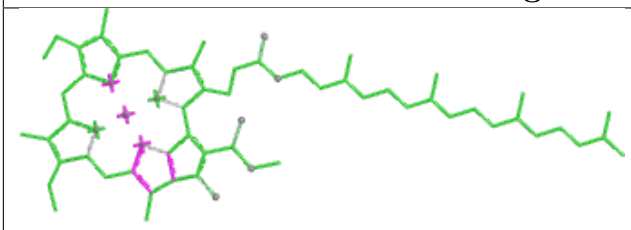


Rings

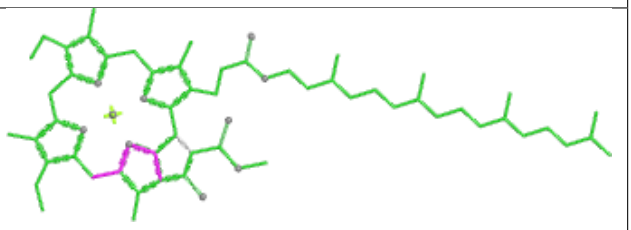
| Ligand CLA 92 603 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 92 612 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

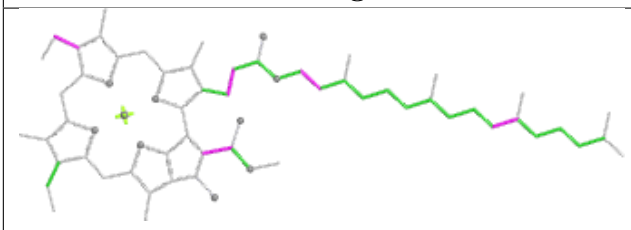
## Ligand CLA A 823



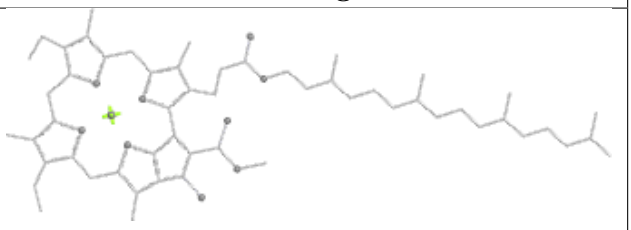
Bond lengths



Bond angles

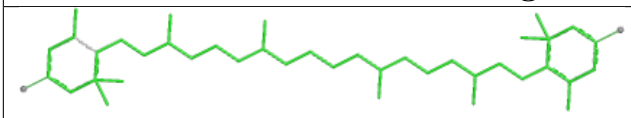


Torsions

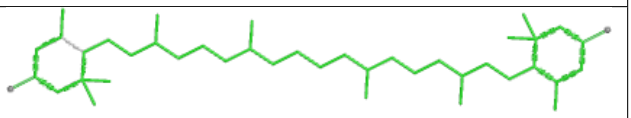


Rings

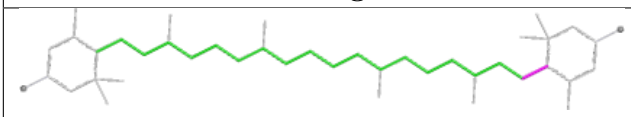
## Ligand LUT 52 620



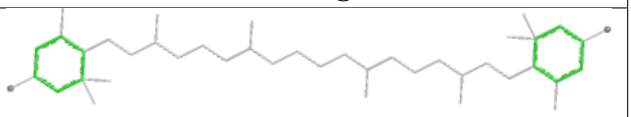
Bond lengths



Bond angles

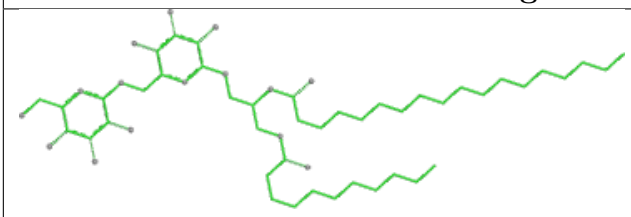


Torsions

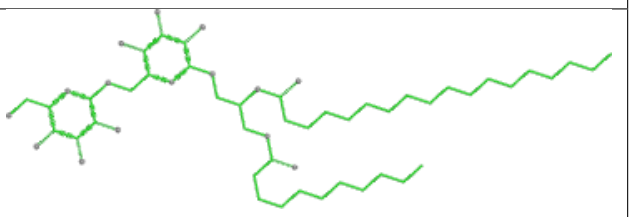


Rings

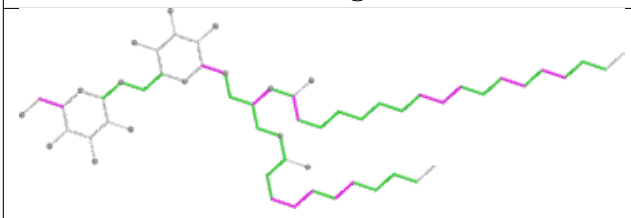
## Ligand DGD B 850



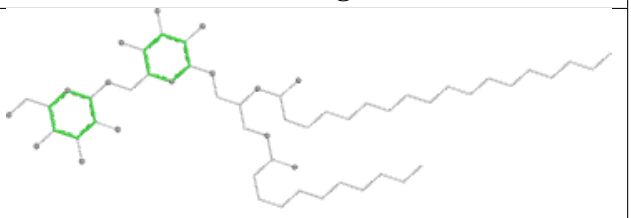
Bond lengths



Bond angles

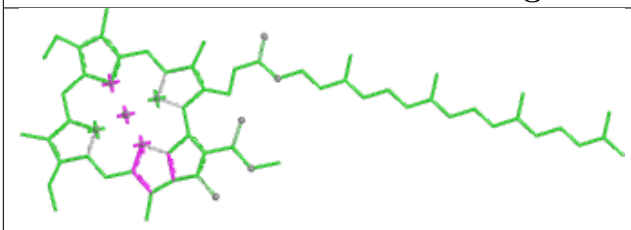


Torsions

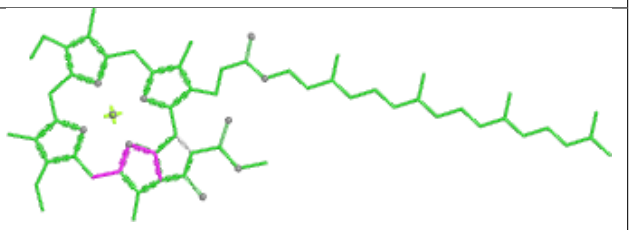


Rings

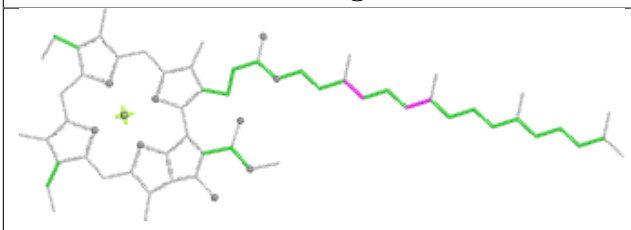
## Ligand CLA A 811



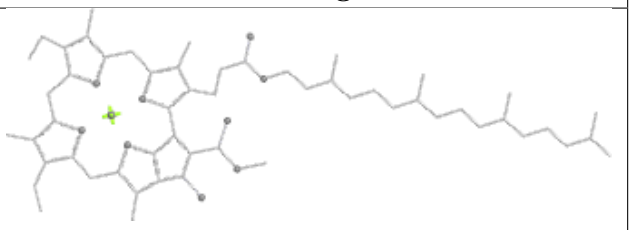
Bond lengths



Bond angles

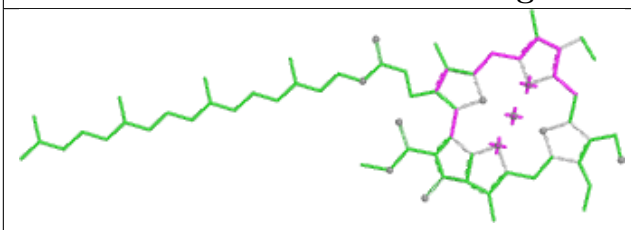


Torsions

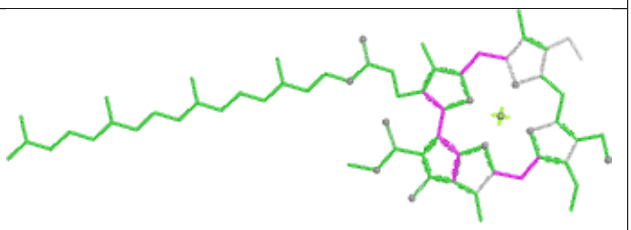


Rings

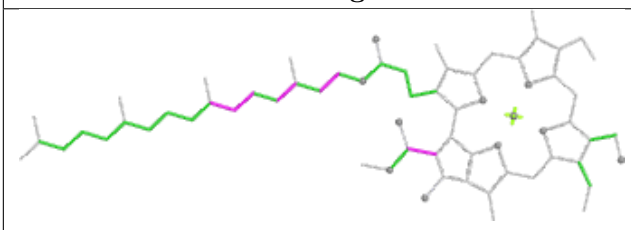
## Ligand CHL Z2 601



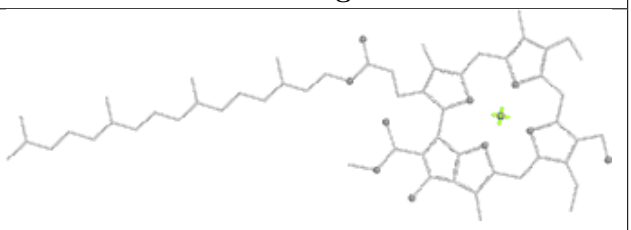
Bond lengths



Bond angles

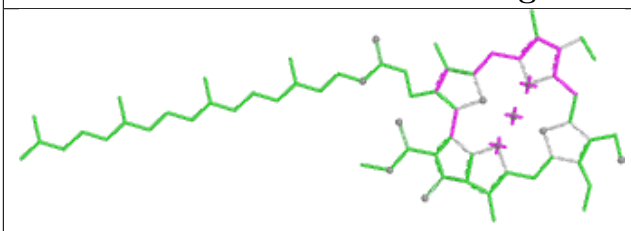


Torsions

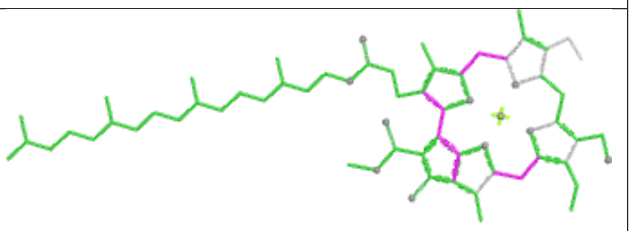


Rings

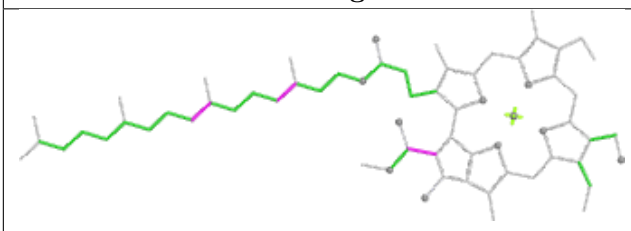
## Ligand CHL 42 601



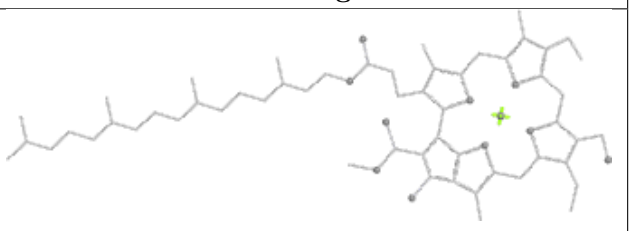
Bond lengths



Bond angles

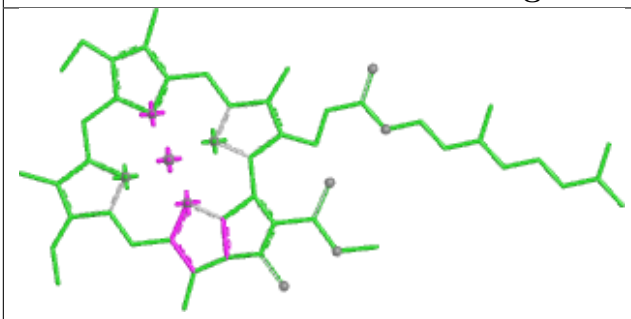


Torsions

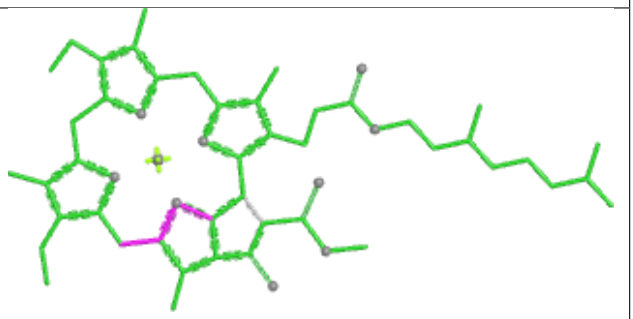


Rings

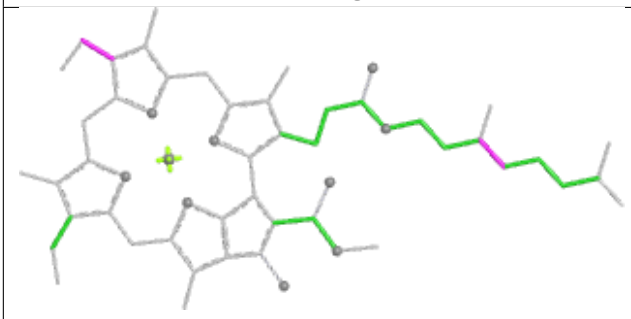
## Ligand CLA A 821



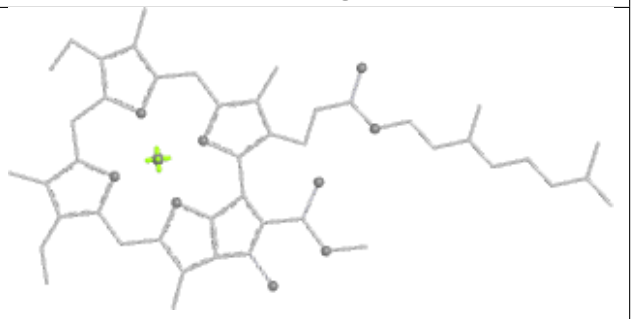
Bond lengths



Bond angles

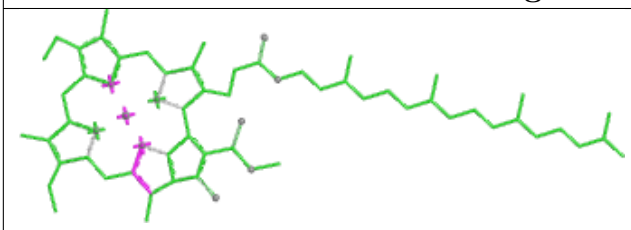


Torsions

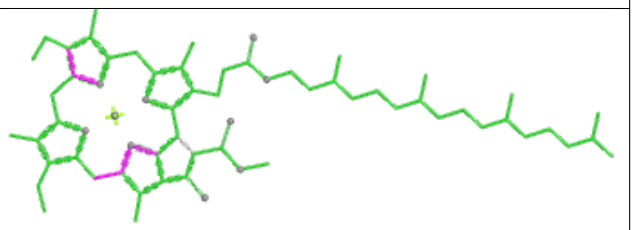


Rings

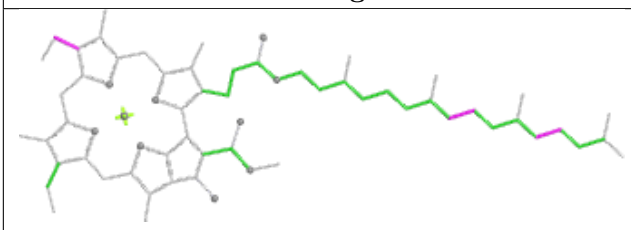
## Ligand CLA B 826



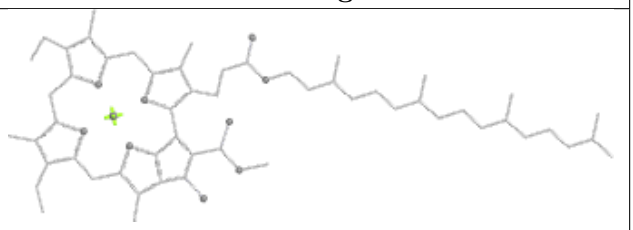
Bond lengths



Bond angles



Torsions

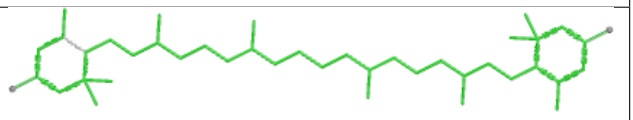


Rings

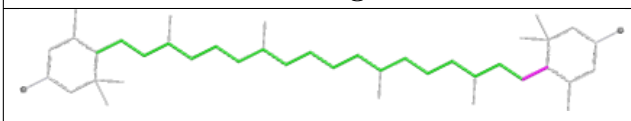
## Ligand LUT 7 621



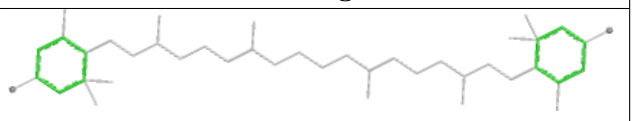
Bond lengths



Bond angles

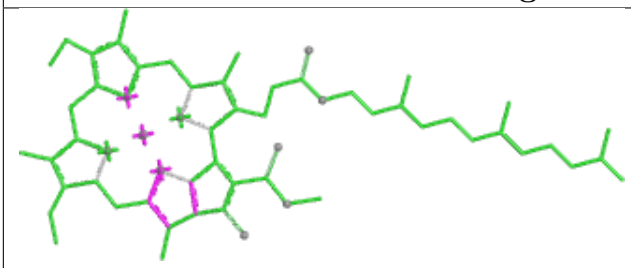


Torsions

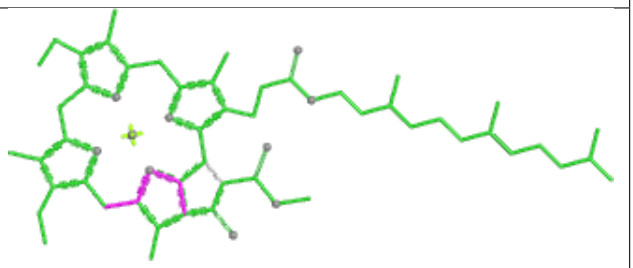


Rings

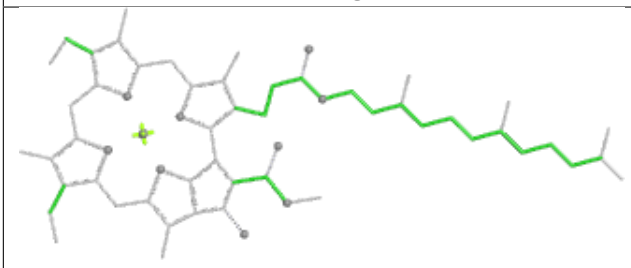
## Ligand CLA 92 610



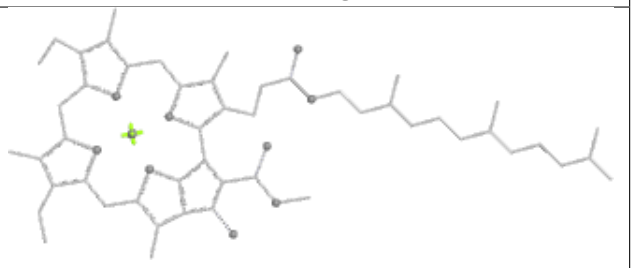
Bond lengths



Bond angles

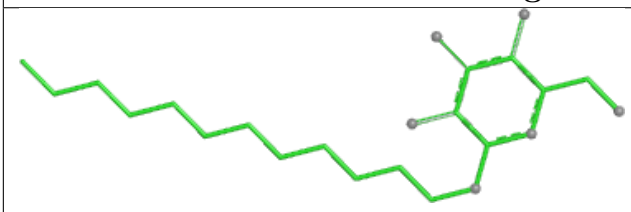


Torsions

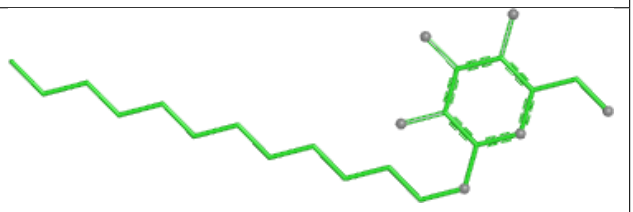


Rings

## Ligand LMU 6 630



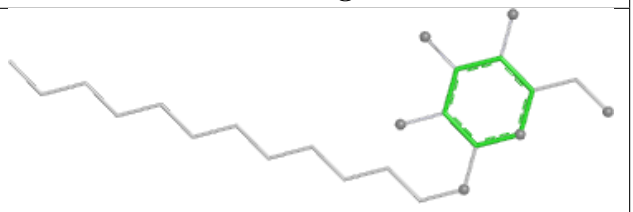
Bond lengths



Bond angles



Torsions

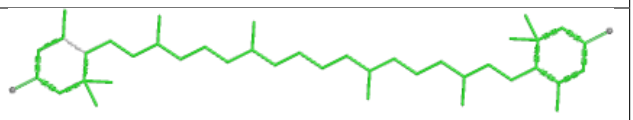


Rings

## Ligand LUT 72 624



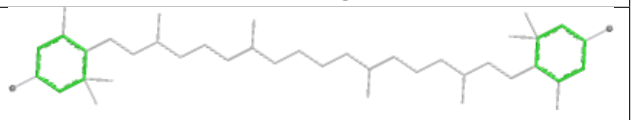
Bond lengths



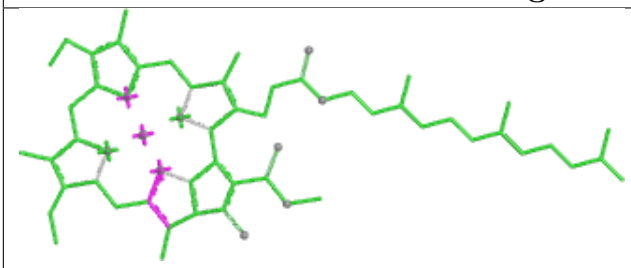
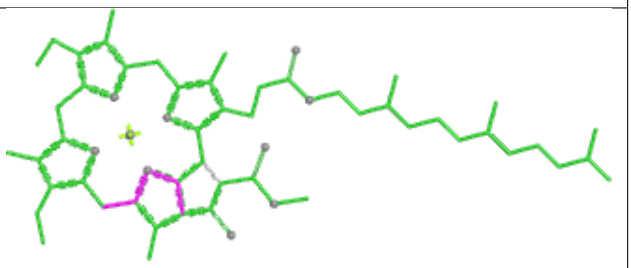
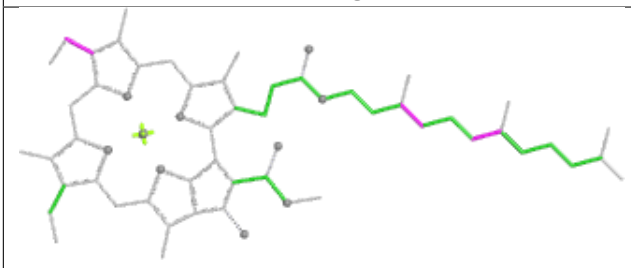
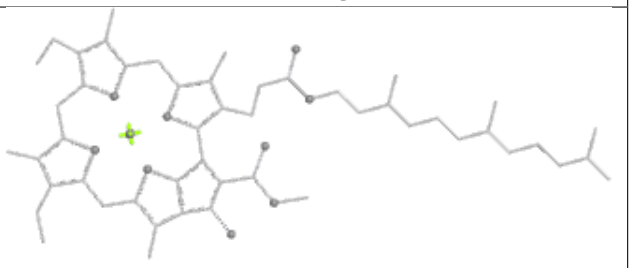
Bond angles

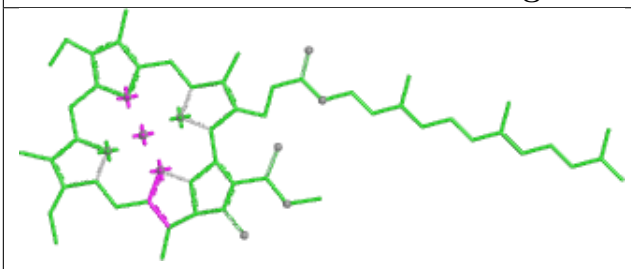
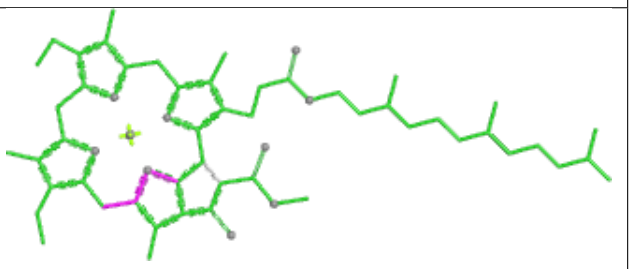
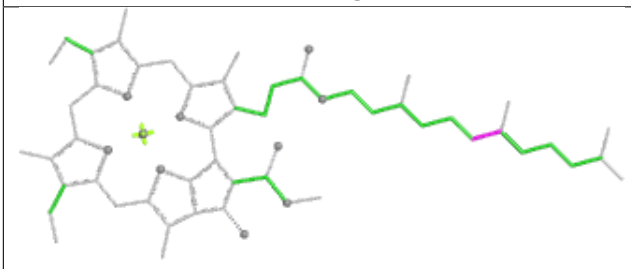
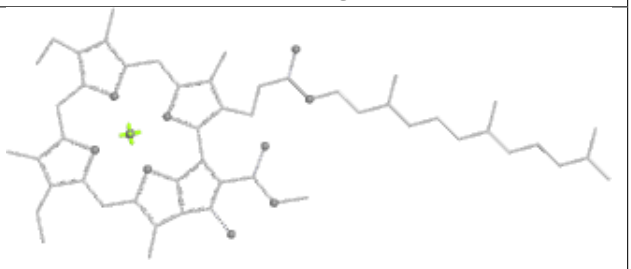


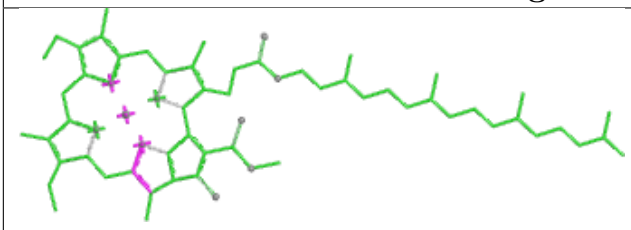
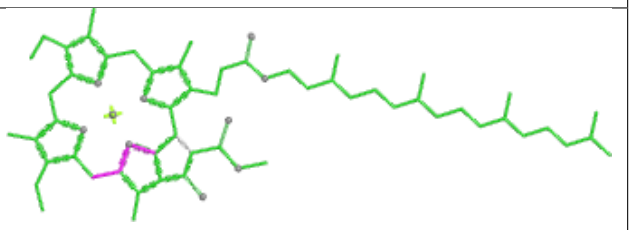
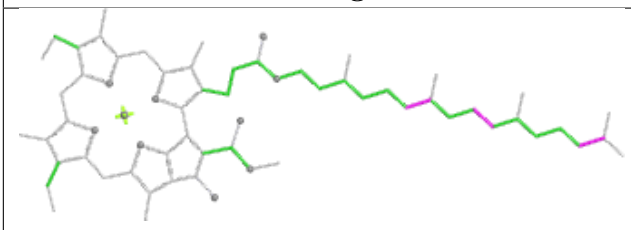
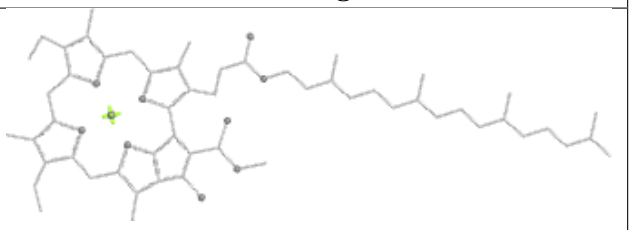
Torsions

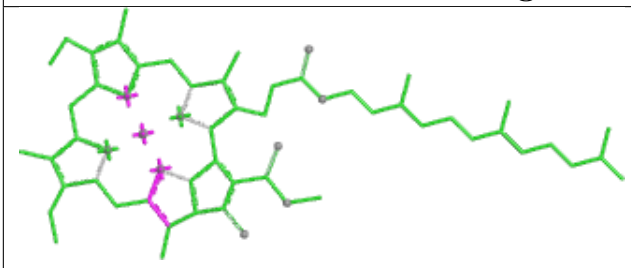
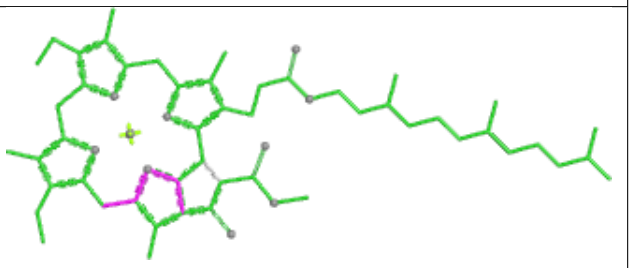
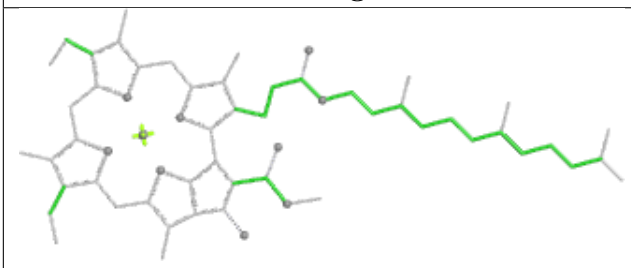
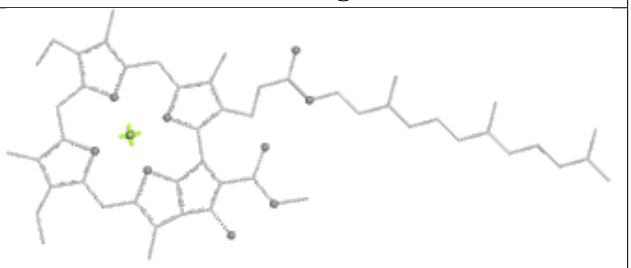


Rings

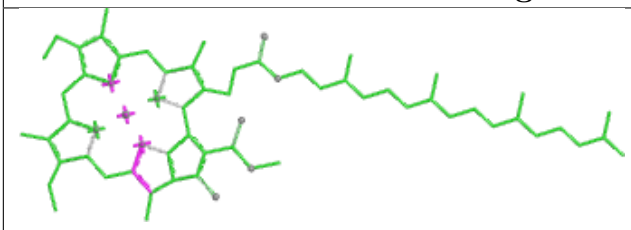
| Ligand CLA 4 611 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

| Ligand CLA G 203 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

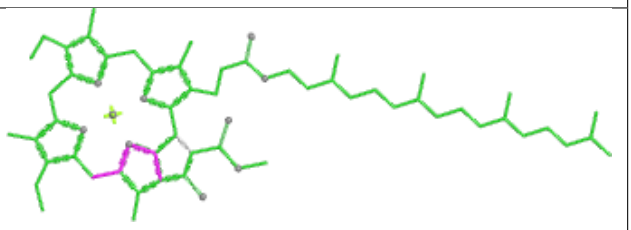
| Ligand CLA 5 601 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA Z2 610 | |
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|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

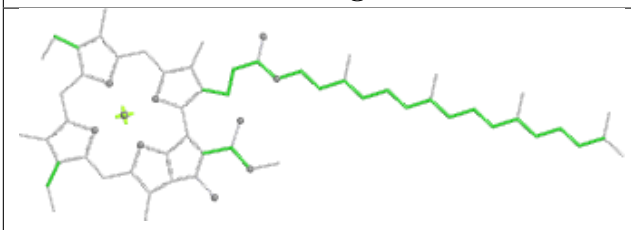
## Ligand CLA B2 816



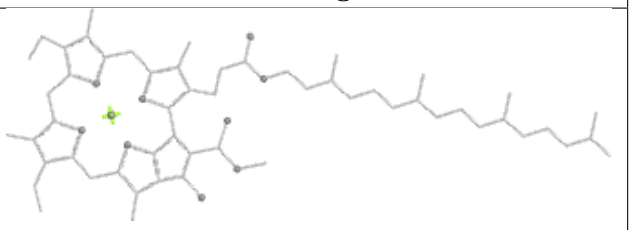
Bond lengths



Bond angles

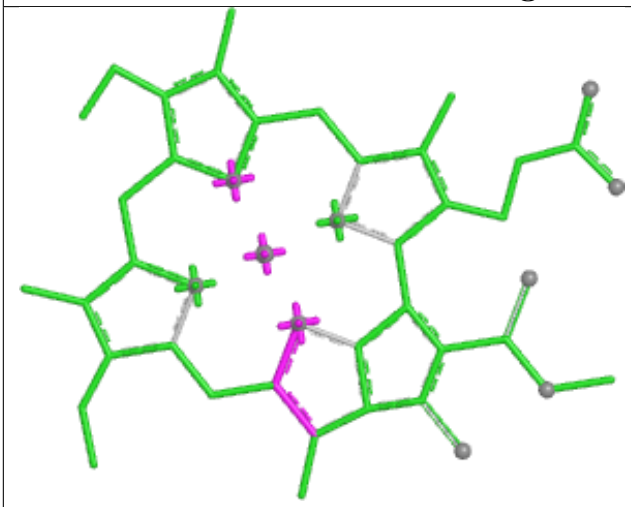


Torsions

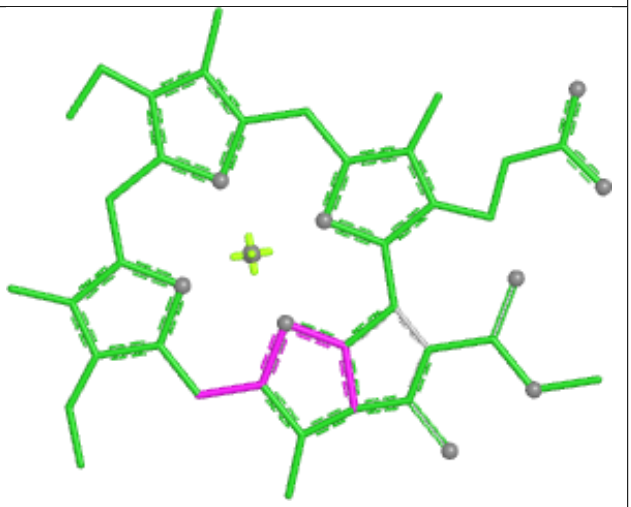


Rings

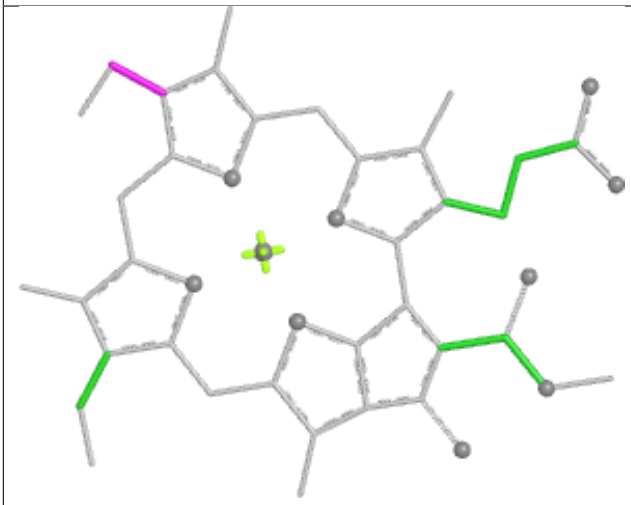
## Ligand CLA 62 617



Bond lengths



Bond angles

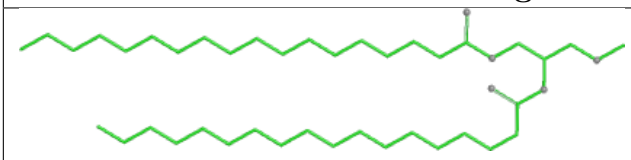


Torsions

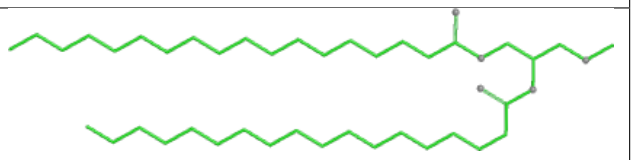


Rings

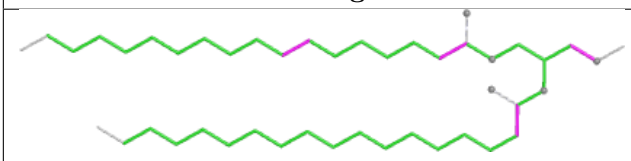
**Ligand LMG 32 722**



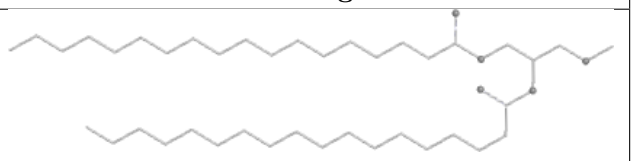
Bond lengths



Bond angles

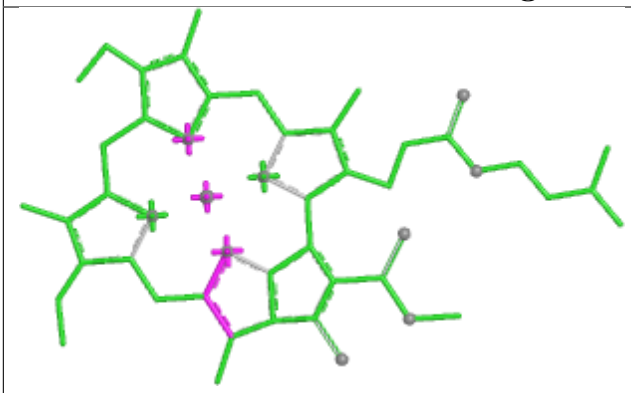


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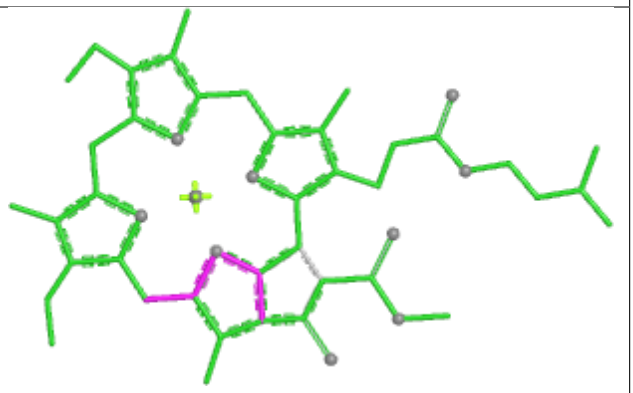


Rings

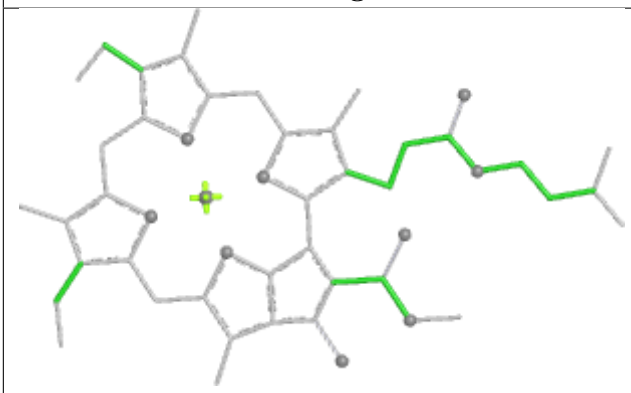
**Ligand CLA 12 604**



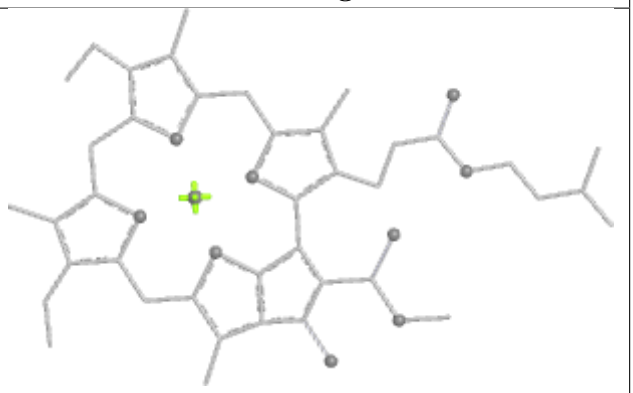
Bond lengths



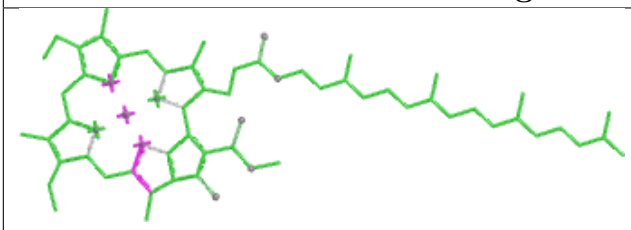
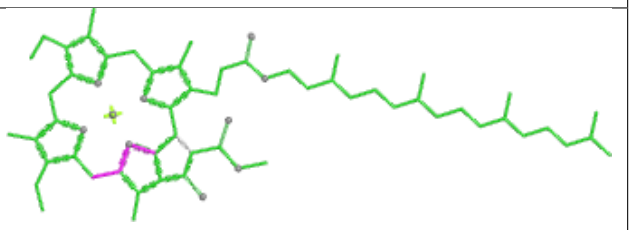
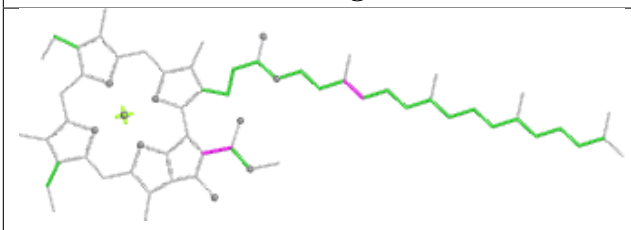
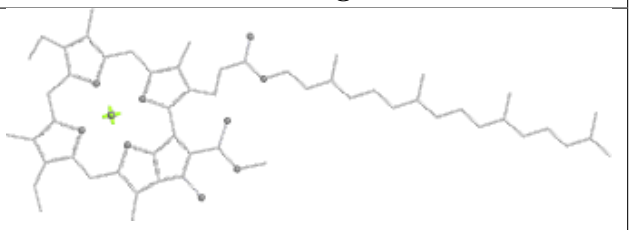
Bond angles

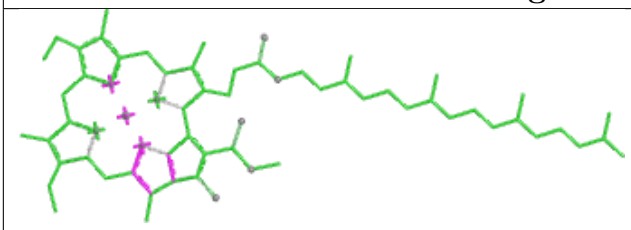
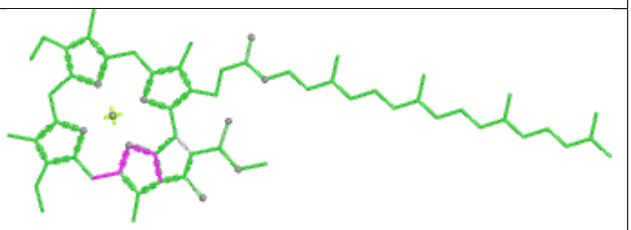
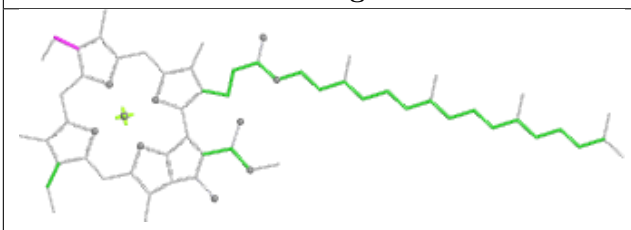
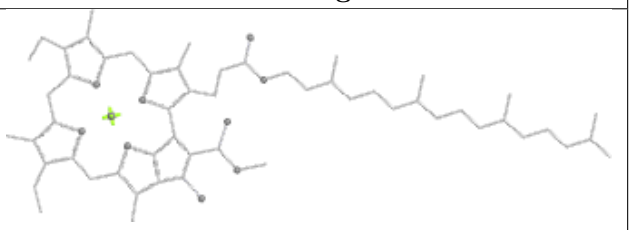


Torsions

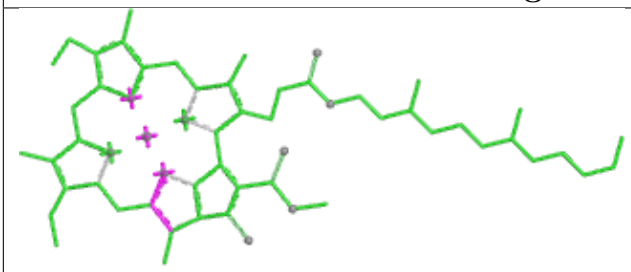


Rings

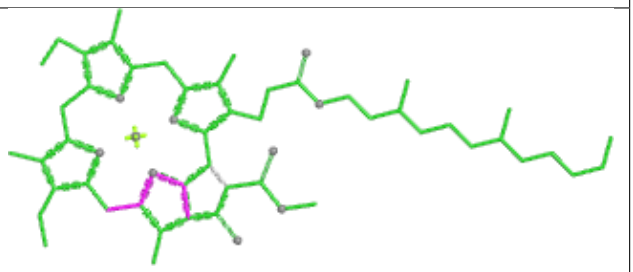
| Ligand CLA B2 815 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 1 610 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

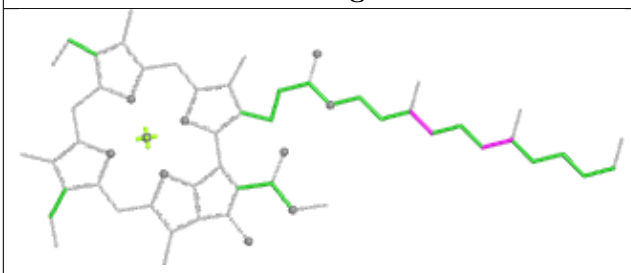
## Ligand CLA B 822



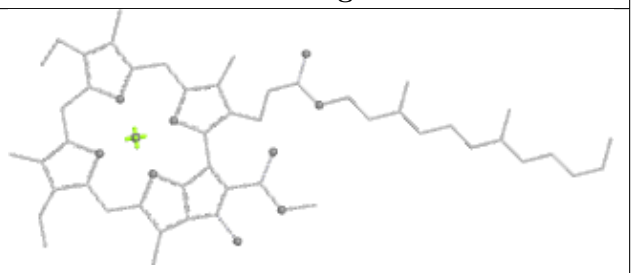
Bond lengths



Bond angles

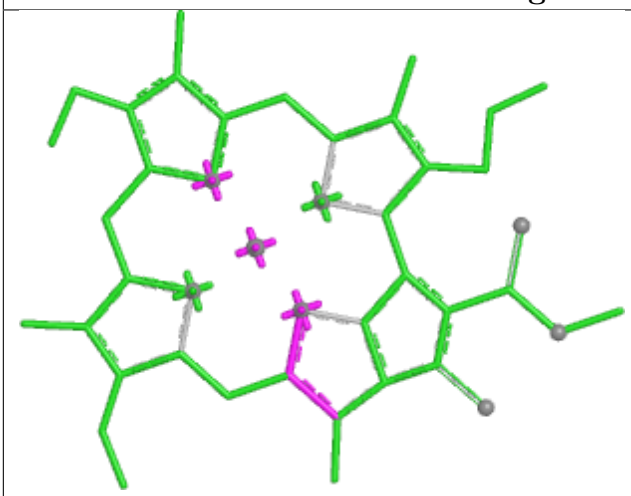


Torsions

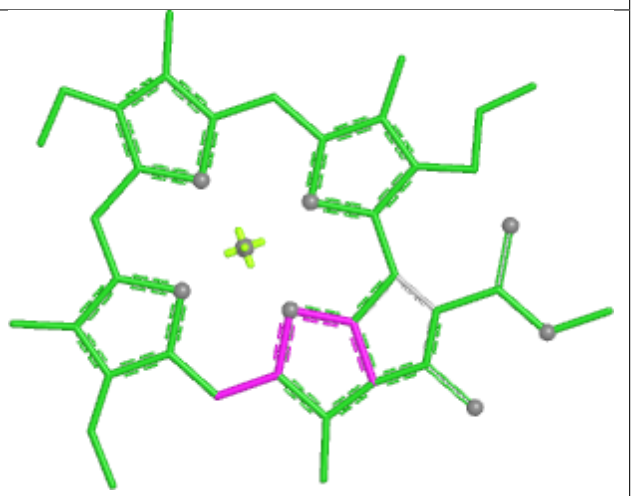


Rings

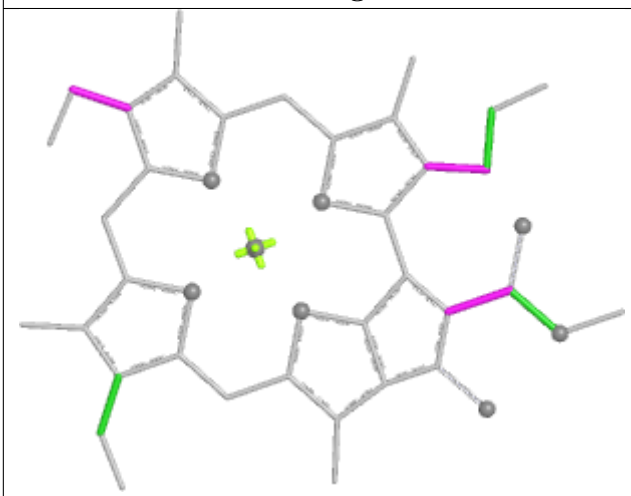
## Ligand CLA 7 614



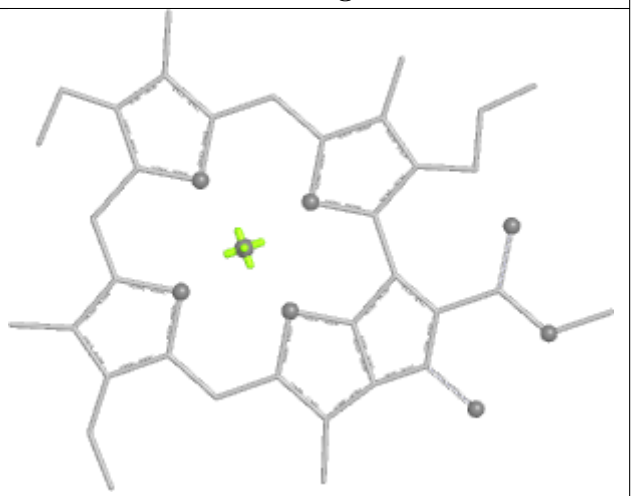
Bond lengths



Bond angles

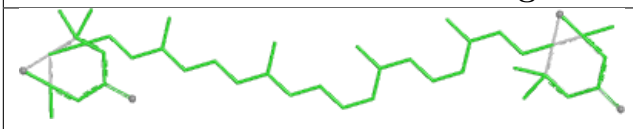


Torsions

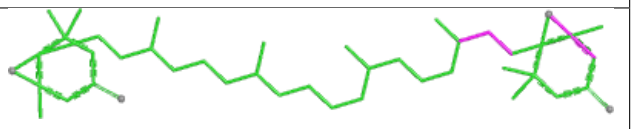


Rings

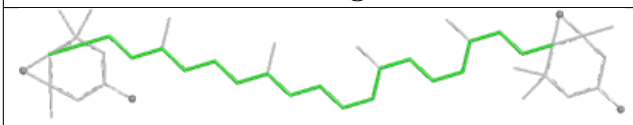
## Ligand XAT 12 618



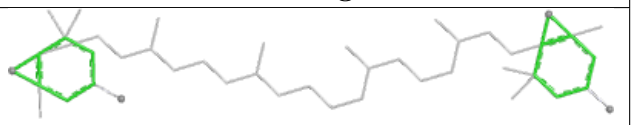
Bond lengths



Bond angles

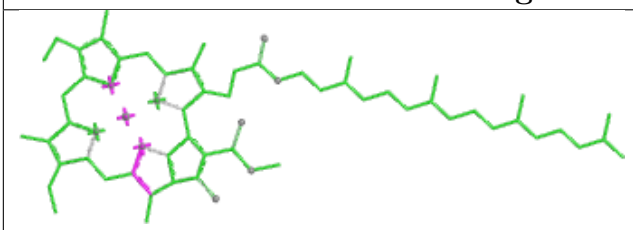


Torsions

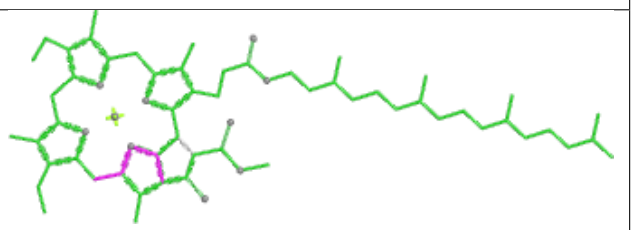


Rings

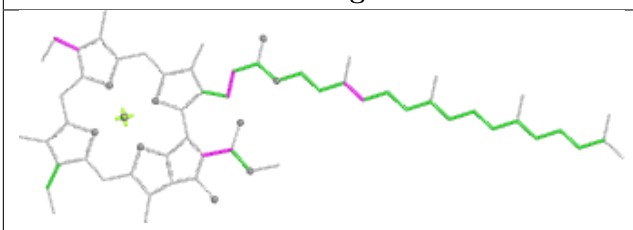
## Ligand CLA B2 839



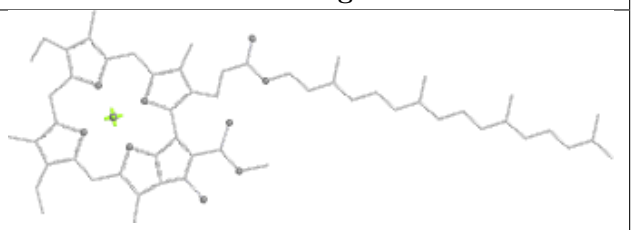
Bond lengths



Bond angles

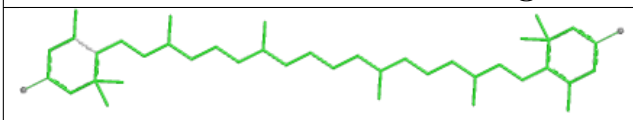


Torsions

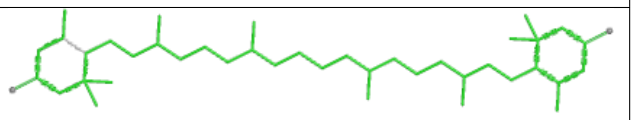


Rings

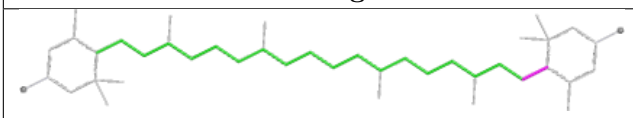
## Ligand LUT Z2 617



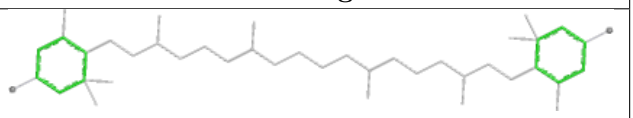
Bond lengths



Bond angles

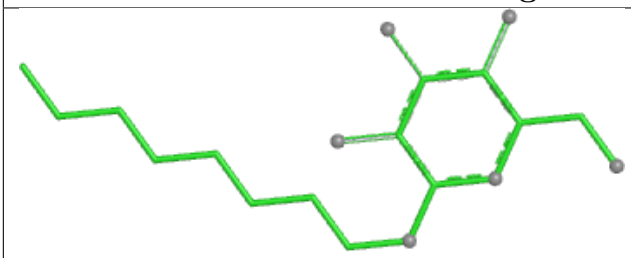


Torsions

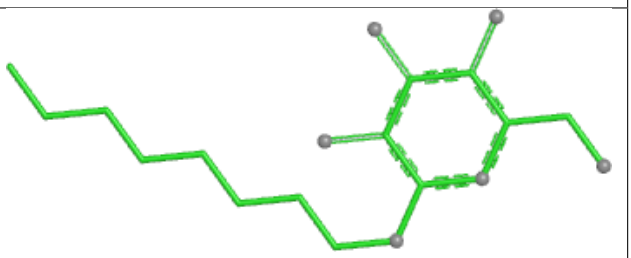


Rings

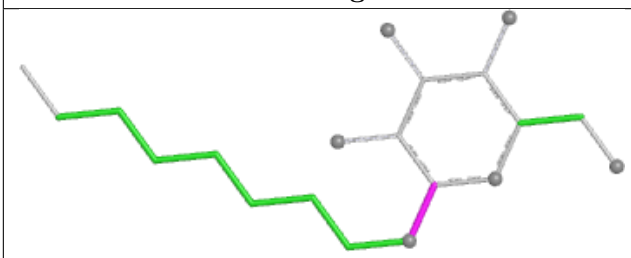
## Ligand LMU A 862



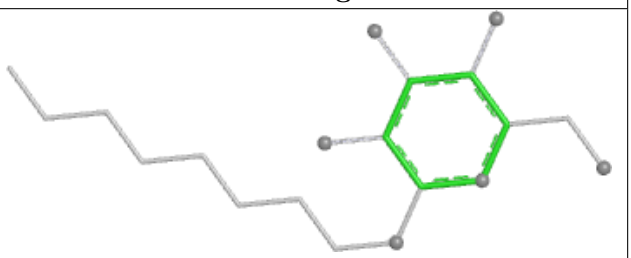
Bond lengths



Bond angles

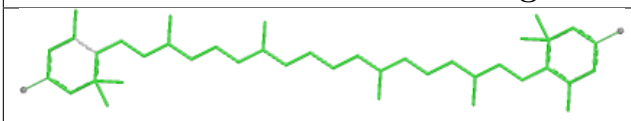


Torsions

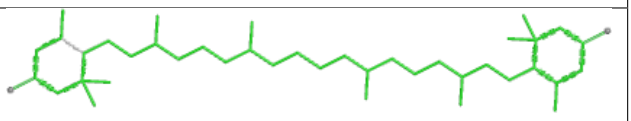


Rings

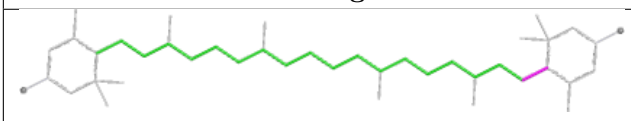
## Ligand LUT 82 617



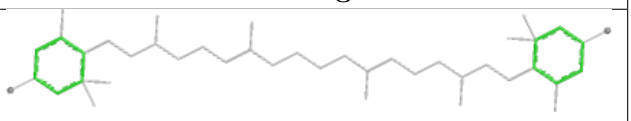
Bond lengths



Bond angles

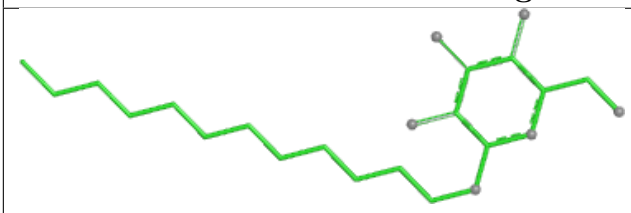


Torsions

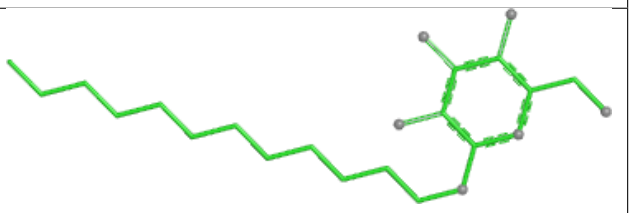


Rings

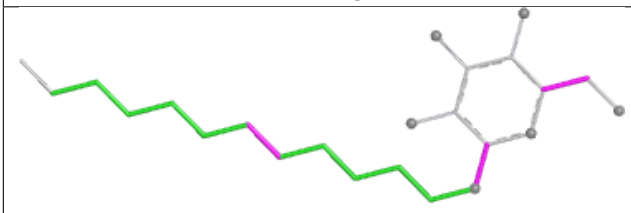
## Ligand LMU 92 624



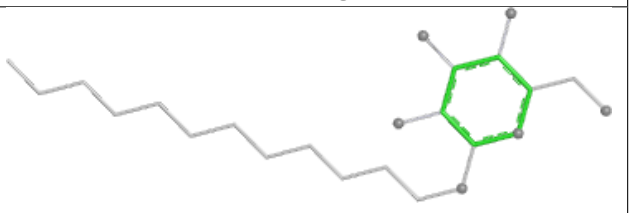
Bond lengths



Bond angles

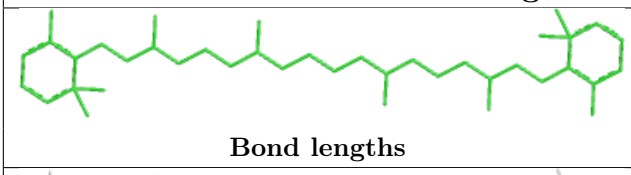


Torsions

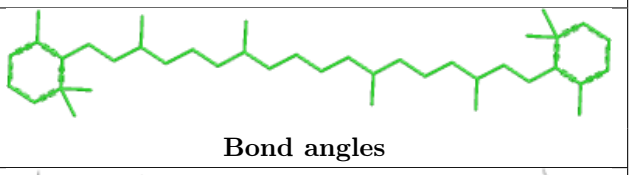


Rings

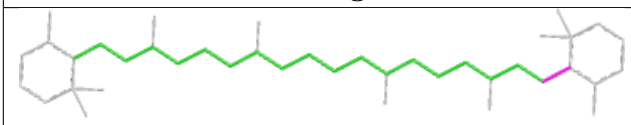
## Ligand BCR A 851



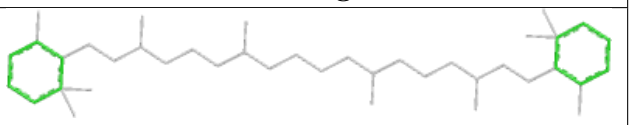
Bond lengths



Bond angles



Torsions

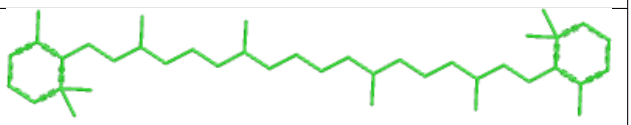


Rings

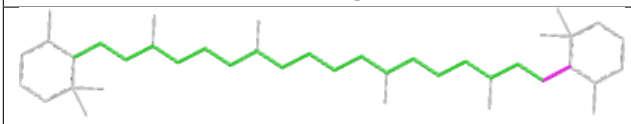
## Ligand BCR K 202



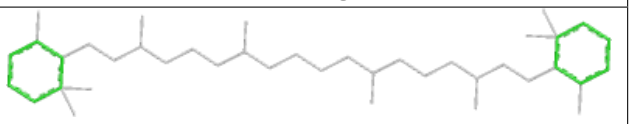
Bond lengths



Bond angles

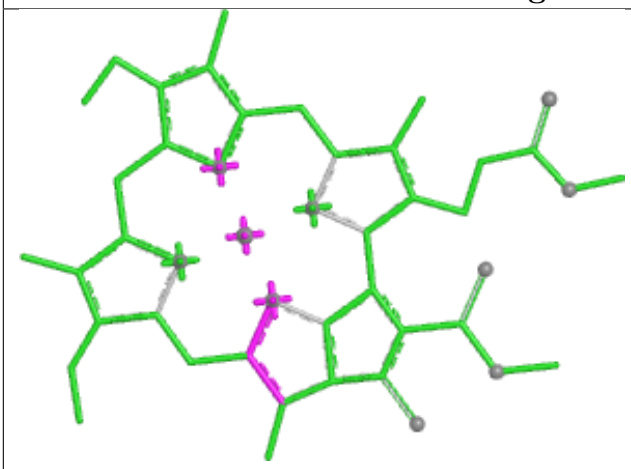


Torsions

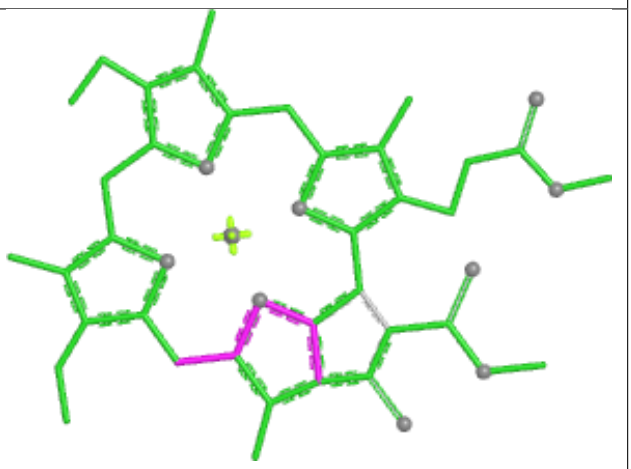


Rings

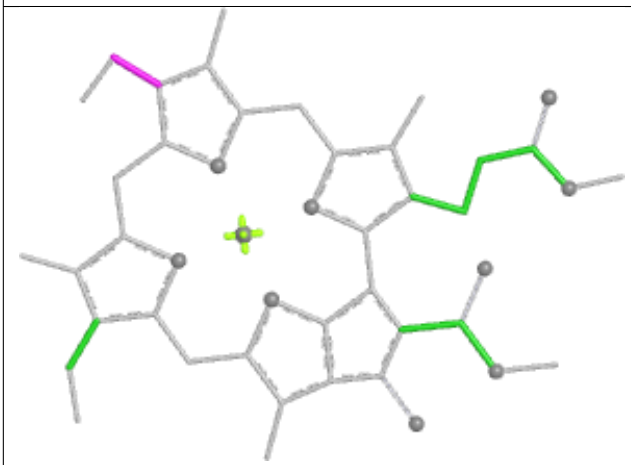
## Ligand CLA 1 616



Bond lengths



Bond angles

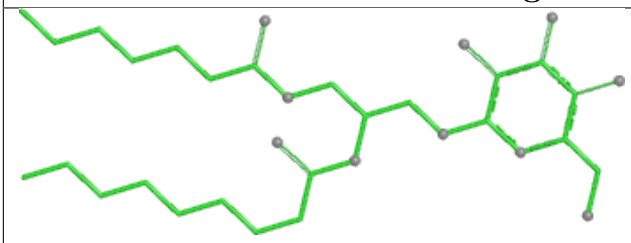


Torsions

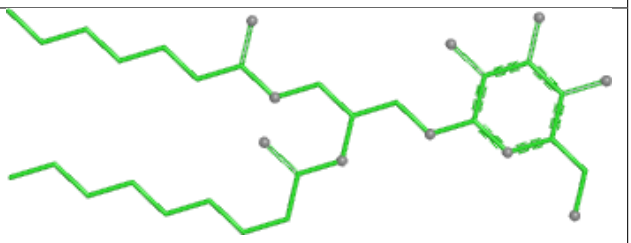


Rings

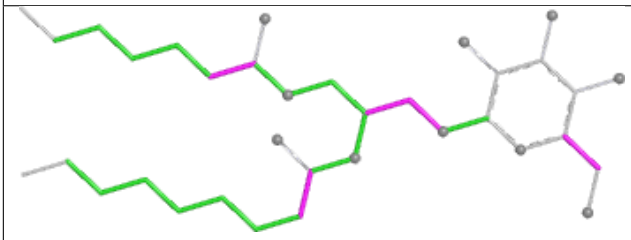
## Ligand LMG J 104



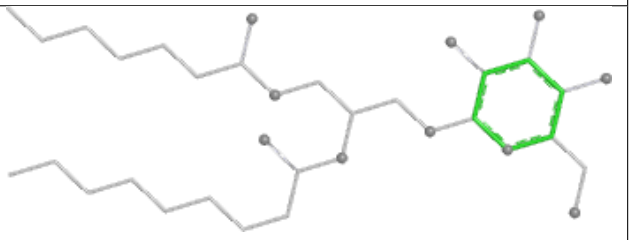
Bond lengths



Bond angles

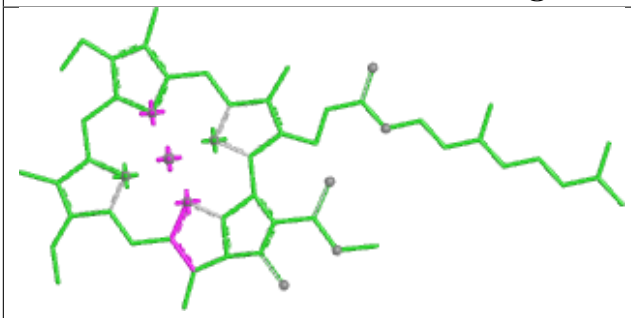


Torsions

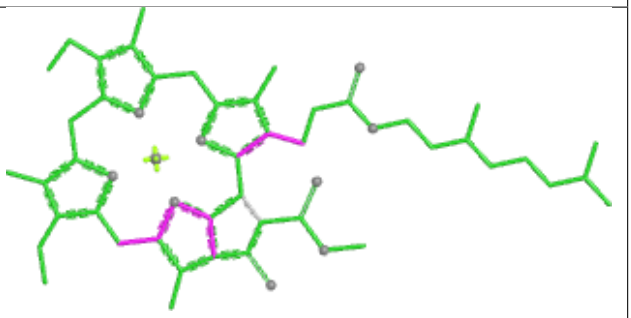


Rings

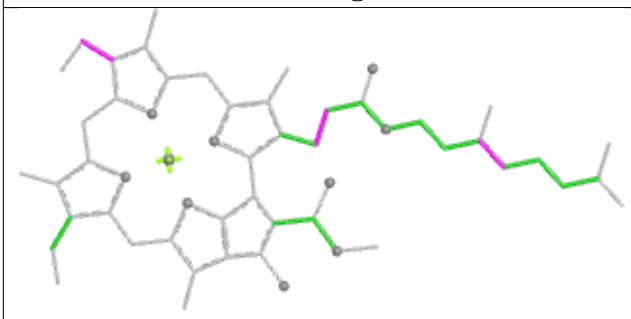
## Ligand CLA 6 609



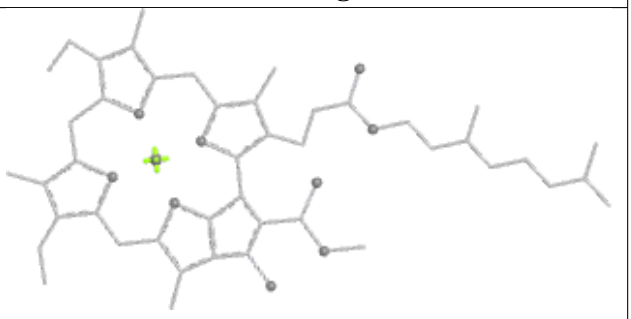
Bond lengths



Bond angles

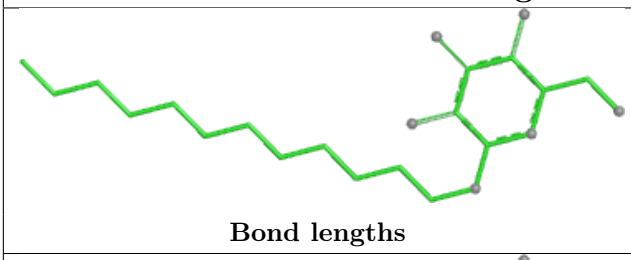


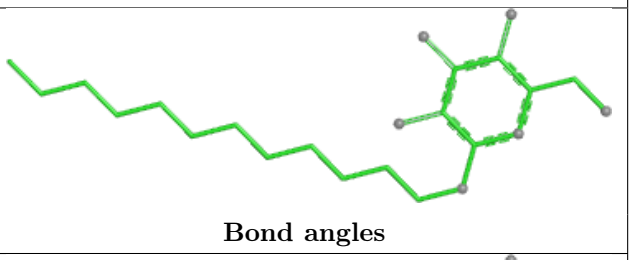
Torsions

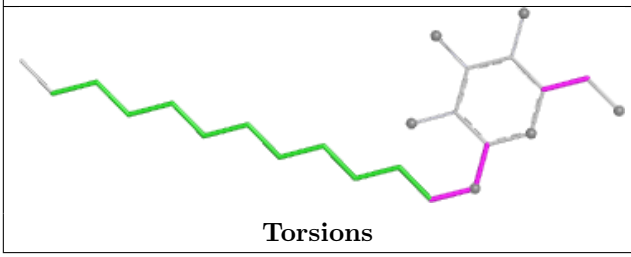


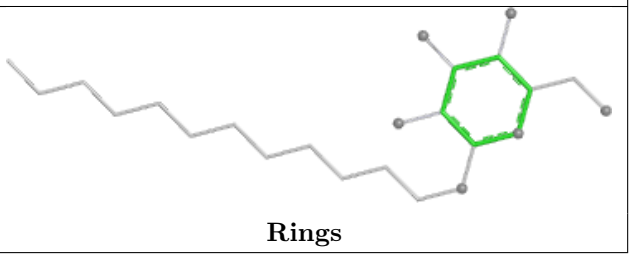
Rings

## Ligand LMU 82 628

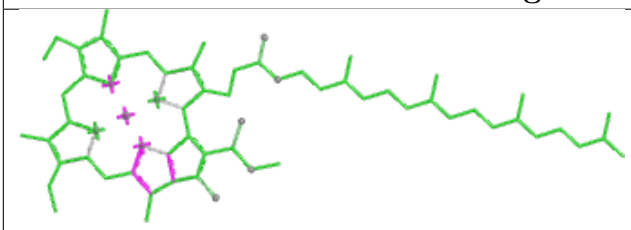

Bond lengths

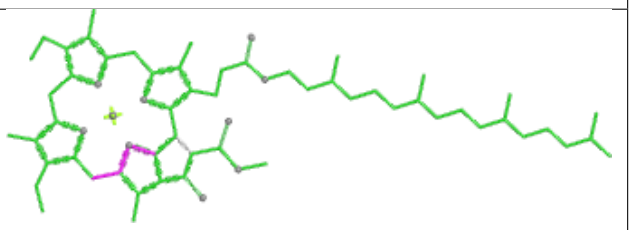

Bond angles

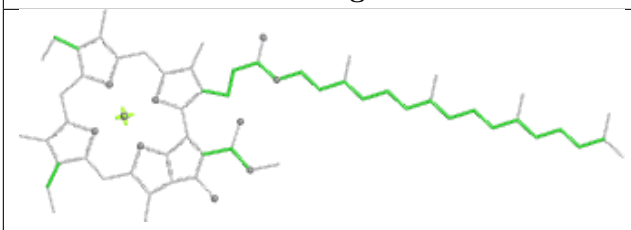

Torsions

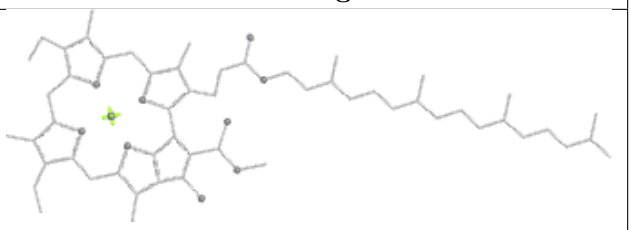

Rings

## Ligand CLA A 802

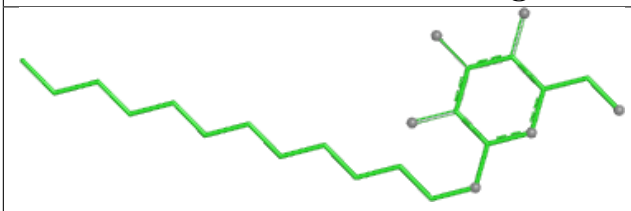

Bond lengths

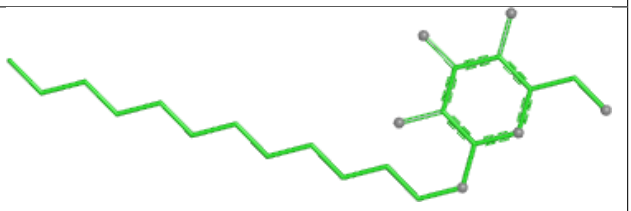

Bond angles


Torsions


Rings

## Ligand LMU A2 865

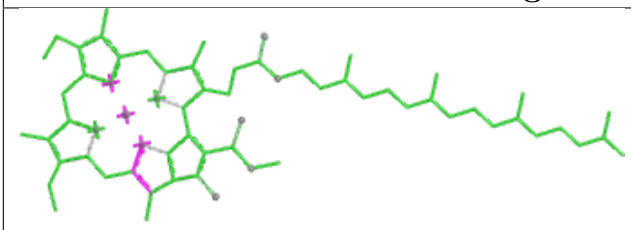

Bond lengths


Bond angles

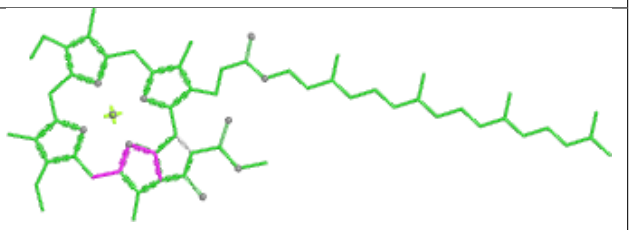

Torsions


Rings

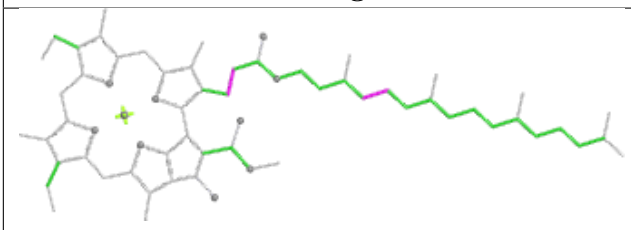
**Ligand CLA A 818**



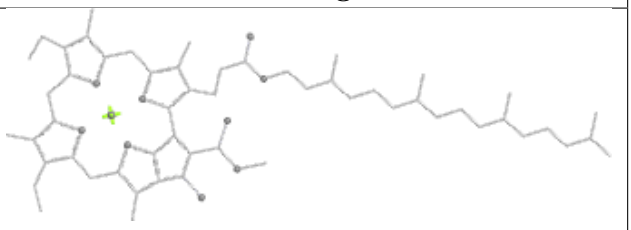
Bond lengths



Bond angles

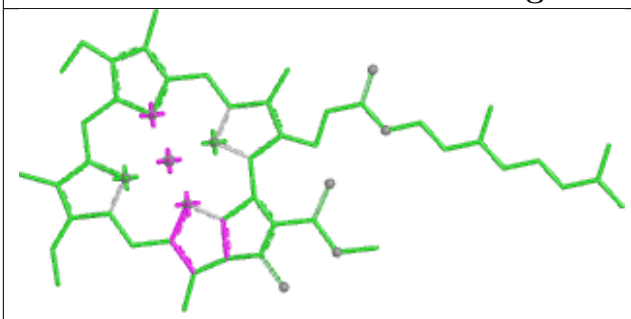


Torsions

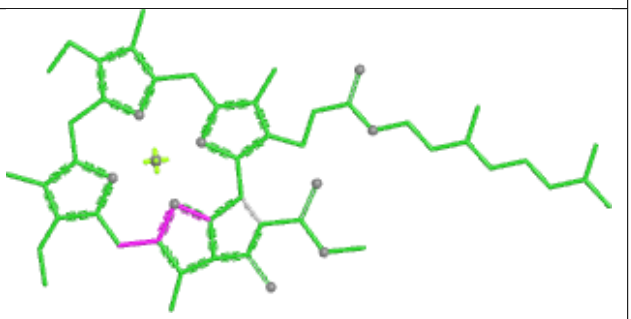


Rings

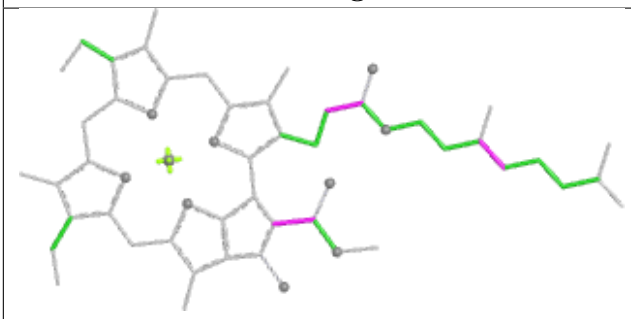
**Ligand CLA Z 603**



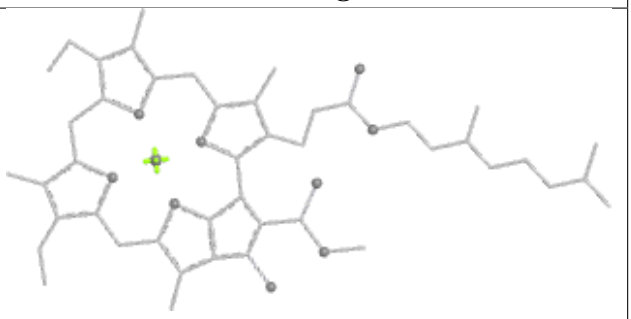
Bond lengths



Bond angles

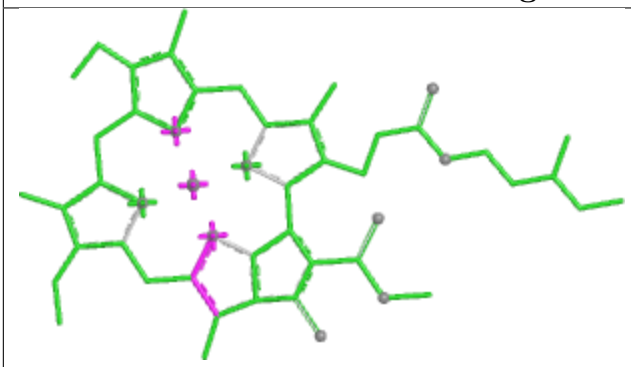


Torsions

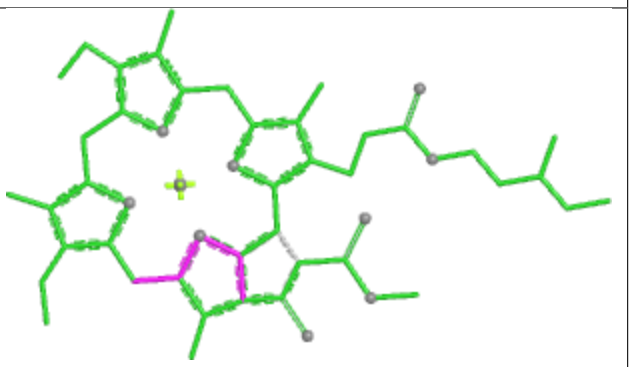


Rings

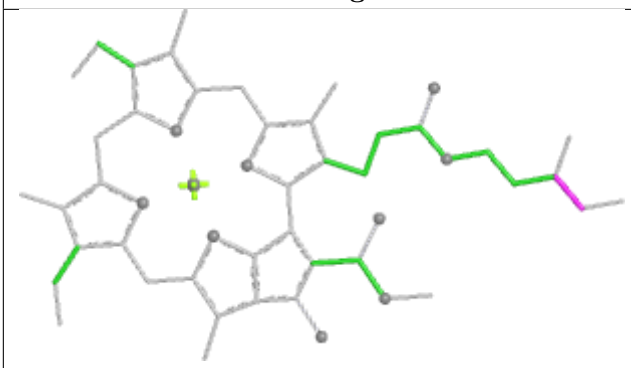
## Ligand CLA 72 604



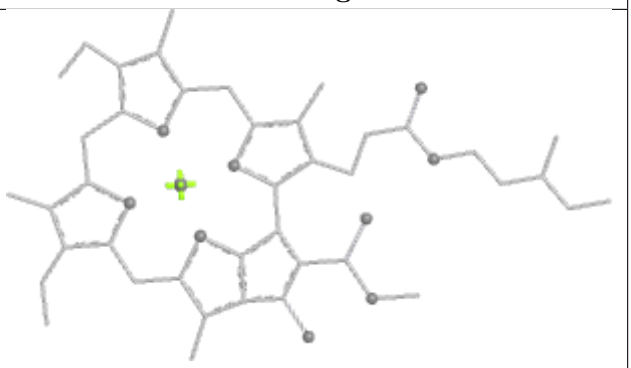
Bond lengths



Bond angles

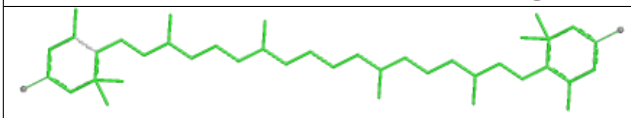


Torsions

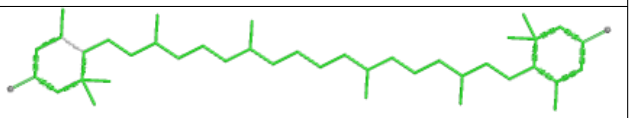


Rings

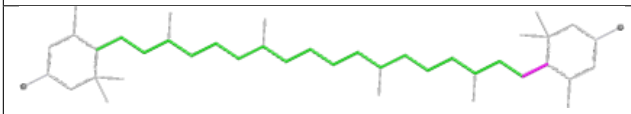
## Ligand LUT 4 619



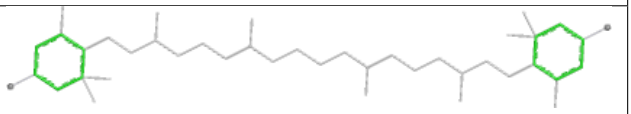
Bond lengths



Bond angles

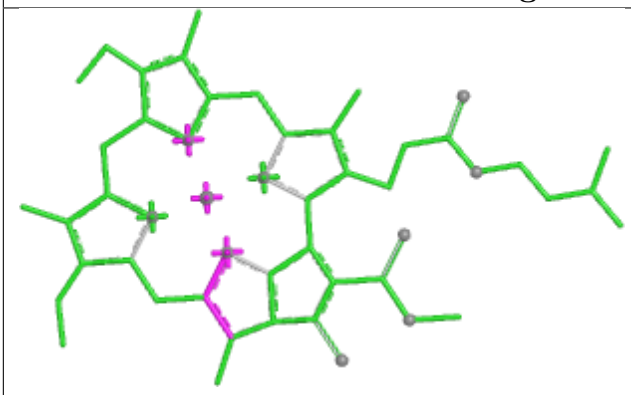


Torsions

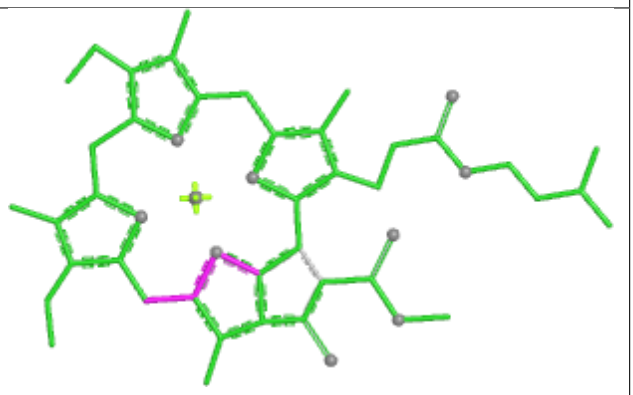


Rings

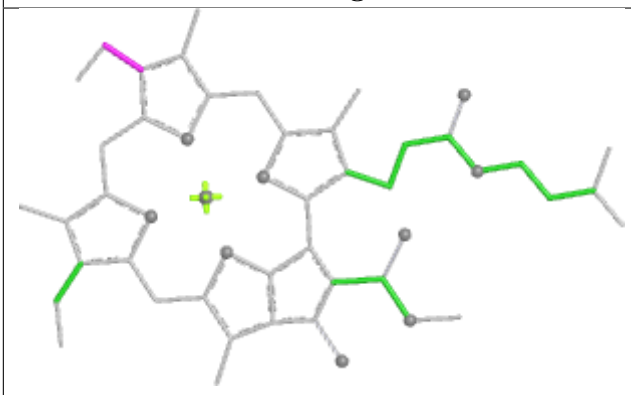
**Ligand CLA 82 608**



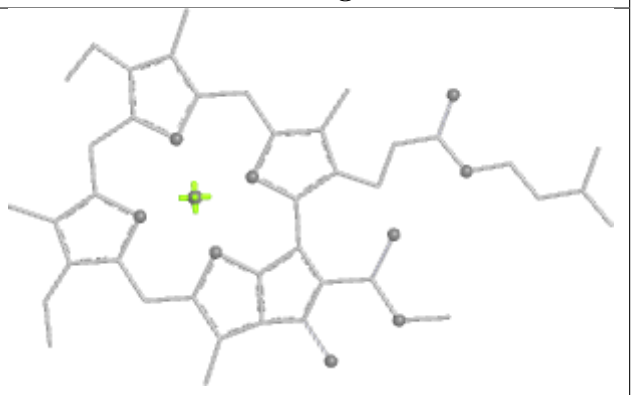
**Bond lengths**



**Bond angles**

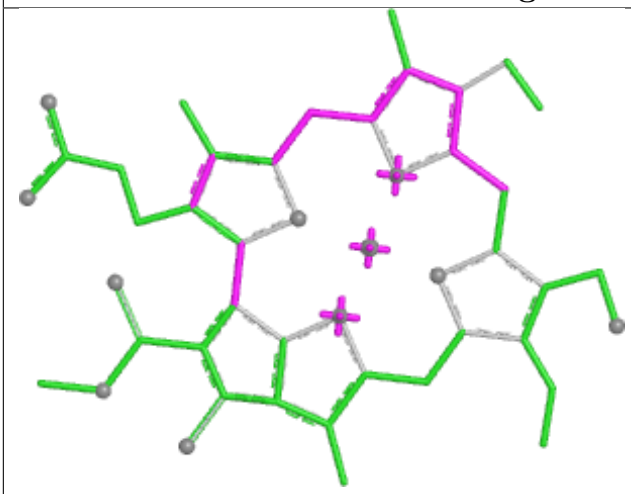


**Torsions**

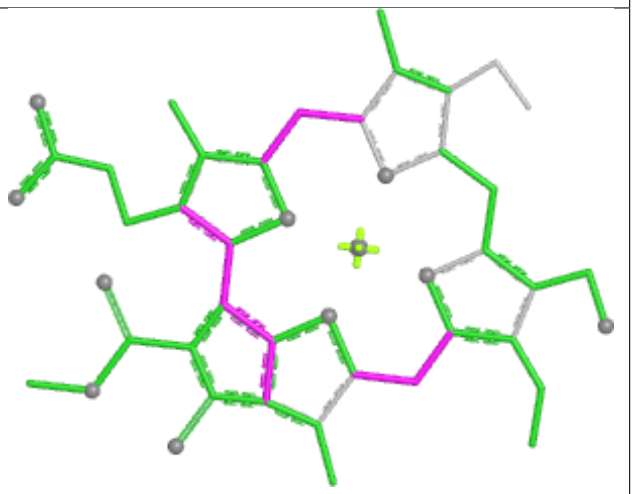


**Rings**

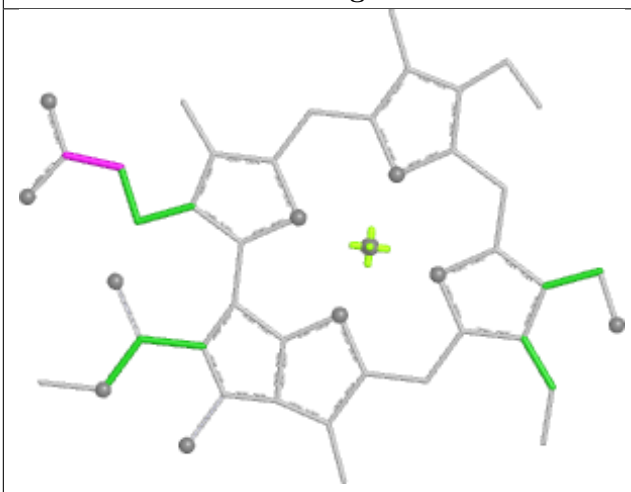
**Ligand CHL 72 606**



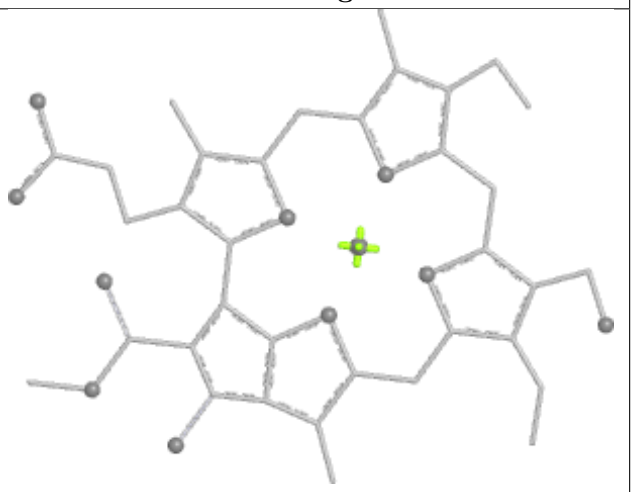
**Bond lengths**



**Bond angles**

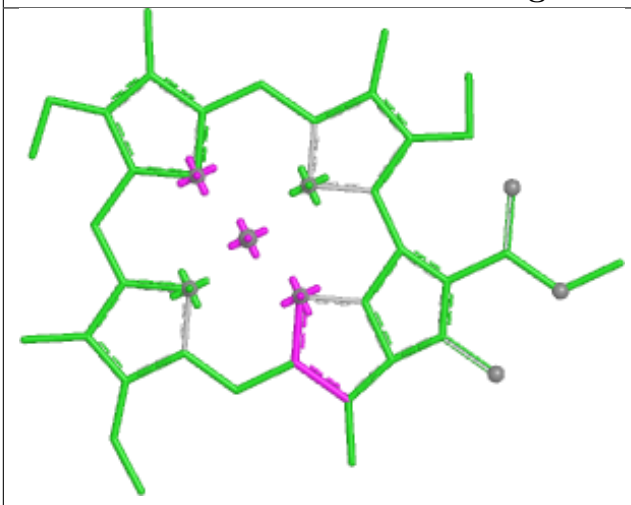


**Torsions**

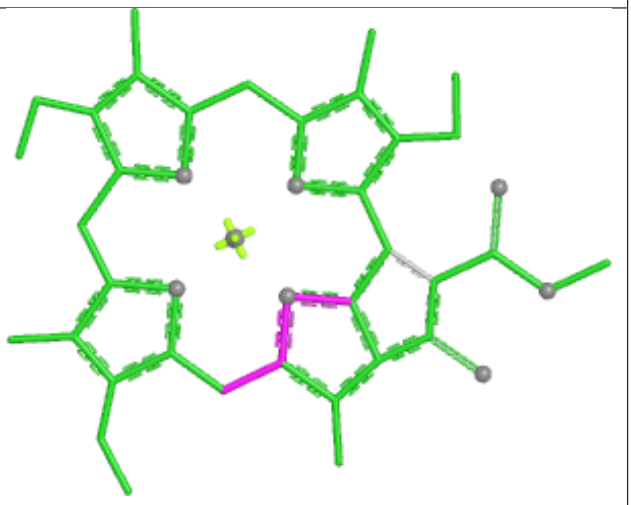


**Rings**

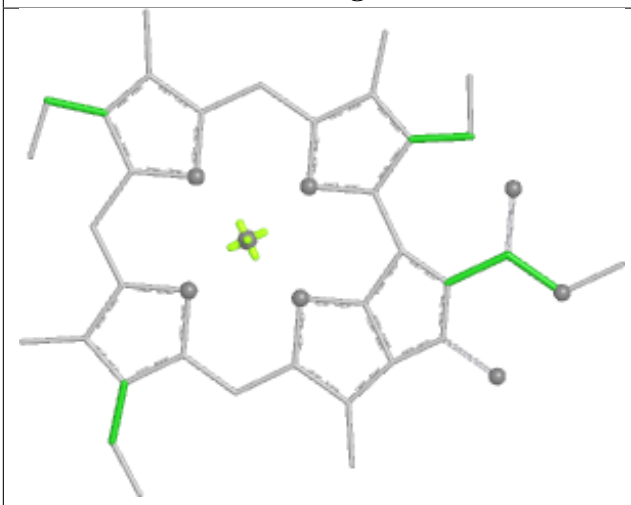
## Ligand CLA 3 606



Bond lengths



Bond angles

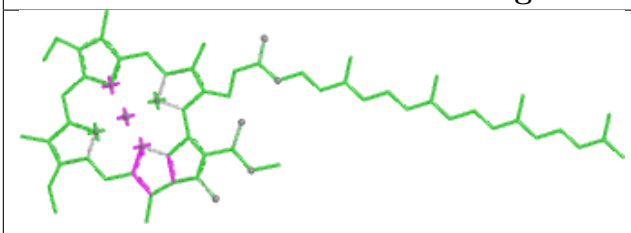


Torsions

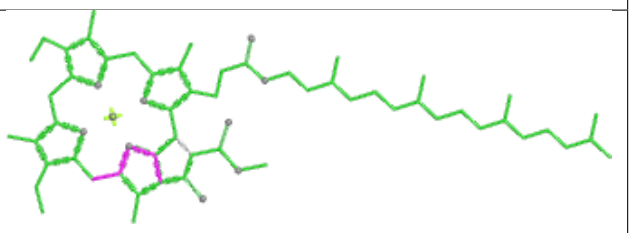


Rings

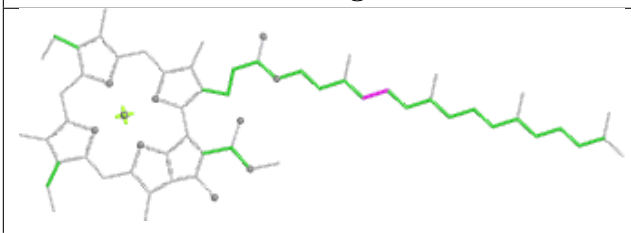
## Ligand CLA A2 833



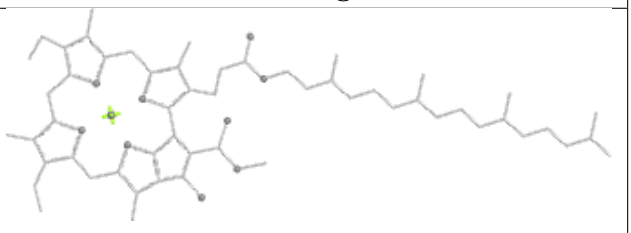
Bond lengths



Bond angles

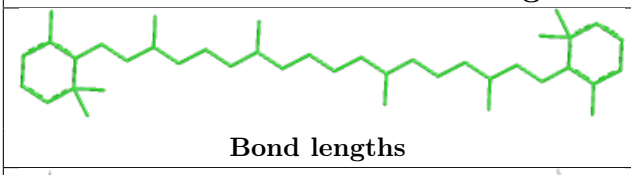


Torsions

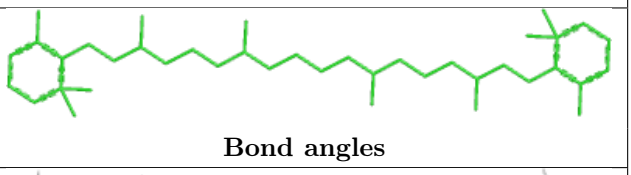


Rings

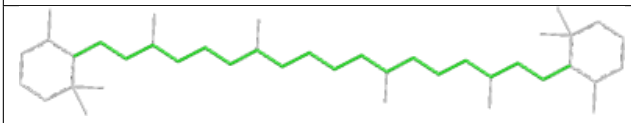
## Ligand BCR B 801



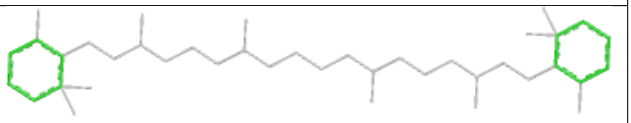
Bond lengths



Bond angles



Torsions

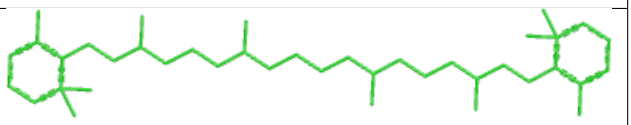


Rings

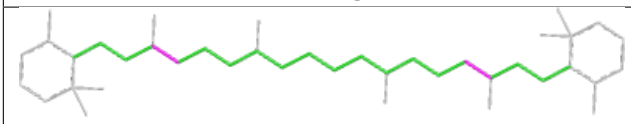
## Ligand BCR B2 845



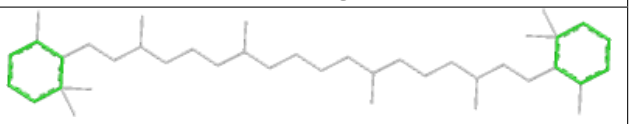
Bond lengths



Bond angles

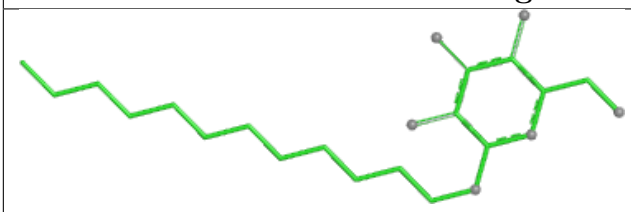


Torsions

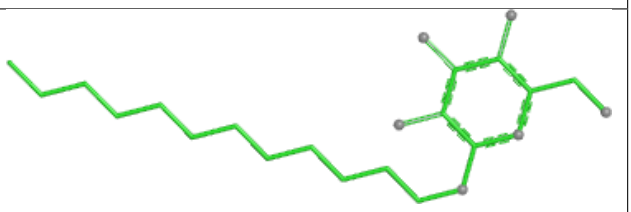


Rings

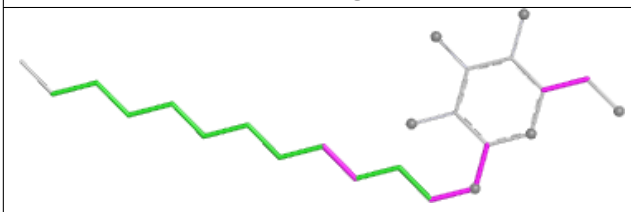
## Ligand LMU 12 625



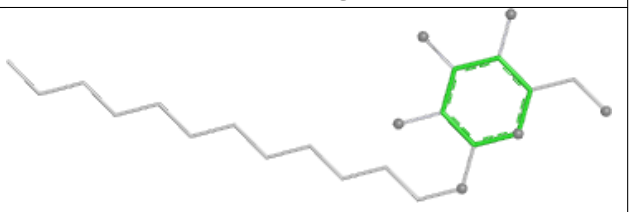
Bond lengths



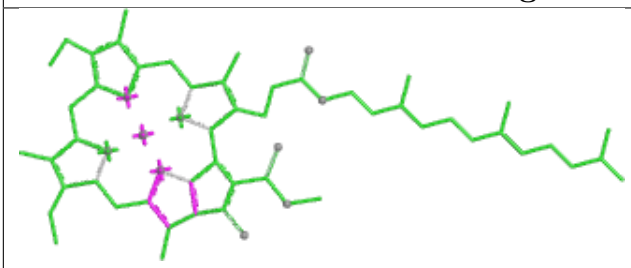
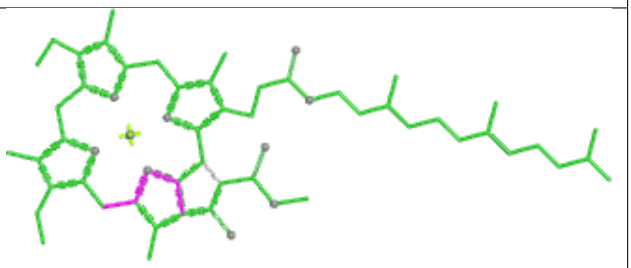
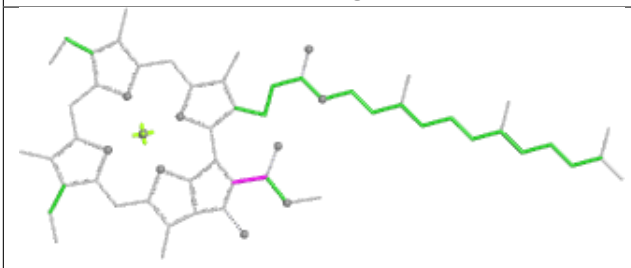
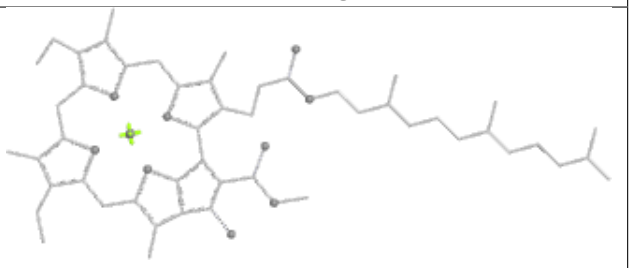
Bond angles

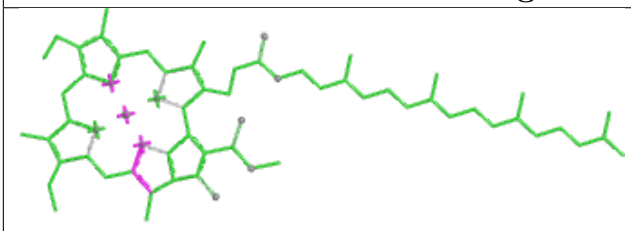
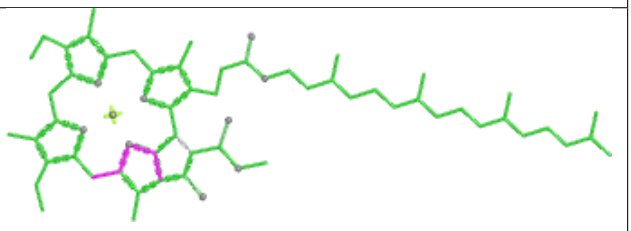
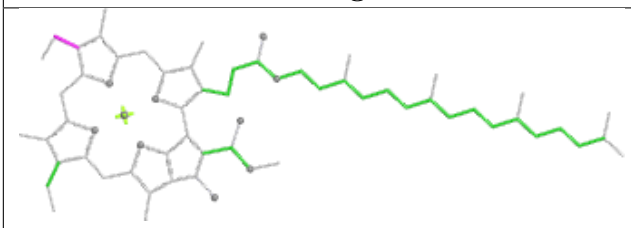
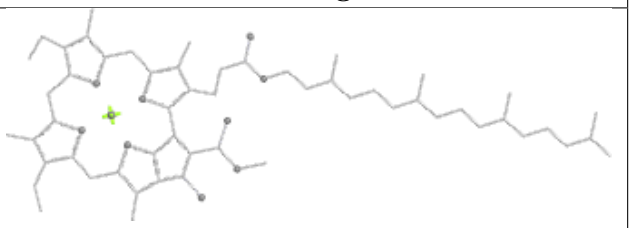


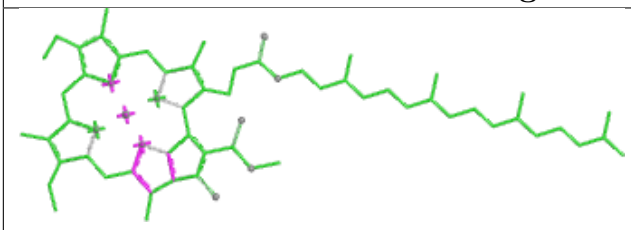
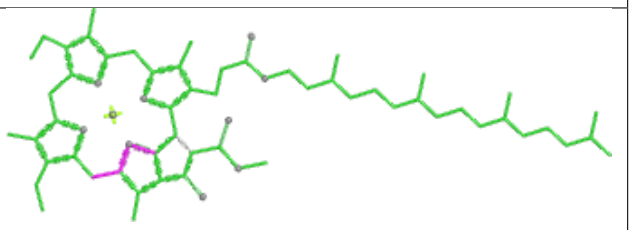
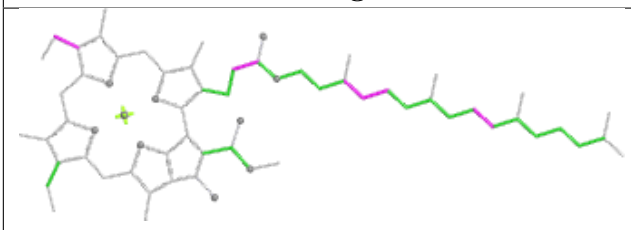
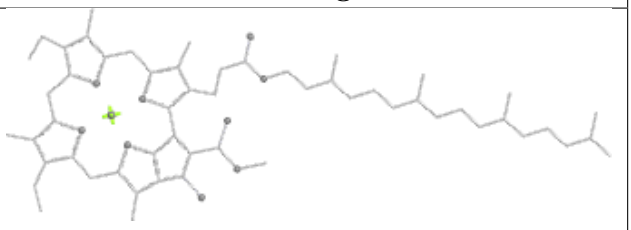
Torsions

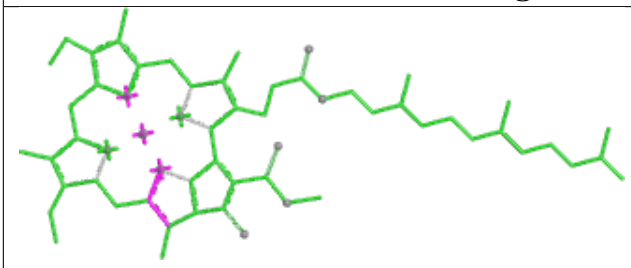
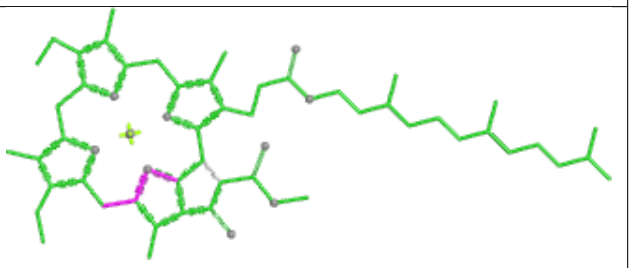
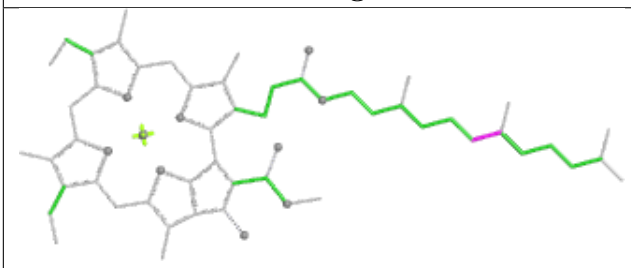
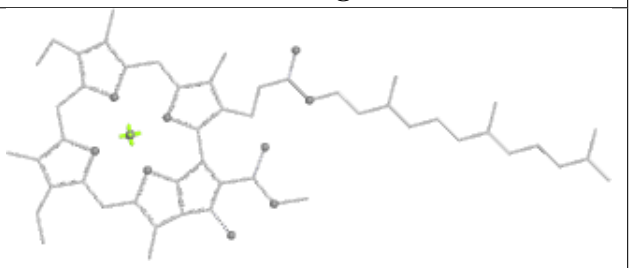


Rings

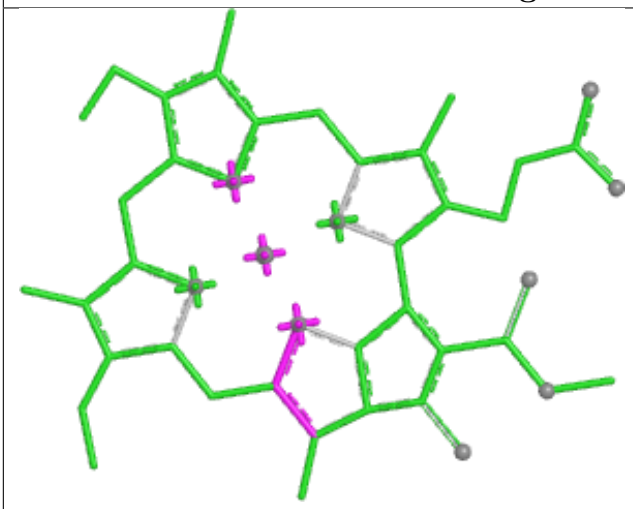
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|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA Z2 613 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

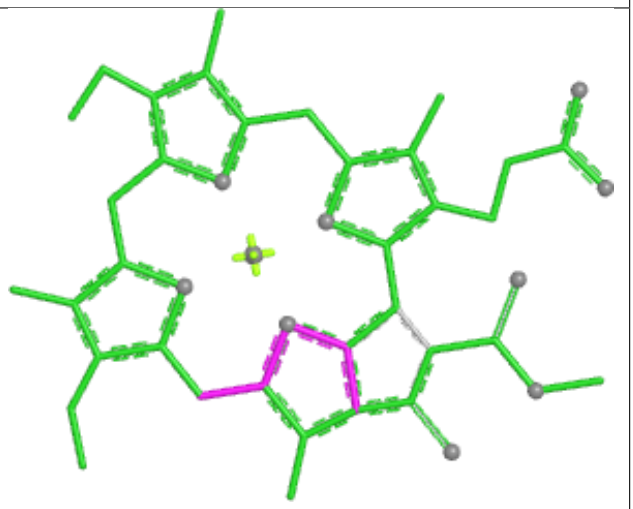
| Ligand CLA 42 603 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA G2 203 | |
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|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

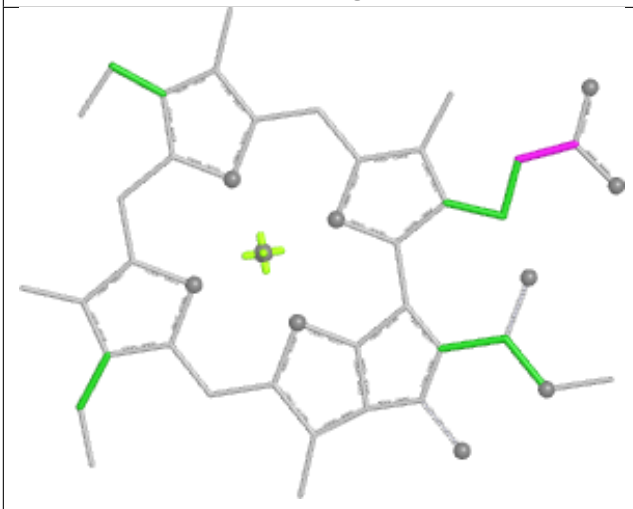
## Ligand CLA 62 612



Bond lengths



Bond angles

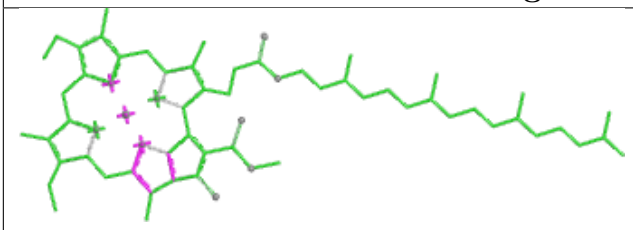


Torsions

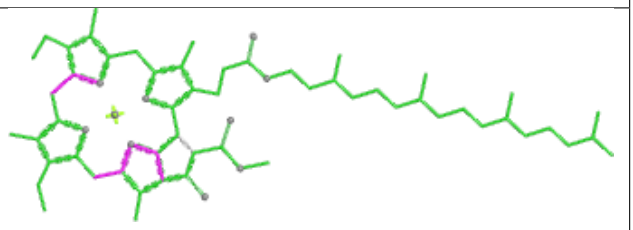


Rings

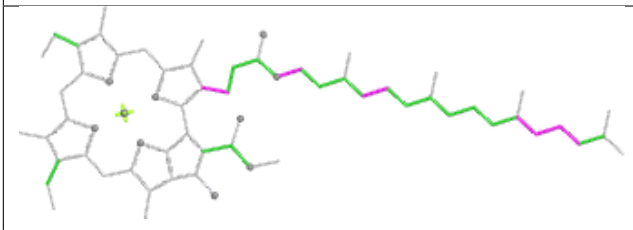
## Ligand CLA A 812



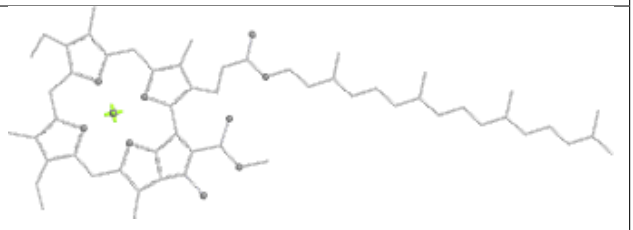
Bond lengths



Bond angles

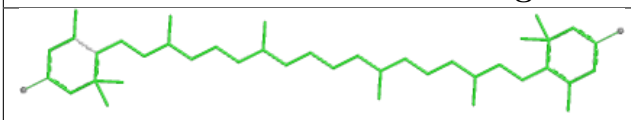


Torsions

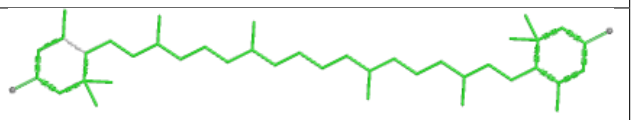


Rings

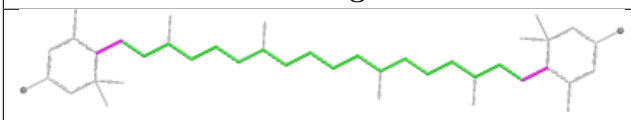
## Ligand LUT A2 856



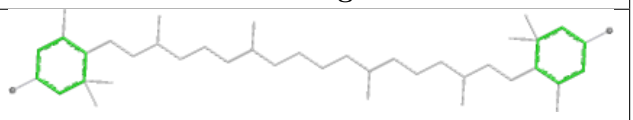
Bond lengths



Bond angles

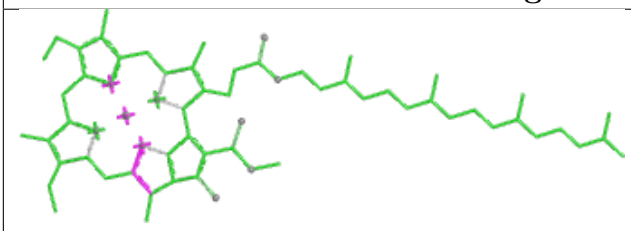


Torsions

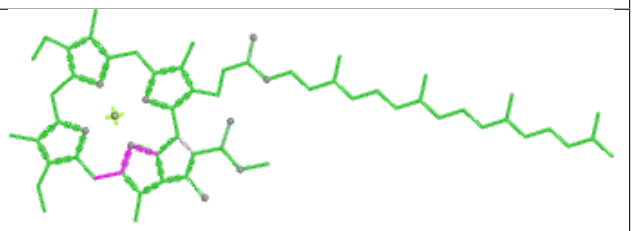


Rings

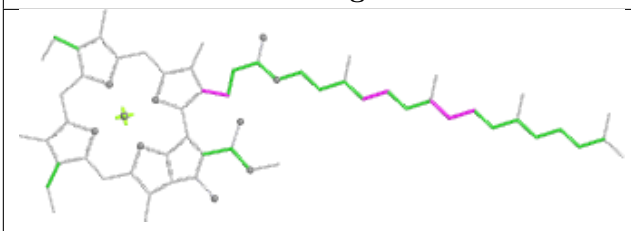
## Ligand CLA B 827



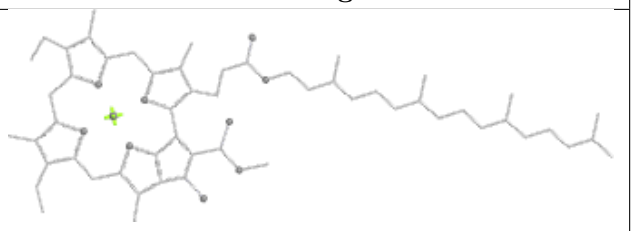
Bond lengths



Bond angles

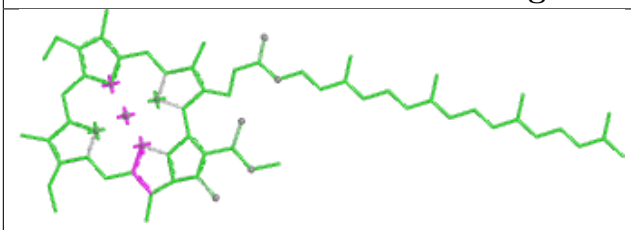


Torsions

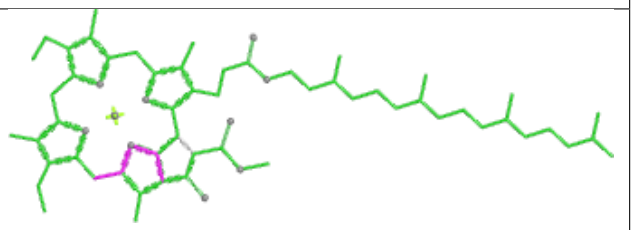


Rings

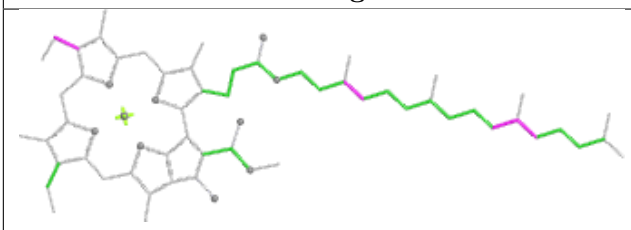
## Ligand CLA 8 613



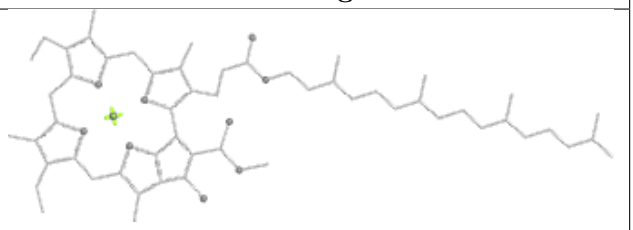
Bond lengths



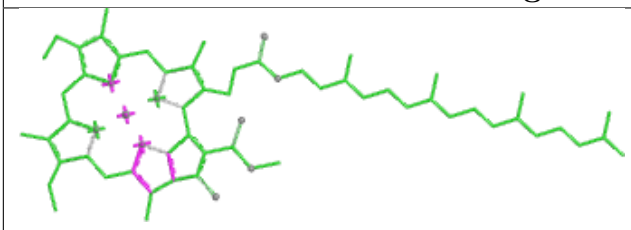
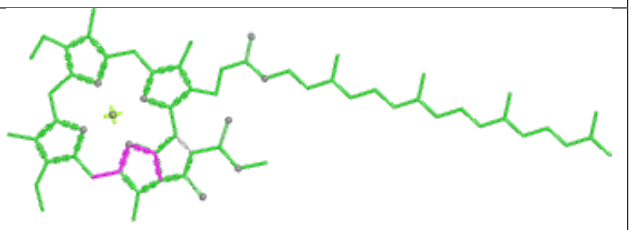
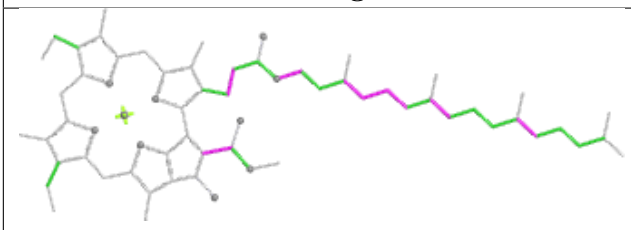
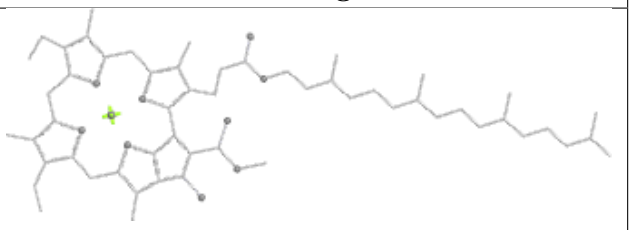
Bond angles

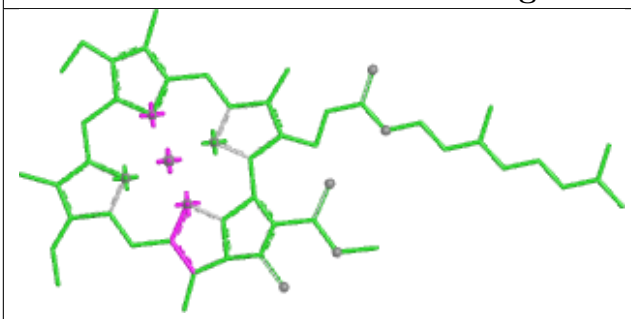
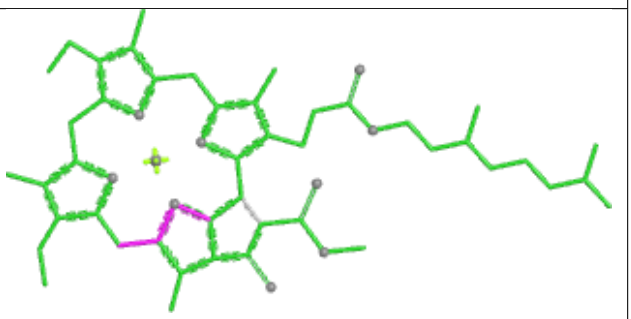
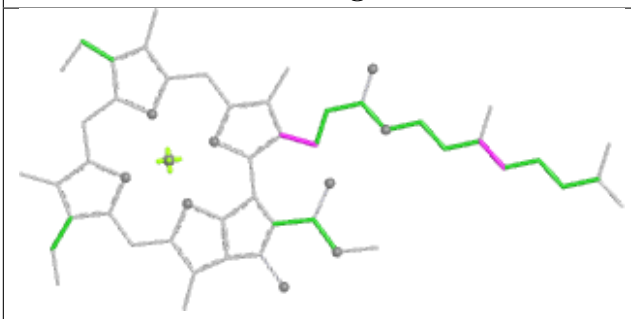
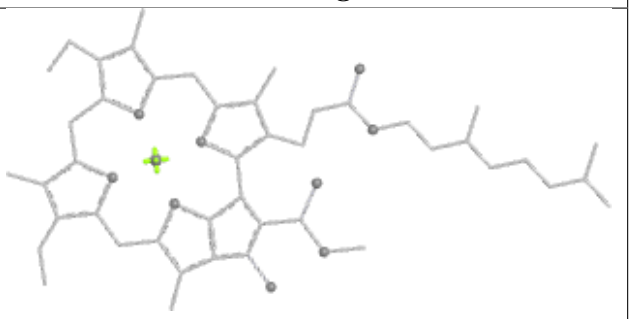


Torsions

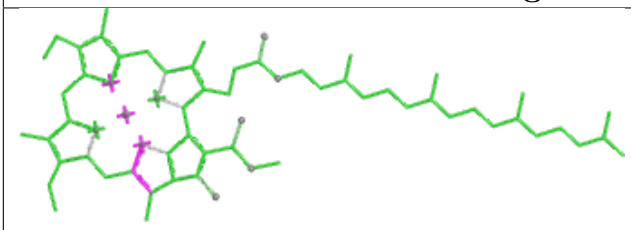


Rings

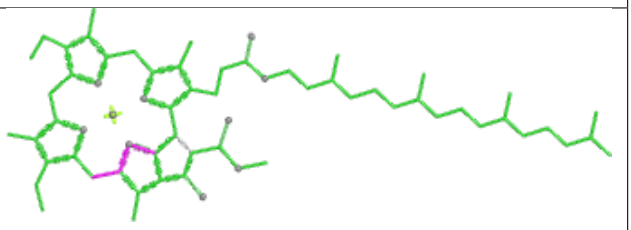
| Ligand CLA A 806 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA J2 101 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

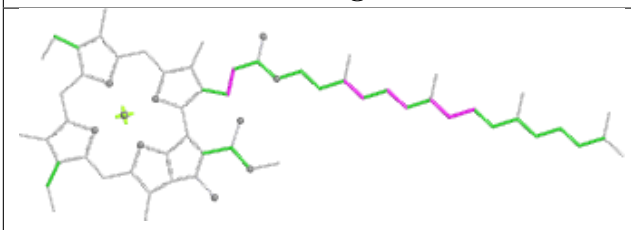
## Ligand CLA A 810



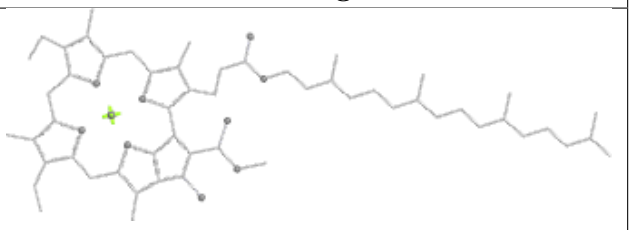
Bond lengths



Bond angles

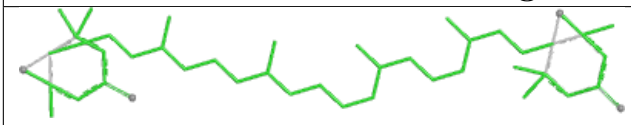


Torsions

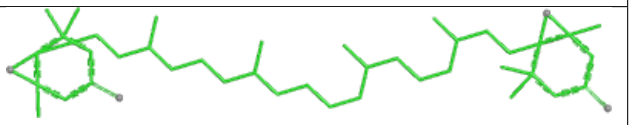


Rings

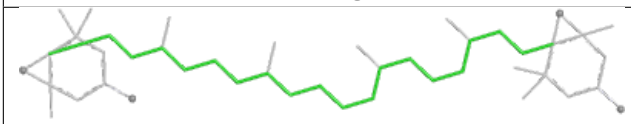
## Ligand XAT 62 624



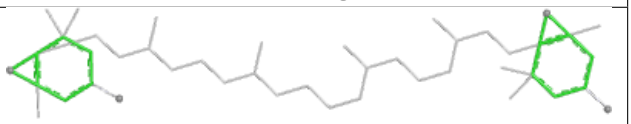
Bond lengths



Bond angles

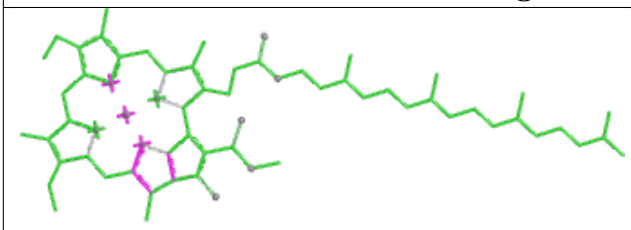


Torsions

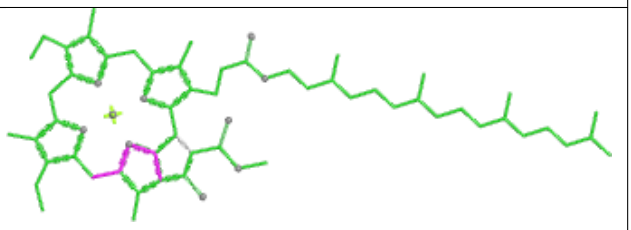


Rings

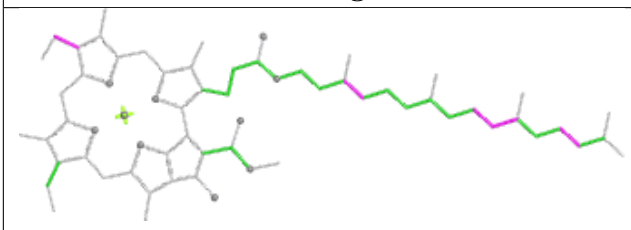
## Ligand CLA B2 840



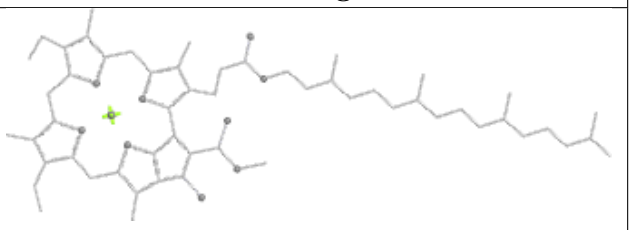
Bond lengths



Bond angles

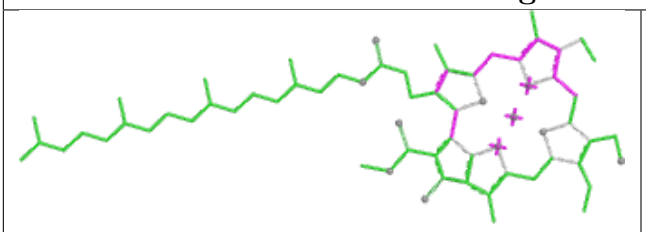


Torsions

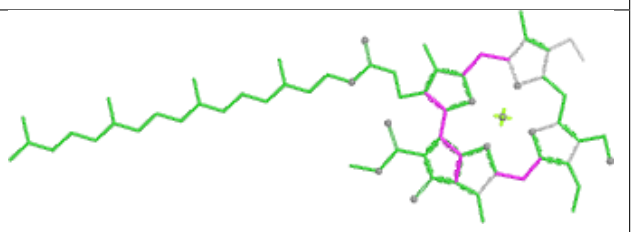


Rings

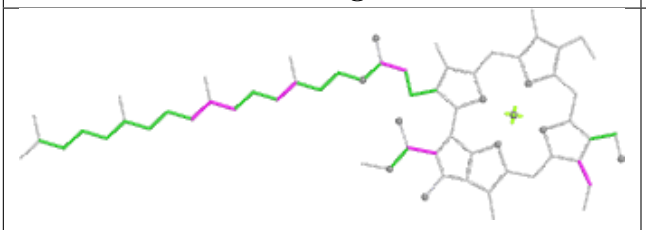
**Ligand CHL 52 607**



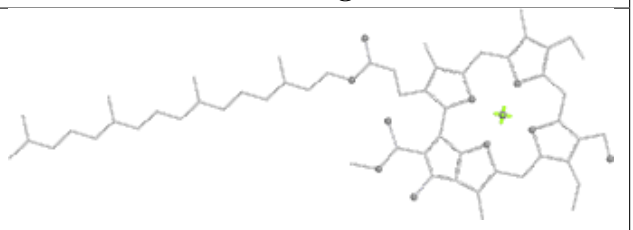
Bond lengths



Bond angles



Torsions

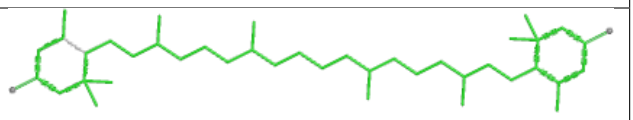


Rings

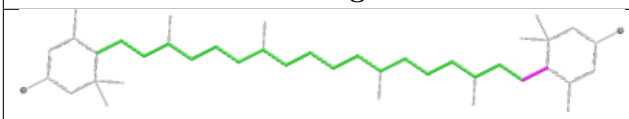
**Ligand LUT 12 617**



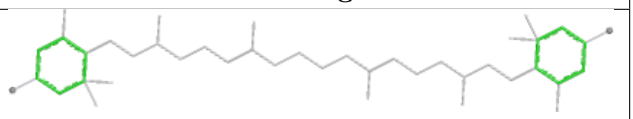
Bond lengths



Bond angles

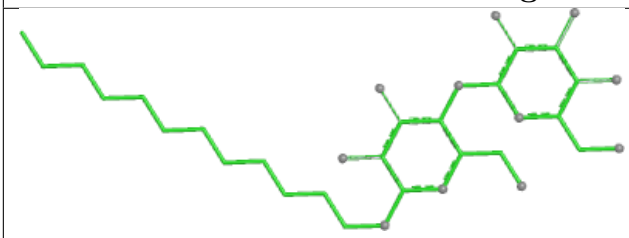


Torsions

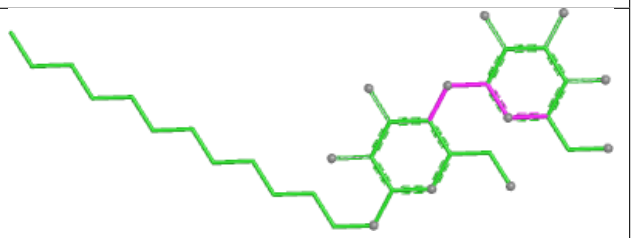


Rings

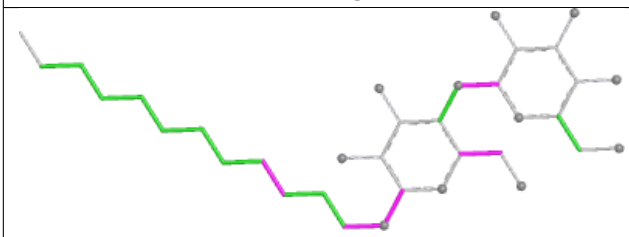
**Ligand LMU B 853**



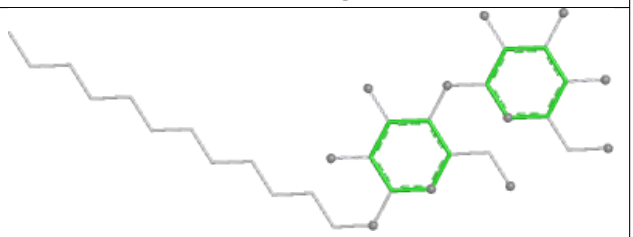
Bond lengths



Bond angles

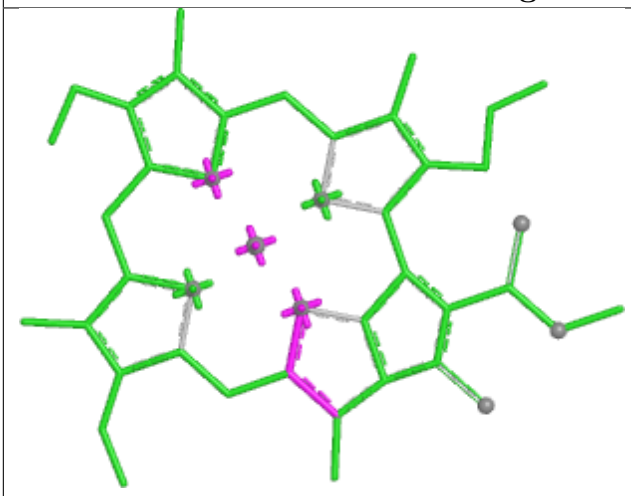


Torsions

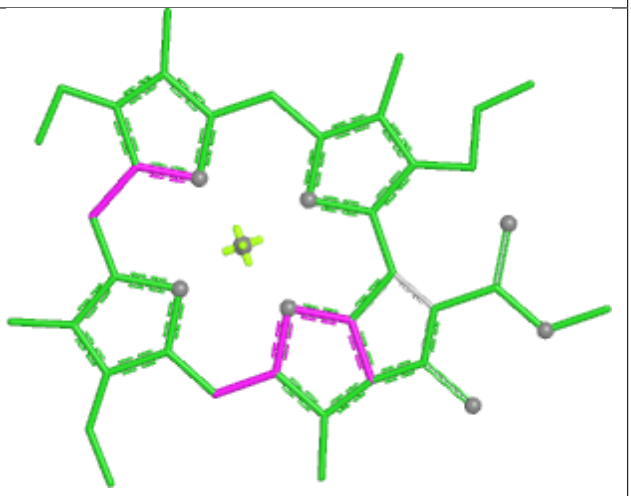


Rings

**Ligand CLA 72 614**



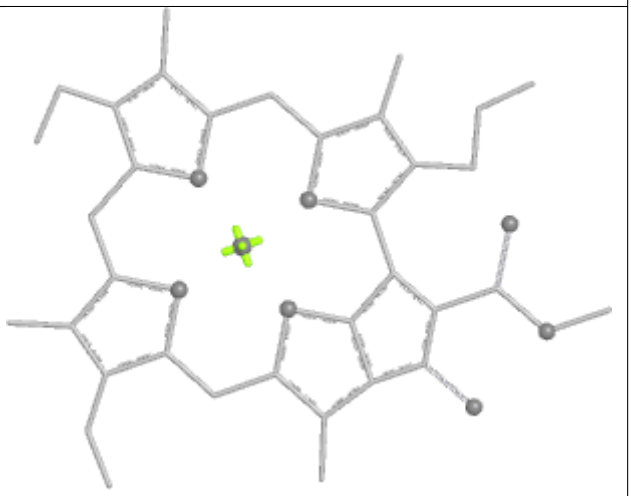
**Bond lengths**



**Bond angles**

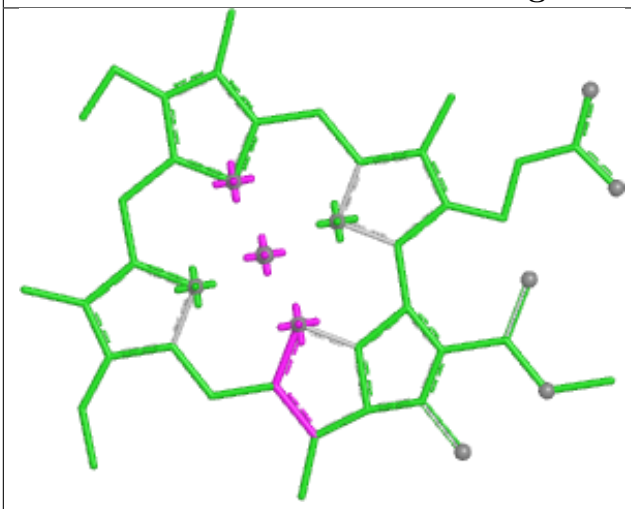


**Torsions**

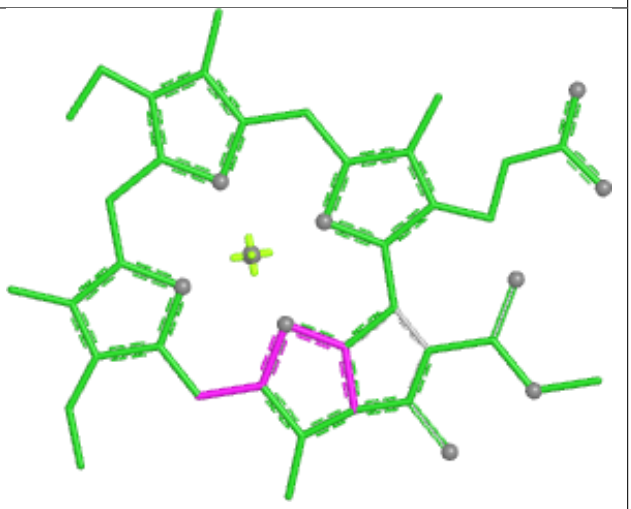


**Rings**

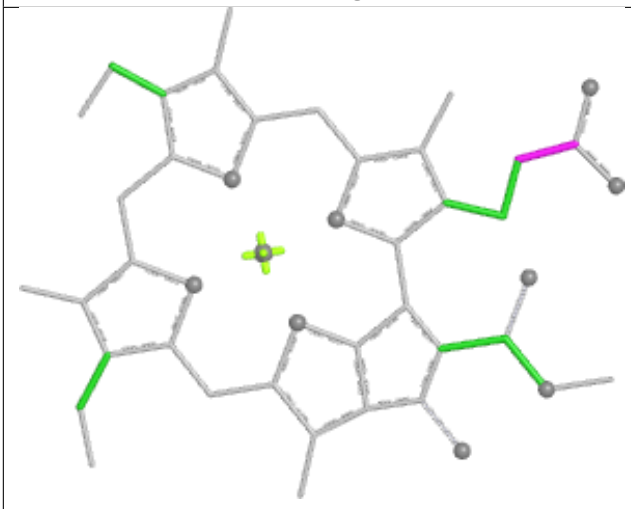
## Ligand CLA 6 612



Bond lengths



Bond angles

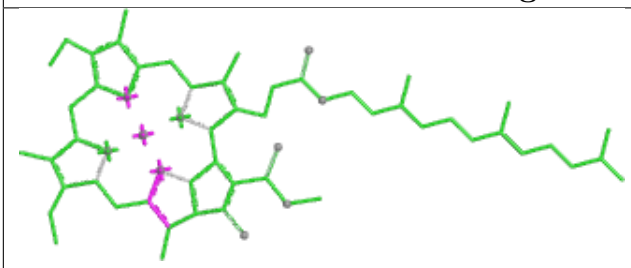


Torsions

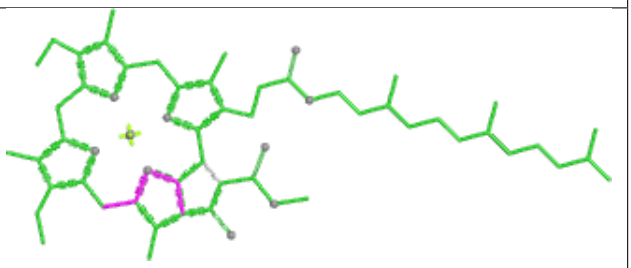


Rings

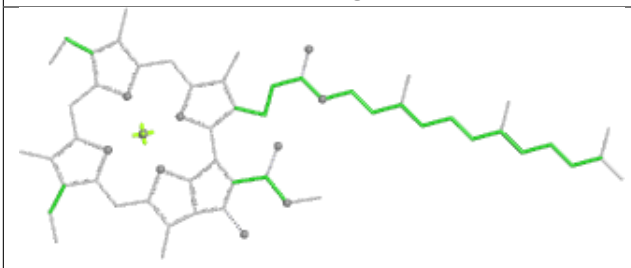
## Ligand CLA 62 610



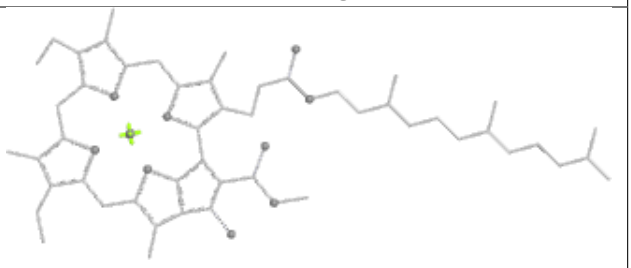
Bond lengths



Bond angles

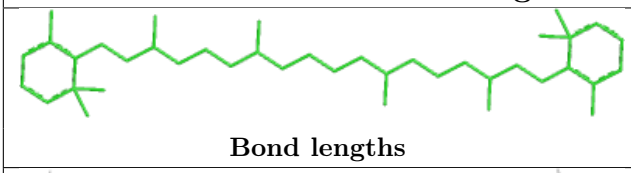


Torsions

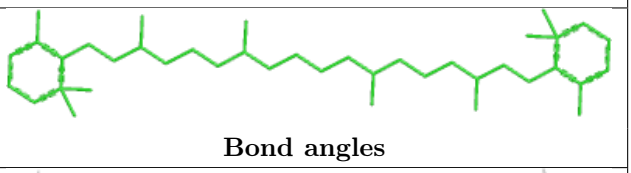


Rings

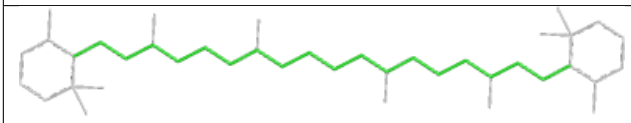
## Ligand BCR B2 843



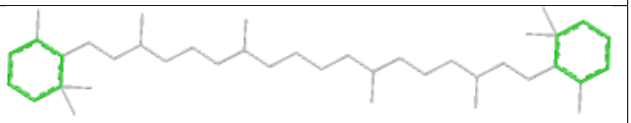
Bond lengths



Bond angles



Torsions



Rings

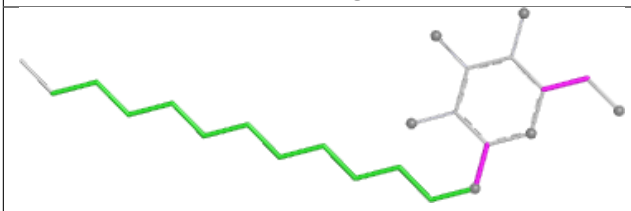
## Ligand LMU A2 864



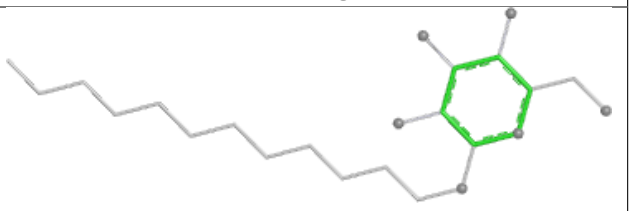
Bond lengths



Bond angles

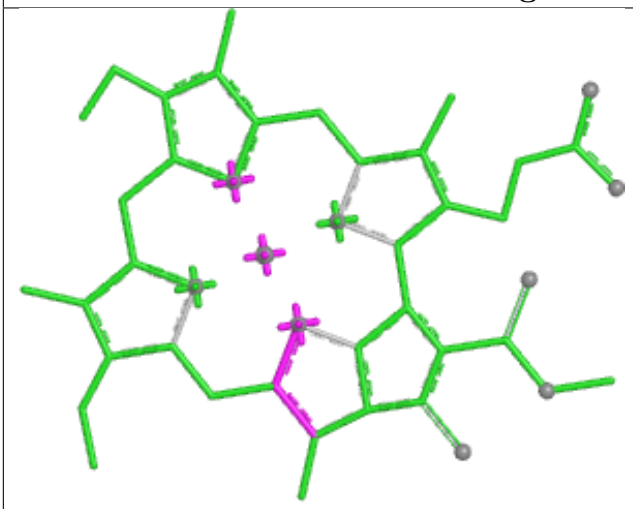


Torsions

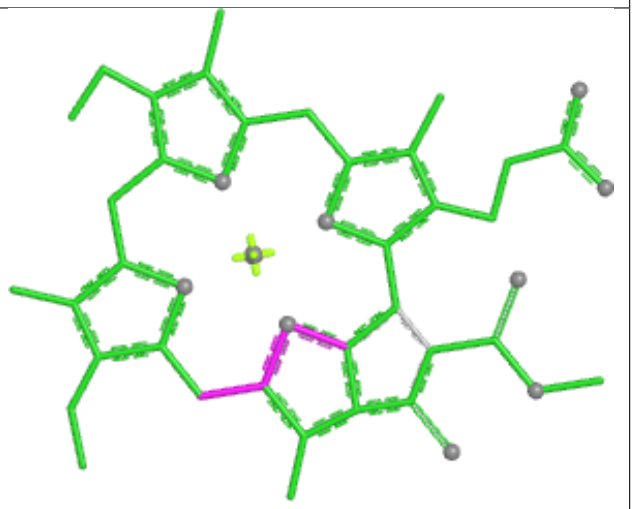


Rings

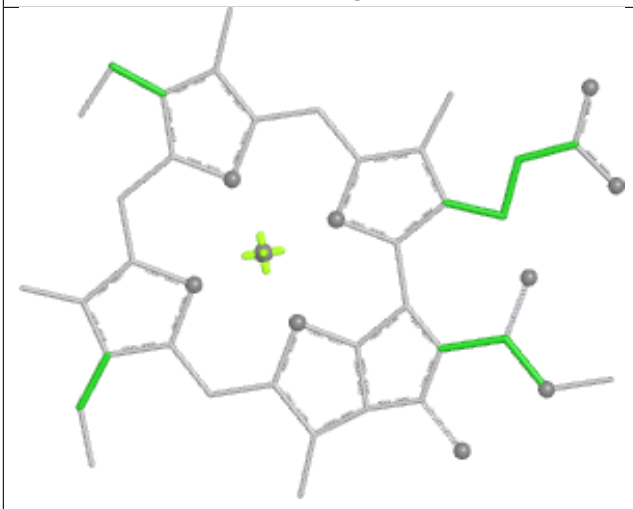
## Ligand CLA 82 609



Bond lengths



Bond angles

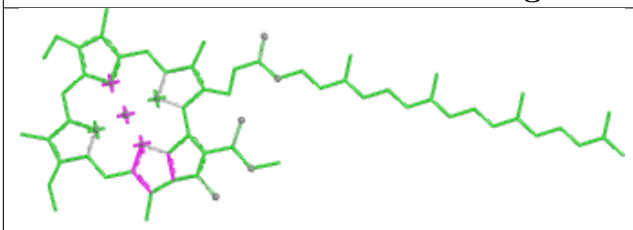


Torsions

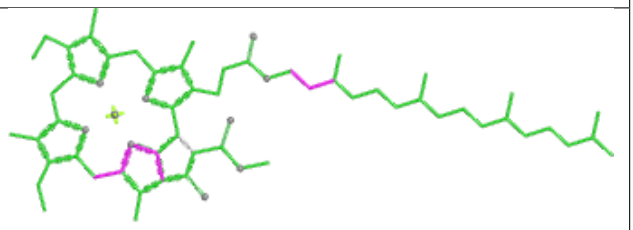


Rings

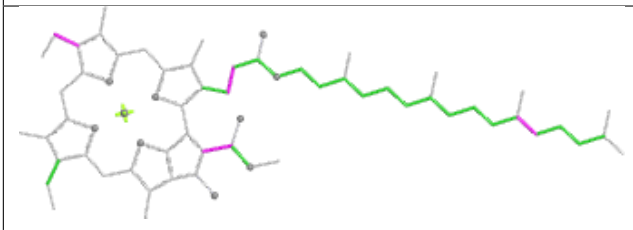
## Ligand CLA A 809



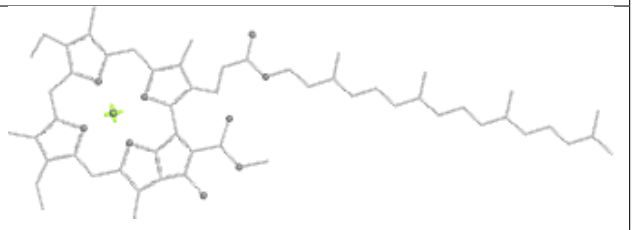
Bond lengths



Bond angles

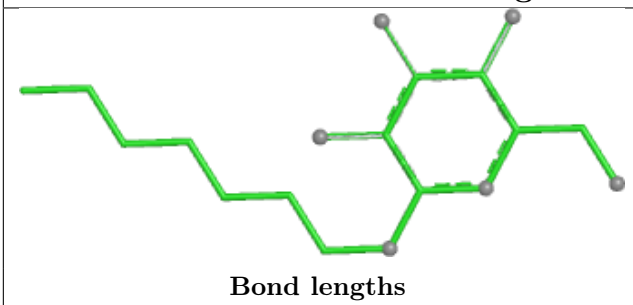


Torsions

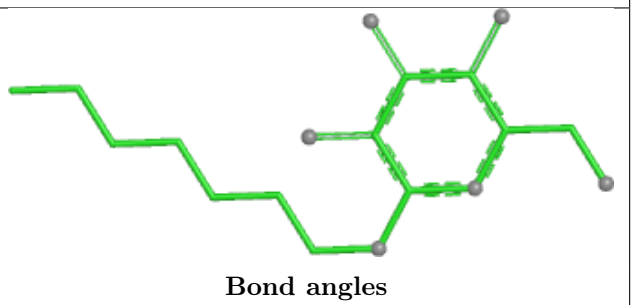


Rings

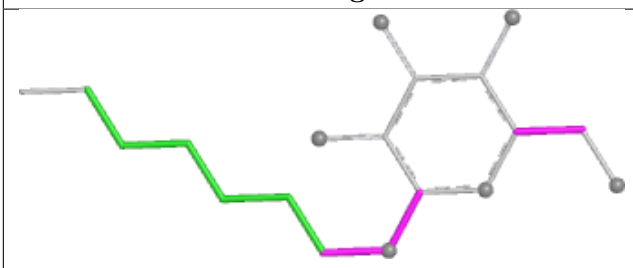
## Ligand LMU 12 622



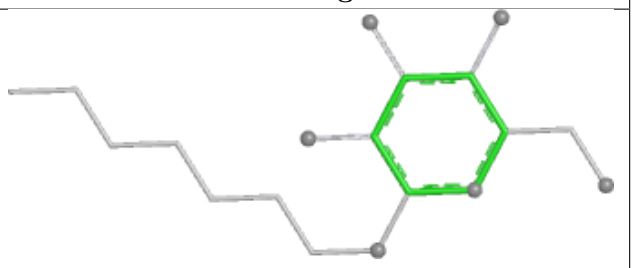
Bond lengths



Bond angles

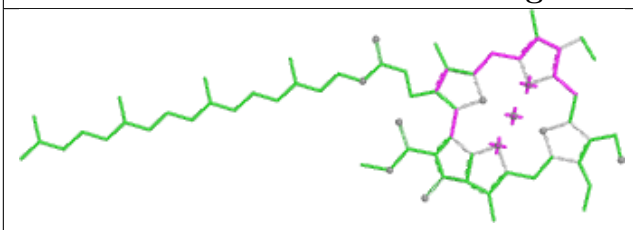


Torsions

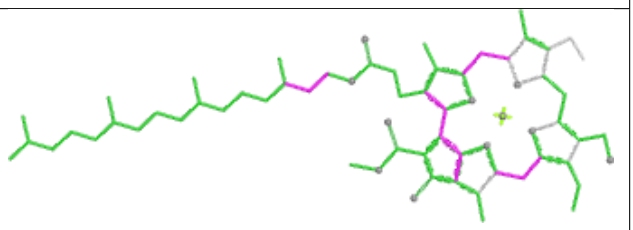


Rings

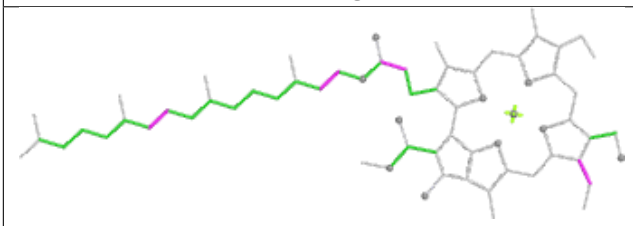
## Ligand CHL Z 607



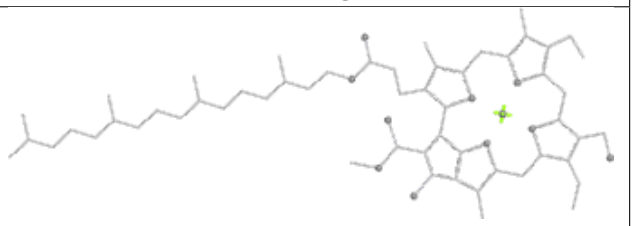
Bond lengths



Bond angles

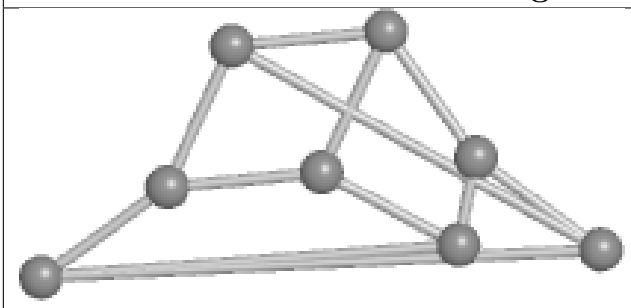


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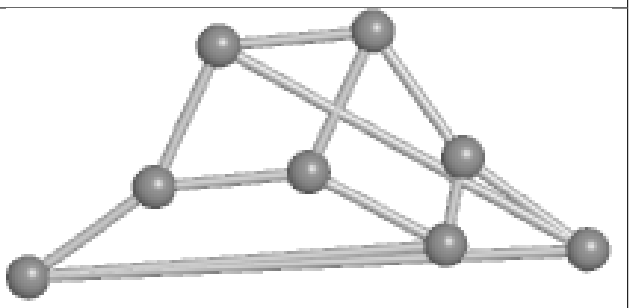


Rings

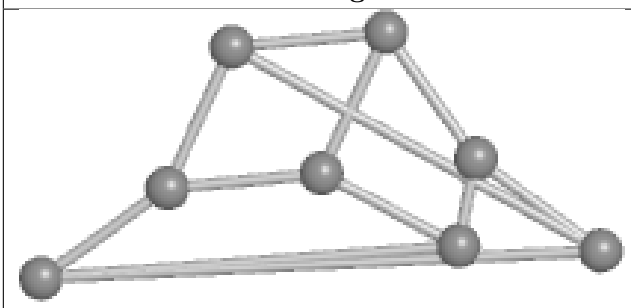
**Ligand SF4 C 101**



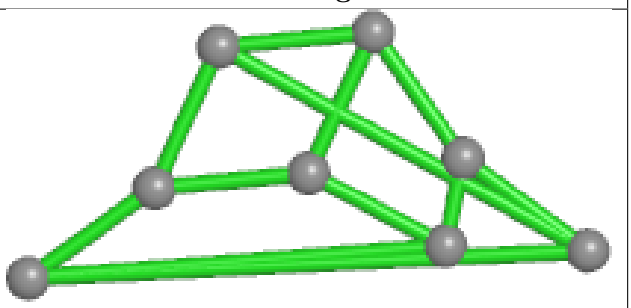
Bond lengths



Bond angles

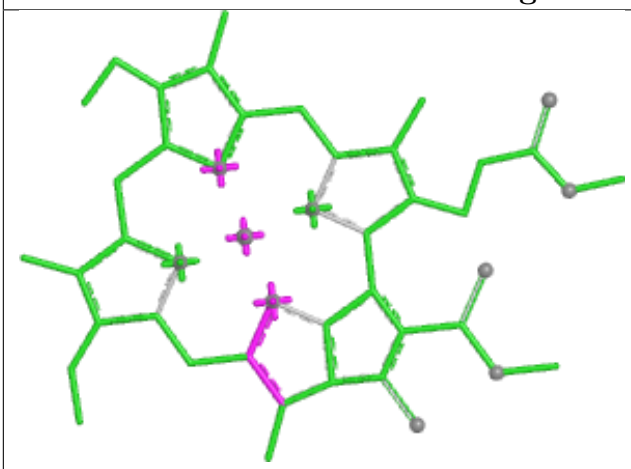


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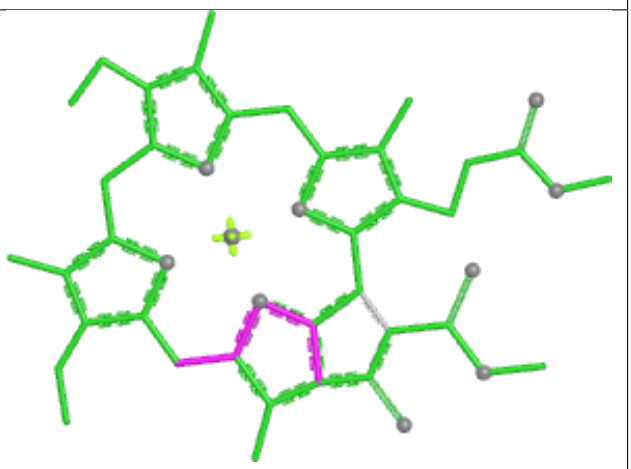


Rings

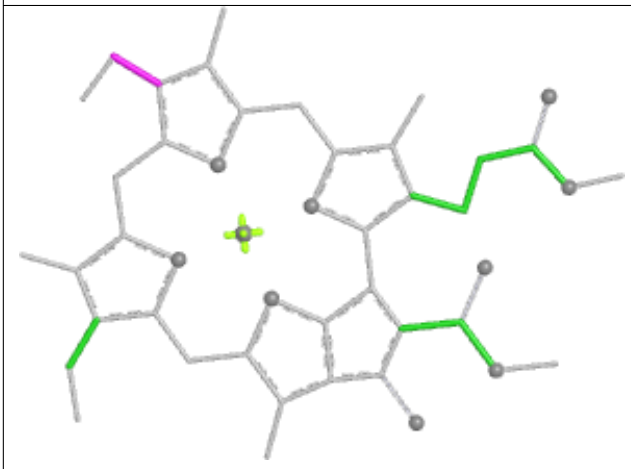
**Ligand CLA 32 612**



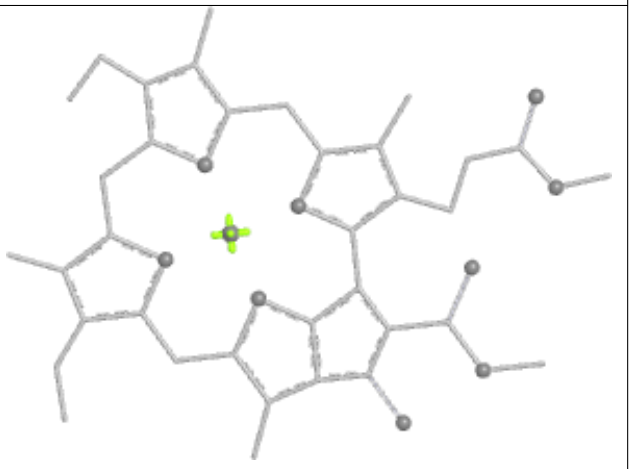
Bond lengths



Bond angles

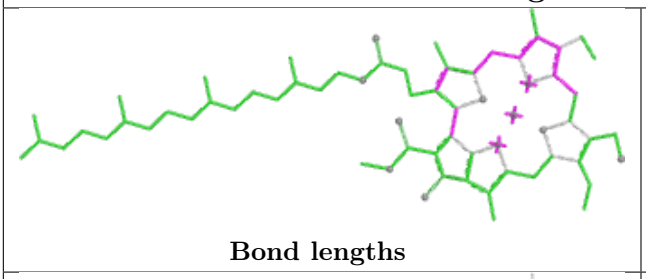


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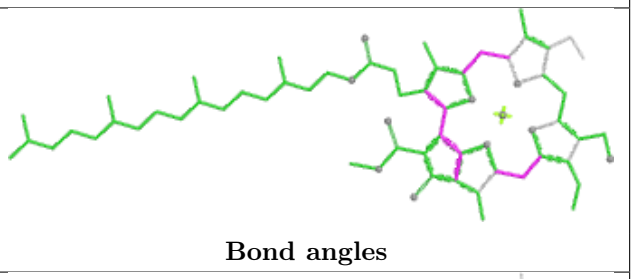


Rings

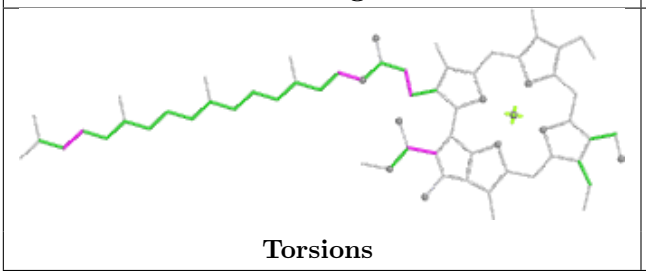
## Ligand CHL 4 608



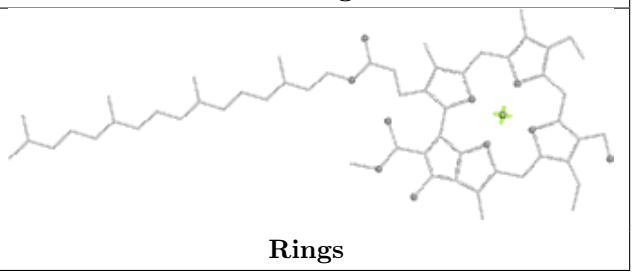
Bond lengths



Bond angles

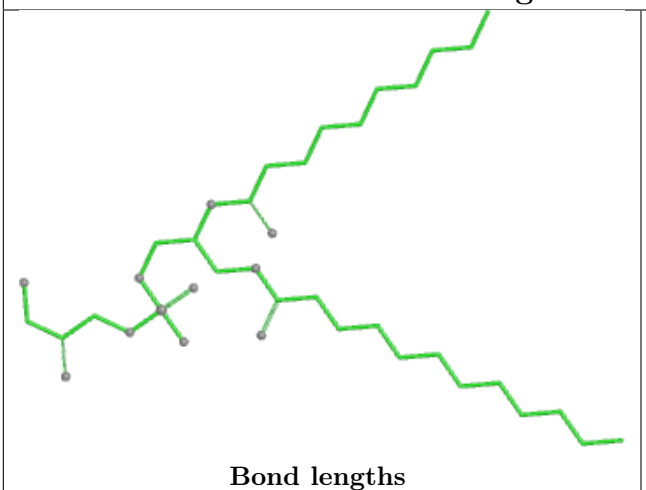


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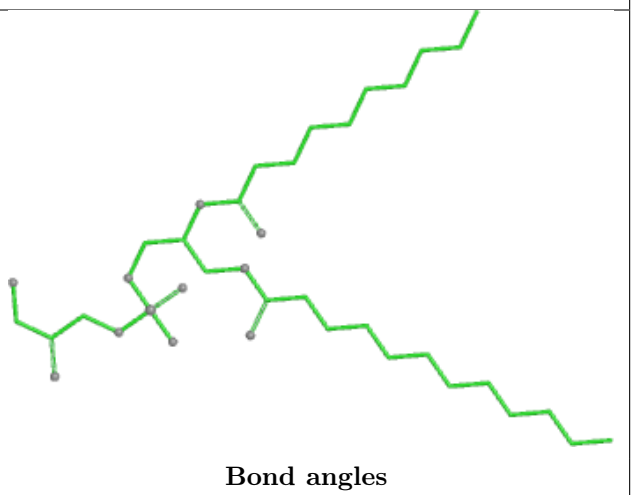


Rings

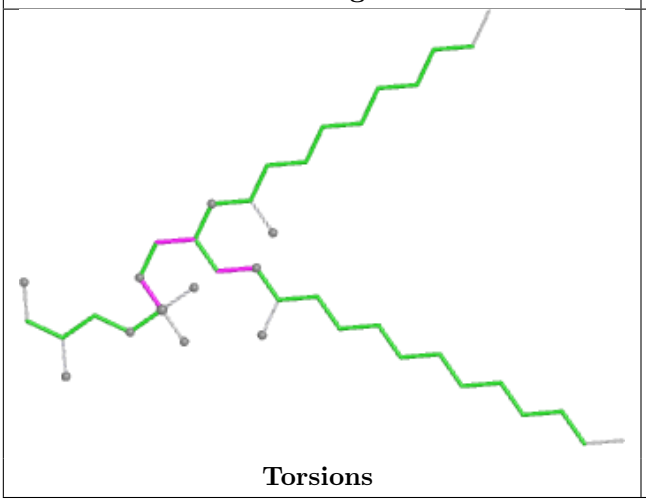
## Ligand LHG Z2 620



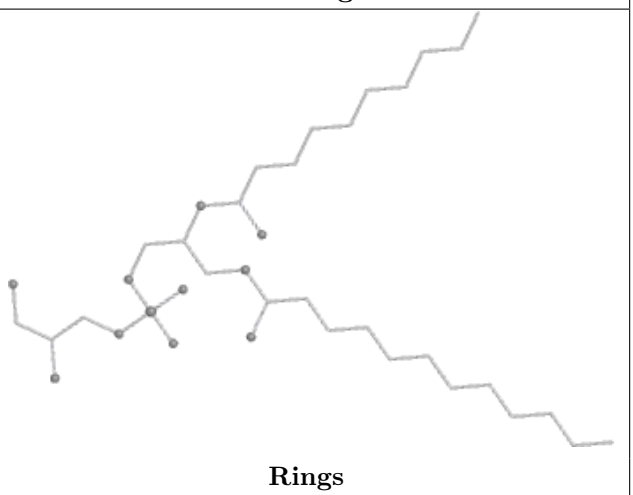
Bond lengths



Bond angles

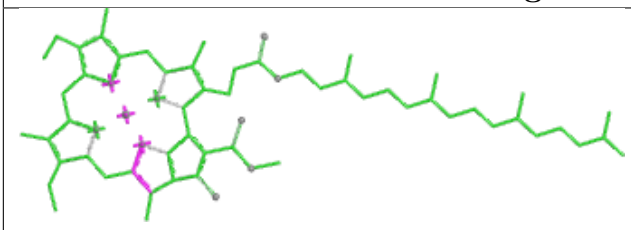


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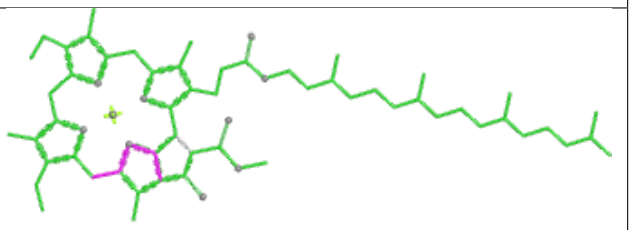


Rings

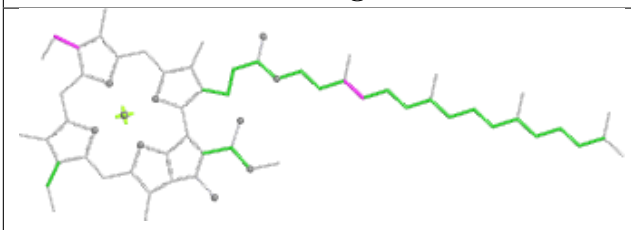
## Ligand CLA B 828



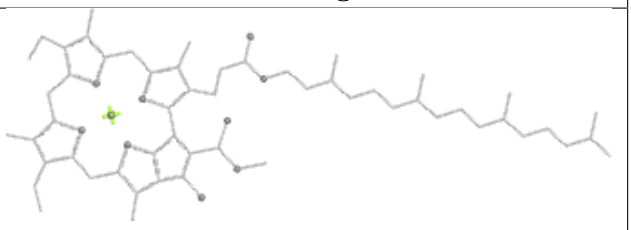
Bond lengths



Bond angles

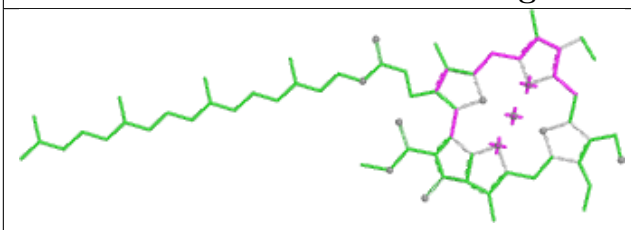


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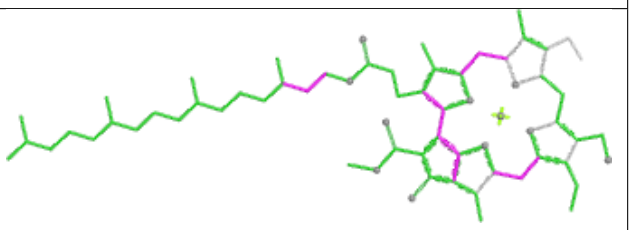


Rings

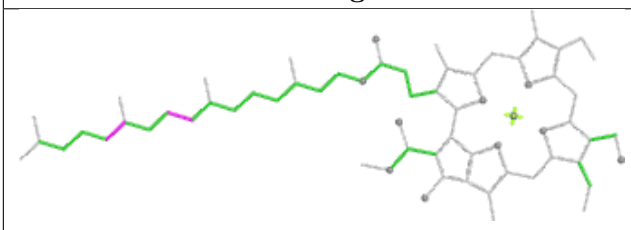
## Ligand CHL 62 616



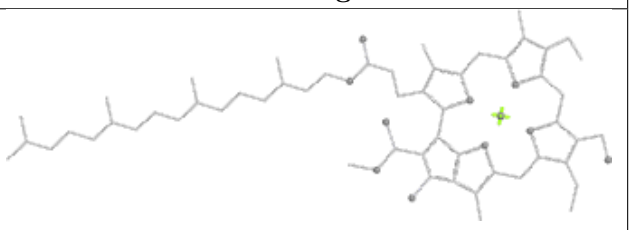
Bond lengths



Bond angles

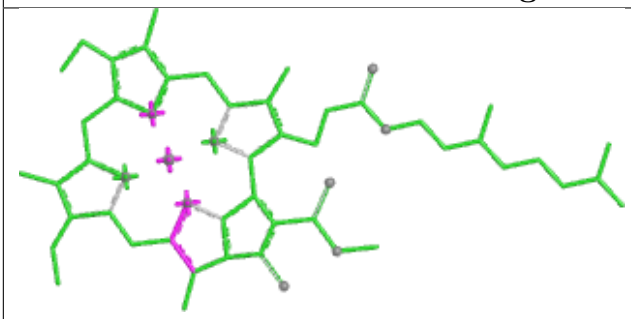


Torsions

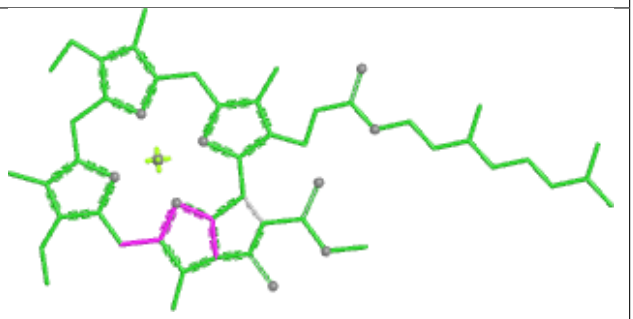


Rings

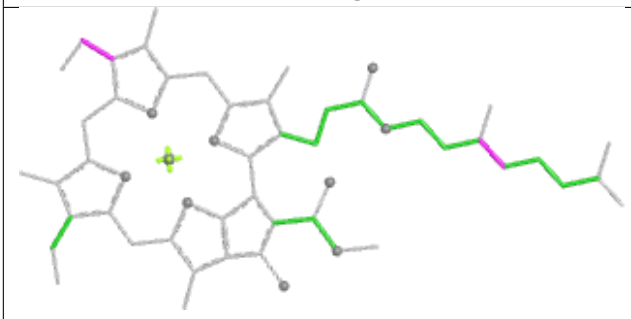
**Ligand CLA 52 611**



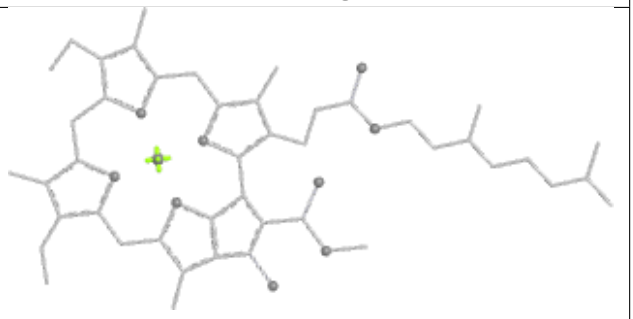
**Bond lengths**



**Bond angles**

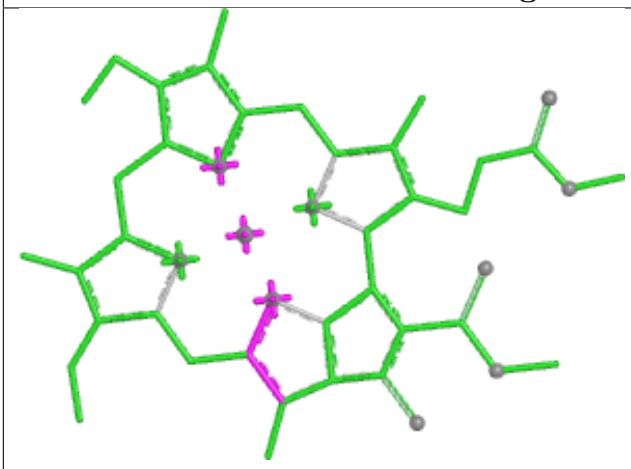


**Torsions**

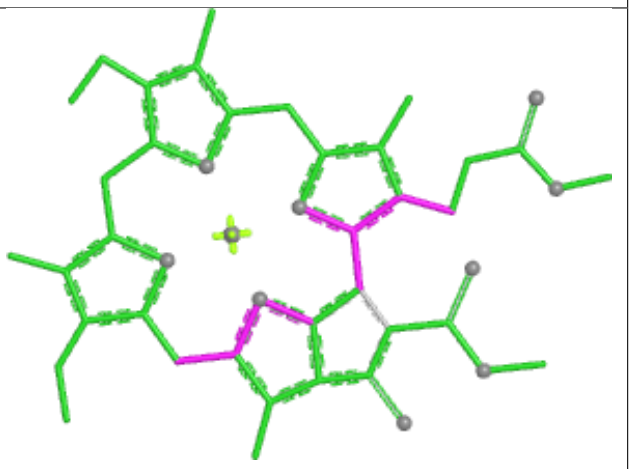


**Rings**

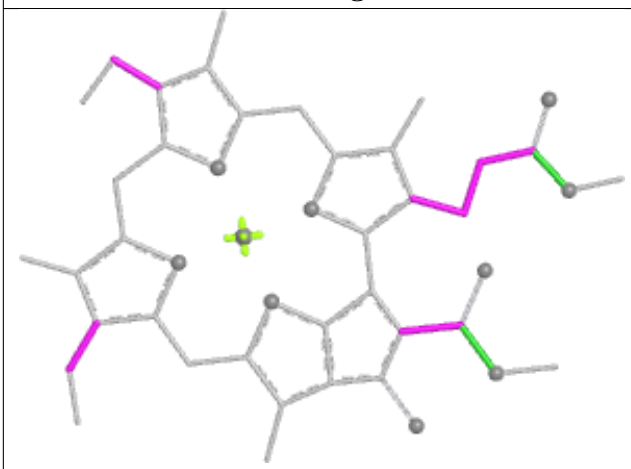
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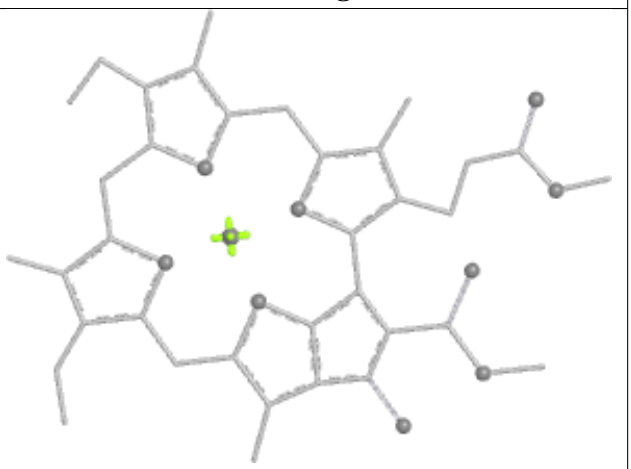
Bond lengths



Bond angles

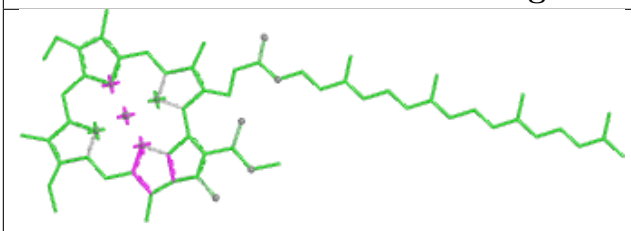


Torsions

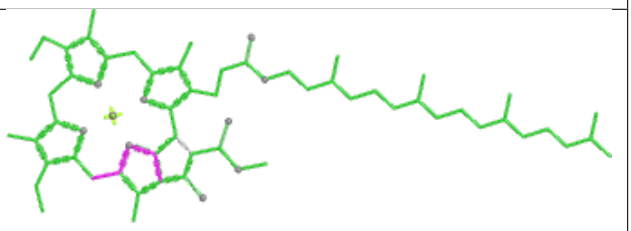


Rings

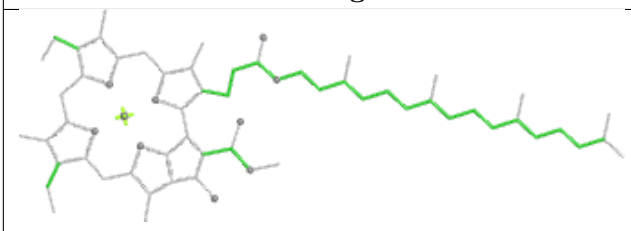
## Ligand CLA 3 610



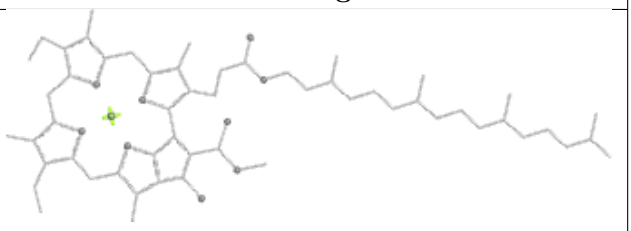
Bond lengths



Bond angles

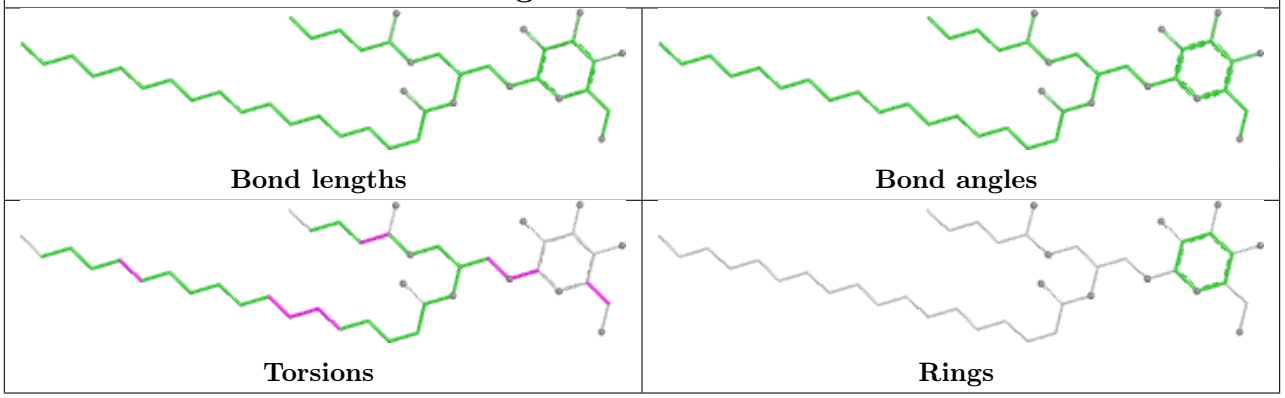


Torsions

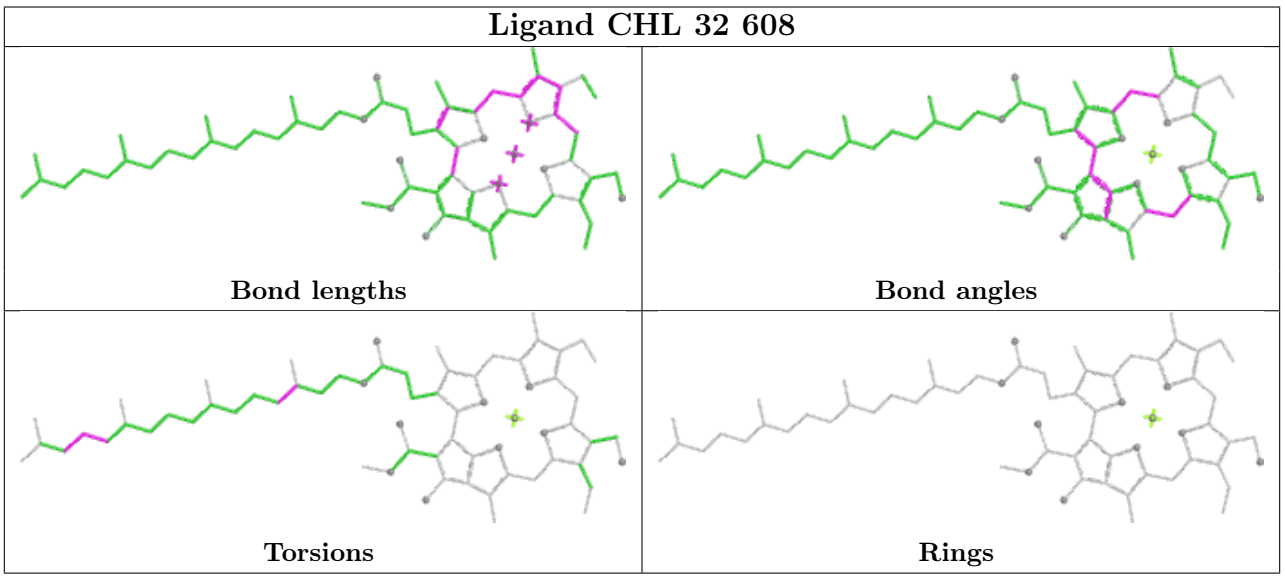


Rings

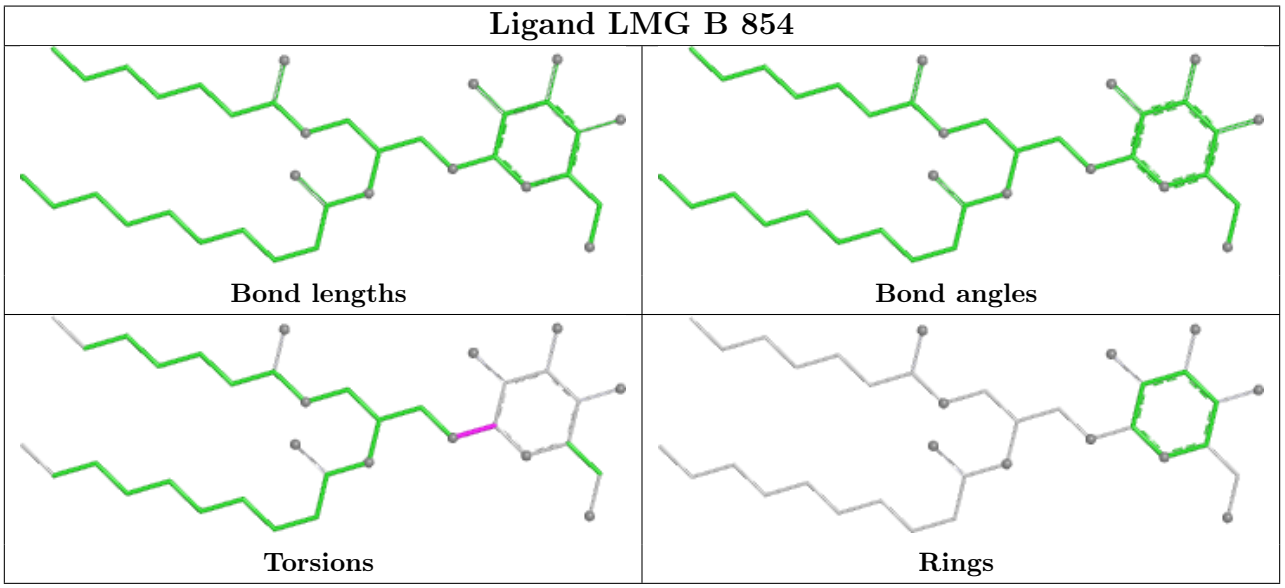
**Ligand LMG 82 629**



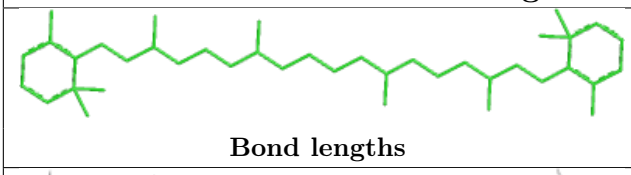

**Ligand CHL 32 608**



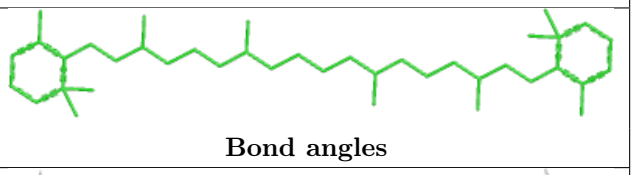

**Ligand LMG B 854**



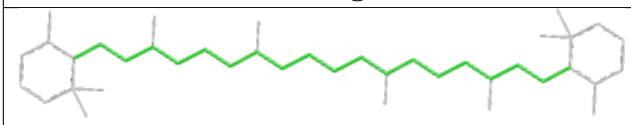
## Ligand BCR A 850



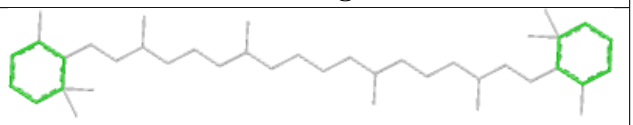
Bond lengths



Bond angles

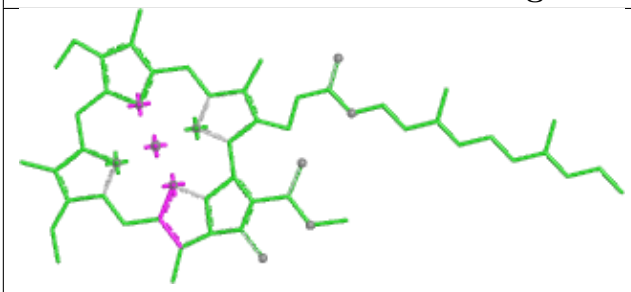


Torsions

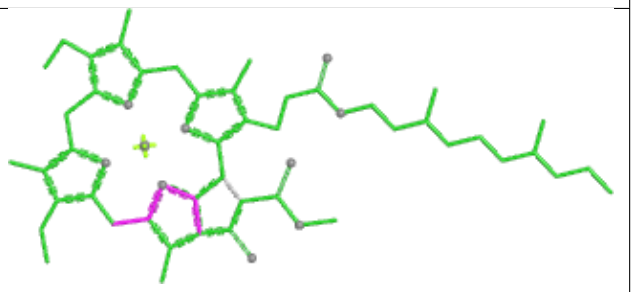


Rings

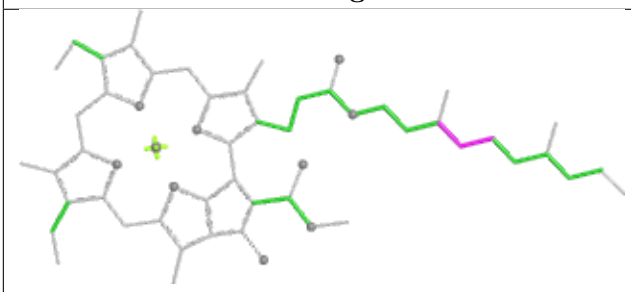
## Ligand CLA Z 604



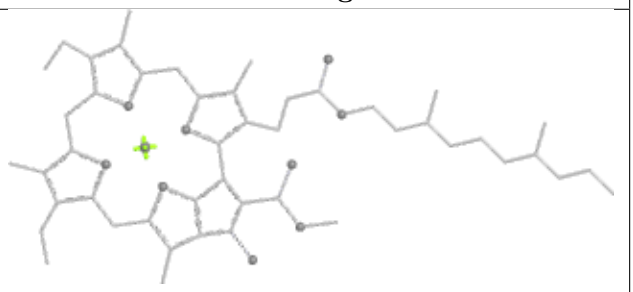
Bond lengths



Bond angles

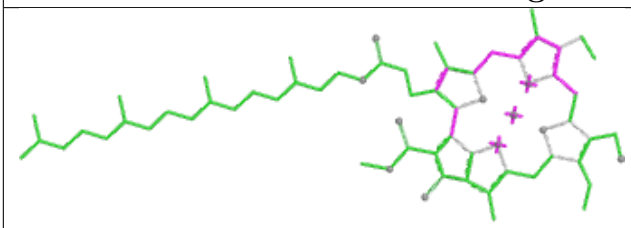


Torsions

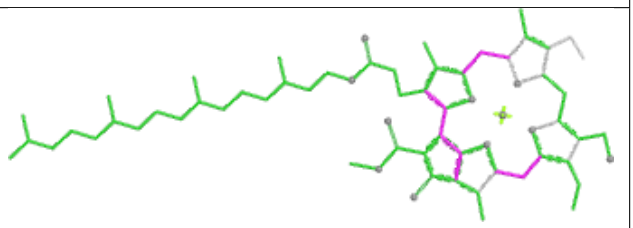


Rings

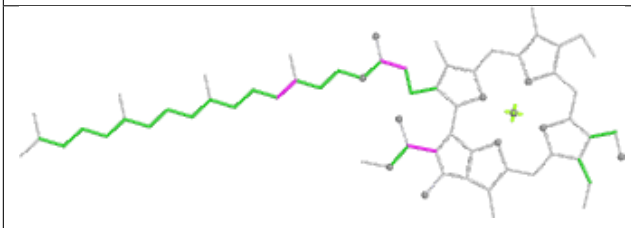
## Ligand CHL 6 601



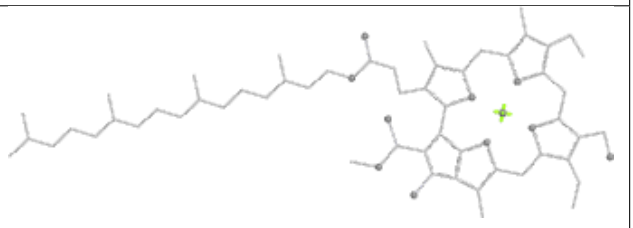
Bond lengths



Bond angles

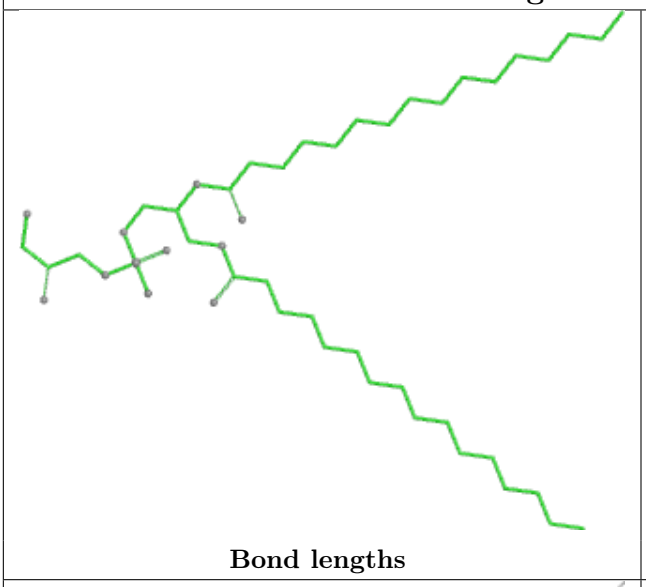


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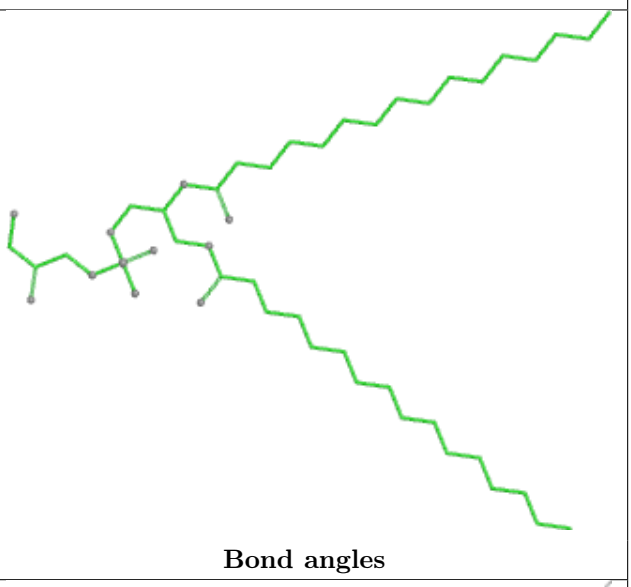


Rings

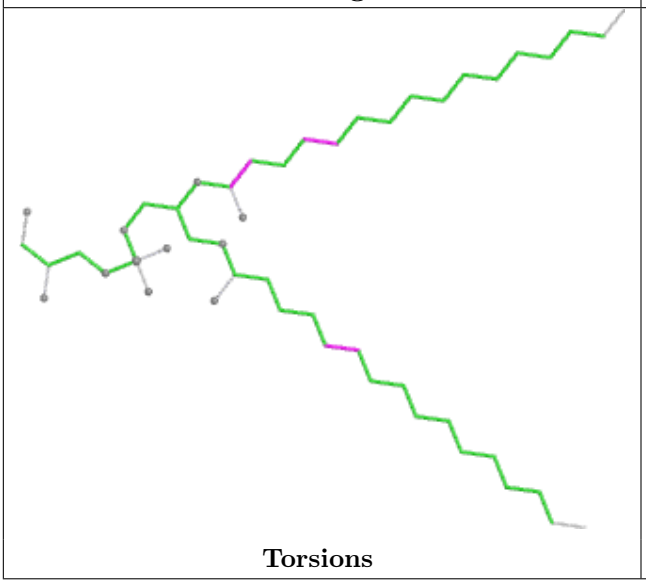
## Ligand LHG 6 619



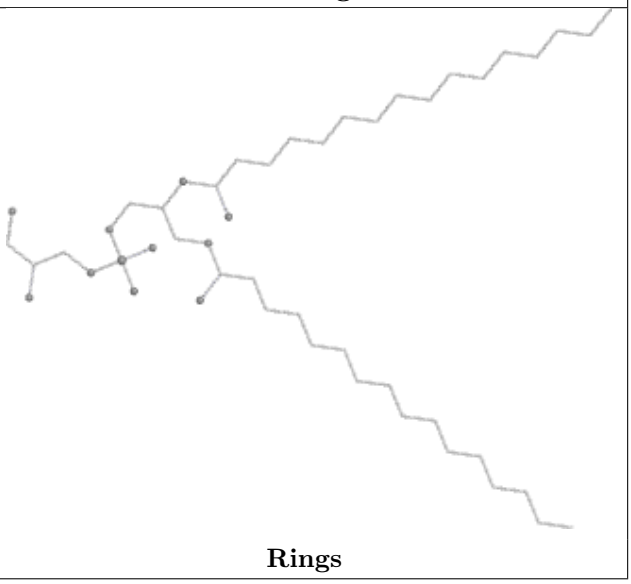
Bond lengths



Bond angles

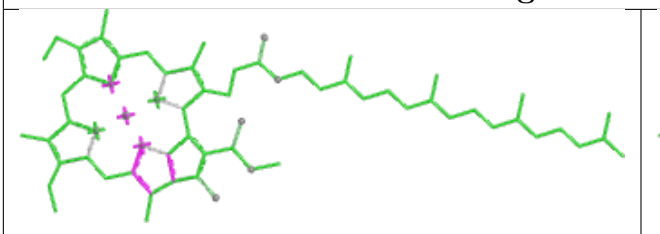


Torsions

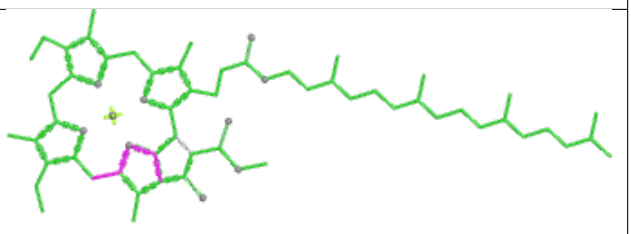


Rings

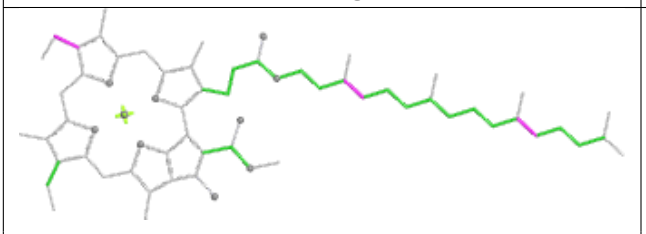
## Ligand CLA L2 203



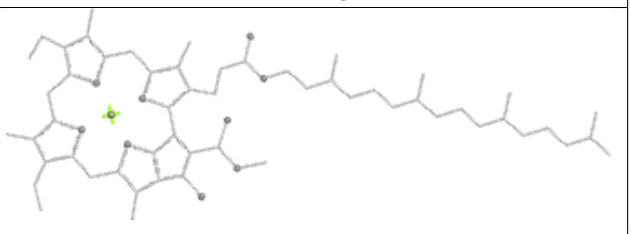
Bond lengths



Bond angles

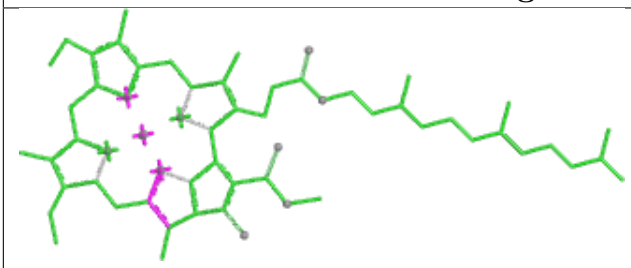


Torsions

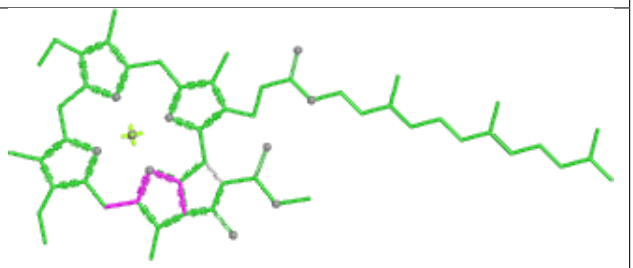


Rings

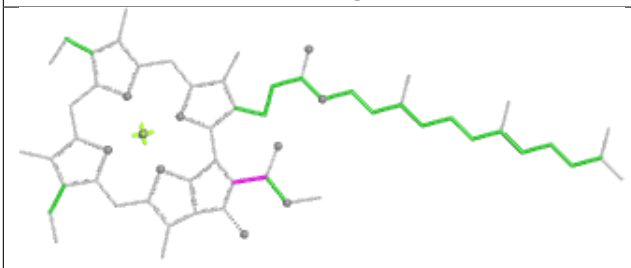
## Ligand CLA Z2 602



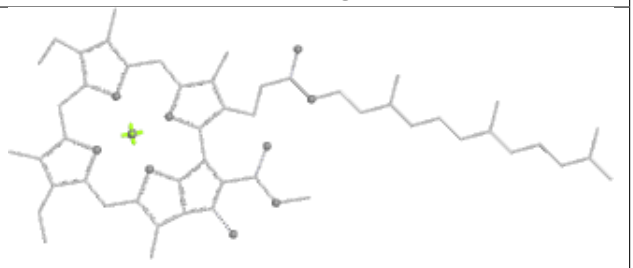
Bond lengths



Bond angles

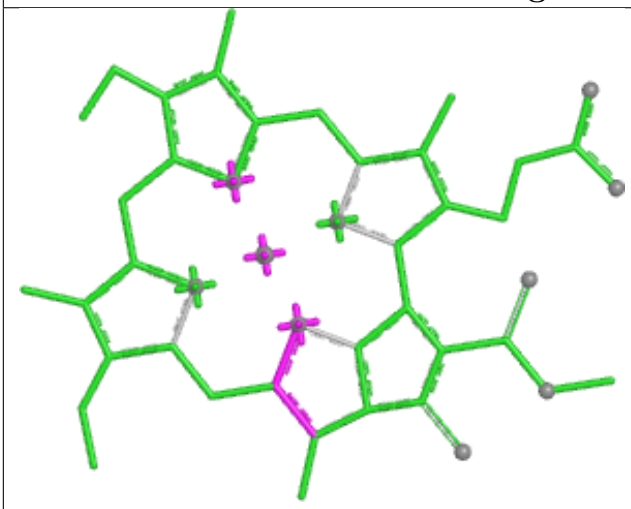


Torsions

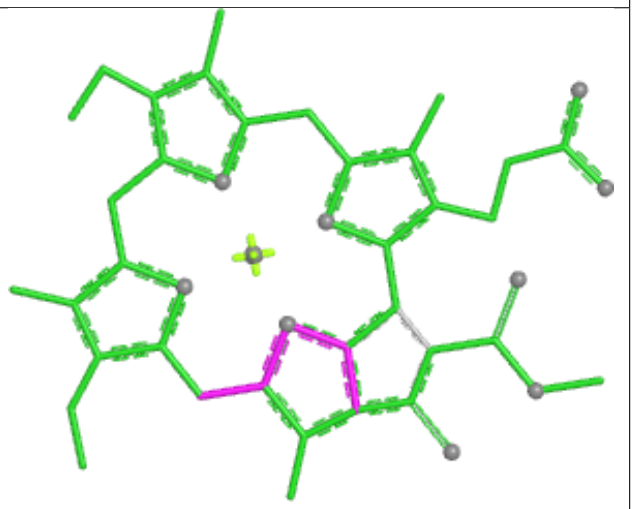


Rings

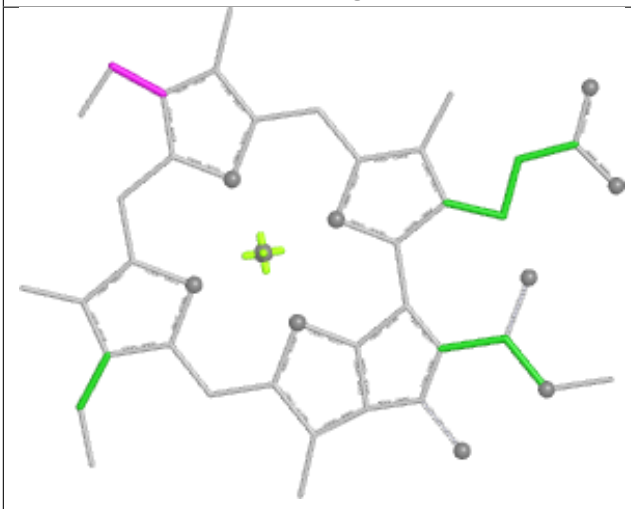
## Ligand CLA 3 614



Bond lengths



Bond angles

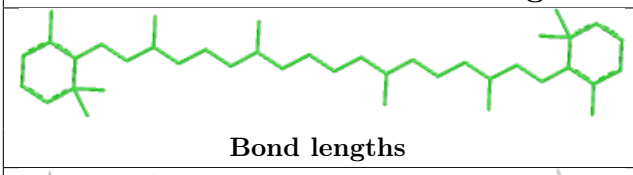


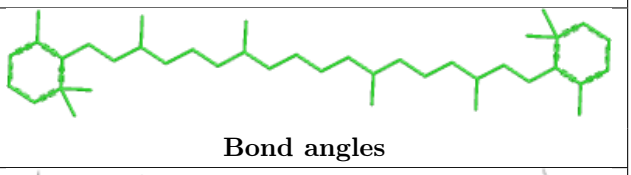
Torsions

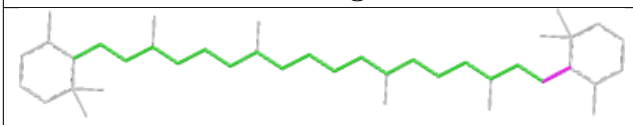


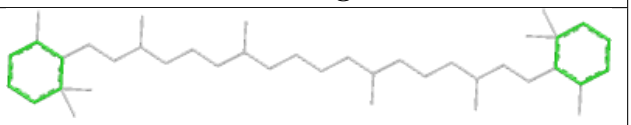
Rings

## Ligand BCR 4 621

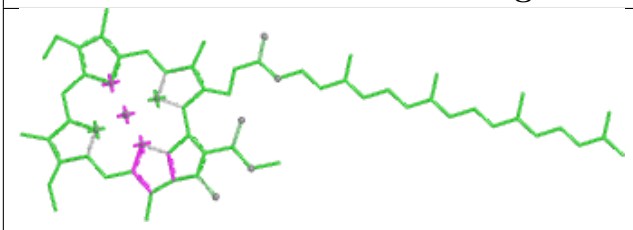

Bond lengths

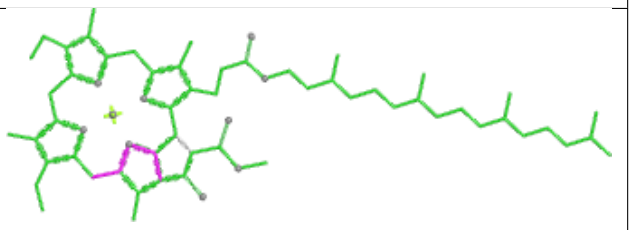

Bond angles

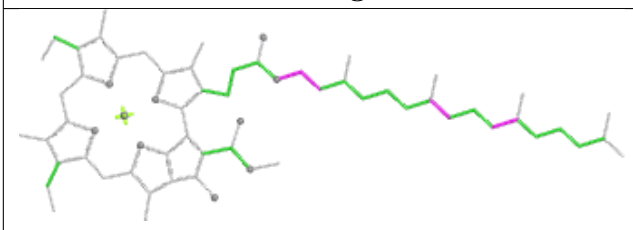

Torsions

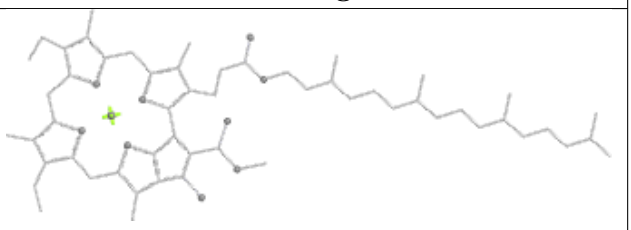

Rings

## Ligand CLA A2 843

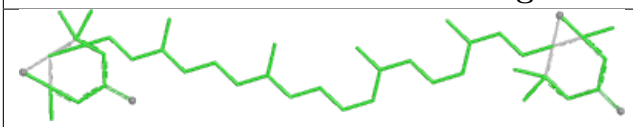

Bond lengths

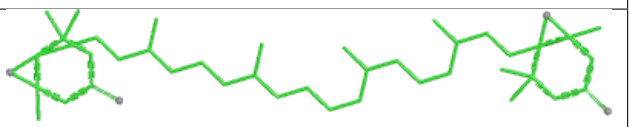

Bond angles

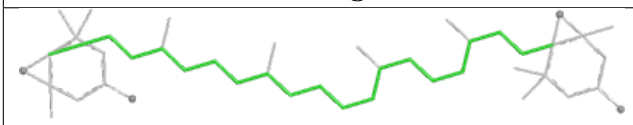

Torsions

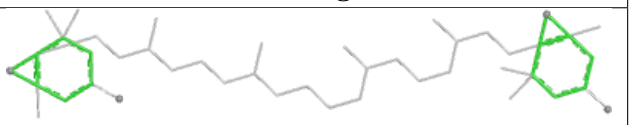

Rings

## Ligand XAT Z2 618

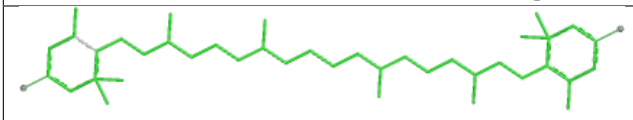

Bond lengths

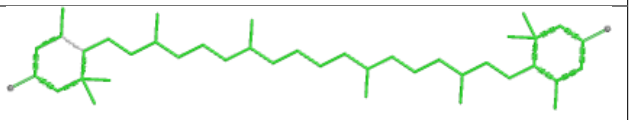

Bond angles

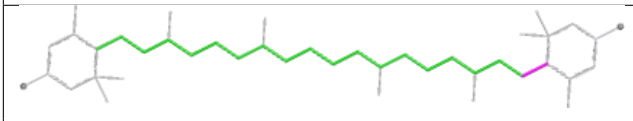

Torsions

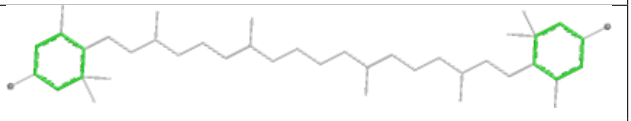

Rings

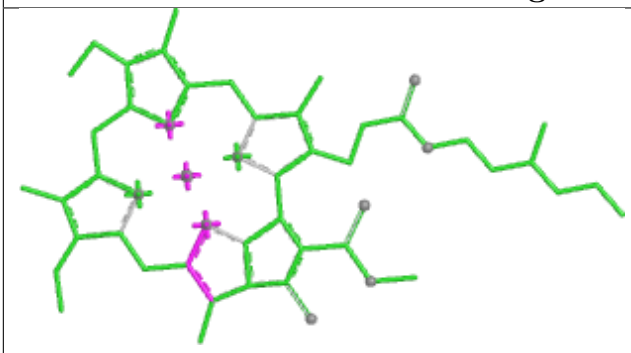
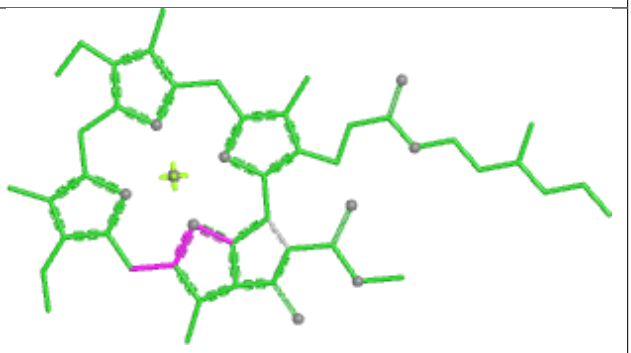
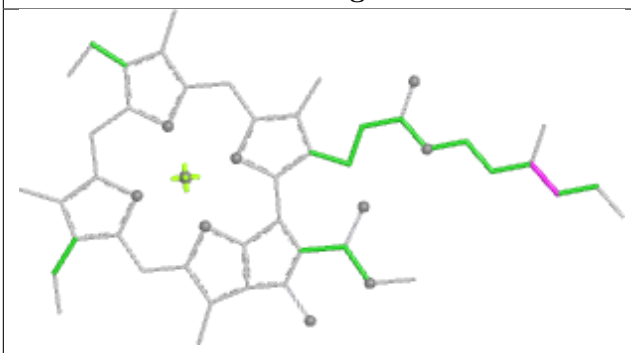
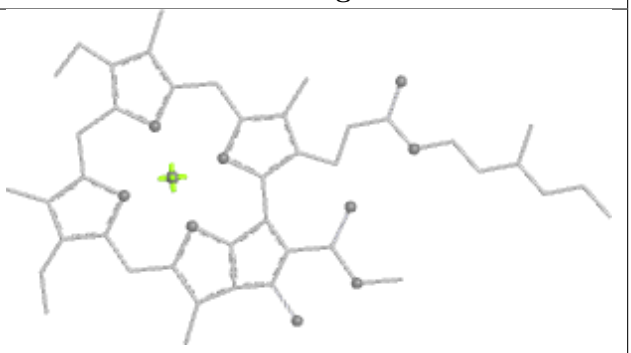
## Ligand LUT 8 617

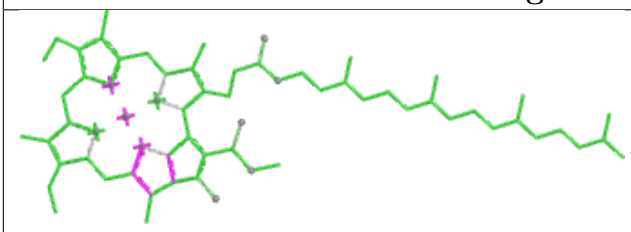
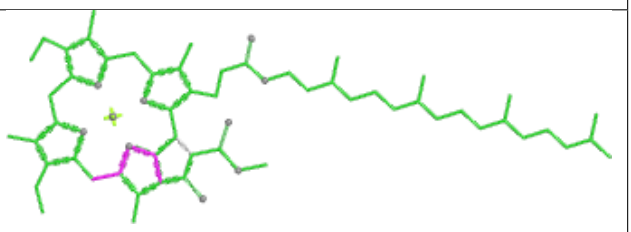
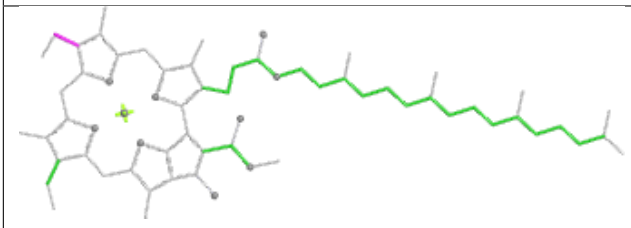
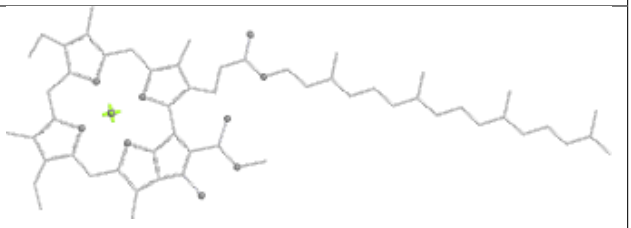

Bond lengths


Bond angles

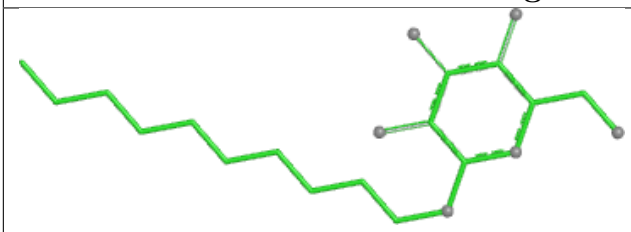

Torsions


Rings

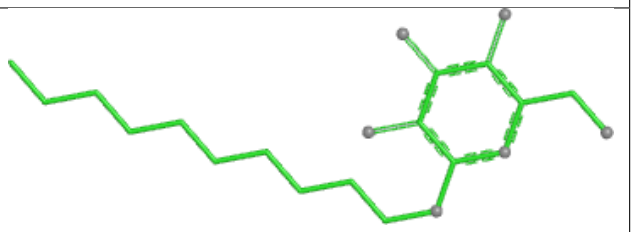
| Ligand CLA 7 612 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA Z 613 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
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| Torsions | Rings |

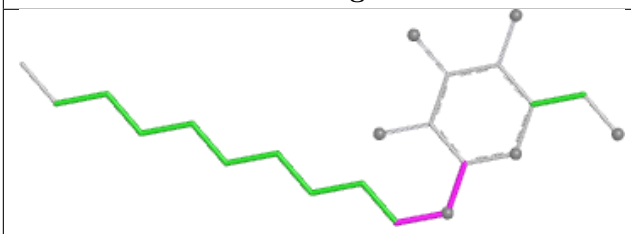
## Ligand LMU 1 627



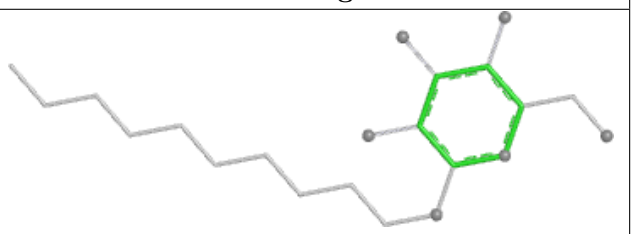
Bond lengths



Bond angles

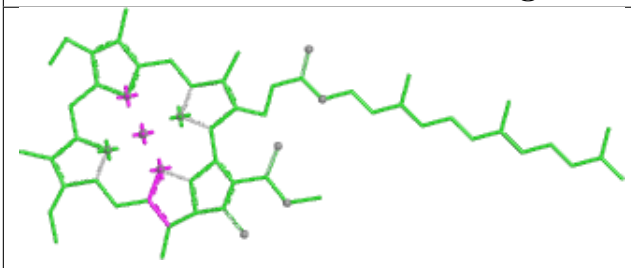


Torsions

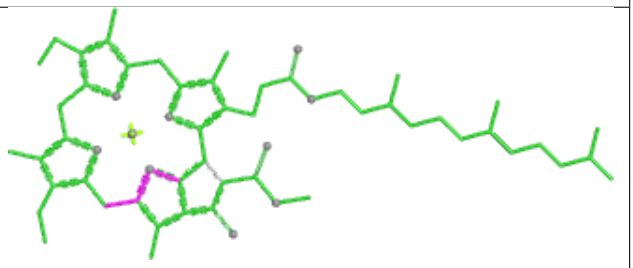


Rings

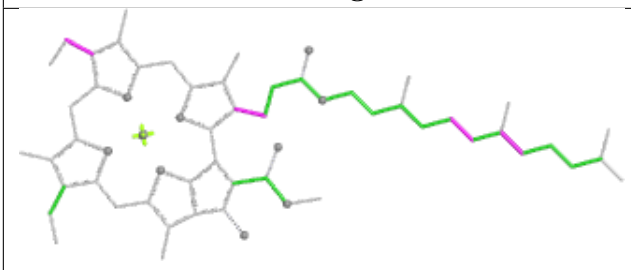
## Ligand CLA 42 609



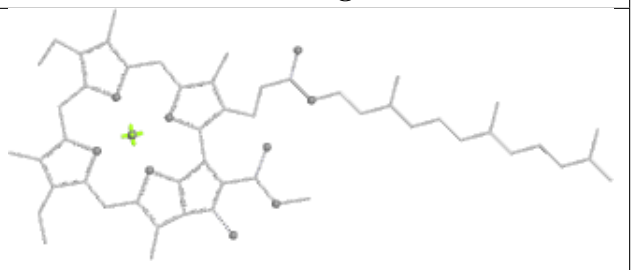
Bond lengths



Bond angles

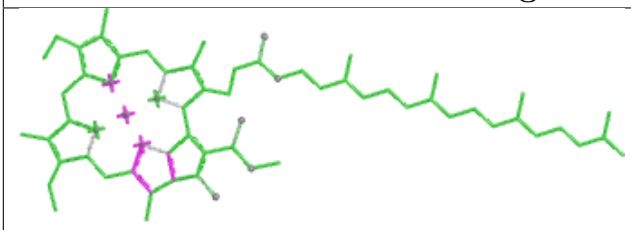


Torsions

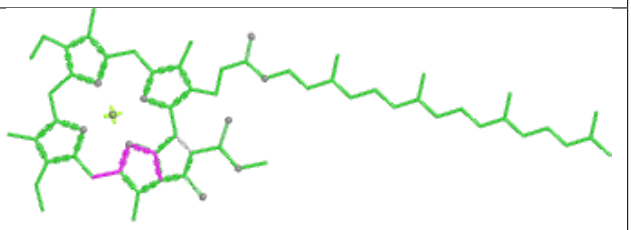


Rings

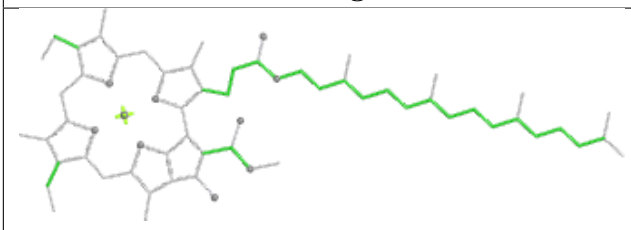
## Ligand CLA 32 610



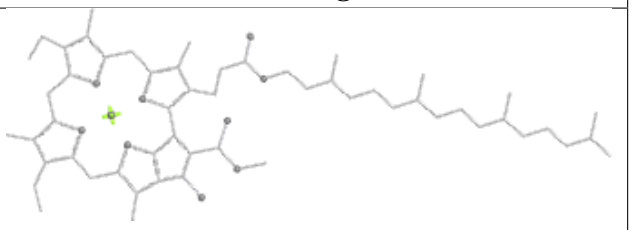
Bond lengths



Bond angles

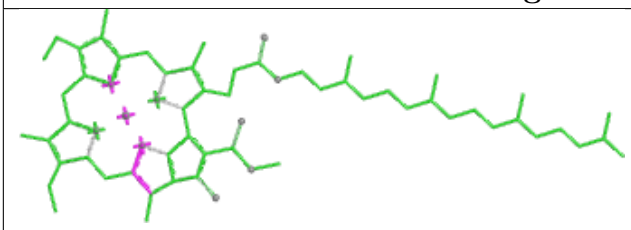


Torsions

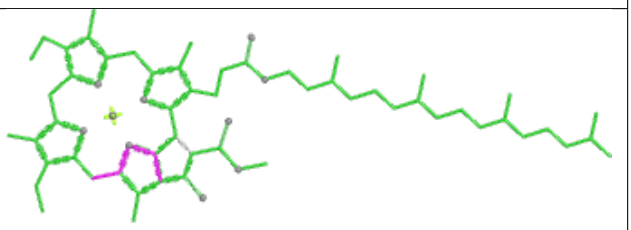


Rings

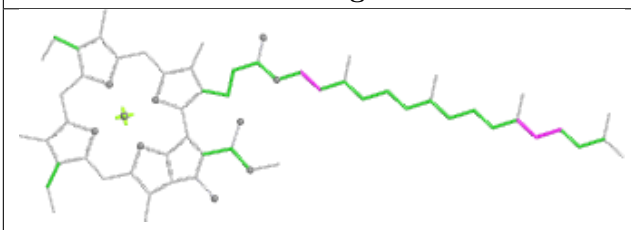
## Ligand CLA A 816



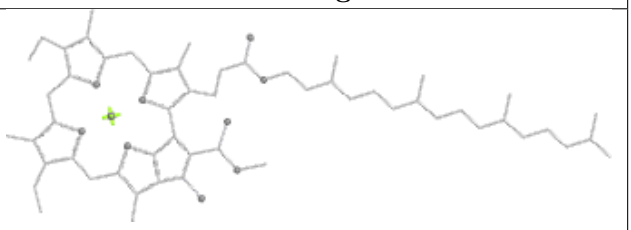
Bond lengths



Bond angles

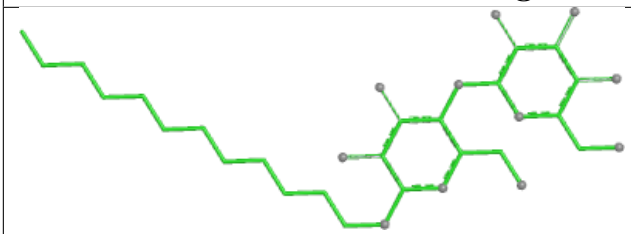


Torsions

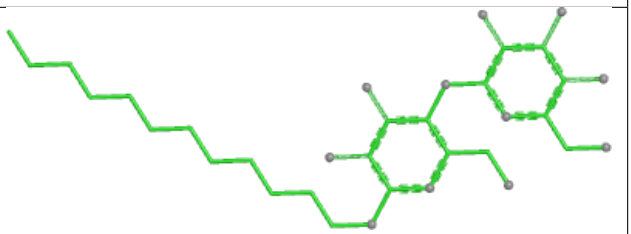


Rings

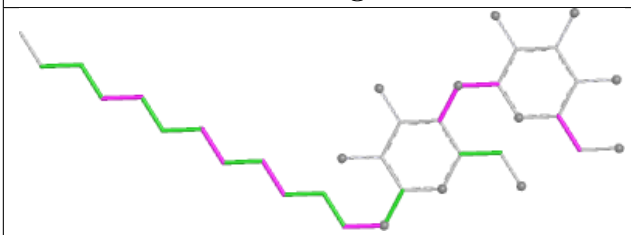
## Ligand LMU 82 627



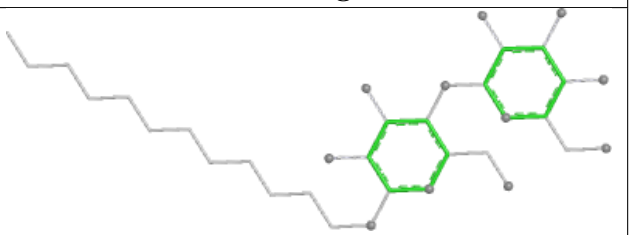
Bond lengths



Bond angles

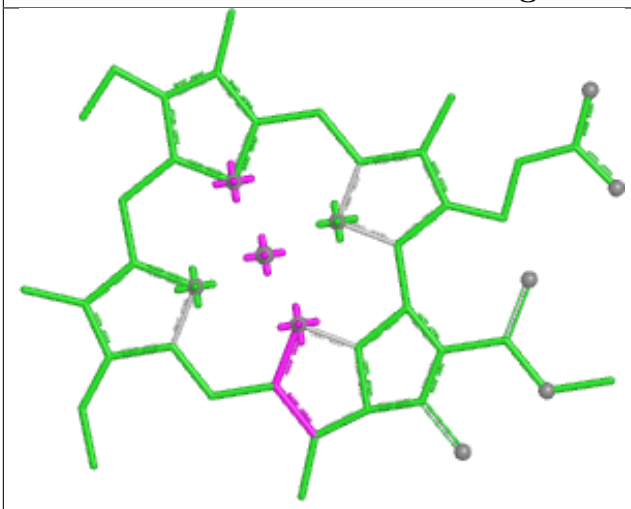


Torsions

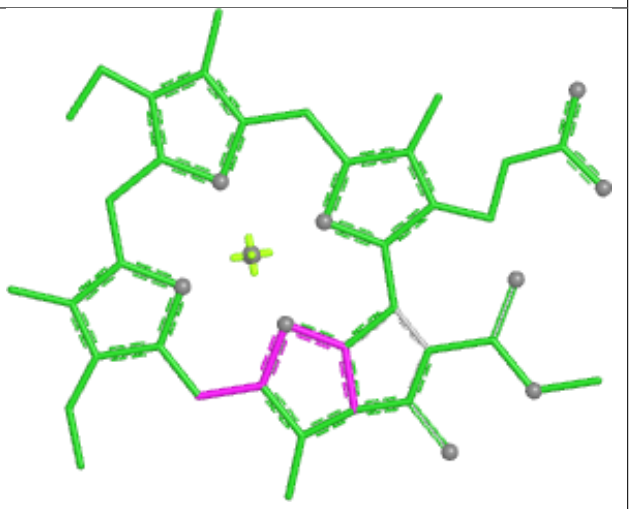


Rings

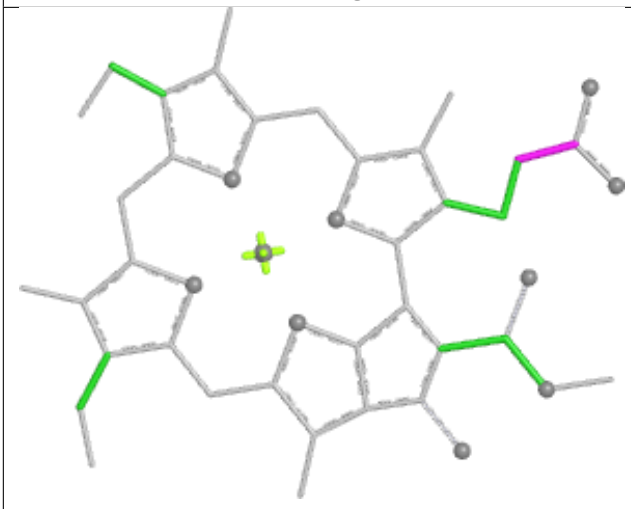
**Ligand CLA 82 611**



**Bond lengths**



**Bond angles**

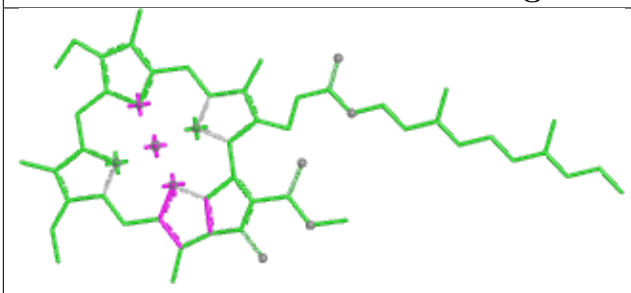


**Torsions**

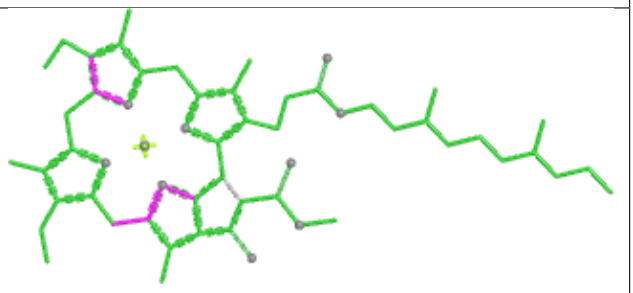


**Rings**

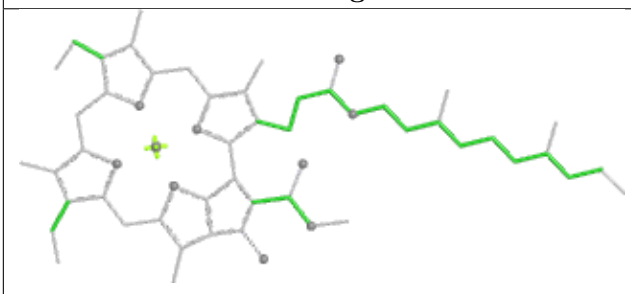
## Ligand CLA A 837



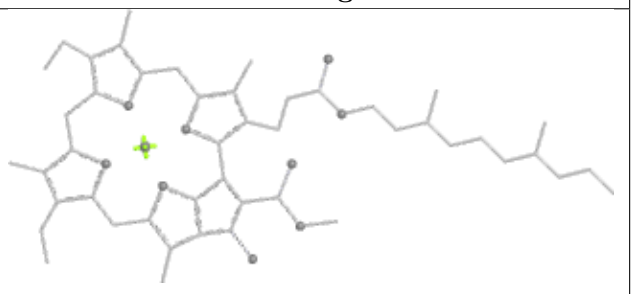
Bond lengths



Bond angles

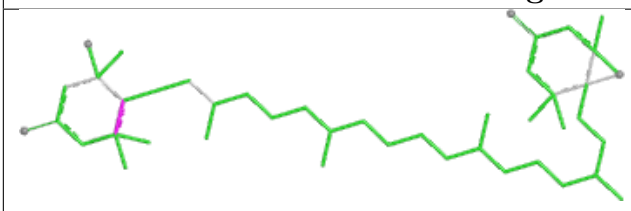


Torsions

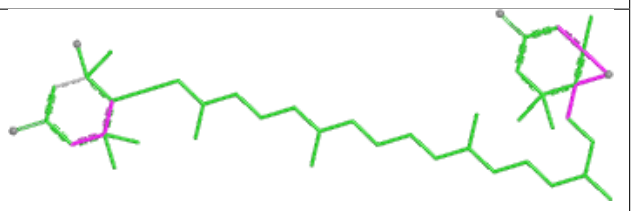


Rings

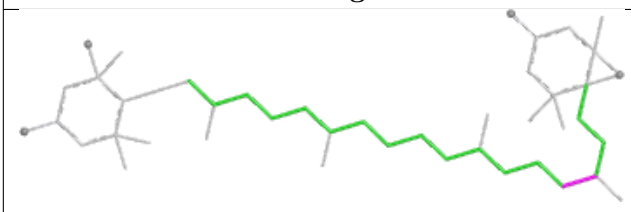
## Ligand NEX 5 625



Bond lengths



Bond angles

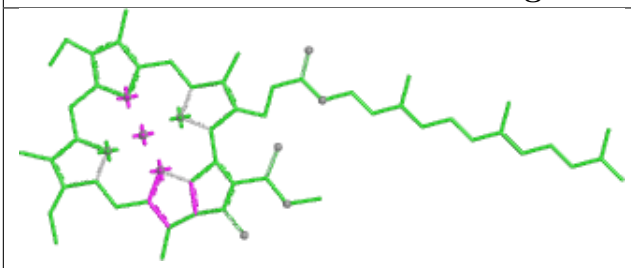


Torsions

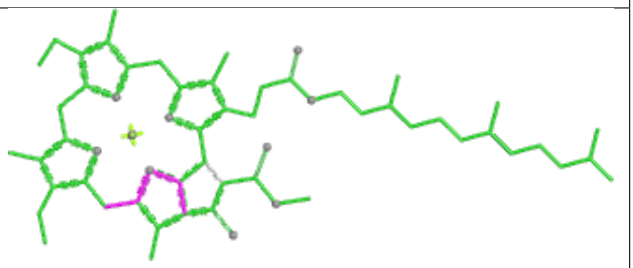


Rings

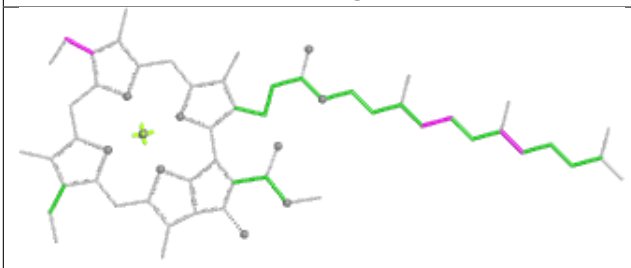
## Ligand CLA B 819



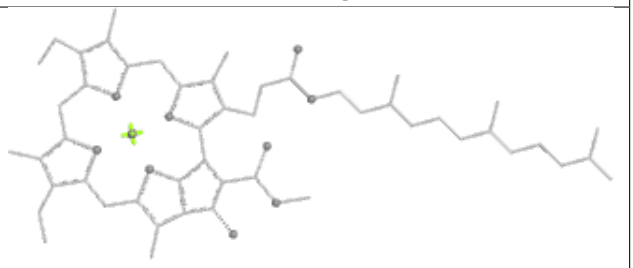
Bond lengths



Bond angles

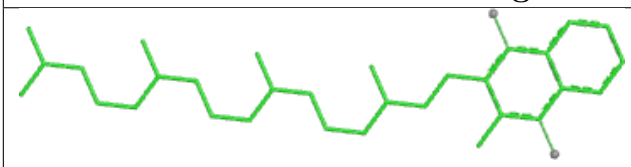


Torsions

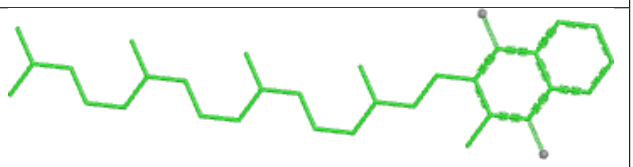


Rings

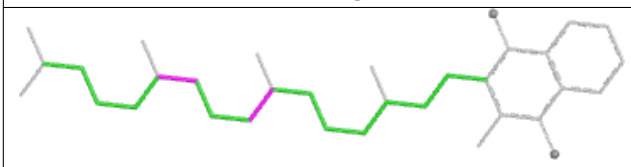
## Ligand PQN A2 844



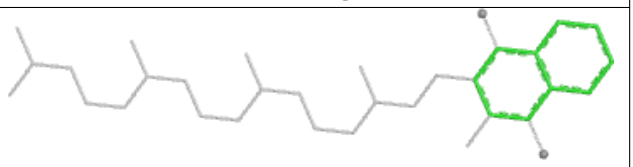
Bond lengths



Bond angles

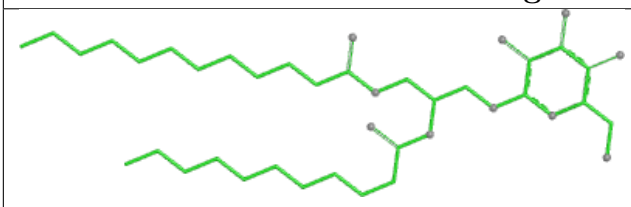


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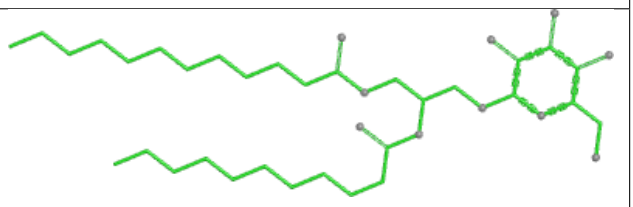


Rings

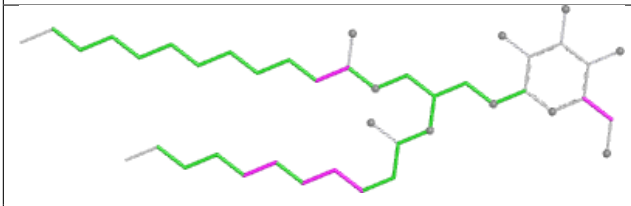
## Ligand LMG 1 628



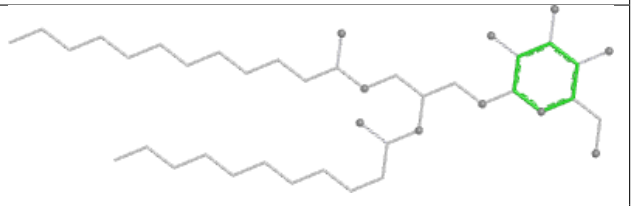
Bond lengths



Bond angles

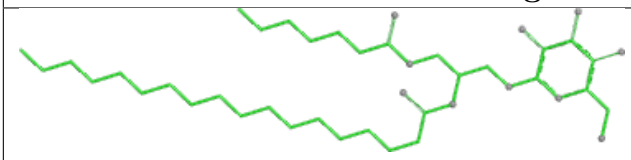


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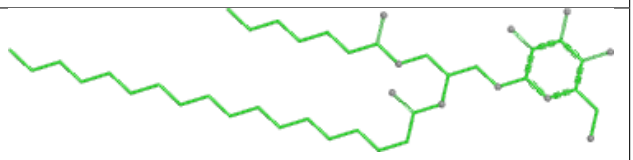


Rings

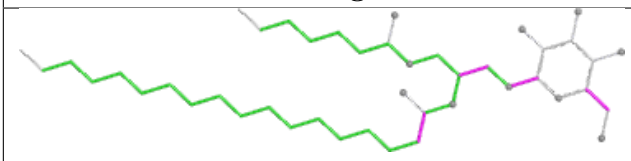
## Ligand LMG 9 620



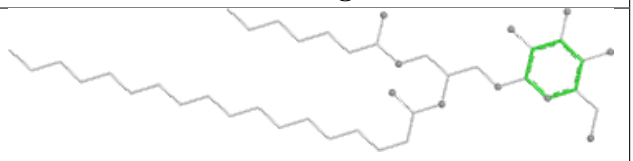
Bond lengths



Bond angles

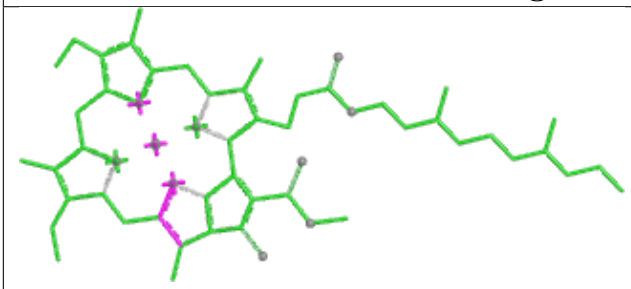


Torsions

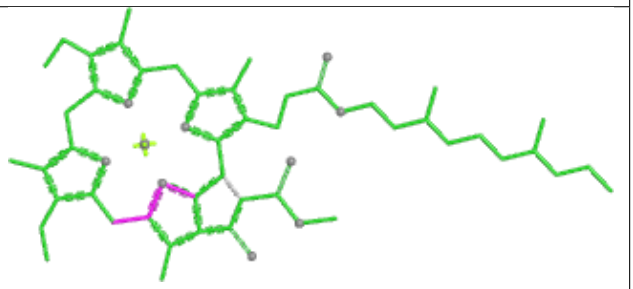


Rings

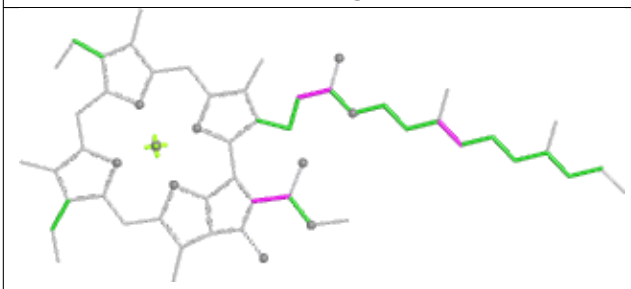
## Ligand CLA 1 603



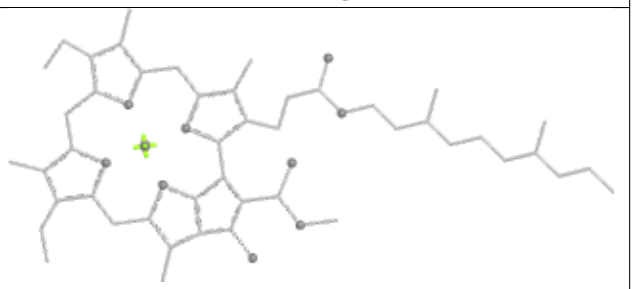
Bond lengths



Bond angles

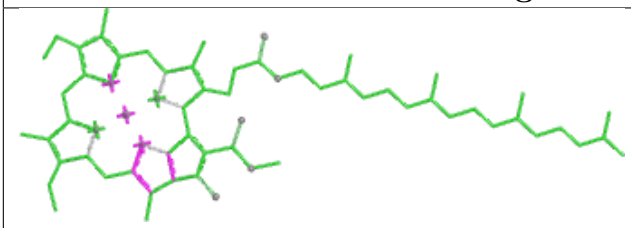


Torsions

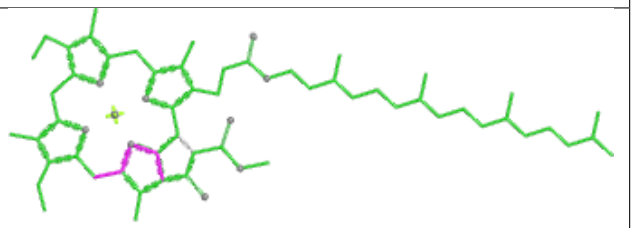


Rings

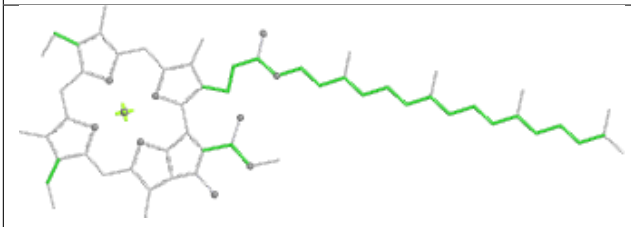
## Ligand CLA B2 837



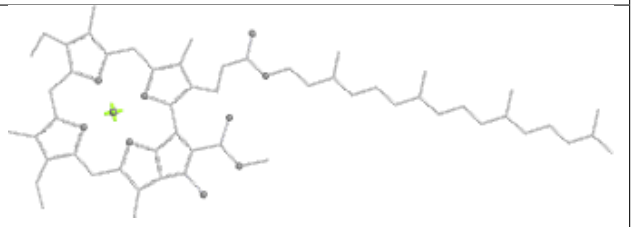
Bond lengths



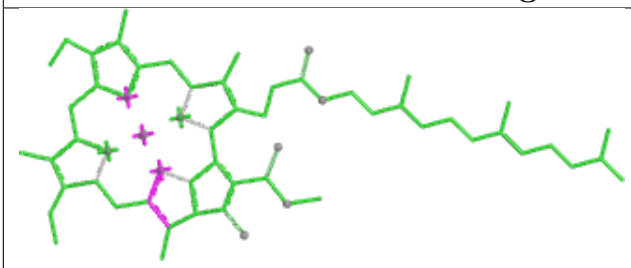
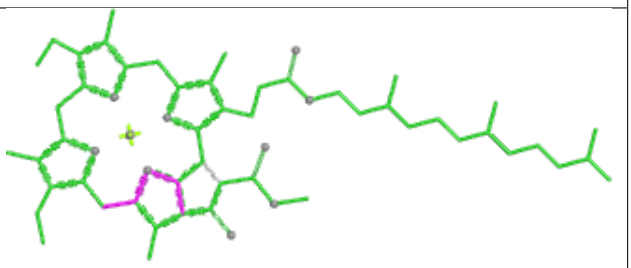
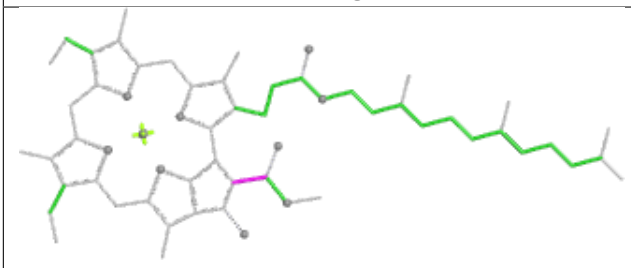
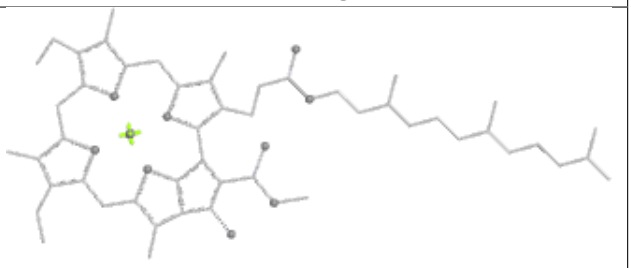
Bond angles

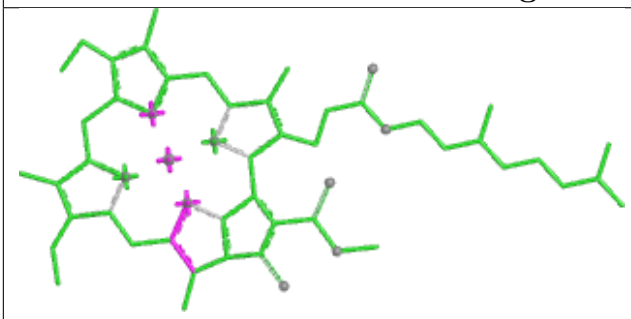
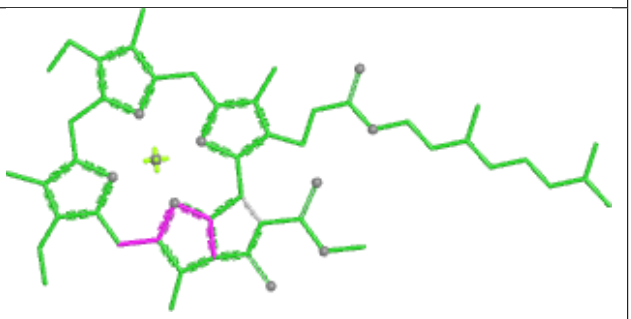
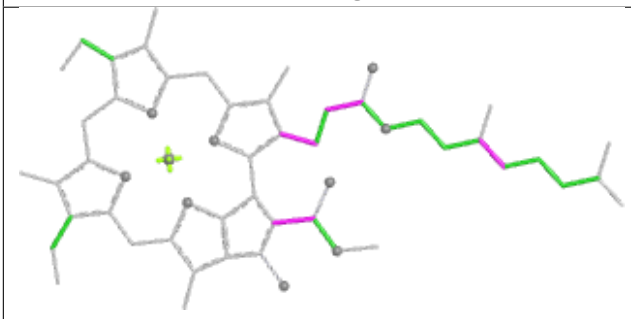
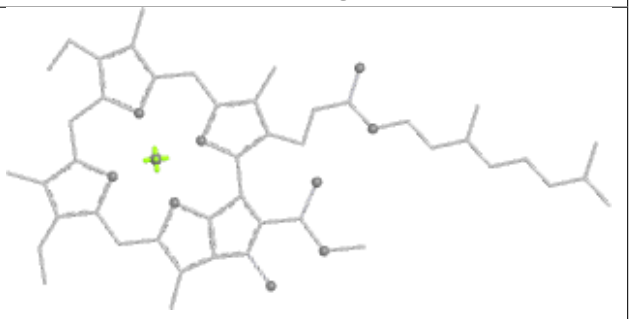


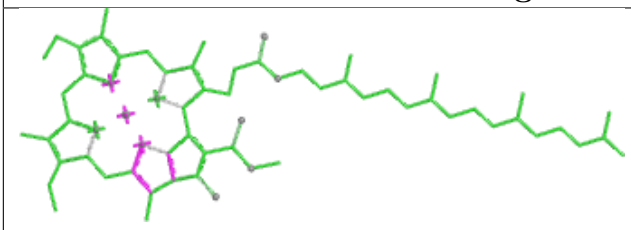
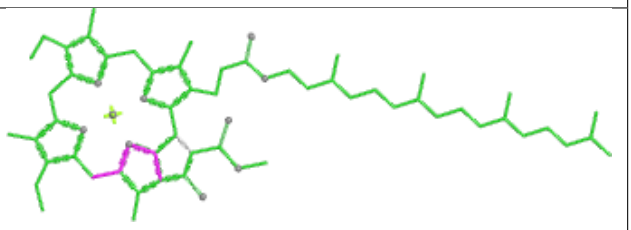
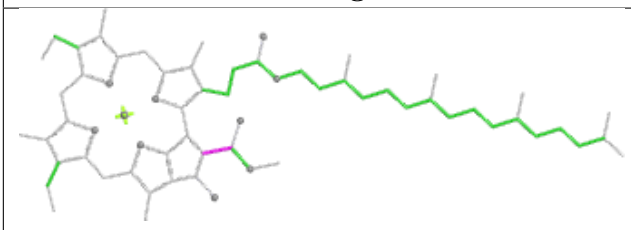
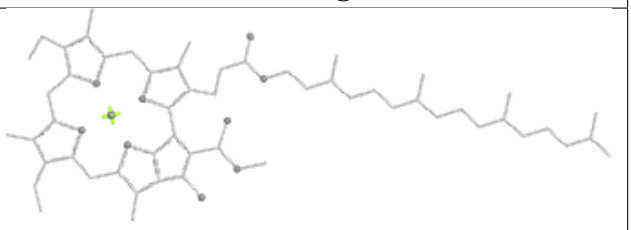
Torsions

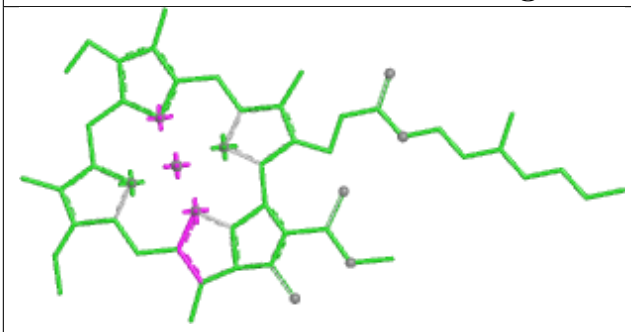
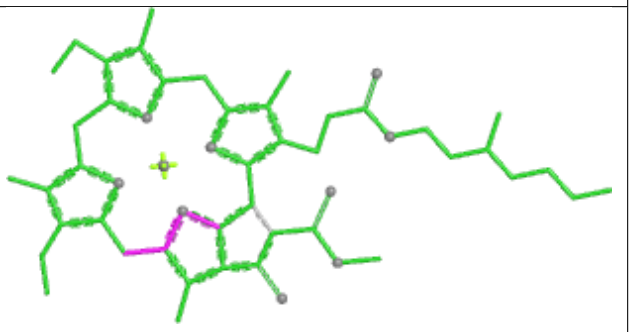
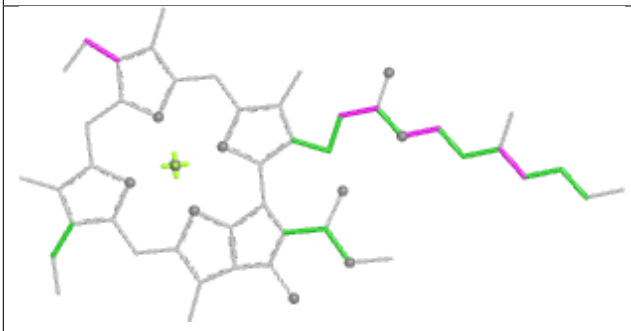
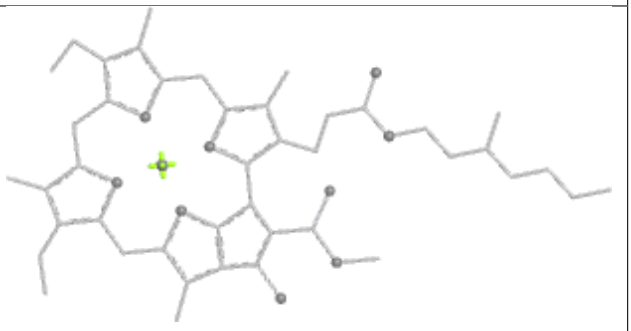


Rings

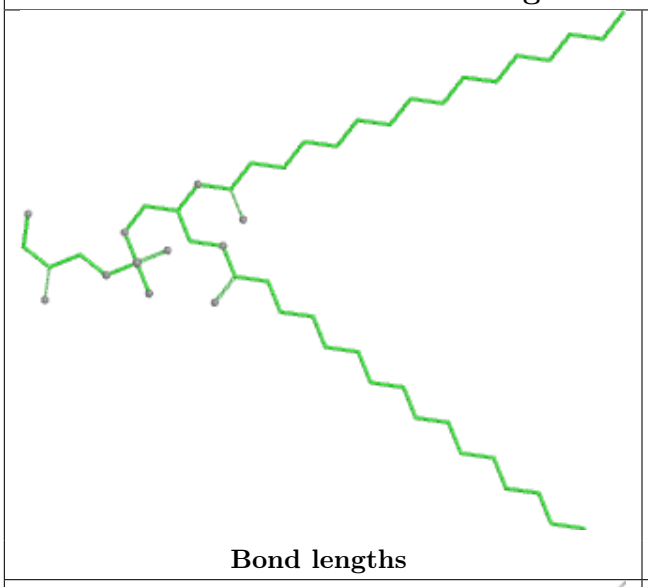
| Ligand CLA 92 602 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 42 614 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

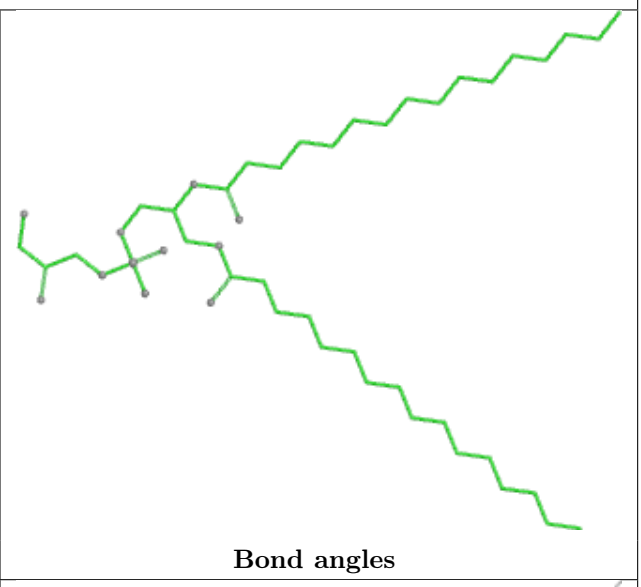
| Ligand CLA A2 831 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CLA 52 616 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

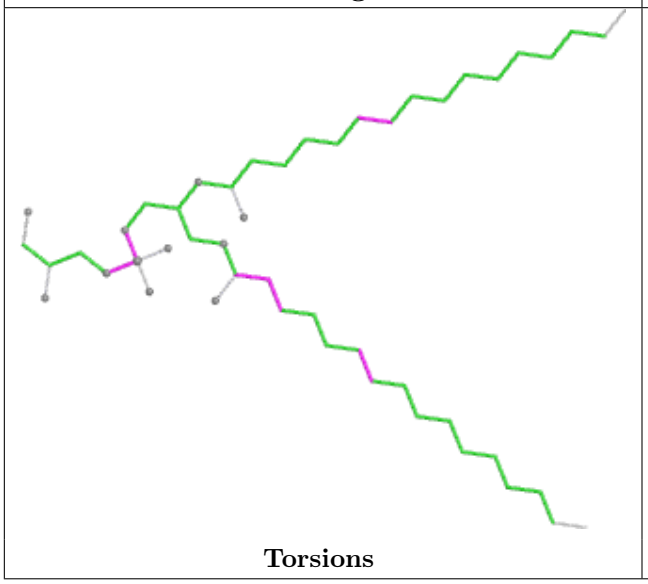
## Ligand LHG A 846



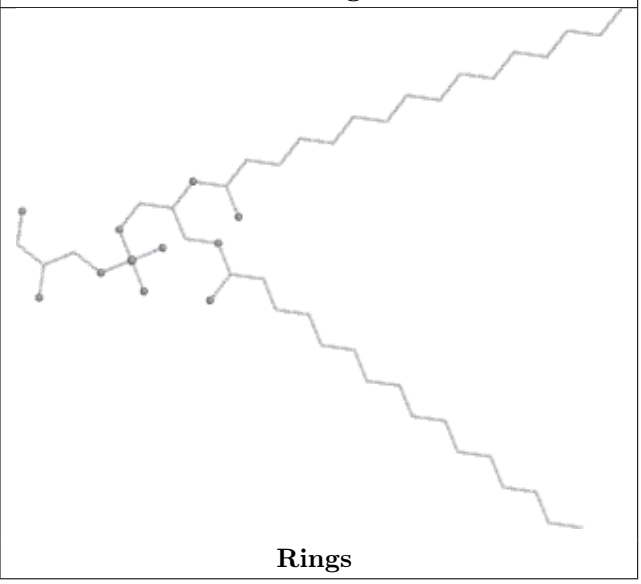
Bond lengths



Bond angles



Torsions



Rings

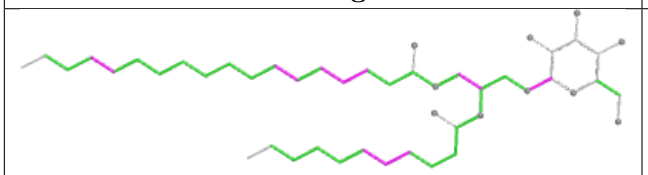
## Ligand LMG A 859



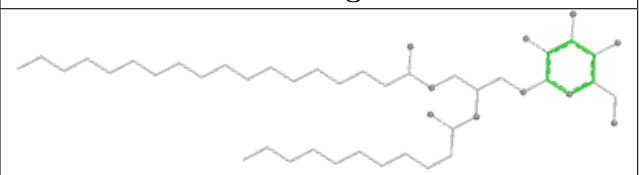
Bond lengths



Bond angles

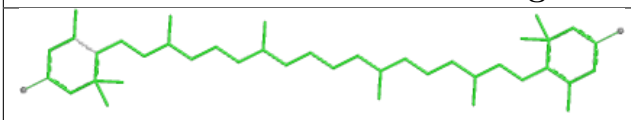


Torsions

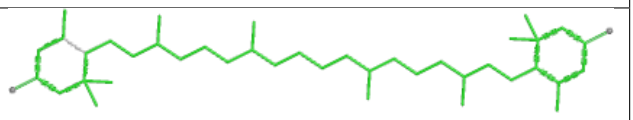


Rings

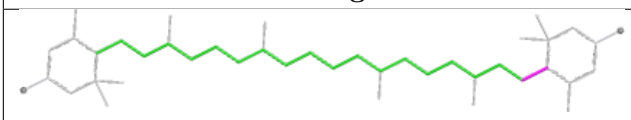
## Ligand LUT 5 620



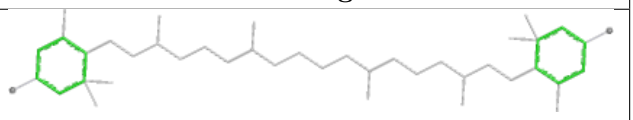
Bond lengths



Bond angles

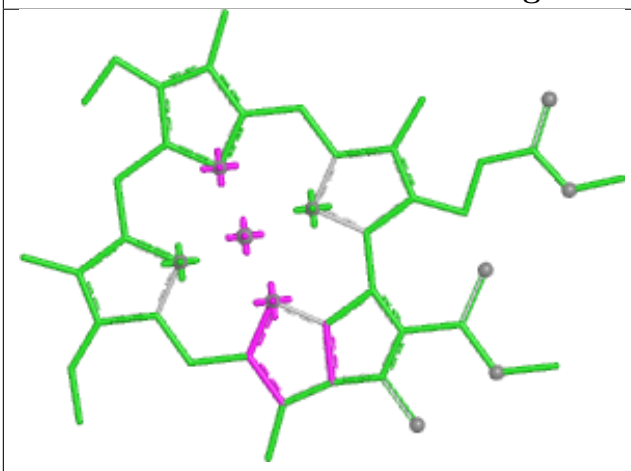


Torsions

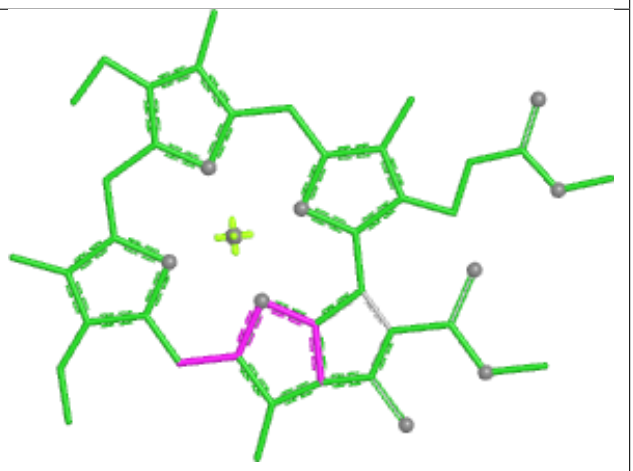


Rings

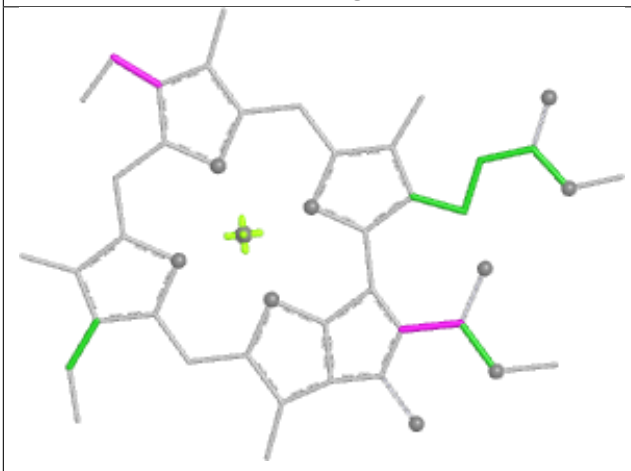
## Ligand CLA K 204



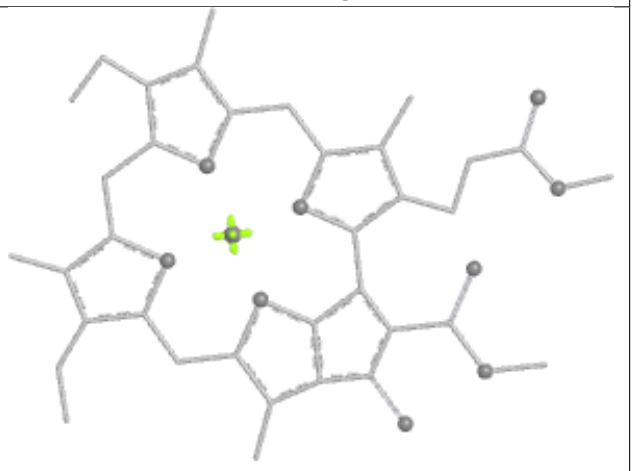
Bond lengths



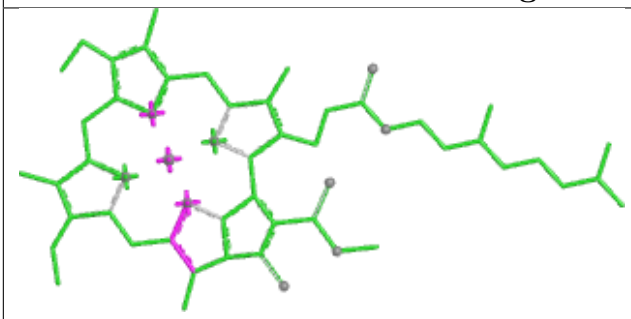
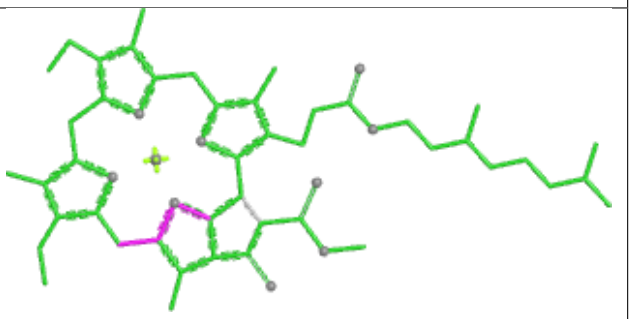
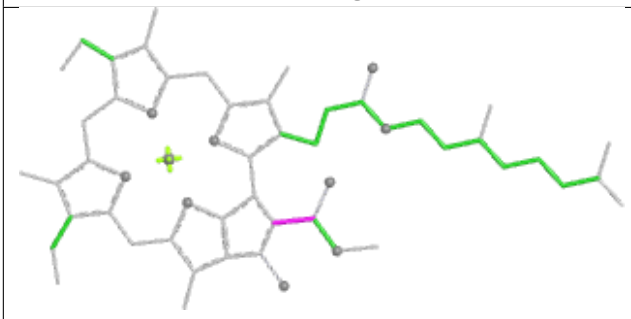
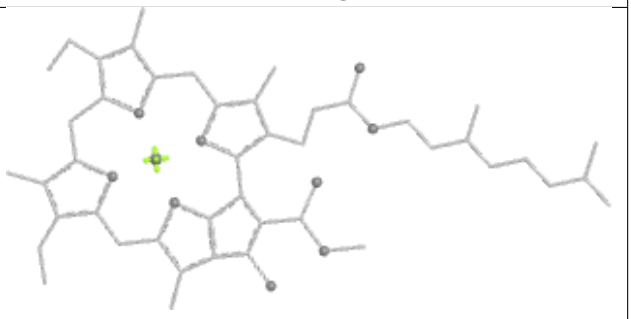
Bond angles

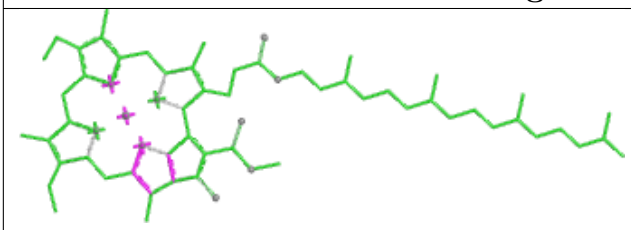
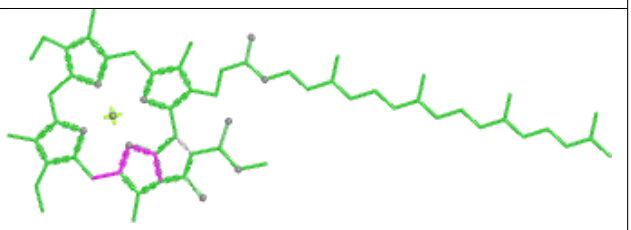
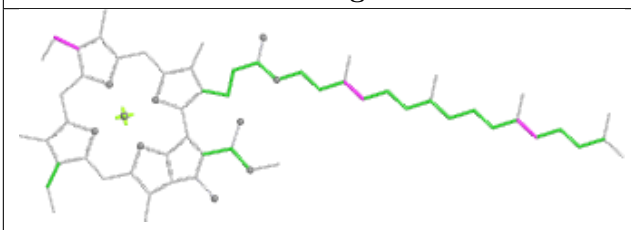
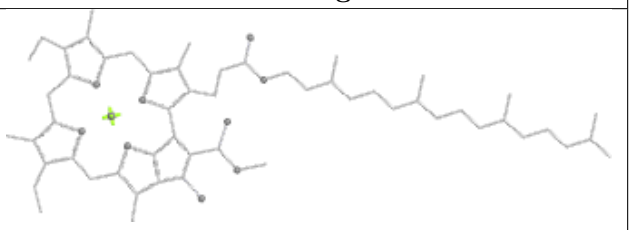


Torsions

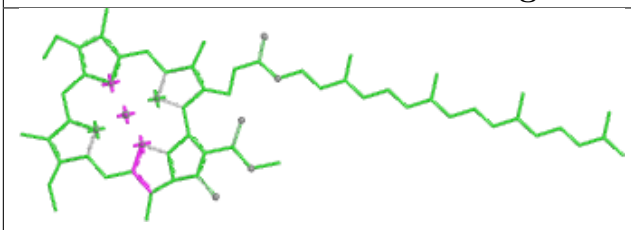


Rings

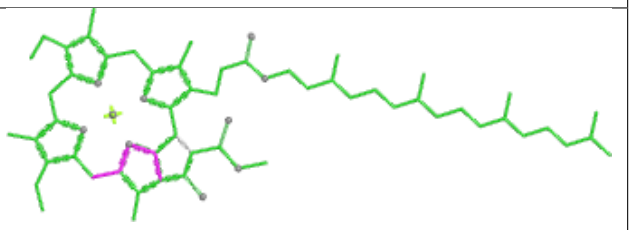
| Ligand CLA 62 622 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA L 203 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

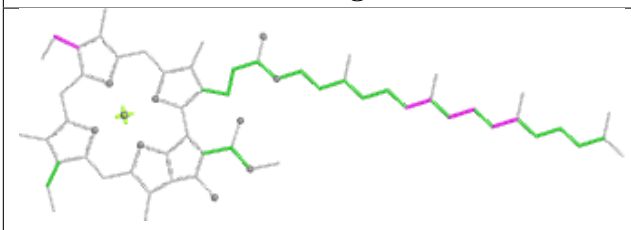
## Ligand CLA 72 611



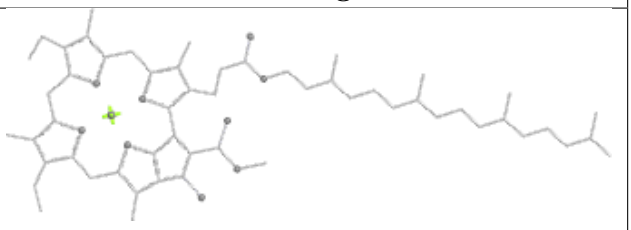
Bond lengths



Bond angles

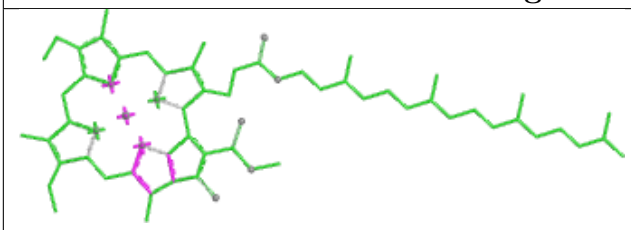


Torsions

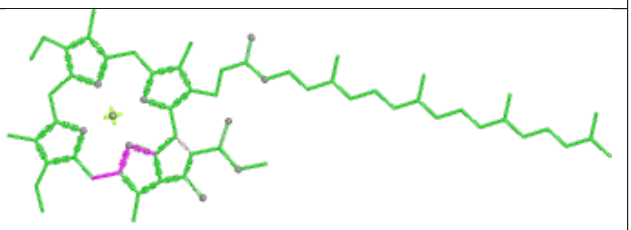


Rings

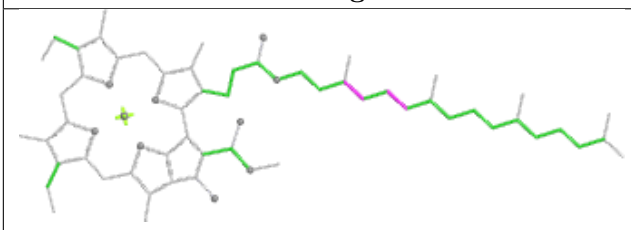
## Ligand CLA B 829



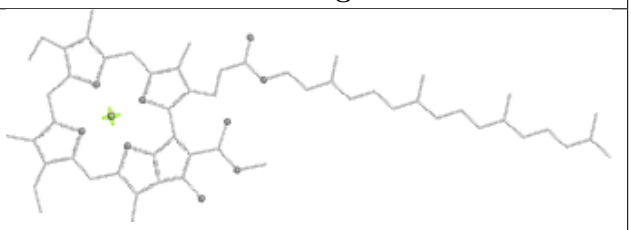
Bond lengths



Bond angles

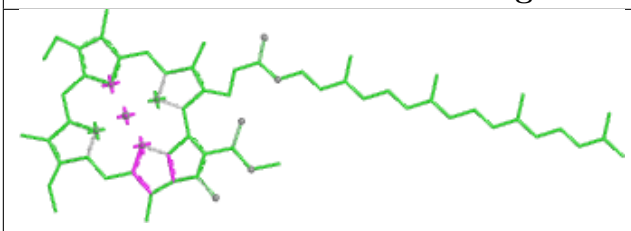


Torsions

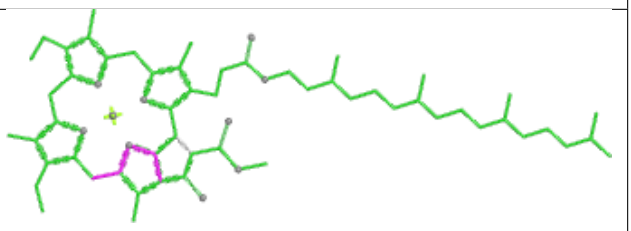


Rings

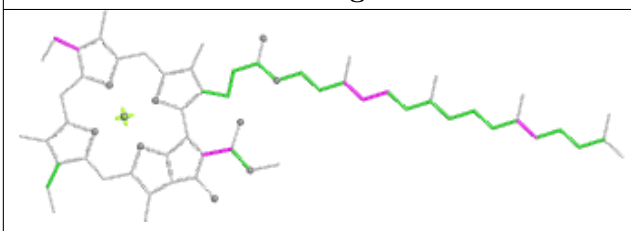
## Ligand CLA B2 808



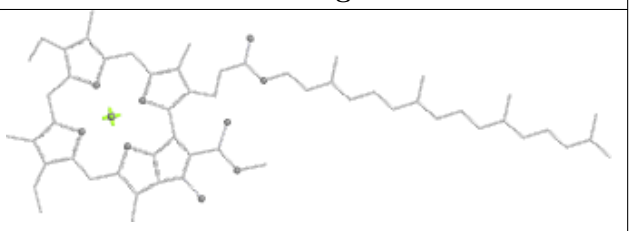
Bond lengths



Bond angles

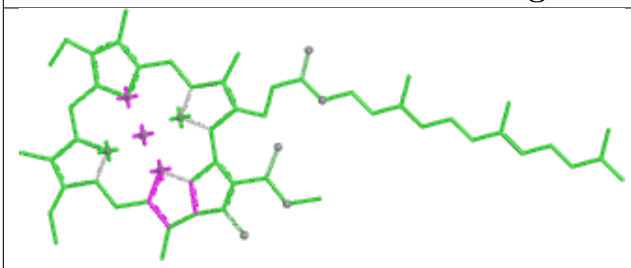


Torsions

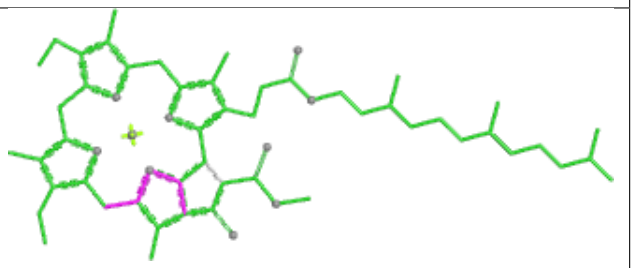


Rings

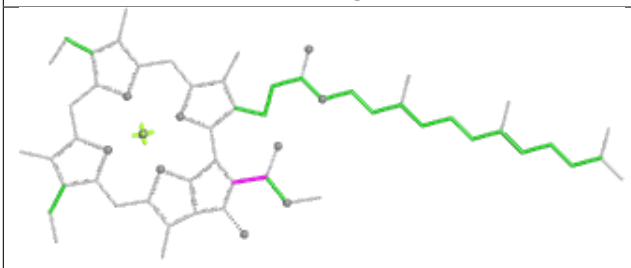
## Ligand CLA 1 602



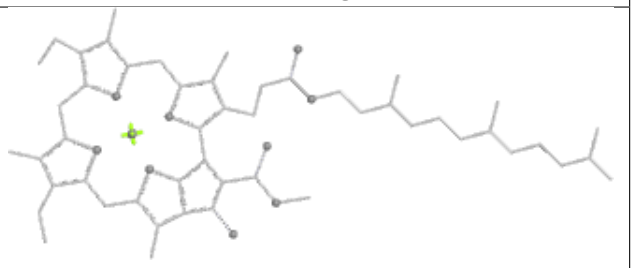
Bond lengths



Bond angles

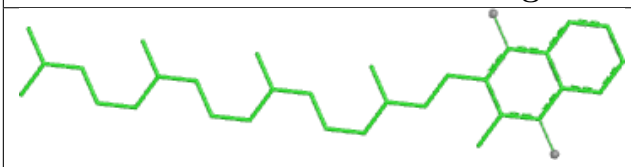


Torsions

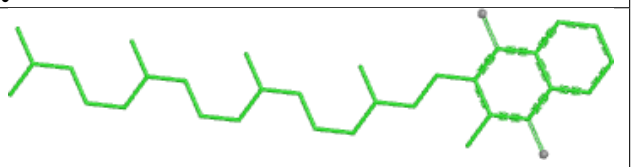


Rings

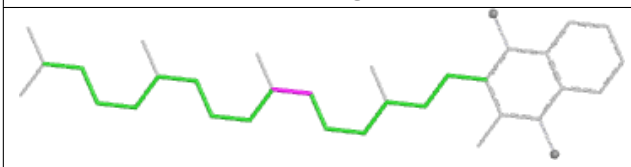
## Ligand PQN B 842



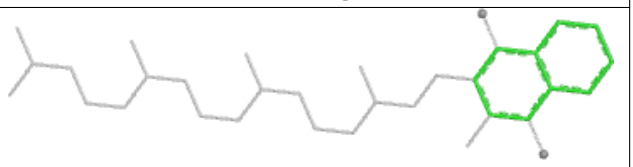
Bond lengths



Bond angles

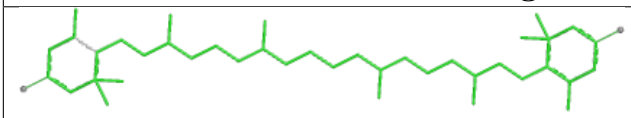


Torsions

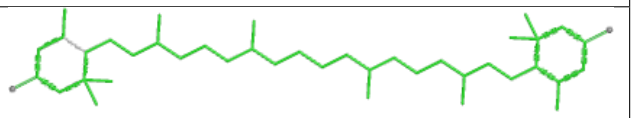


Rings

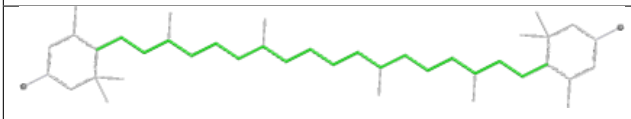
## Ligand LUT 32 720



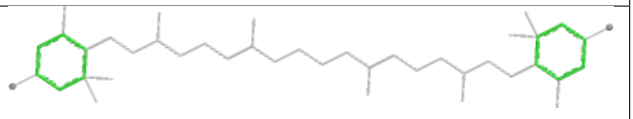
Bond lengths



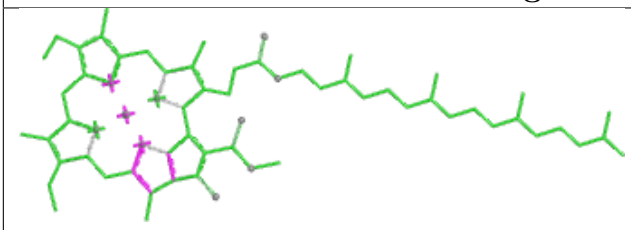
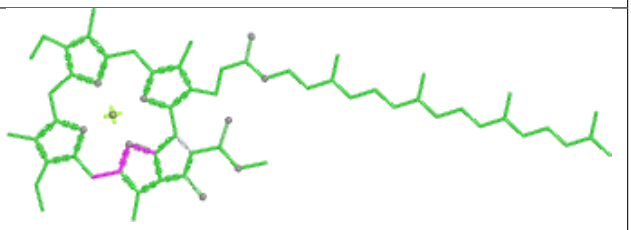
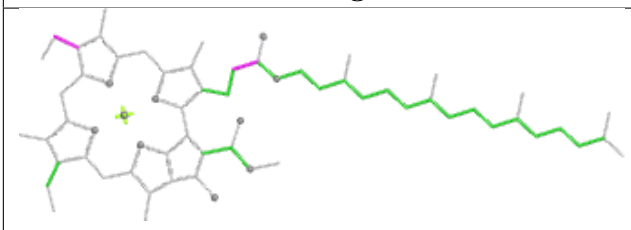
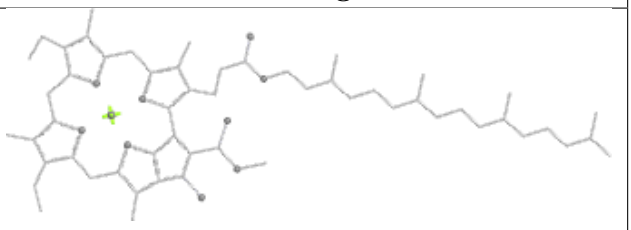
Bond angles

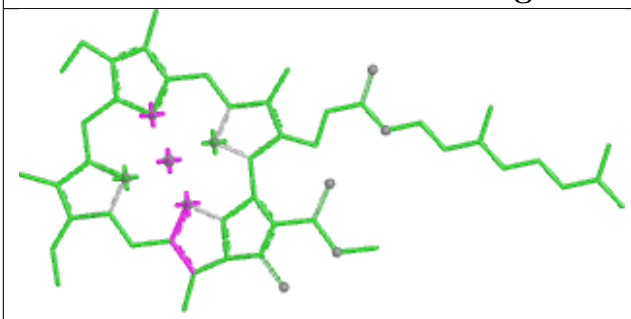
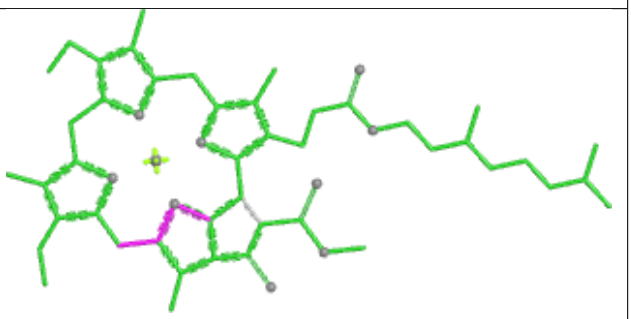
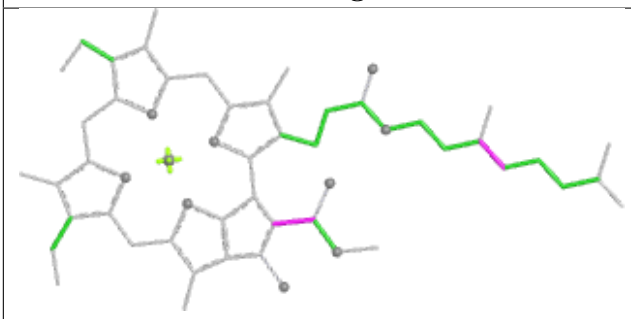
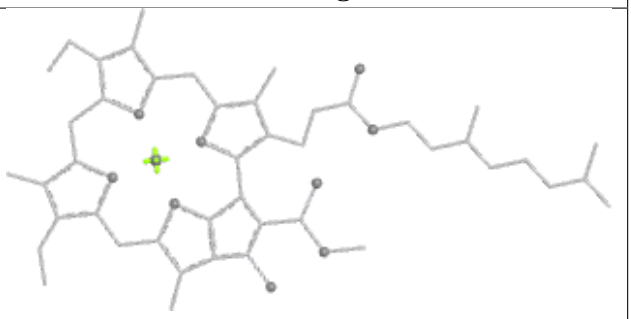


Torsions

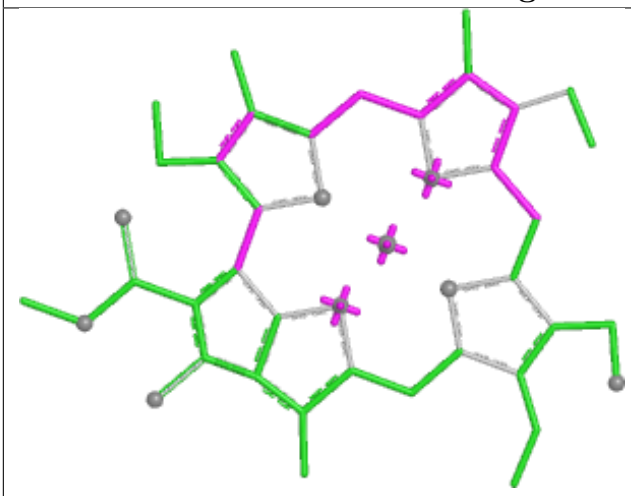


Rings

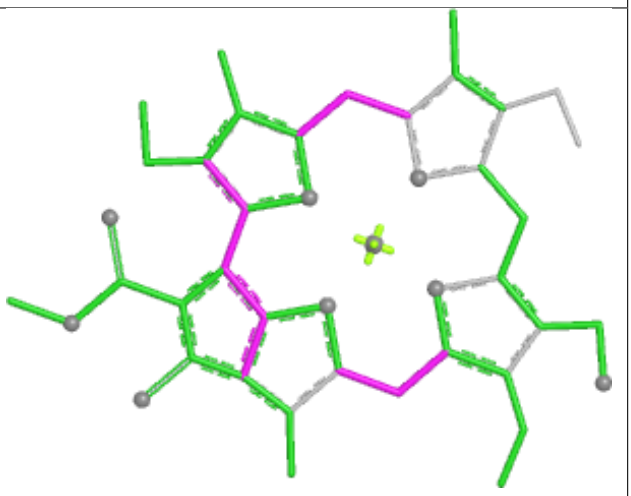
| Ligand CLA A 807 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA A2 817 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

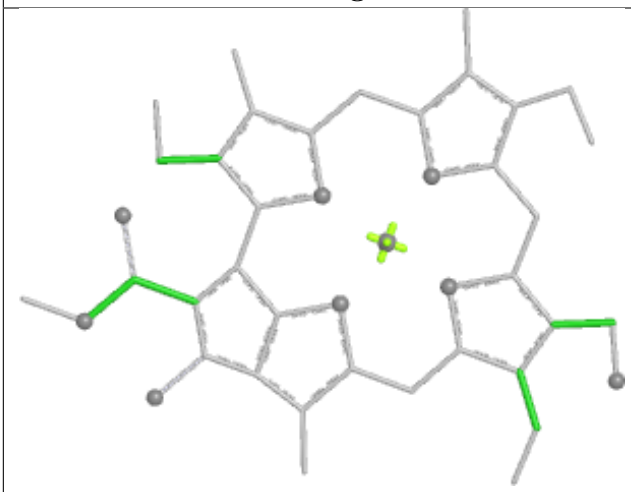
**Ligand CHL 62 618**



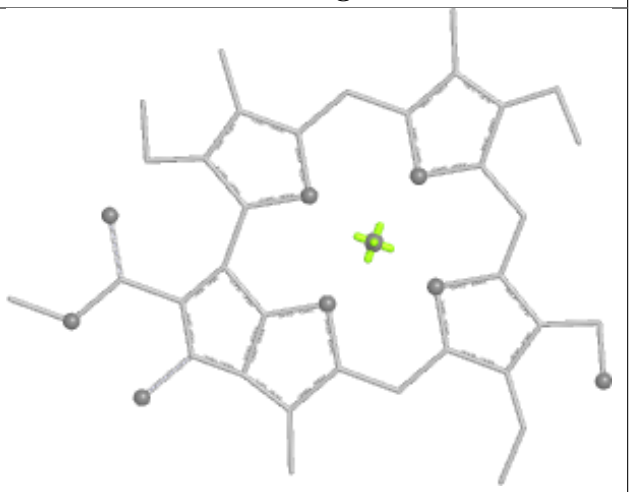
**Bond lengths**



**Bond angles**

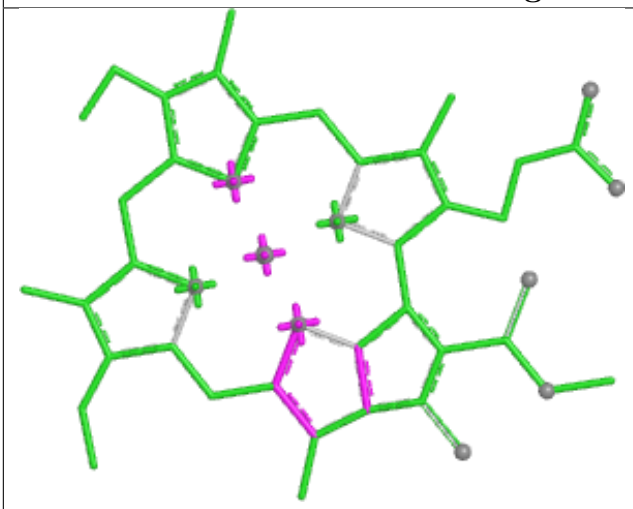


**Torsions**

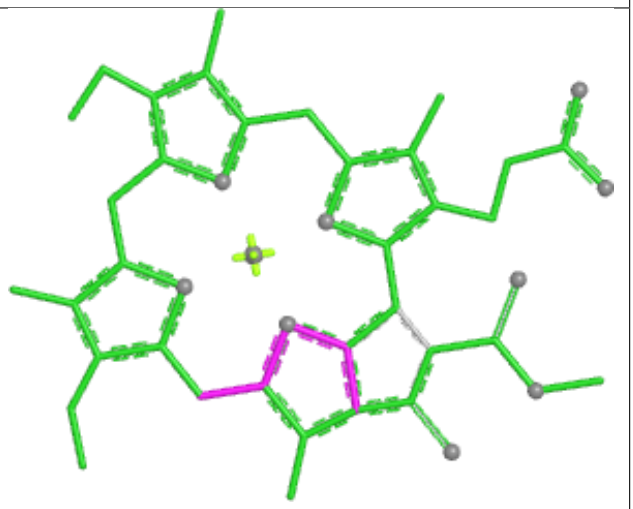


**Rings**

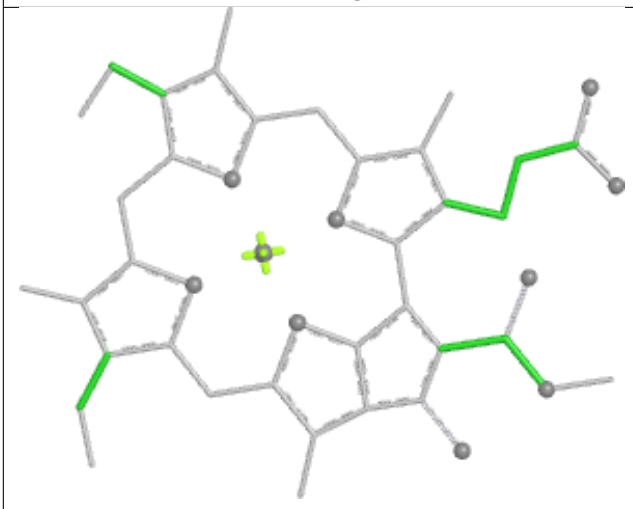
**Ligand CLA B 830**



**Bond lengths**



**Bond angles**

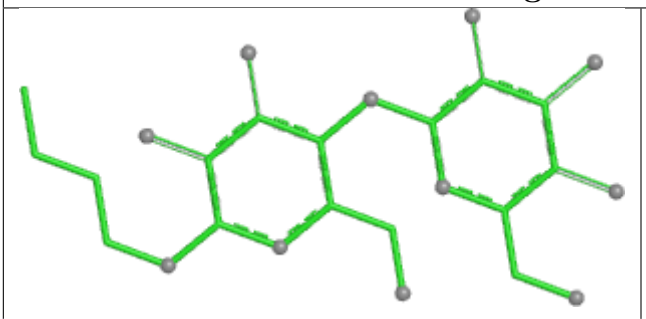


**Torsions**

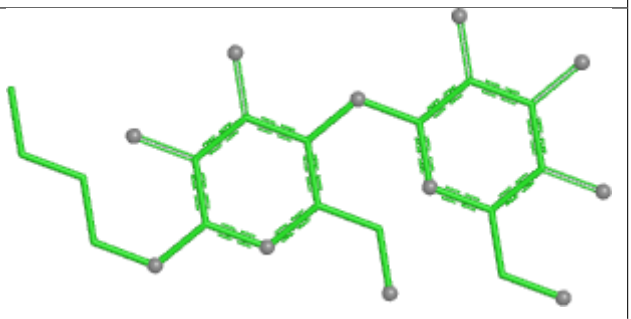


**Rings**

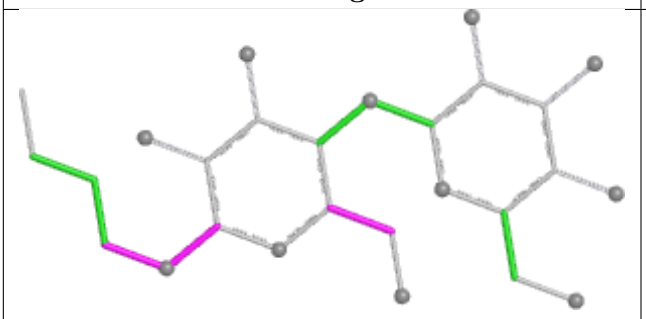
## Ligand LMU 7 629



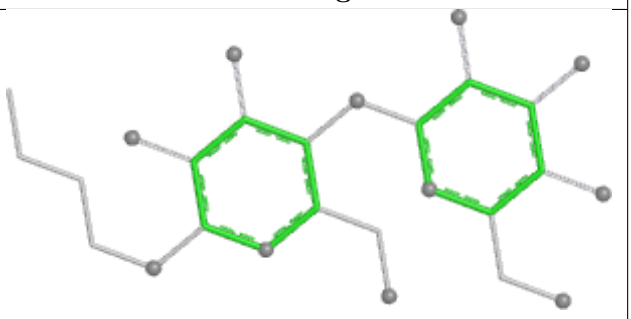
Bond lengths



Bond angles

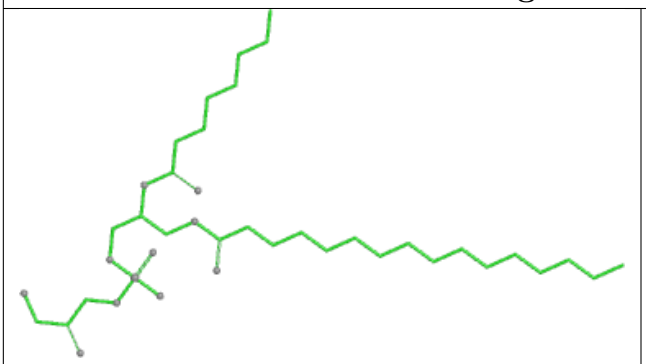


Torsions

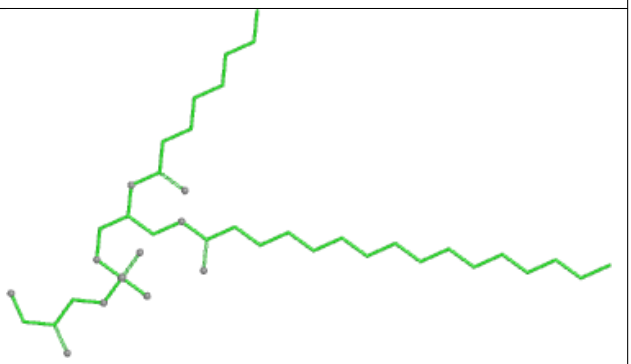


Rings

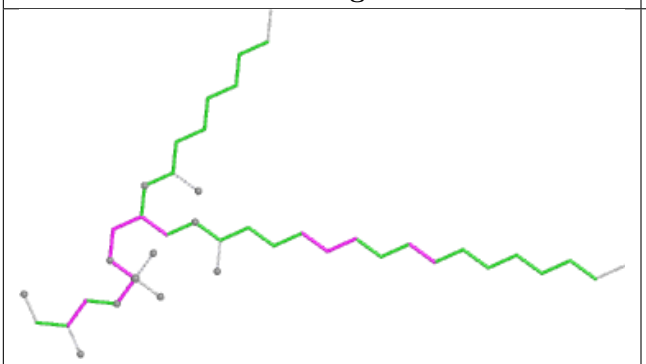
## Ligand LHG 92 622



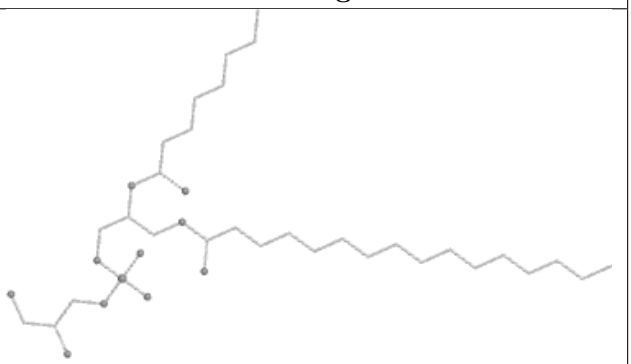
Bond lengths



Bond angles

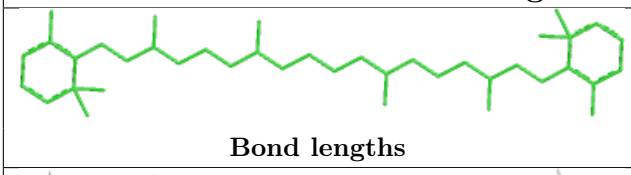


Torsions

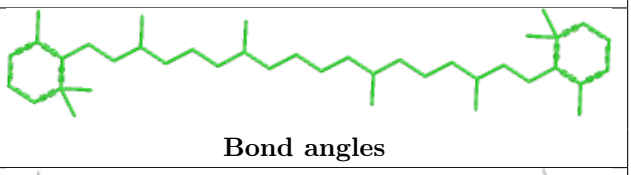


Rings

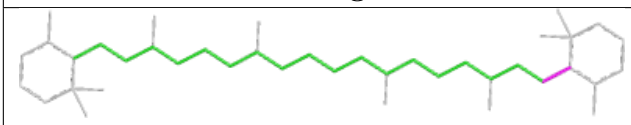
## Ligand BCR 3 719



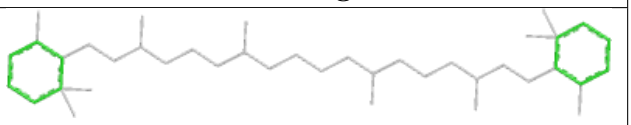
Bond lengths



Bond angles

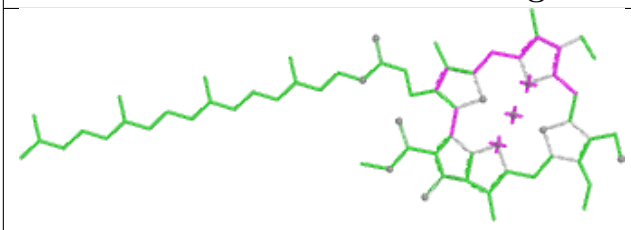


Torsions

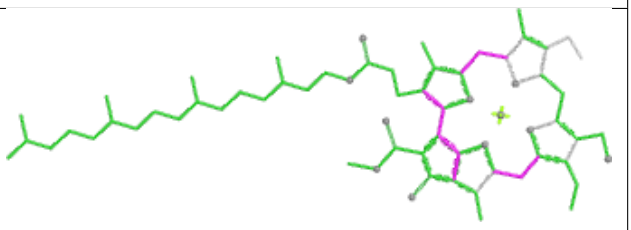


Rings

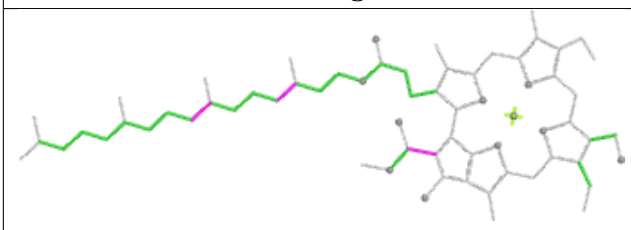
## Ligand CHL 4 601



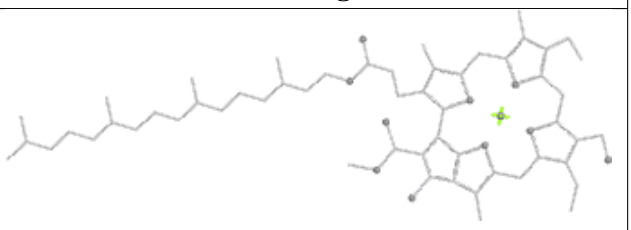
Bond lengths



Bond angles

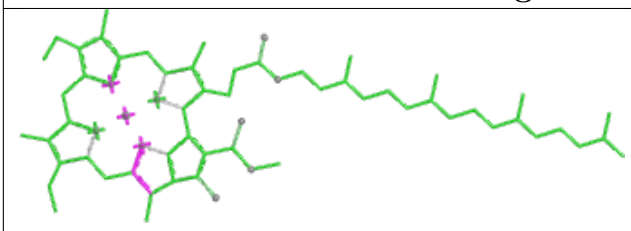


Torsions

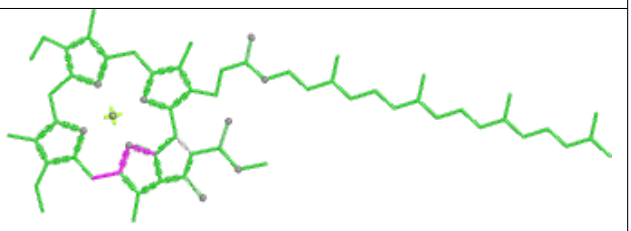


Rings

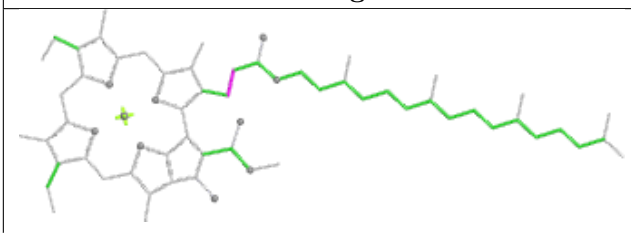
## Ligand CLA A2 854



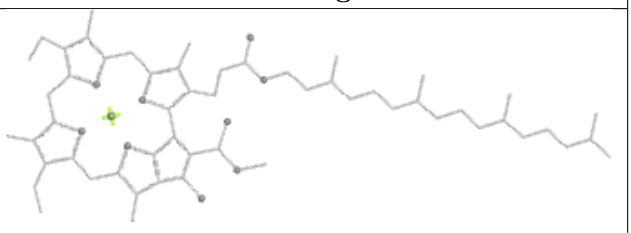
Bond lengths



Bond angles

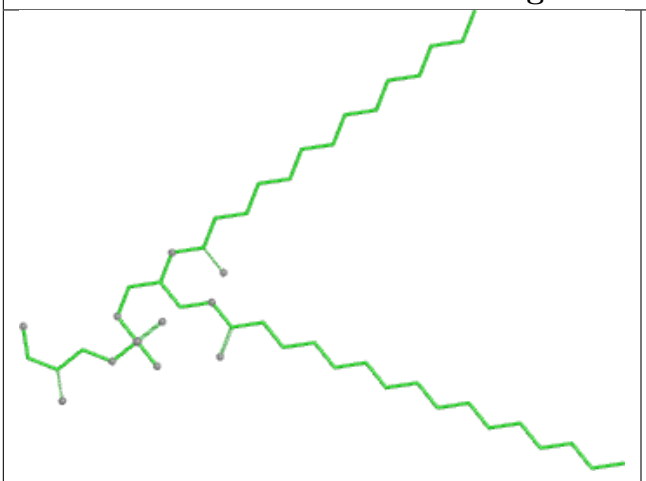


Torsions

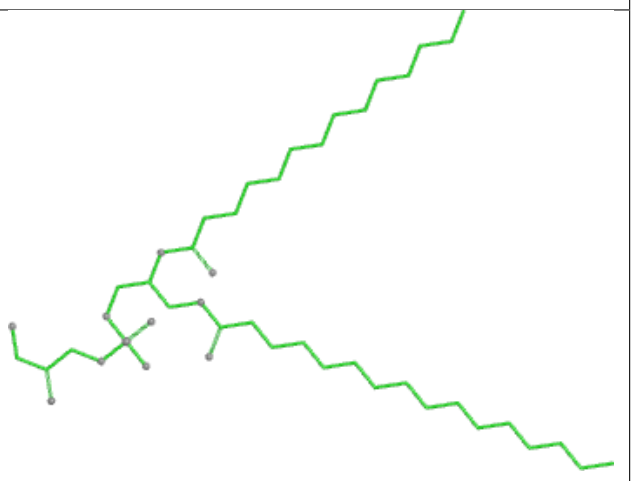


Rings

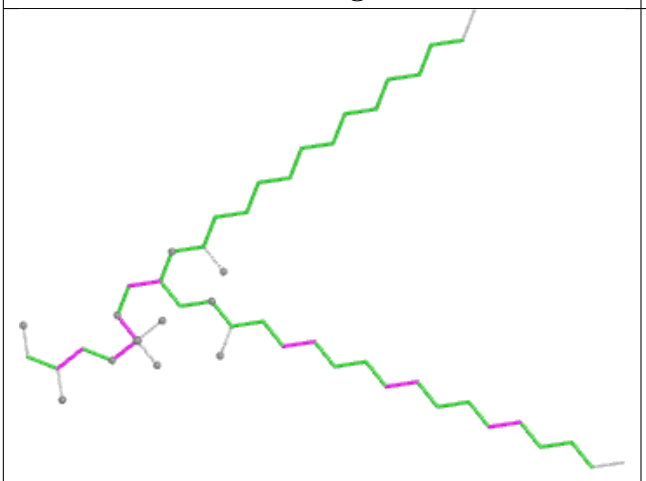
**Ligand LHG 3 623**



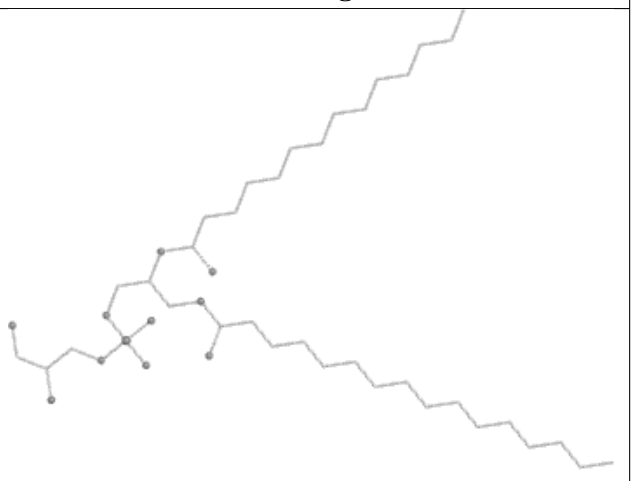
**Bond lengths**



**Bond angles**

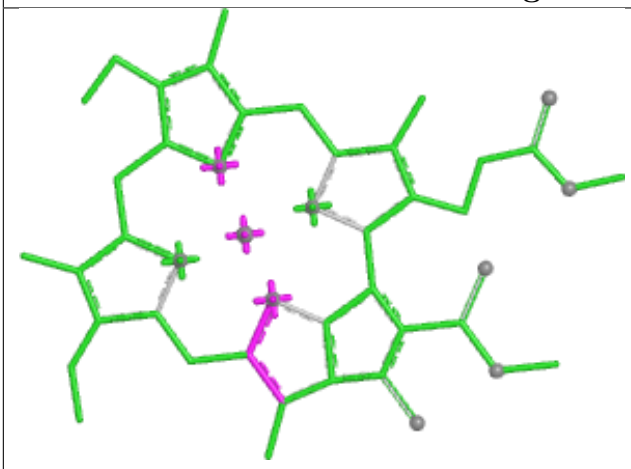


**Torsions**

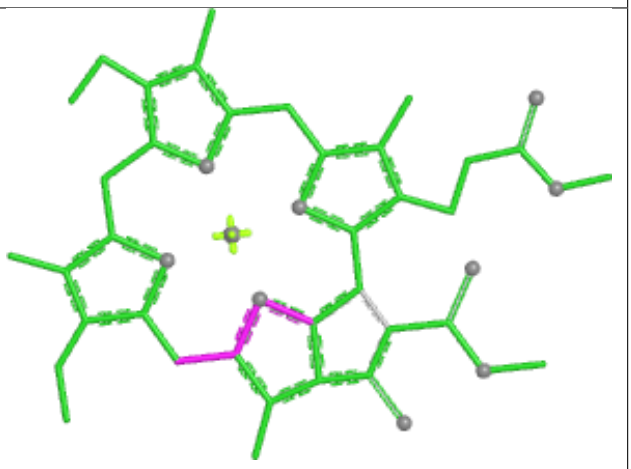


**Rings**

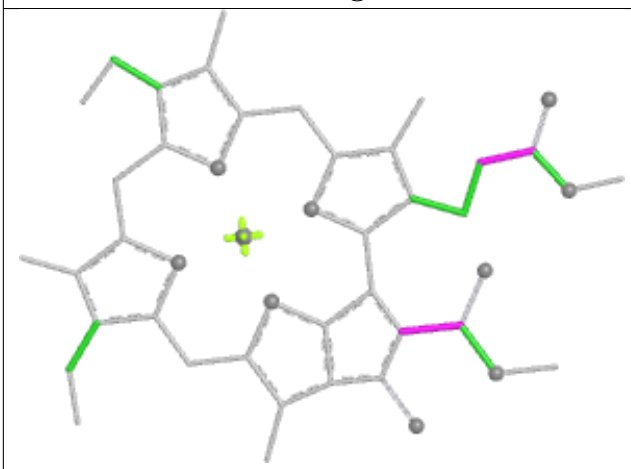
## Ligand CLA G 204



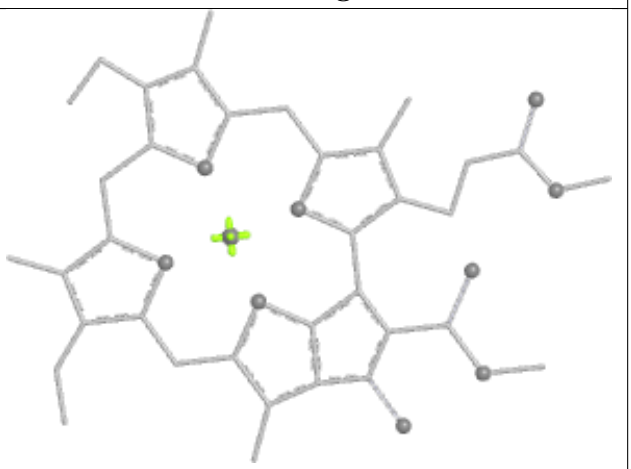
Bond lengths



Bond angles

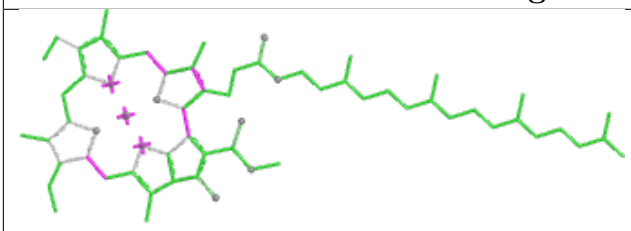


Torsions

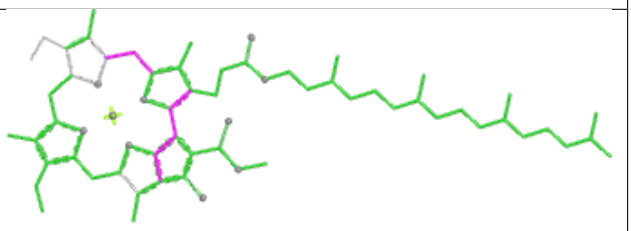


Rings

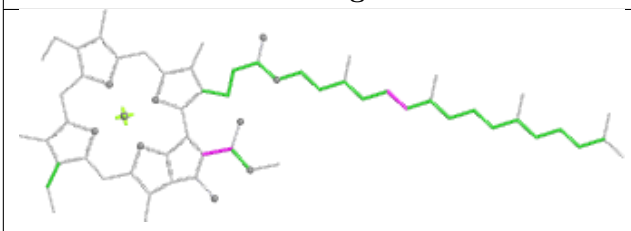
## Ligand CL0 A 801



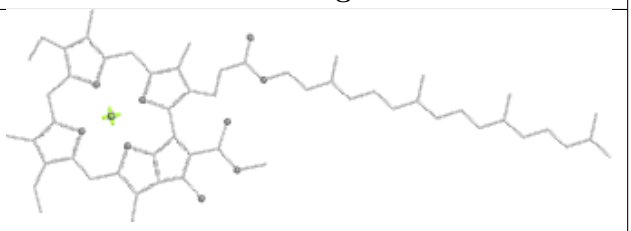
Bond lengths



Bond angles

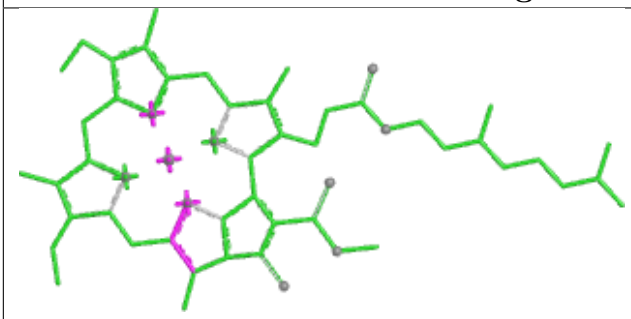


Torsions

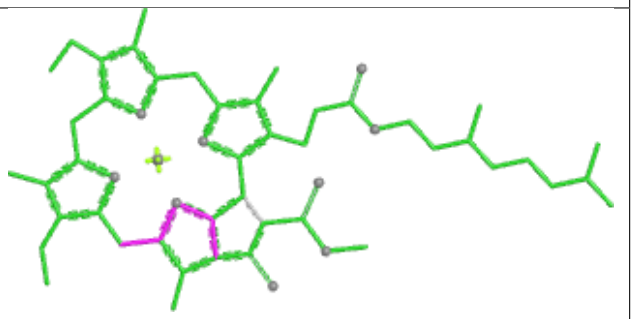


Rings

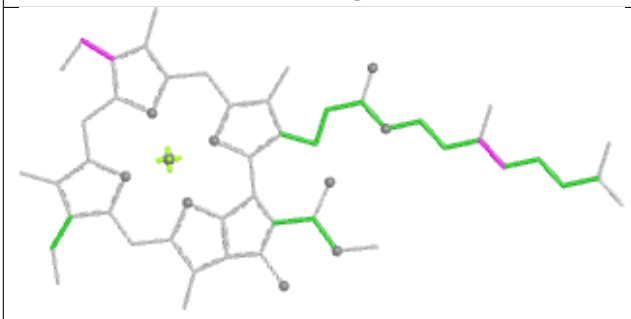
**Ligand CLA B2 807**



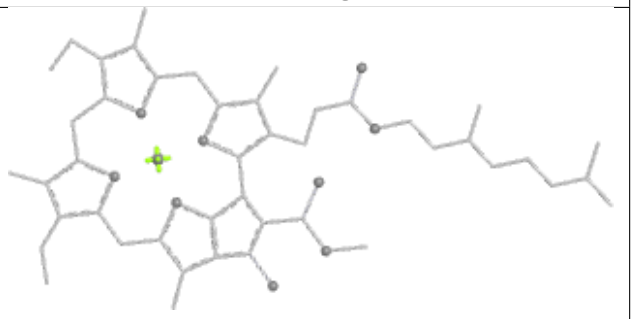
**Bond lengths**



**Bond angles**

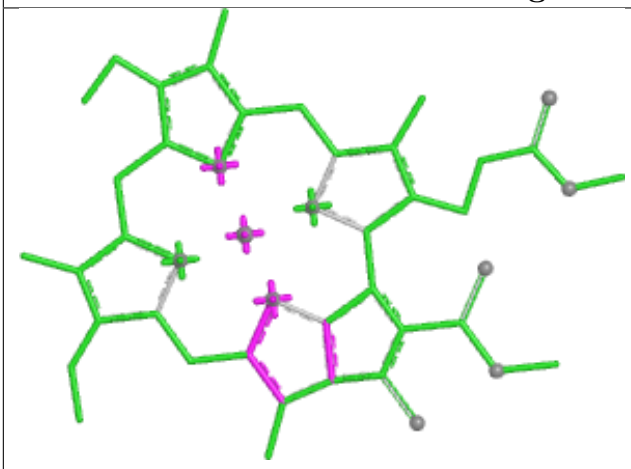


**Torsions**

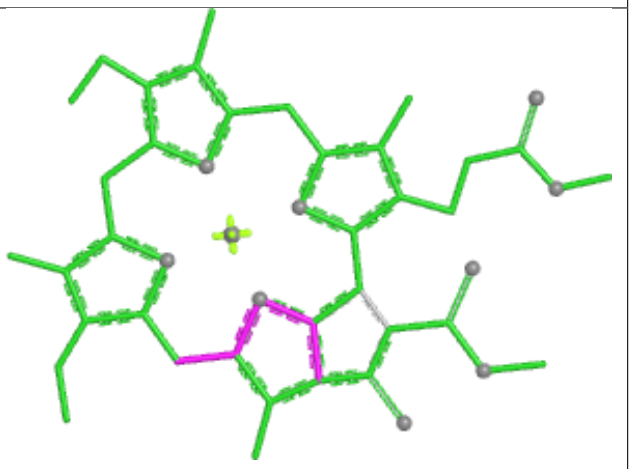


**Rings**

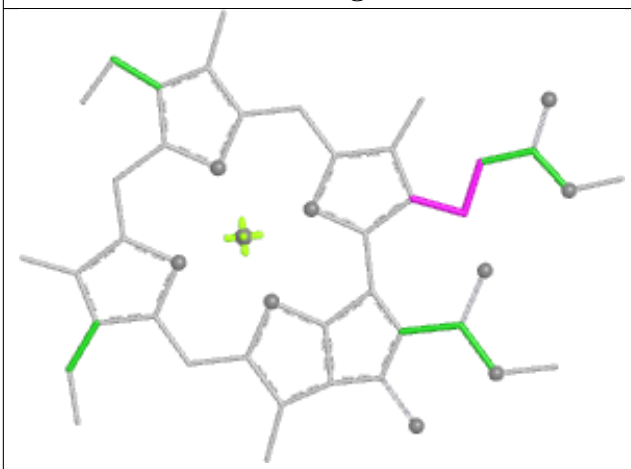
## Ligand CLA 7 616



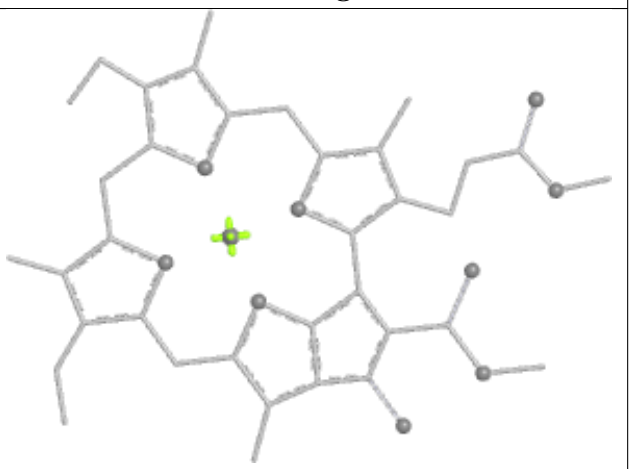
Bond lengths



Bond angles

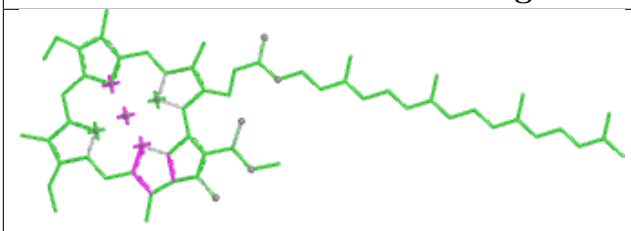


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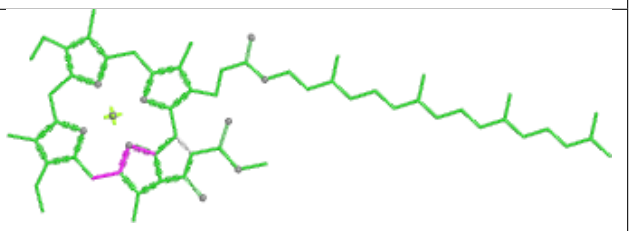


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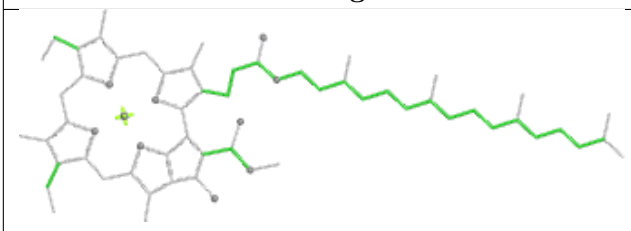
## Ligand CLA A2 802



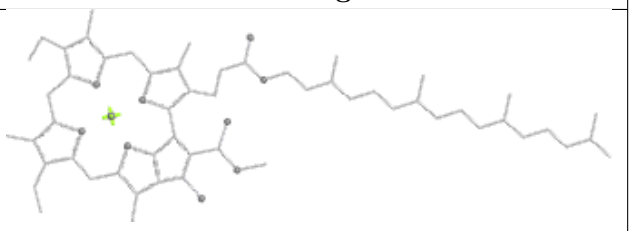
Bond lengths



Bond angles

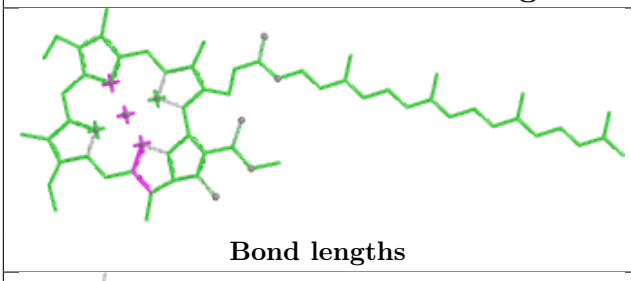


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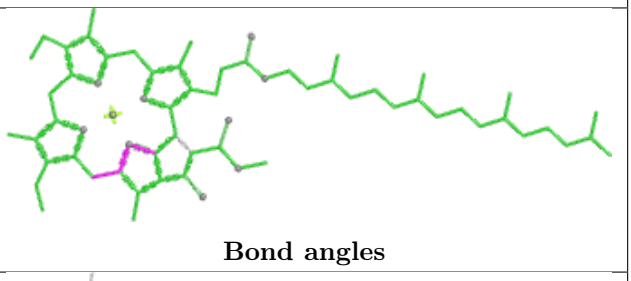


Rings

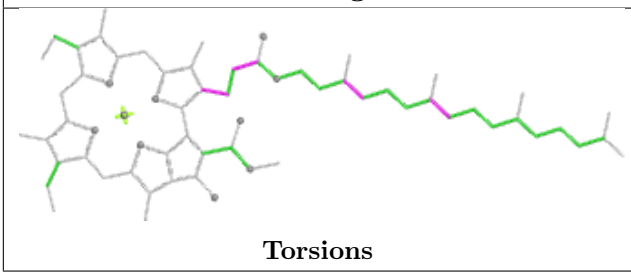
## Ligand CLA 32 615



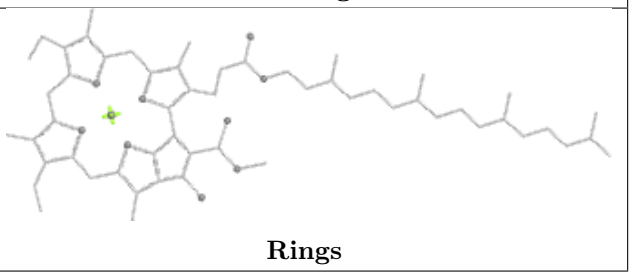
Bond lengths



Bond angles

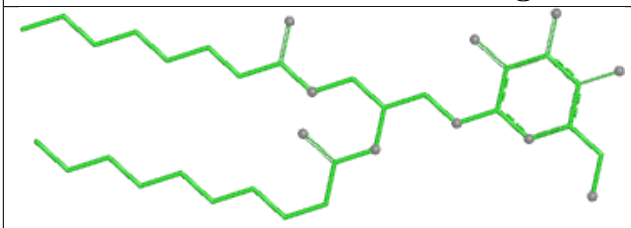


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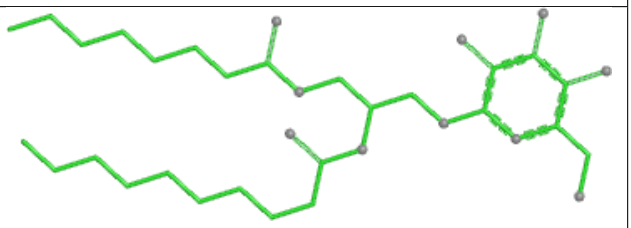


Rings

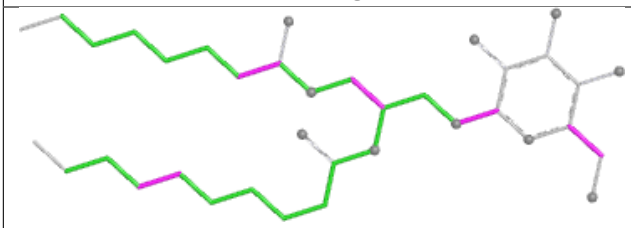
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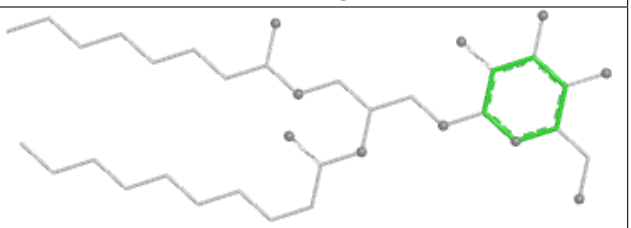
Bond lengths



Bond angles

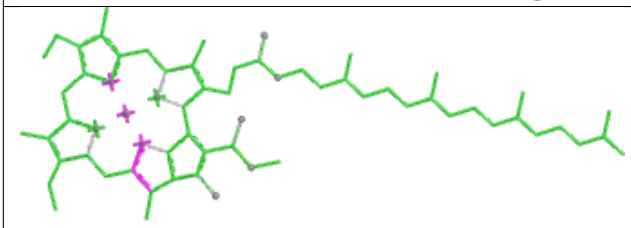


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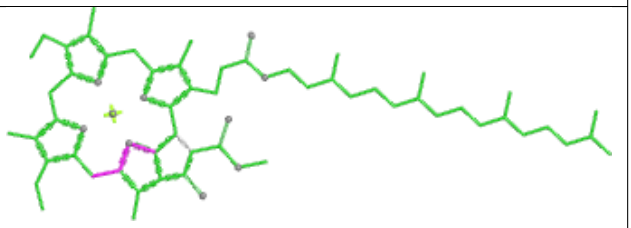


Rings

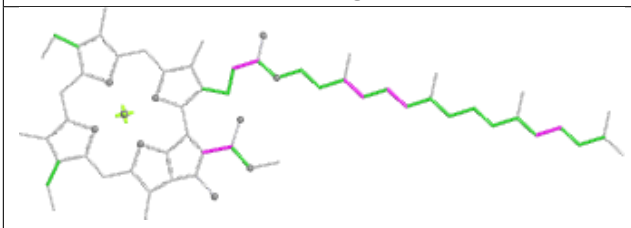
## Ligand CLA 6 603



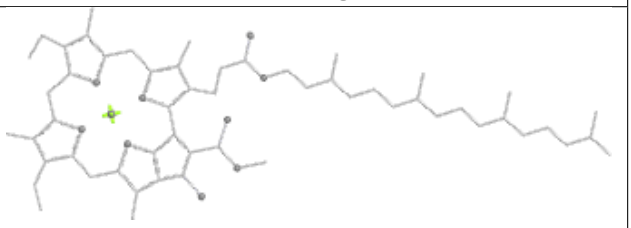
Bond lengths



Bond angles

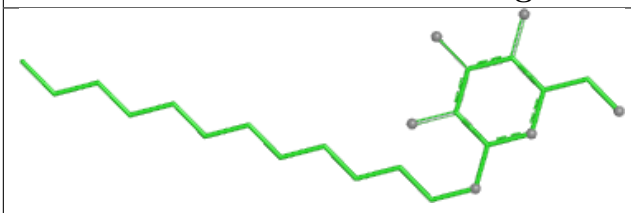


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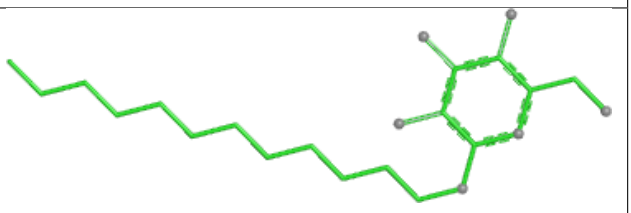


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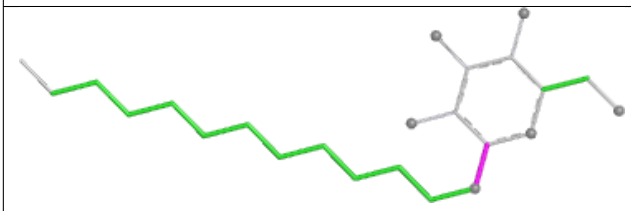
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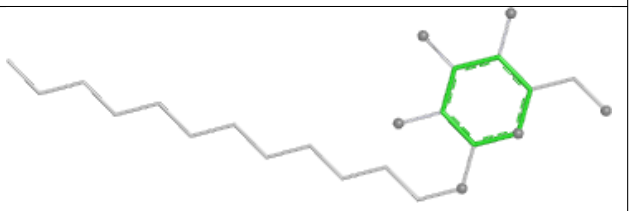
Bond lengths



Bond angles



Torsions

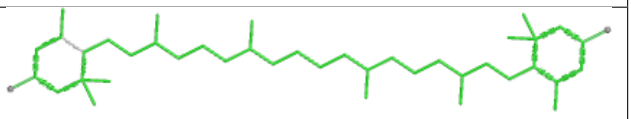


Rings

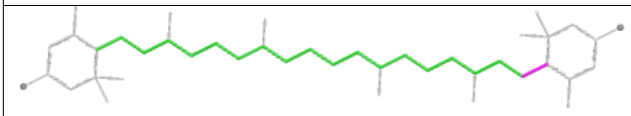
## Ligand LUT 3 622



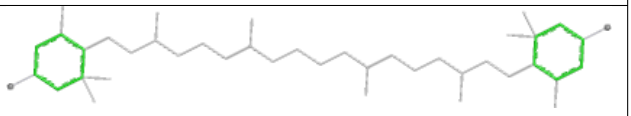
Bond lengths



Bond angles

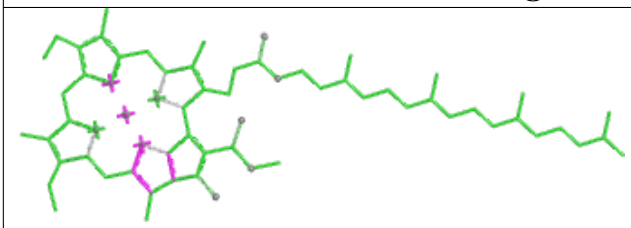


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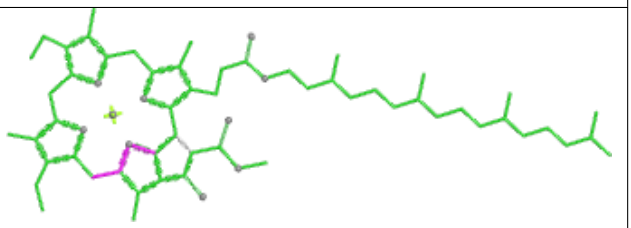


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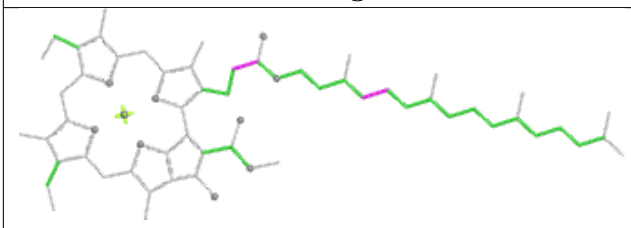
## Ligand CLA B 806



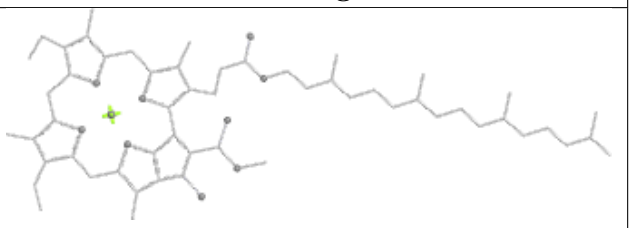
Bond lengths



Bond angles

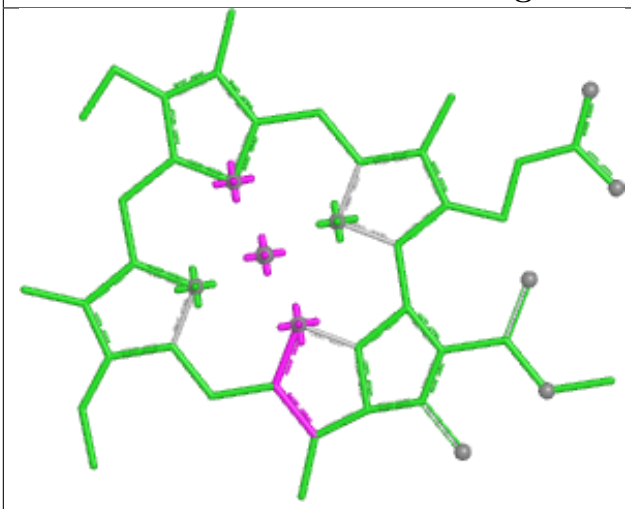


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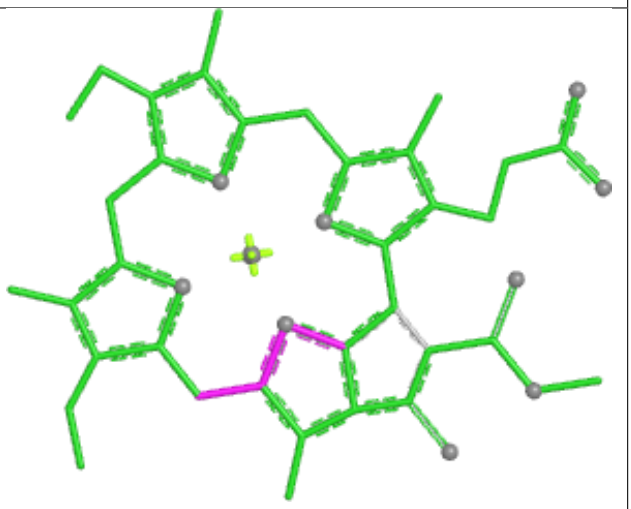


Rings

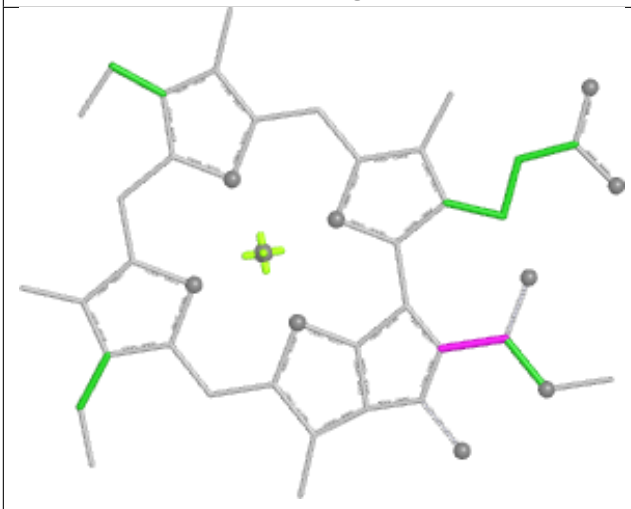
**Ligand CLA A2 845**



**Bond lengths**



**Bond angles**

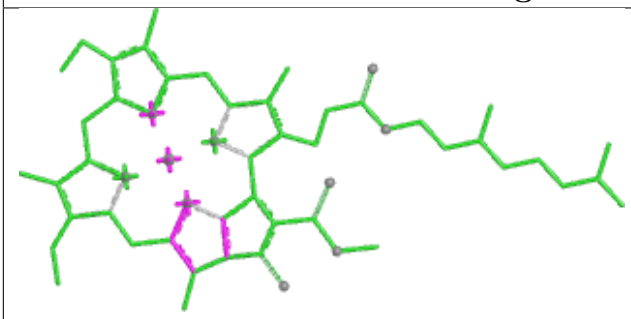


**Torsions**

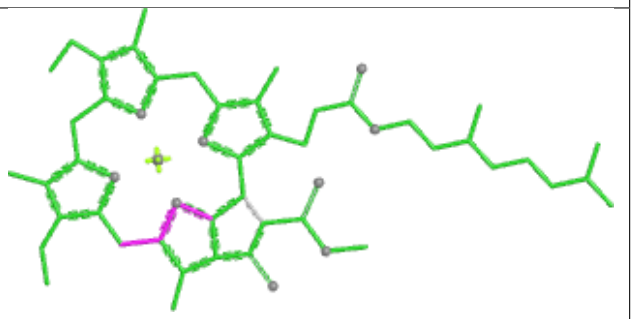


**Rings**

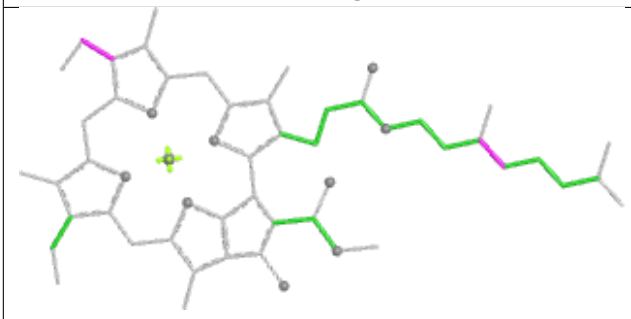
## Ligand CLA A2 821



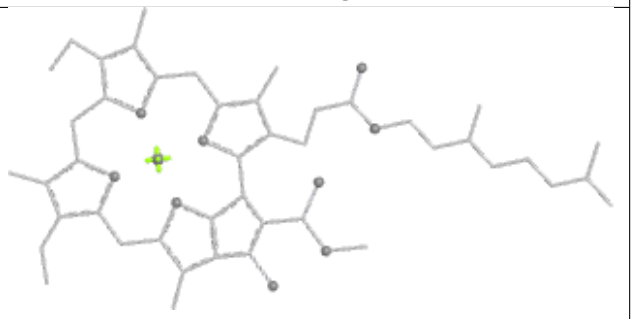
Bond lengths



Bond angles

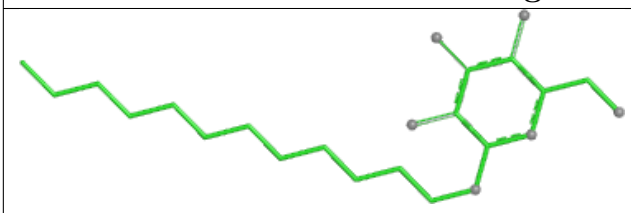


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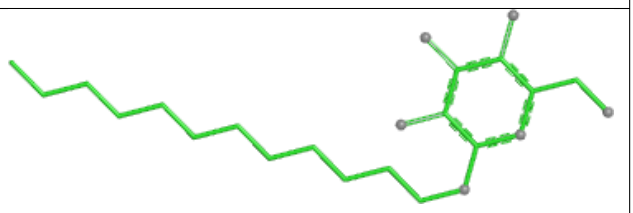


Rings

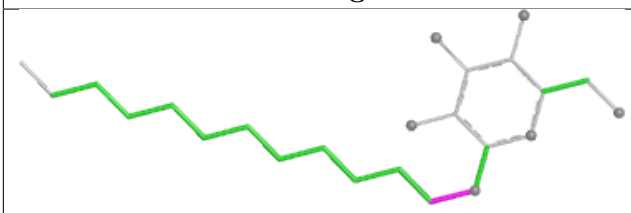
## Ligand LMU 8 624



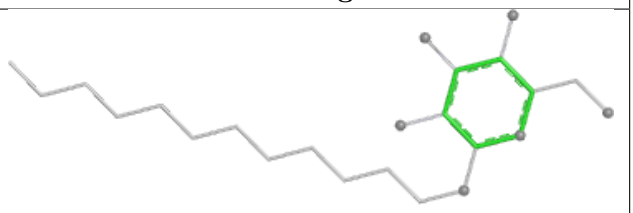
Bond lengths



Bond angles

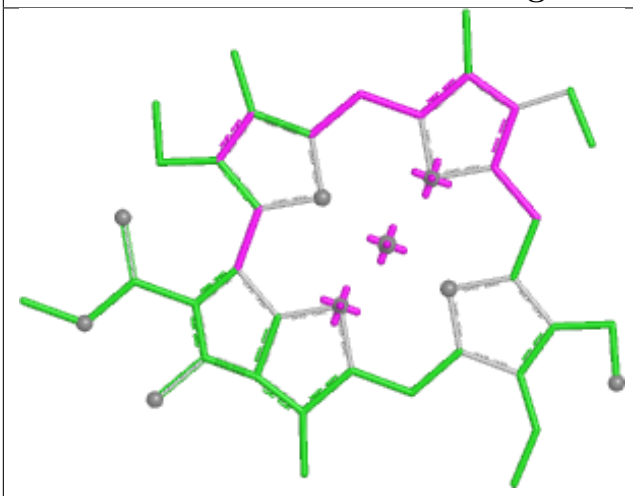


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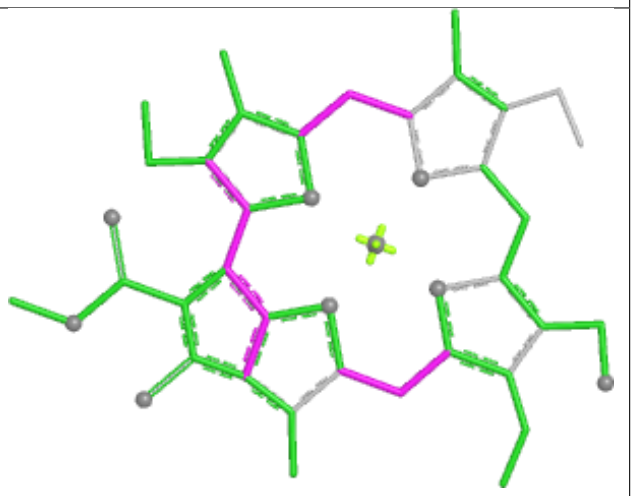


Rings

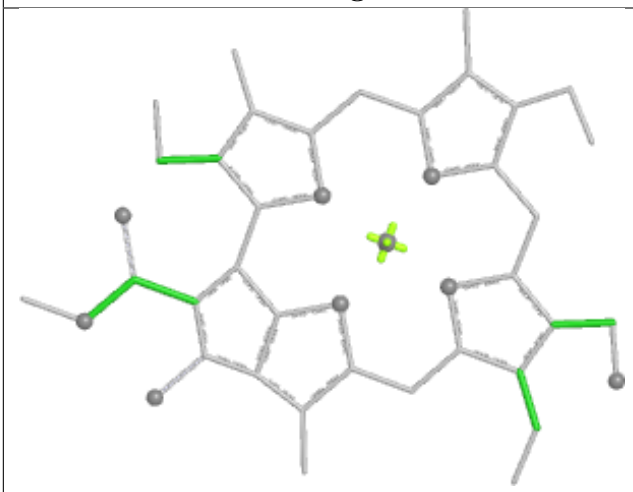
## Ligand CHL 6 618



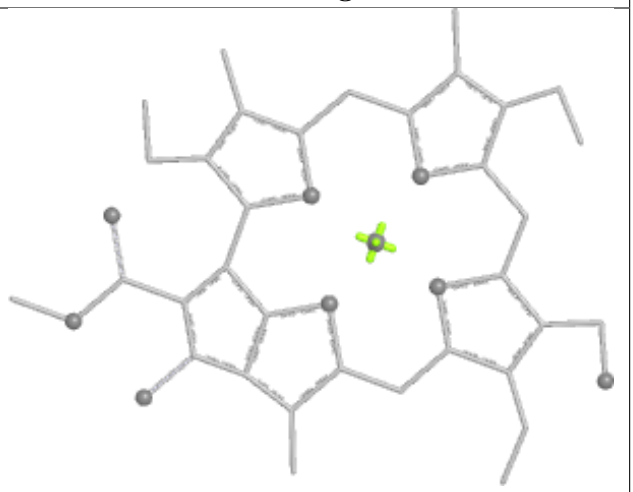
Bond lengths



Bond angles

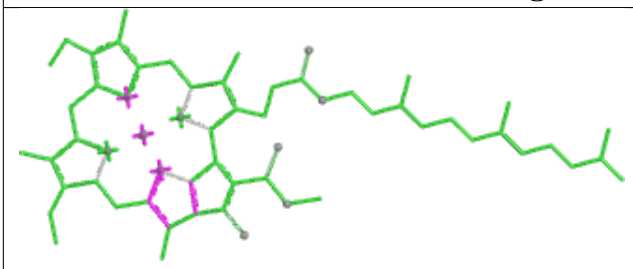


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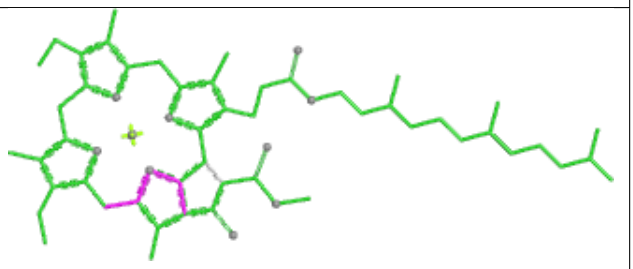


Rings

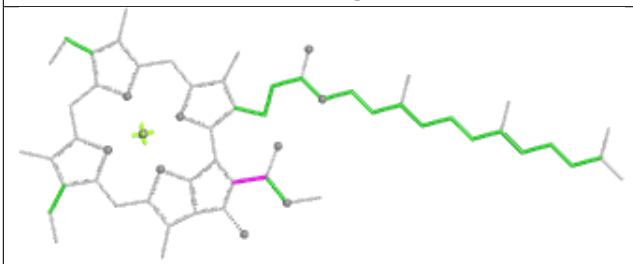
## Ligand CLA 9 602



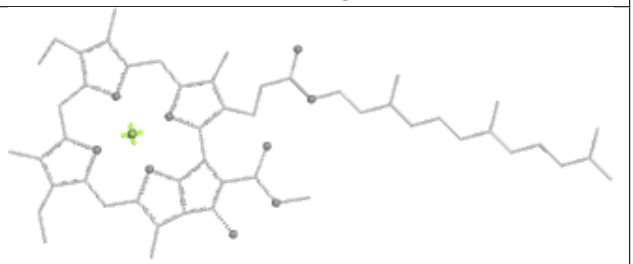
Bond lengths



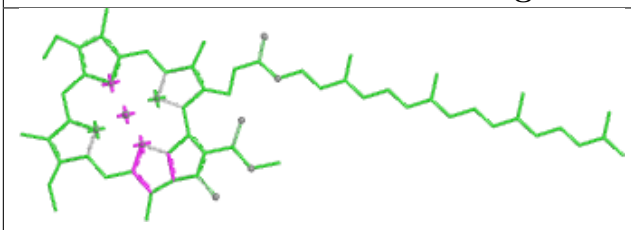
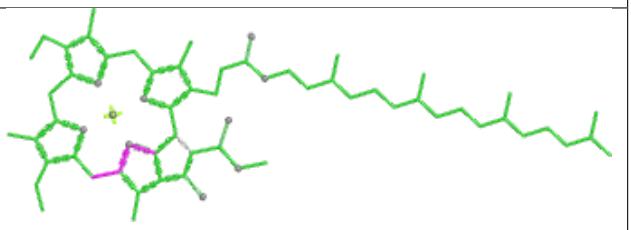
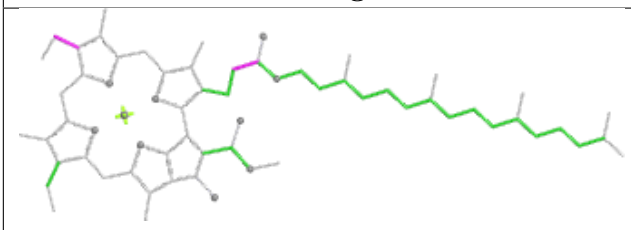
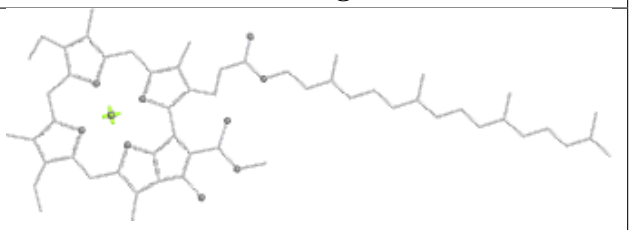
Bond angles

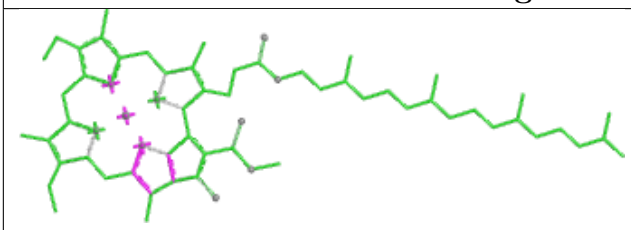
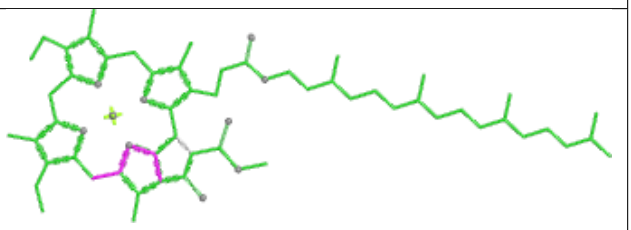
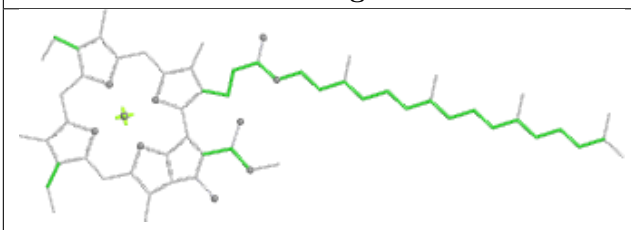
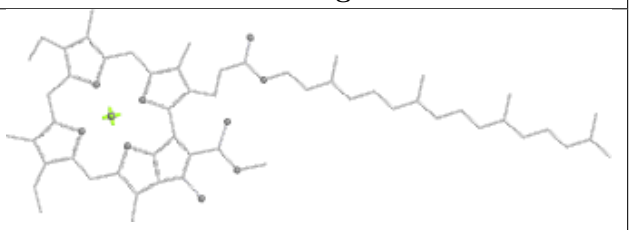


Torsions

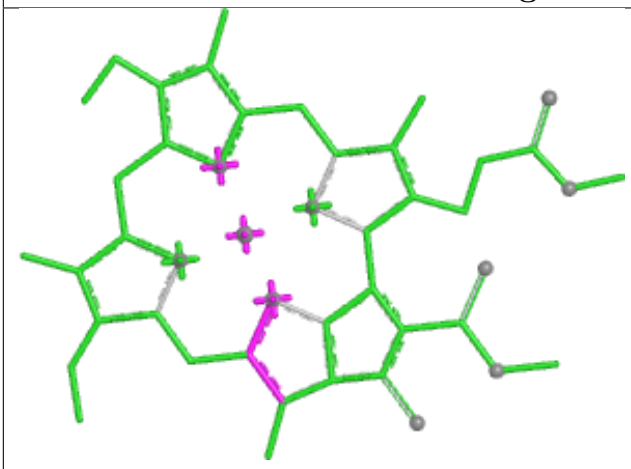


Rings

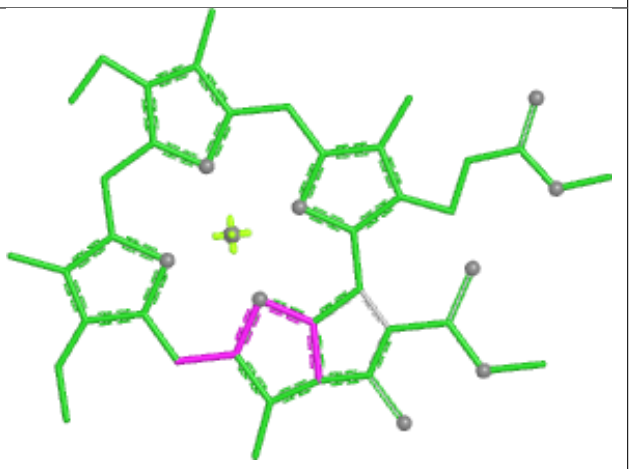
| Ligand CLA A2 807 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA A2 822 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

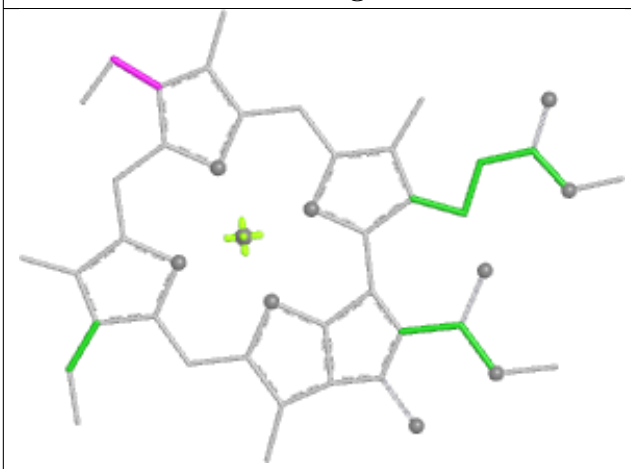
## Ligand CLA 12 616



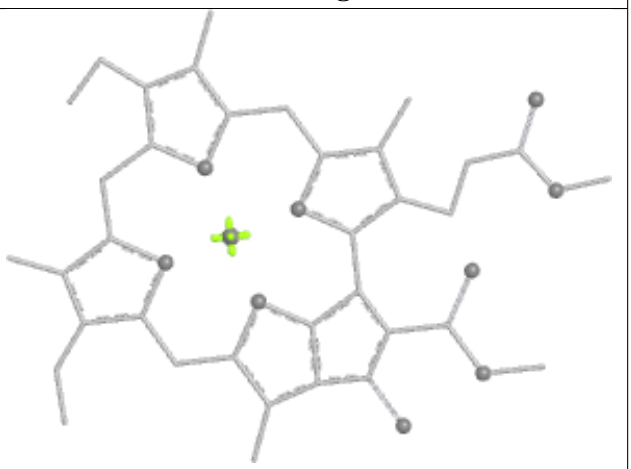
Bond lengths



Bond angles

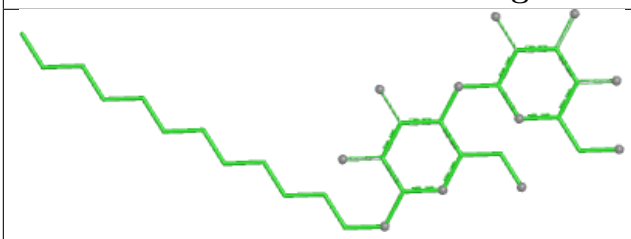


Torsions

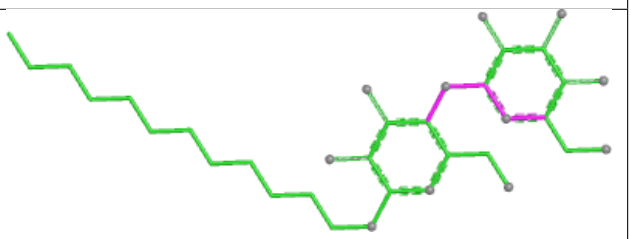


Rings

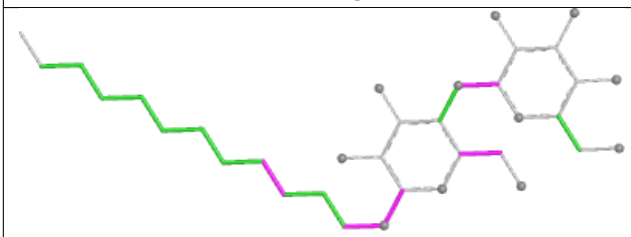
## Ligand LMU B2 853



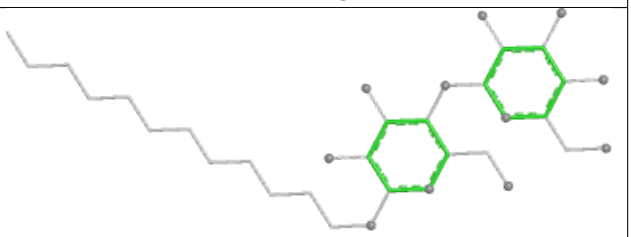
Bond lengths



Bond angles

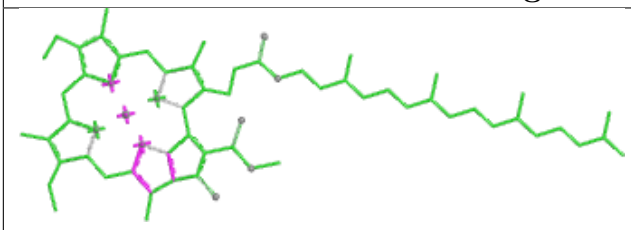


Torsions

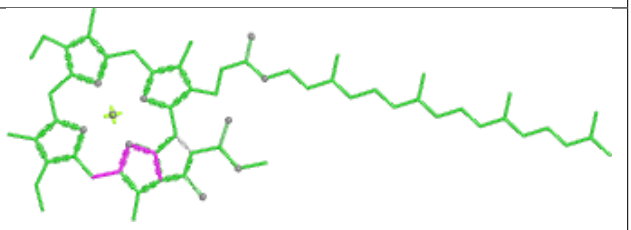


Rings

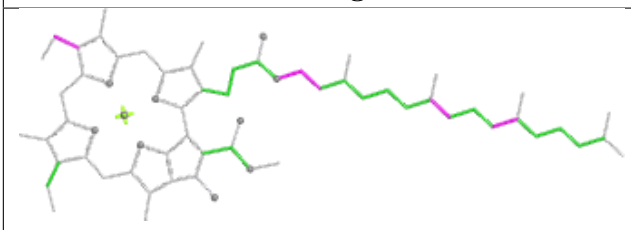
## Ligand CLA A 843



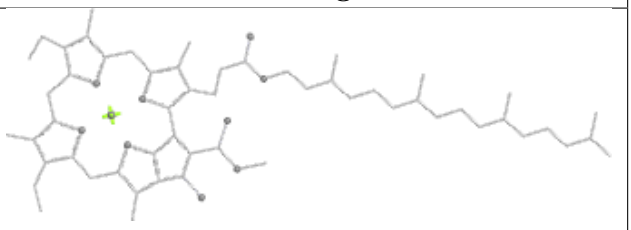
Bond lengths



Bond angles

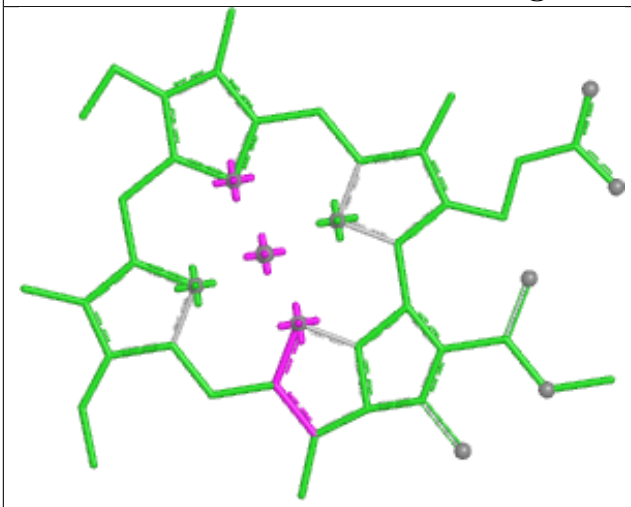


Torsions

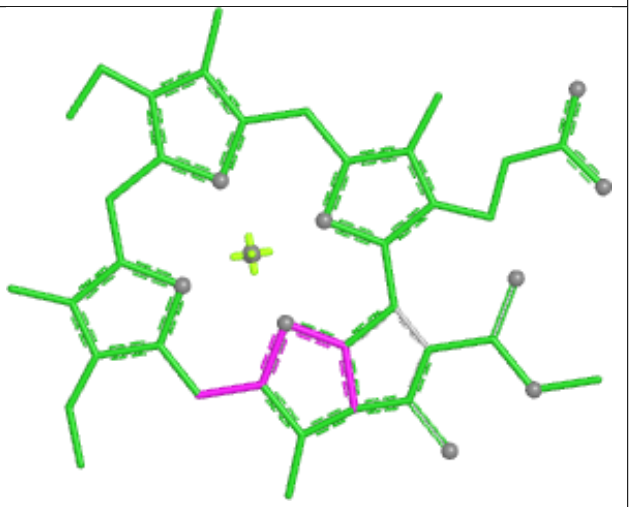


Rings

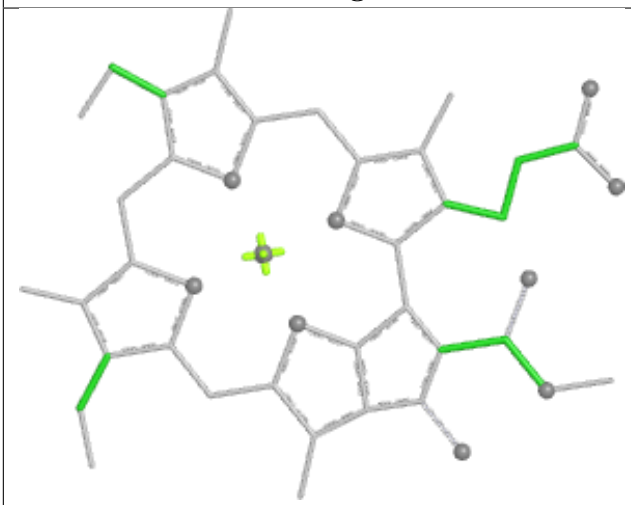
## Ligand CLA 8 609



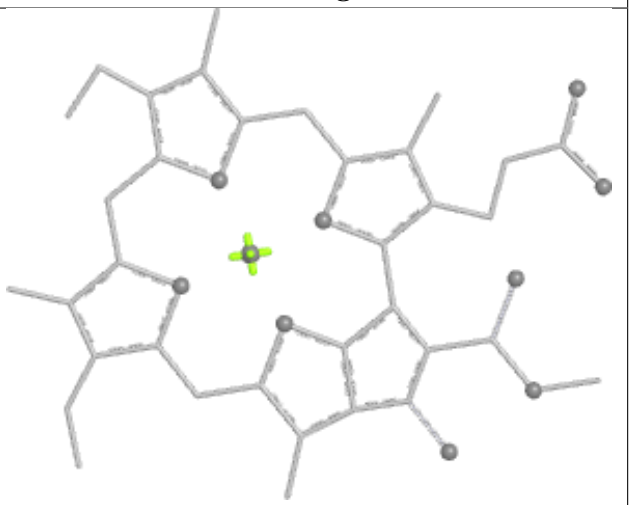
Bond lengths



Bond angles

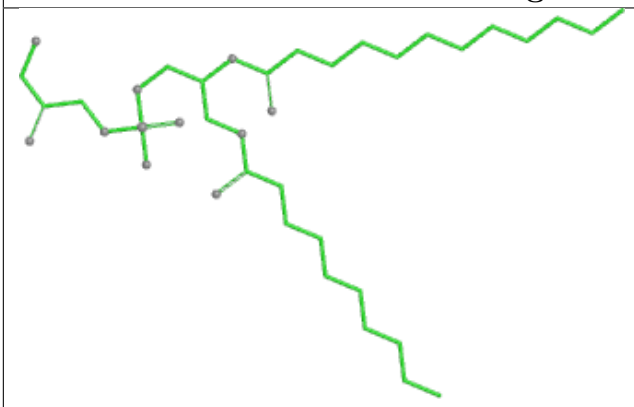


Torsions

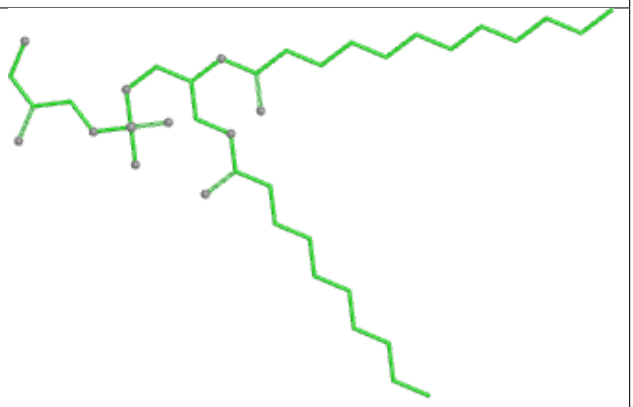


Rings

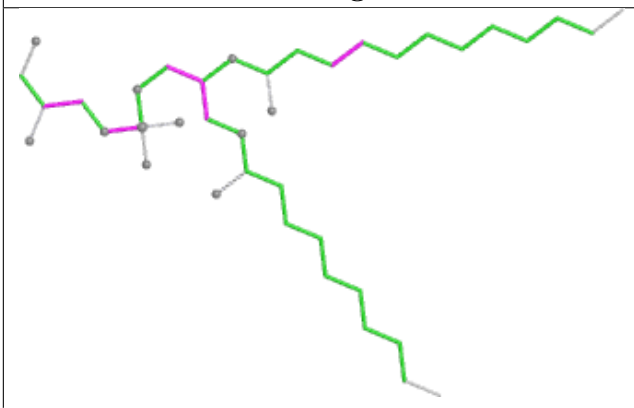
## Ligand LHG 1 620



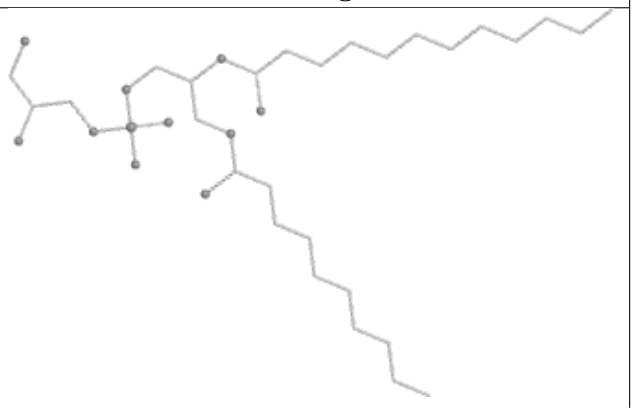
Bond lengths



Bond angles

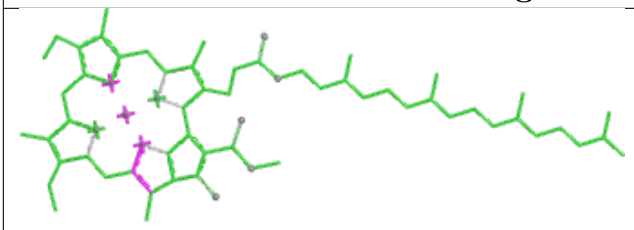


Torsions

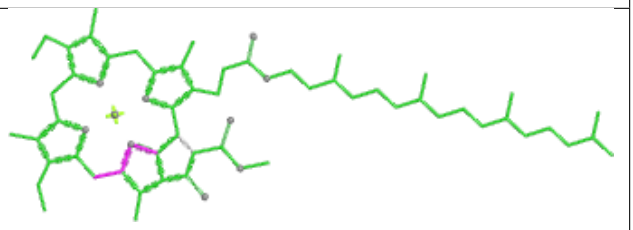


Rings

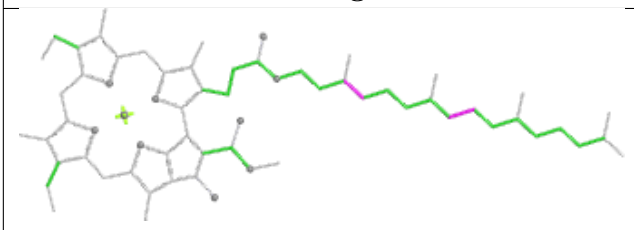
## Ligand CLA B2 813



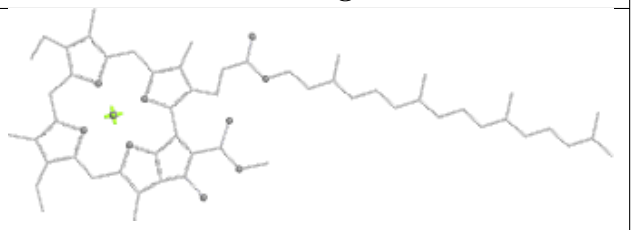
Bond lengths



Bond angles

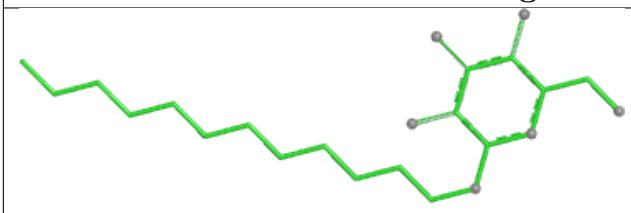


Torsions

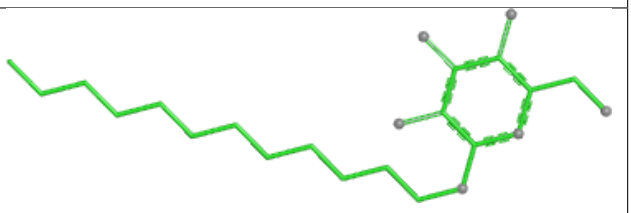


Rings

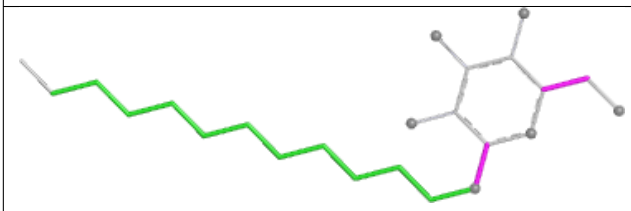
## Ligand LMU A 861



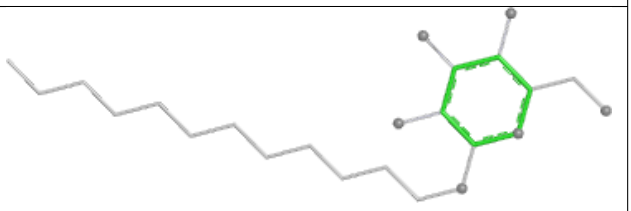
Bond lengths



Bond angles

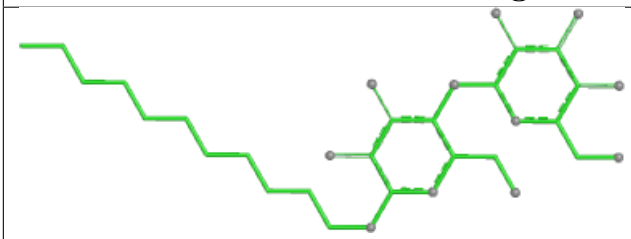


Torsions

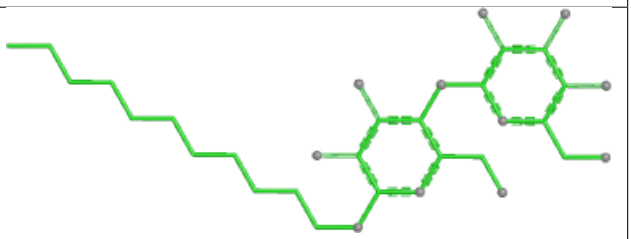


Rings

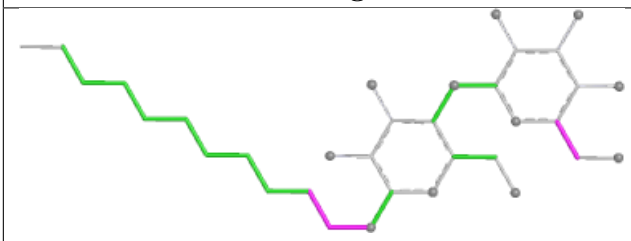
## Ligand LMU A2 857



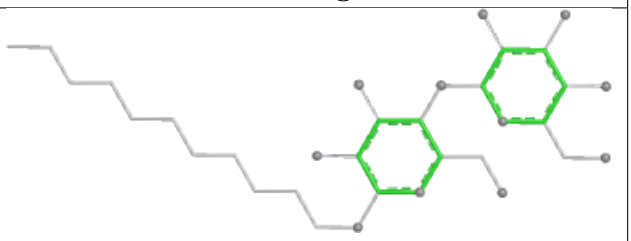
Bond lengths



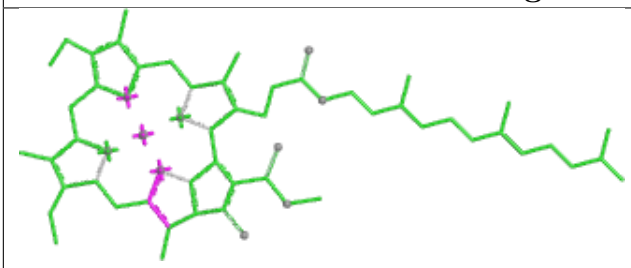
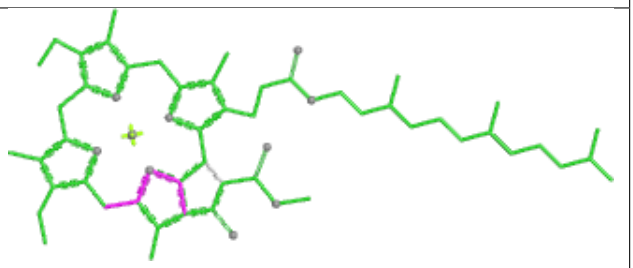
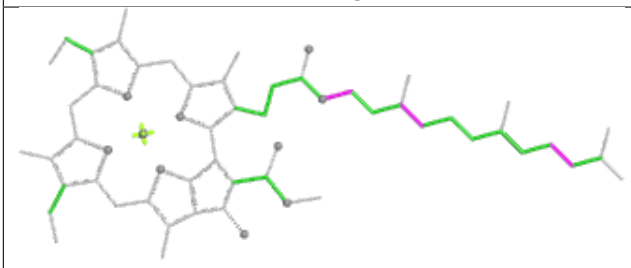
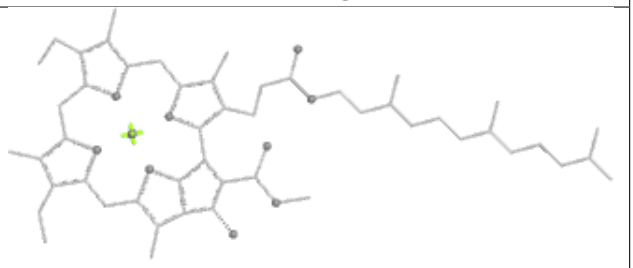
Bond angles

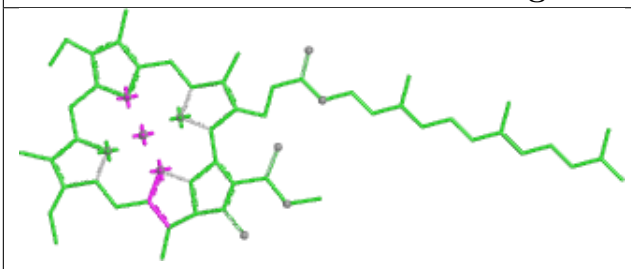
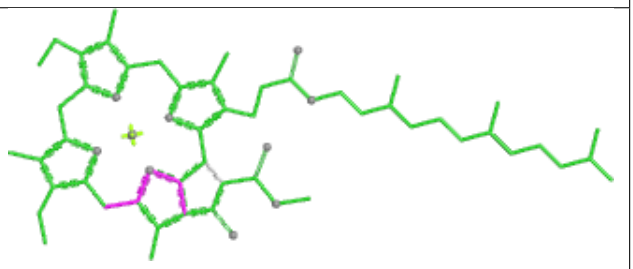
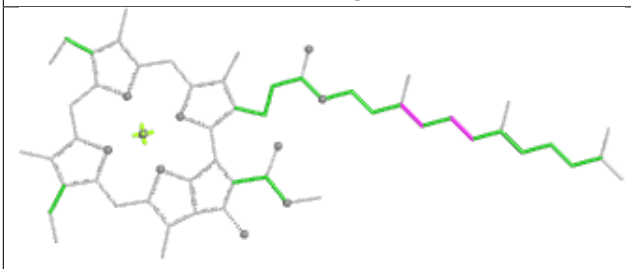
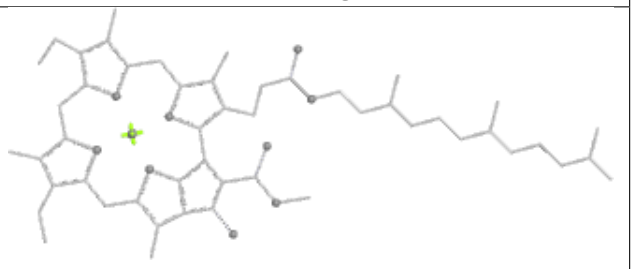


Torsions

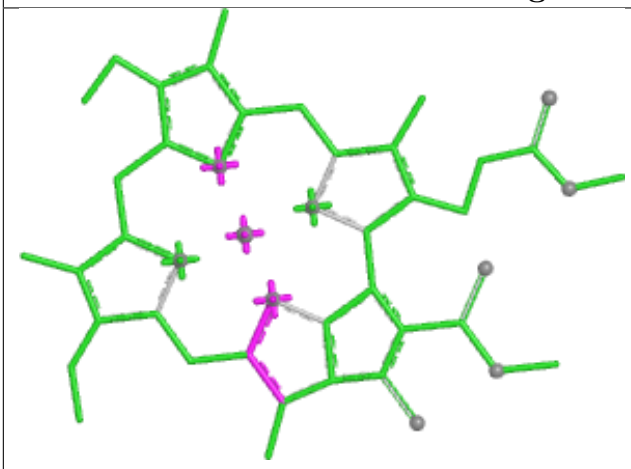


Rings

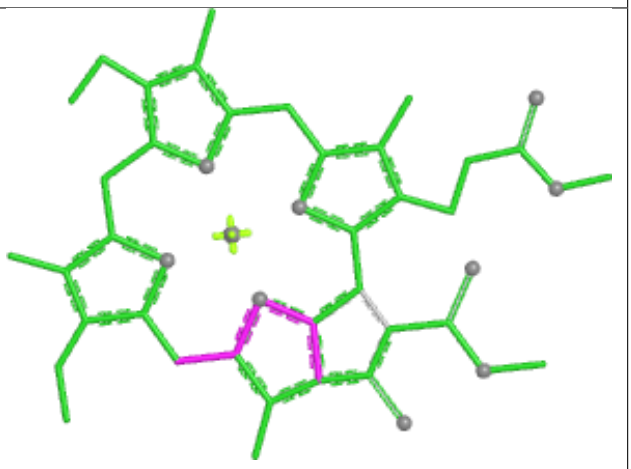
| Ligand CLA B 836 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand CLA 4 610 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

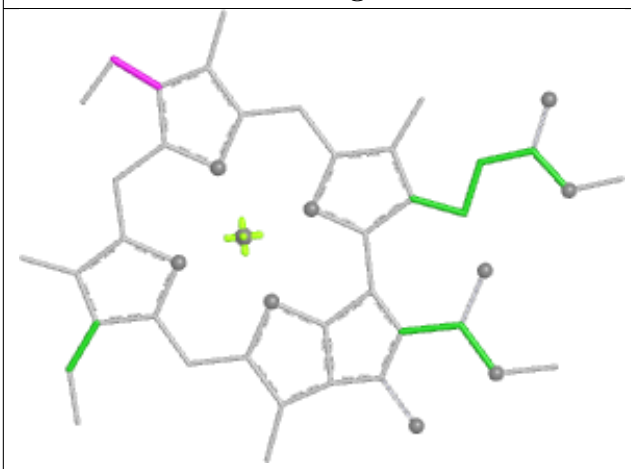
**Ligand CLA 3 612**



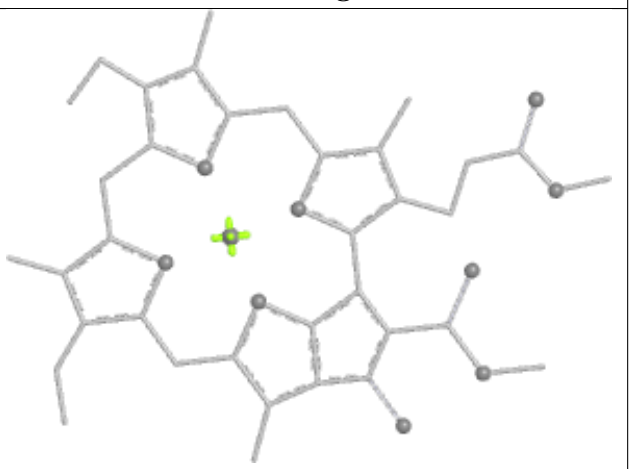
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

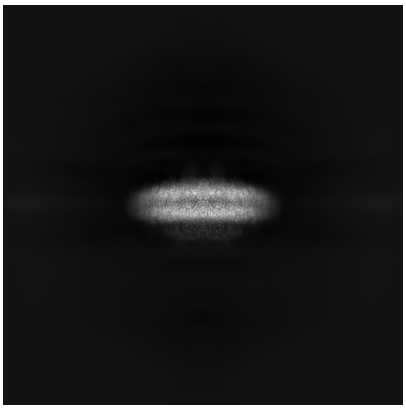
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14871. These allow visual inspection of the internal detail of the map and identification of artifacts.

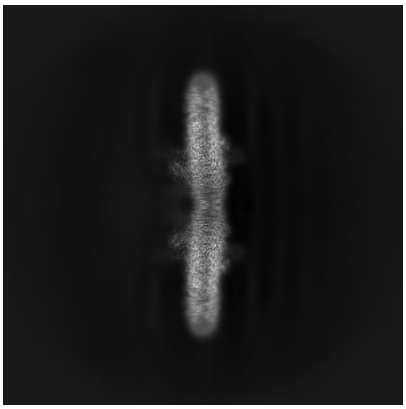
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

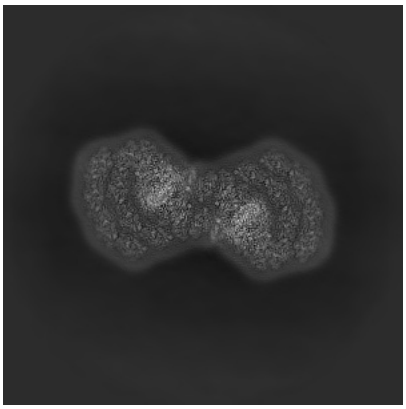
### 6.1.1 Primary map



X

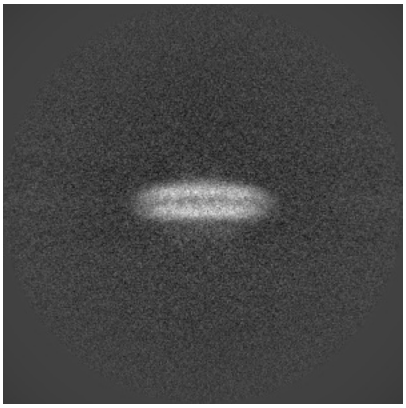


Y

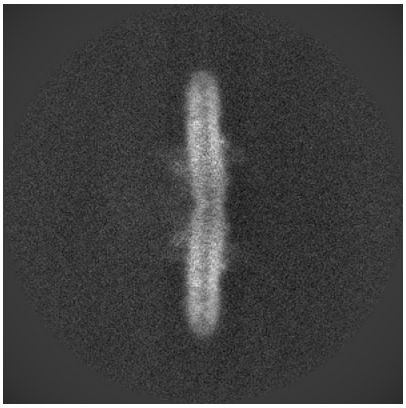


Z

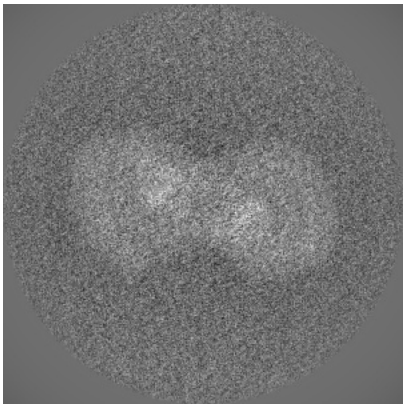
### 6.1.2 Raw map



X



Y

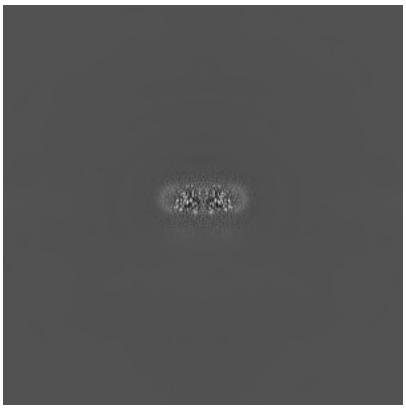


Z

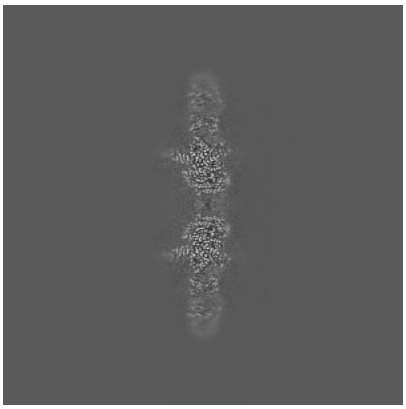
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

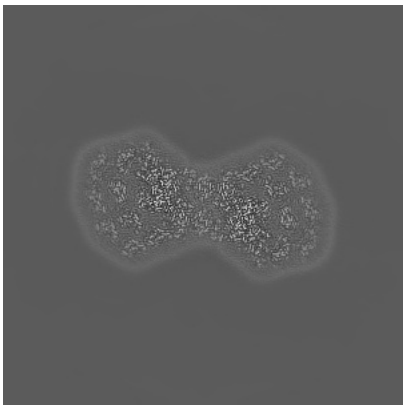
### 6.2.1 Primary map



X Index: 350

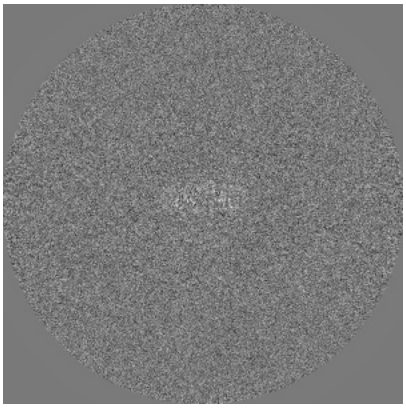


Y Index: 350

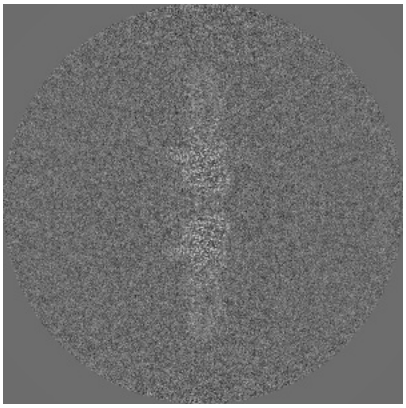


Z Index: 350

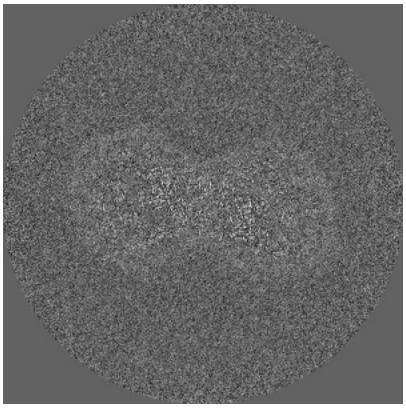
### 6.2.2 Raw map



X Index: 350



Y Index: 350

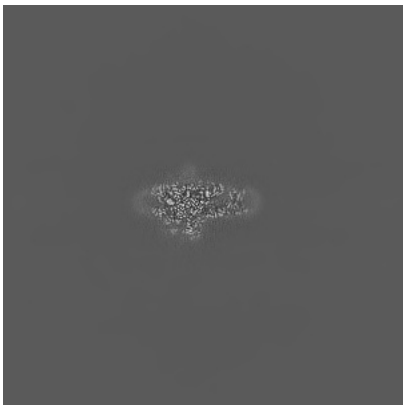


Z Index: 350

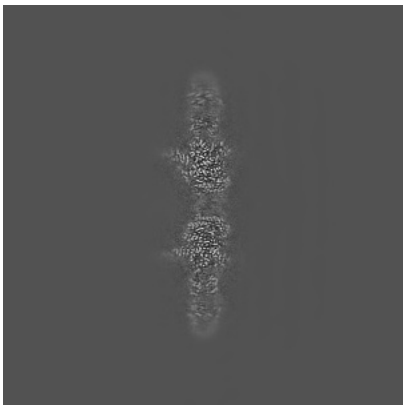
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

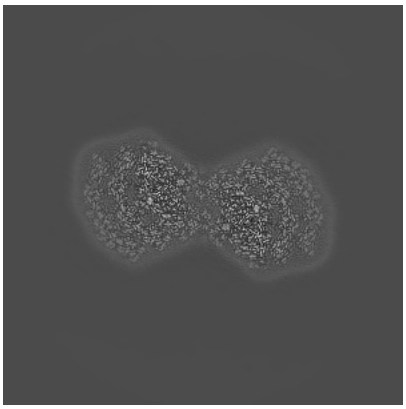
### 6.3.1 Primary map



X Index: 422

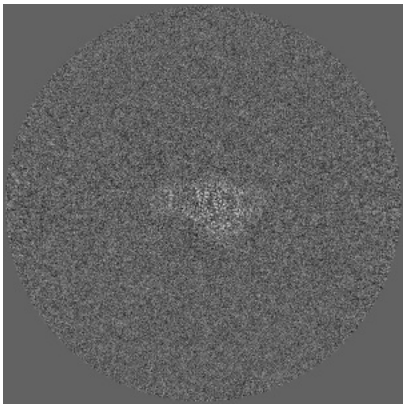


Y Index: 349

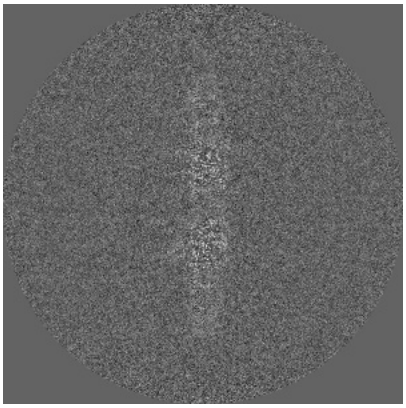


Z Index: 340

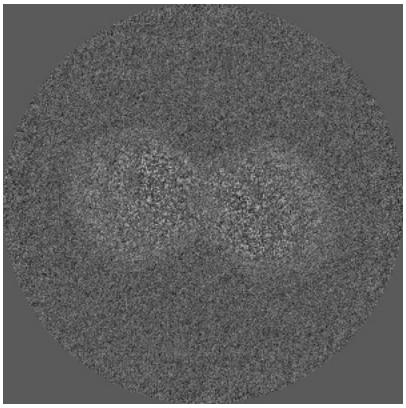
### 6.3.2 Raw map



X Index: 292



Y Index: 355

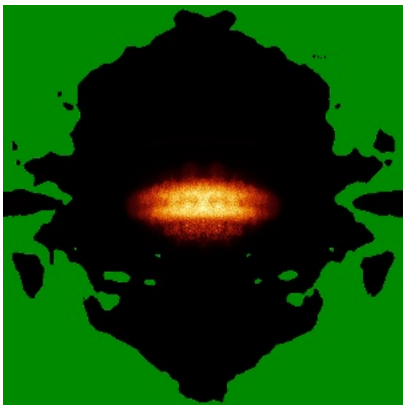


Z Index: 339

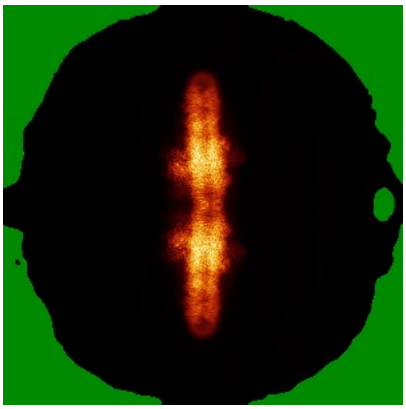
The images above show the largest variance slices of the map in three orthogonal directions.

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

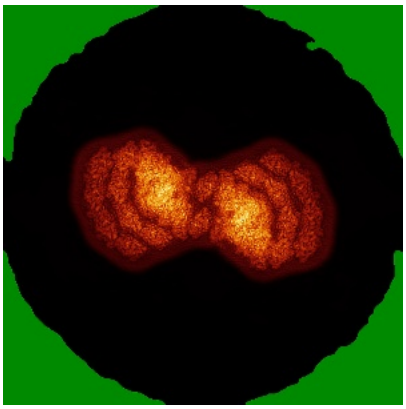
### 6.4.1 Primary map



X

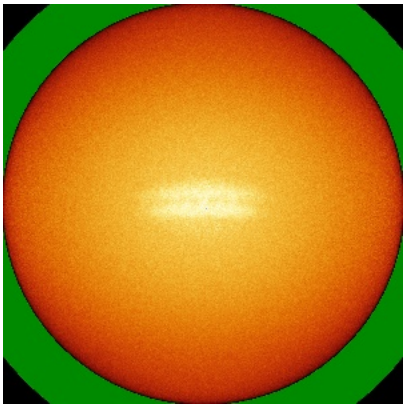


Y

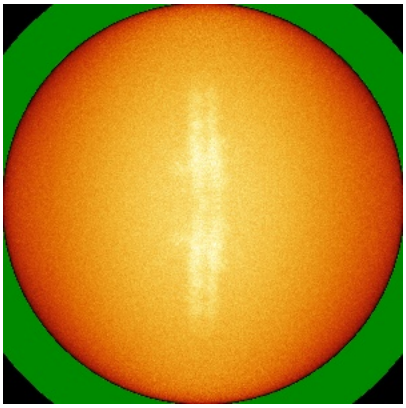


Z

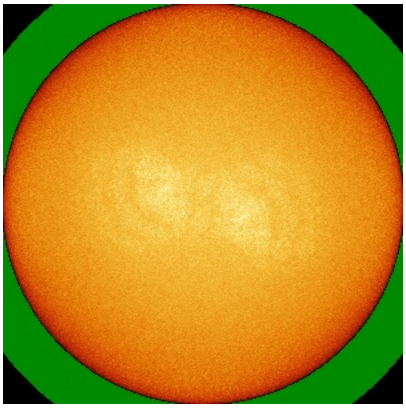
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

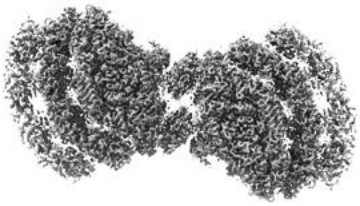
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

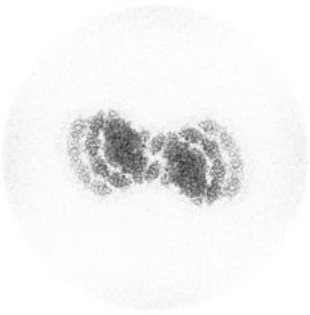
### 6.5.2 Raw map



X



Y



Z

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

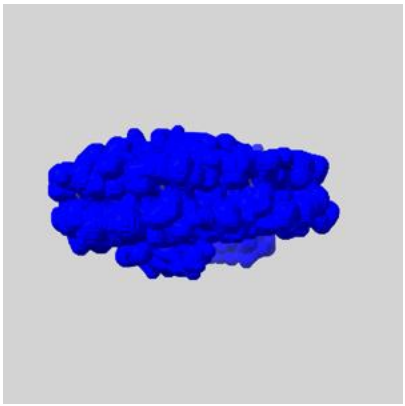
## 6.6 Mask visualisation (i)

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

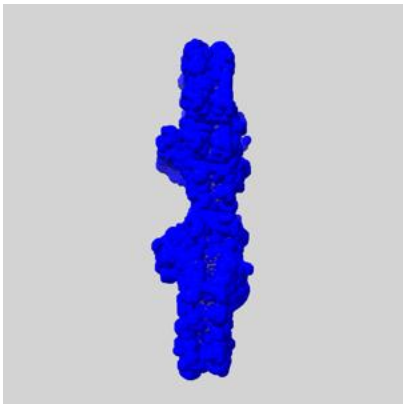
A mask typically either:

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

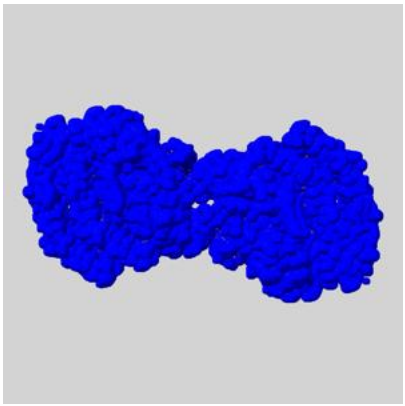
### 6.6.1 emd_14871_msk_1.map (i)



X



Y

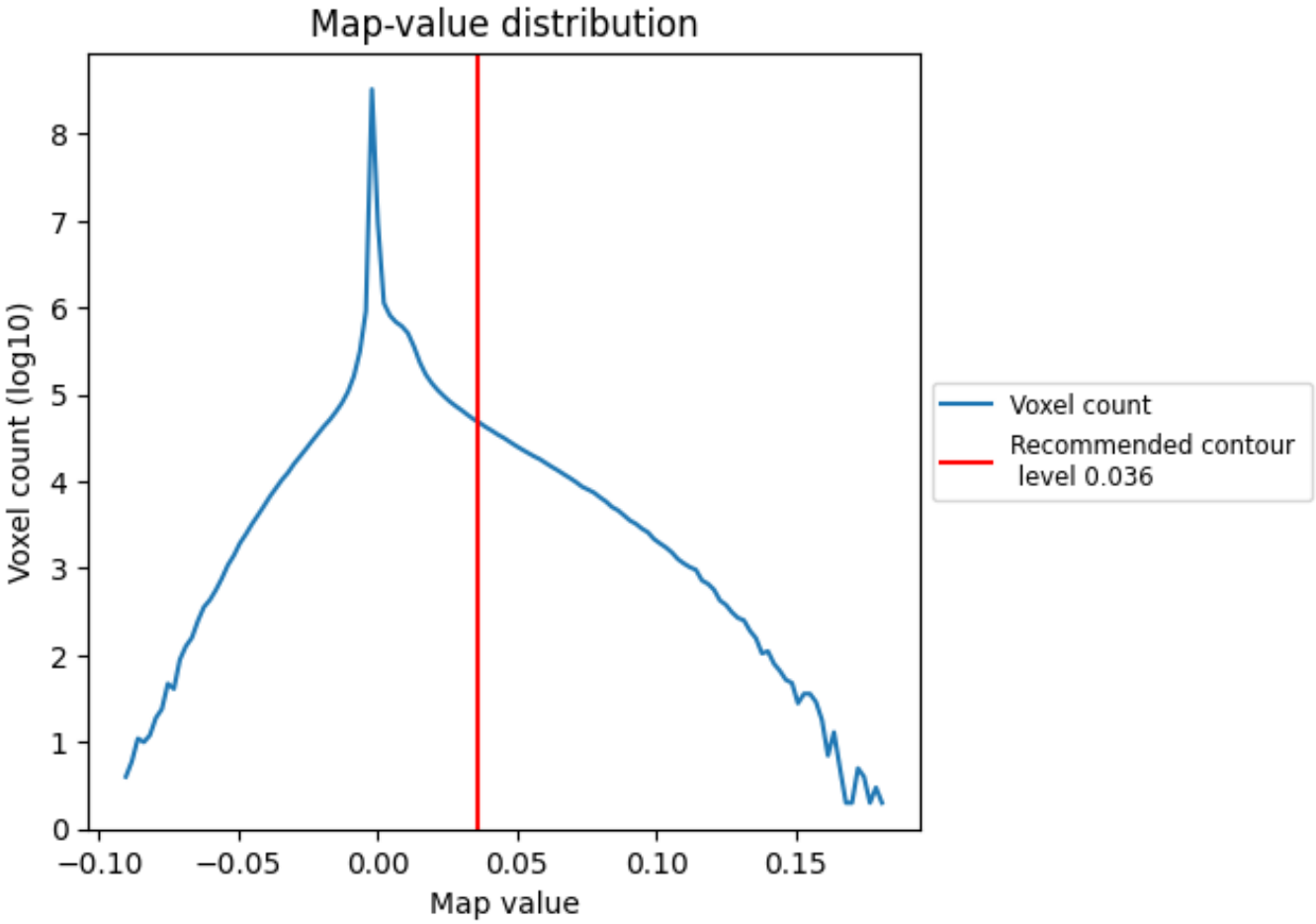


Z

# 7 Map analysis

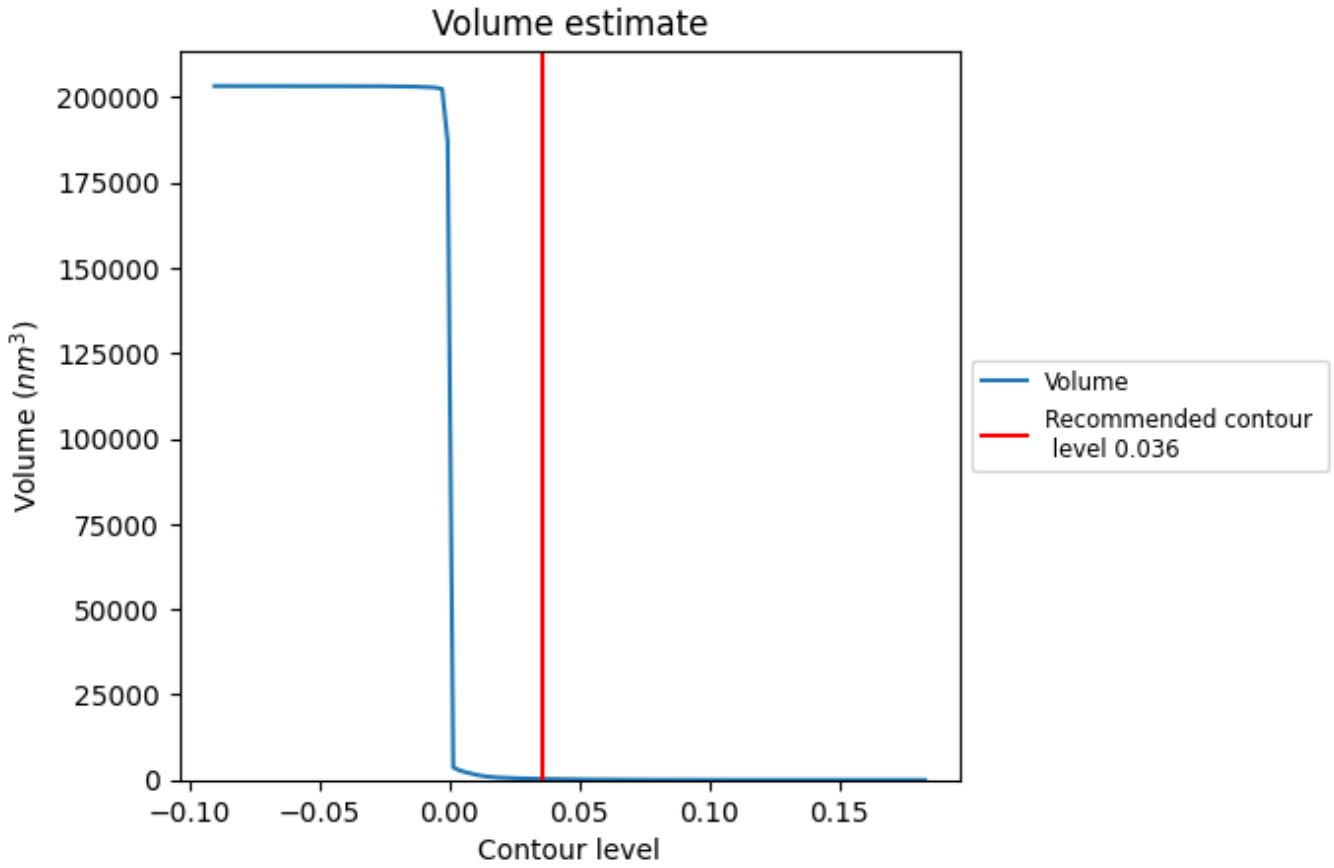
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

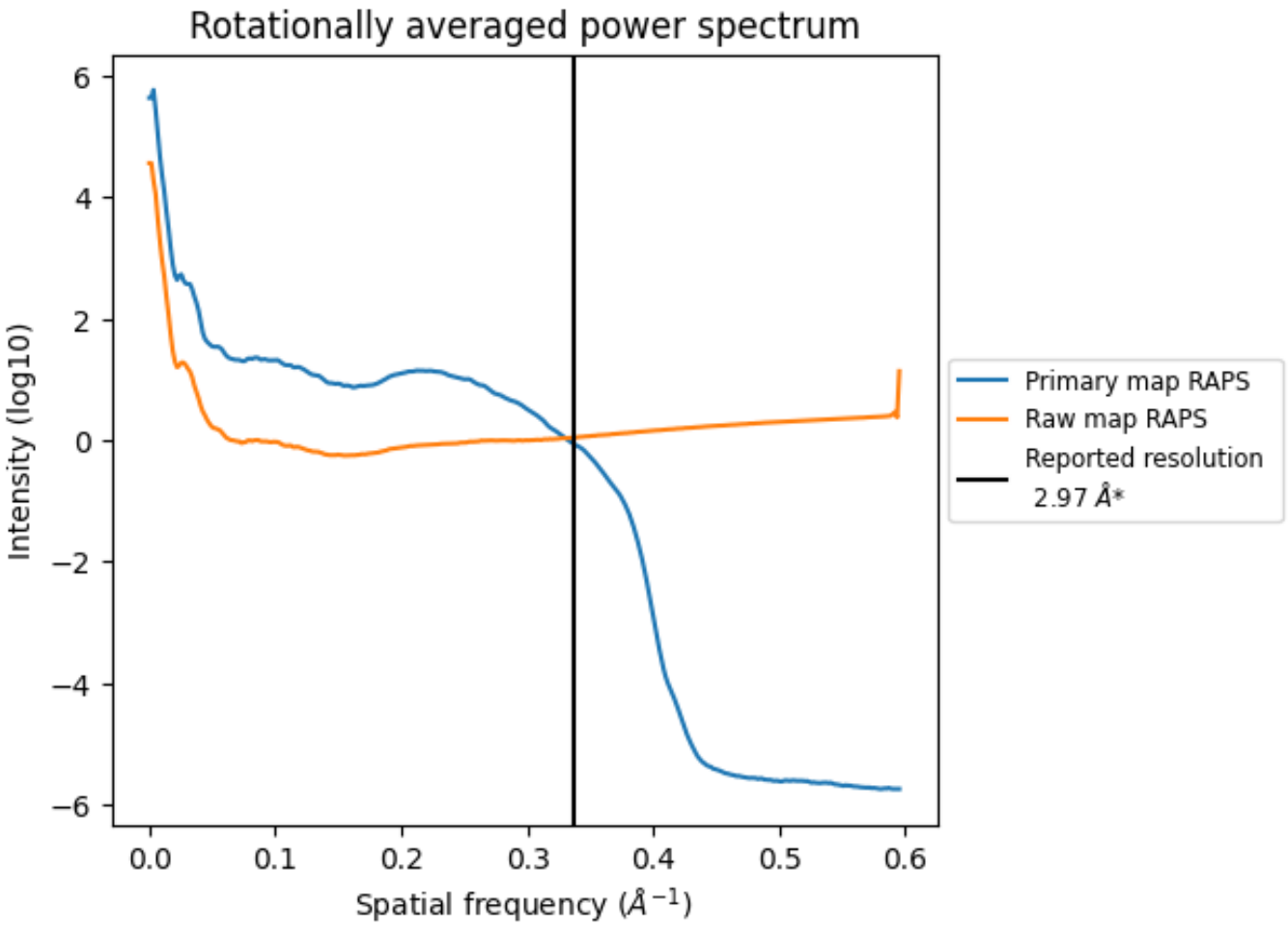
## 7.2 Volume estimate




The volume at the recommended contour level is 297 $nm^3$; this corresponds to an approximate mass of 268 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)

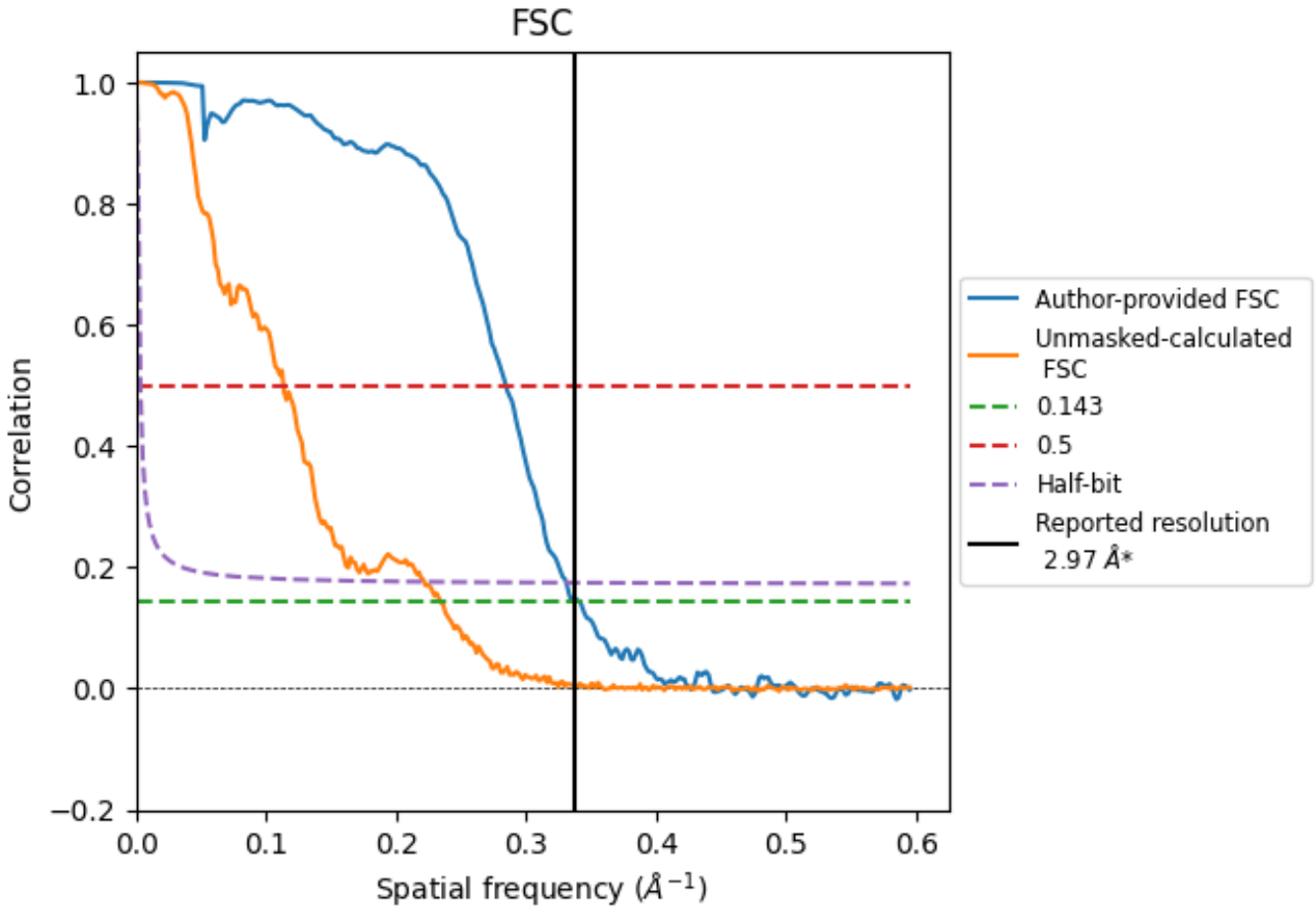



*Reported resolution corresponds to spatial frequency of 0.337 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.337 Å$^{-1}$

## 8.2 Resolution estimates (i)

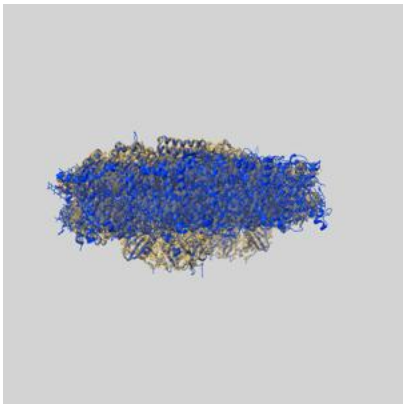
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.97 | - | - |
| Author-provided FSC curve | 2.92 | 3.51 | 3.02 |
| Unmasked-calculated* | 4.27 | 8.82 | 4.51 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.97 by more than 10 %

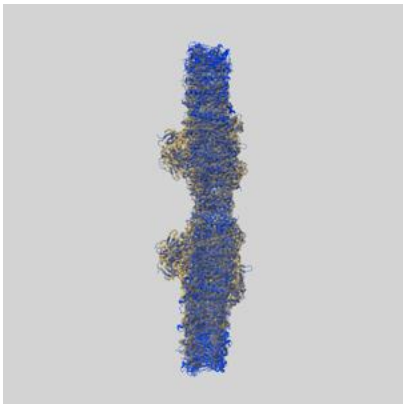
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14871 and PDB model 7ZQD. Per-residue inclusion information can be found in section 3 on page 62.

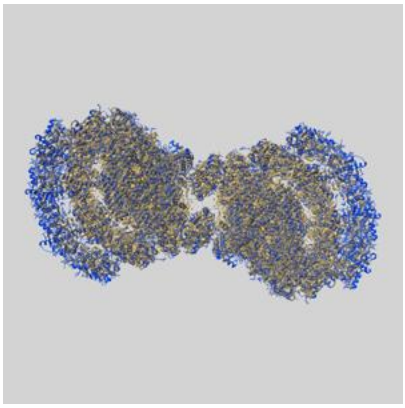
## 9.1 Map-model overlay



X



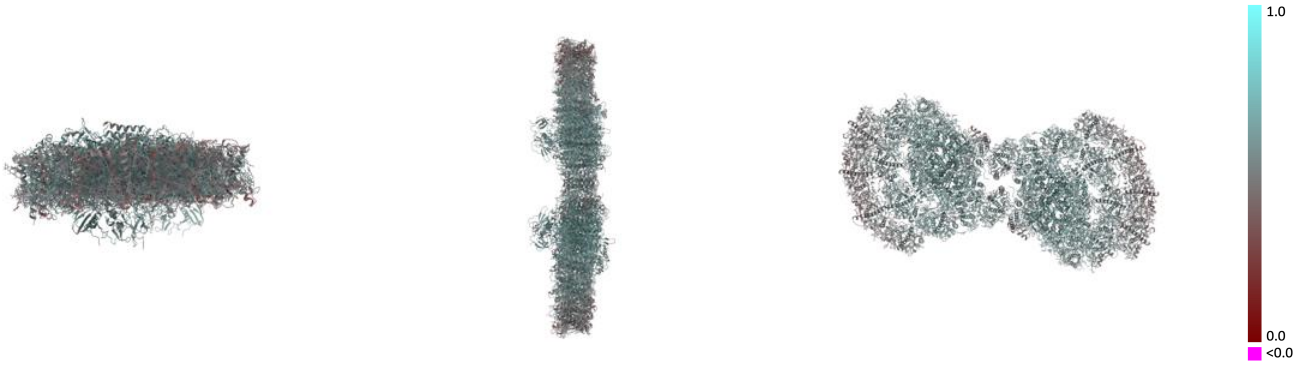
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.036 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.

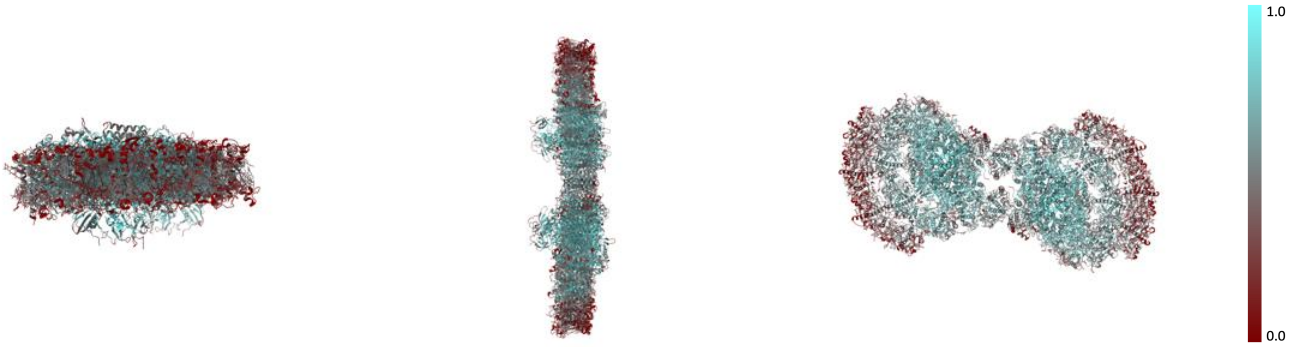
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

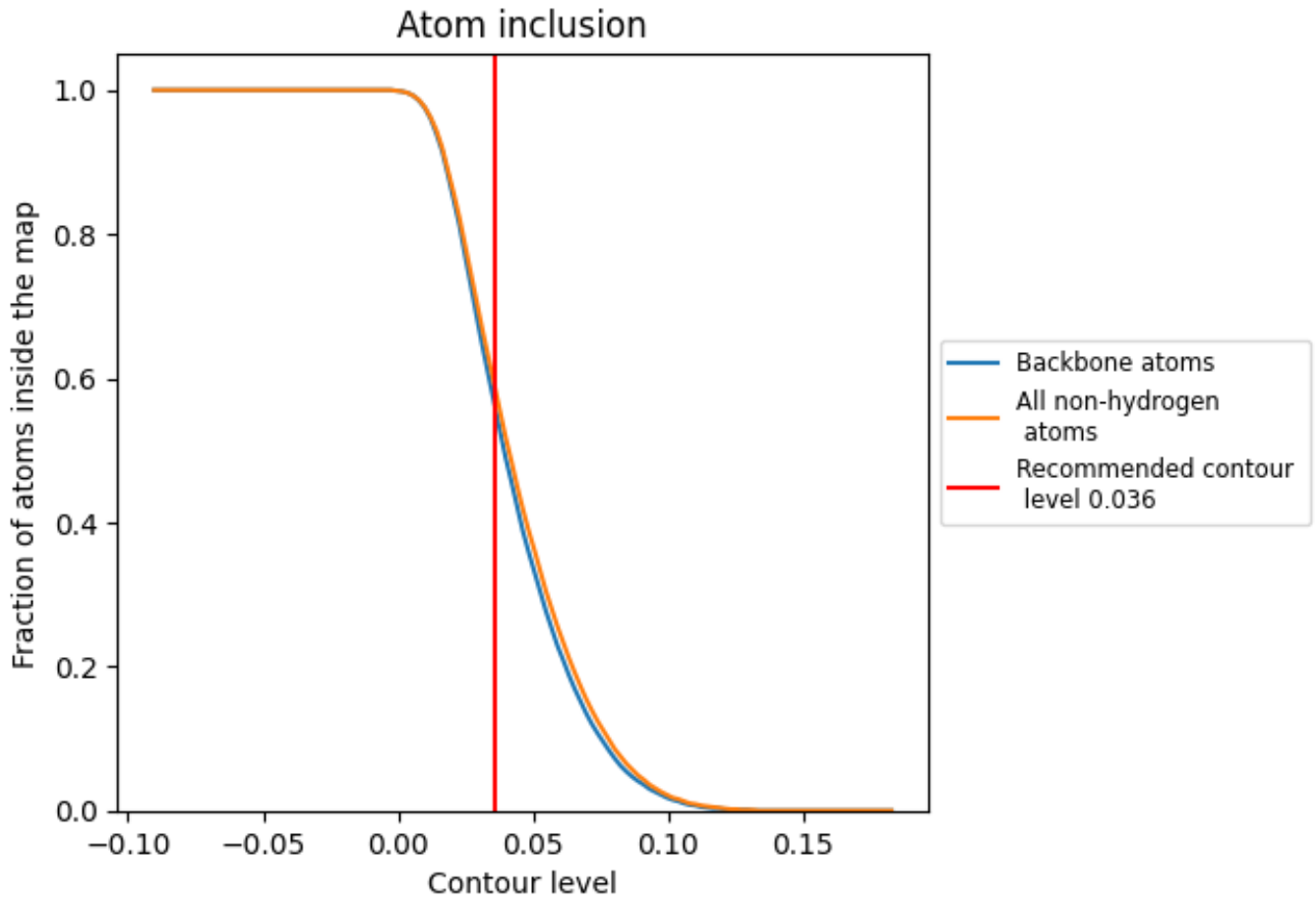
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (0.036).

## 9.4 Atom inclusion (i)




At the recommended contour level, 56% of all backbone atoms, 59% 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 (0.036) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.5860 | 0.5590 |
| 1 | 0.5840 | 0.5670 |
| 12 | 0.5940 | 0.5700 |
| 3 | 0.5550 | 0.5510 |
| 32 | 0.5540 | 0.5520 |
| 4 | 0.2170 | 0.4530 |
| 42 | 0.2180 | 0.4540 |
| 5 | 0.2790 | 0.4730 |
| 52 | 0.2720 | 0.4740 |
| 6 | 0.1970 | 0.4450 |
| 62 | 0.2040 | 0.4470 |
| 7 | 0.5830 | 0.5540 |
| 72 | 0.5770 | 0.5510 |
| 8 | 0.6230 | 0.5710 |
| 82 | 0.6220 | 0.5700 |
| 9 | 0.5400 | 0.5400 |
| 92 | 0.5430 | 0.5420 |
| A | 0.7970 | 0.6210 |
| A2 | 0.7980 | 0.6200 |
| B | 0.8060 | 0.6190 |
| B2 | 0.8070 | 0.6190 |
| C | 0.7500 | 0.6000 |
| C2 | 0.7510 | 0.5950 |
| D | 0.5600 | 0.5630 |
| D2 | 0.5610 | 0.5590 |
| E | 0.6130 | 0.5730 |
| E2 | 0.6050 | 0.5720 |
| F | 0.6940 | 0.5900 |
| F2 | 0.6890 | 0.5870 |
| G | 0.5060 | 0.5480 |
| G2 | 0.5050 | 0.5490 |
| I | 0.5740 | 0.5470 |
| I2 | 0.5740 | 0.5440 |
| J | 0.7280 | 0.5920 |
| J2 | 0.7340 | 0.5950 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| K | 0.3470 | 0.5380 |
| K2 | 0.3190 | 0.5390 |
| L | 0.3930 | 0.5010 |
| L2 | 0.3890 | 0.5010 |
| Z | 0.3190 | 0.4950 |
| Z2 | 0.3190 | 0.4960 |